Many-Body Invariants for Super Spin Chains with Antiunitary Symmetries

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Kurzzusammenfassung

Es werden Vorschläge für Vielteilcheninvarianten in Superspinketten geprüft. Durch Symmetrie geschützte Phasen werden als Homotopieklassen von Grundzuständen mit Anregungslücke modelliert. Der Matrixproduktzustandsformalismus wird systematisch auf fermionische Systeme mit antiunitären Symmetrien ausgeweitet. Ein basisunabhängiger diagrammatischer Zugang, der mit anti-unitären Symmetrien kompatibel ist, wird entwickelt. Vorschlägen aus der Literatur folgend werden Observablen vom Typus der Verschränkungsentropien mit Modifikationen für fermionische Matrixproduktzustände berechnet und ihre Homotopieinvarianz bewiesen. Die Nützlichkeit von Klassifikationen durch diese und ähnliche Observablen wird im Lichte der Klassifikation eindimensionaler fermionischer durch Symmetrie geschützter Phasen mit Gruppenkohomologie bewertet. Die Homotopieinvarianz wird im Limes divergierender virtueller Dimension bei beschränkter Korrelationslänge gezeigt.

Abstract

Proposals for many-body invariants for super-spin chains with anti-unitary symmetries are evaluated. Symmetry protected phases are modeled as homotopy classes of gapped ground states. The formalism of matrix product states is systematically extended to fermionic systems with anti-unitary symmetries. A basis-independent diagrammatic approach capable of handling anti-unitary symmetries is developed. Suggestions from the literature for observables of a twisted entanglement entropy type are calculated and proven to be topological invariants of fermionic matrix product states. The viability of classifications via these invariants is discussed as well as the connection to the cohomology classification of one-dimensional fermionic symmetry protected phases. Taking the limit of diverging bond dimension while controlling the correlation length, the homotopy invariance is proved to persist.

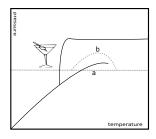
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Introduction

Matter at equilibrium is characterized by only a few variables, rather than the myriads of degrees of freedom specifying the configuration of its constituents.



Sketch of the phase diagram of water. The straight dashed line (a) cuts two phase transition lines at atmospheric pressure; the ice melting transition, and the liquid-vapor transition. For the latter, however, one can use path (b) to avoid the phase transition. This is possible by the continuity of the order parameter.

The behavior of water in equilibrium, be it in a water glass or a steam engine, can be characterized by such a small set of variables as temperature and pressure. All other observables, like compressibility or density, are functions of these two. Continuously varying the variables will, in general, produce continuous variations of the observables, with exceptions: Due to the large number of constituents involved, it is possible for the observables to acquire jumps or kinks — a phase transition.

This is a most happy fact of nature, for it allows us to cool our cocktails: At atmospheric pressure and 273 Kelvin, the melting transition binds a specific enthalpy of fusion of around 300 Joules per Gram, enough to cool water by 80 Kelvin. Thus, ice cubes can cool a drink considerably without diluting it much

If an observable with a continuous target space shows non-analytic behavior, then there might be another path through the phase diagram avoiding the transition. For example, liquid water and vapor are connected by the boiling transition, but also through the supercritical state of water.

On the other hand, observables taking values in a discrete set can vary only in jumps. Therefore, there are patches characterized by the value of that quantized observable, which are separated from others by phase transitions: Discrete observables are homotopy invariants of non-critical states of matter.

Often, symmetries are necessary to stabilize quantization. This is the case for the systems considered in this thesis. For illustration, consider the *Haldane phase* of integer-valued spin chains [70], or, less generally, the AKLT chain [2]. In the AKLT construction, onsite vector degrees of freedom are presented as the symmetrization of two virtual spinors. The two half-spins across any bond are projected into their singlet state. This results, for a finite chain, in an unpaired spinor at each edge of the chain. This feature of *fractionalization* is generic in the presence of a symmetry protecting the edge modes, and it is particularly significant in the case of uneven integer spins, where it yields spinors at

the edge as in the AKLT case. For example, a time-reversing symmetry T in the bulk forces a Kramers degeneracy at the boundary. The edge modes of two identical chains combine to a non-anomalous representation of the symmetry, rendering the degeneracy removable. Thus, the number of half-spins at the edge modulo two is the quantized observable. By breaking the symmetry, for example by coupling the chain to an external magnetic field, the edge modes can get removed without any phase transition.

These two examples should indicate already the versatility of so-called *topological* phases. In order to bring this variability into a common framework, it is helpful to turn again to the idea of paths in a phase diagram alluded to in the beginning – now enlarged by all possible couplings consistent with a prescribed set of symmetries.

By considering deformations by smooth paths in this infinite-dimensional space, states with widely different phenomenology can be joined by paths not crossing any phase transition line. Can all states be joined by such a smooth path, or are there disconnected states? Which? And – how to detect to which of such sets a given state belongs? More formally, what is the set of path-connected components of the set of ground states? If there is more than one such component, some states are necessarily separated by a phase transition.

In recent years, a multitude of methods has been developed to compute such groups. There is now a complete and mathematically rigorous understanding of such phases in one and two spatial dimension [17, 120]. In two space dimensions, an important distinction arises, whether or not anyonic quasiparticles are present in the system. Anyons, however, are out of the scope of this thesis and are ignored in the following discussion. The method used is a refinement or re-application of methods first developed in the context of matrix product states (MPS). To represent the AKLT state, the physical spin was augmented by two virtual spins. In analogy, a larger number of virtual degrees of freedom can be introduced to represent more general states – in fact, any state can be approximated by states constructed in this manner [50]. Imposing invariance of the state under a group action G on the physical spins is manifested by a projective symmetry action on the virtual spins. For a finite chain, in general, the two ends together form a proper representation of G. Since projective representations are classified by group cohomology, this yields an algebraic classification of topological phases, in particular in one spatial dimension. In the AKLT-chain, the time-reversal symmetry with $T^2 = 1$ factorizes to two projective representations with $\widehat{T}^2 = -1$.

Another line of inquiry, not so encumbered with microscopic details, has advanced to similar results. There, topological phases are modeled by *invertible* topological field theories (TFTs). A general motivation why this could work are the observations that (a) the partition sums of invertible TFTs can be computed on triangulated manifolds, and, for suitable choice of manifold, yield states that are representatives of certain topological phases [85, 86]. Secondly, since the formulation of the problem of classification of topological phases with unique ground states allows for a quite large range of deformations of the initial Hamiltonian and even the degrees of freedom present in the system, one can hope that it is (b) possible to deform *any* state to one of the type mentioned in

(a). This intuition is difficult to formulate precisely, let alone to prove. In the context of tensor networks, a more limited claim is investigated under the program of *entanglement renormalization* [171], a coarse graining procedure. The states mentioned in (a) are then thought to arise as fixed points of this renormalization procedure, that is, invertible TFTs would characterize the long-range behaviour of topological phases with unique ground states.

The arguments in this thesis do not depend on the subscription to the above belief. Rather, the claim is used in the following way: A given invertible TFT is completely characterized by its value on a relatively small set of manifolds. Therefore, if it is true that invertible TFTs characterize topological phases, then it should be possible to diagnose topological phases by computing expressions corresponding to these partition sums. Once these expressions are found, it is no longer necessary to know that they are motivated by TFT. Instead, this thesis proves that they are, in fact, topological invariants of gapped ground states, without using field theoretic methods. As it turns out, this TFT-inspired program gives a good picture at least of one-dimensional topological phases which is why this approach is introduced shortly in the following.

If $G_{\text{TFT}} \to O(d)$ is a group homomorphism (with some additional constraints), certain d-manifolds can be equipped with G_{TFT} -structures, similar to how certain Riemannian manifolds can be endowed with a spin structure. G_{TFT} is related to the condensed-matter symmetry group G and contains space-time symmetries. The bordism group is the set of all closed d-manifolds with G_{TFT} -structures, where those manifolds are considered equivalent that are the boundary of a (d+1)-manifold with G_{TFT} -structure, with appropriate gluing conditions. Then unitary invertible TFTs – and, by the assumption of a continuum limit, topological phases with G-symmetry – are classified by their partition sum, a homomorphism Z: bordism group $\to U(1)$ [176]. The classifications obtained in this way agree with more rigorous results in one spatial dimension, while in higher dimensions some phases seem to not be captured by TFTs [120].

It is also quite straightforward to determine to which class a given TFT belongs. If $X_1, ..., X_n$ are generators of the bordism group, the set of unit complex numbers

$$Z(X_1),...,Z(X_n)$$

completely determines the theory.

From the perspective of condensed matter physics, this of course is quite abstract. What is the Hubbard model on a Klein bottle? To motivate the meaningfulness of these words, recall that in the path integral formalism, the reduced density matrix on a region A is represented pictorially by a torus with slits along A, in the continuum limit. Taking powers and tracing produces higher-genus surfaces, as has been first exploited to analyze the entanglement properties of conformal field theories [27]. Non-orientable surfaces can be realized through anti-unitary operations like motion-reversal or particle-hole transformations [154]. In this way, one obtains, for generating manifolds $X_1, ..., X_n$, a set of polynomial expressions $P_1(\rho), ..., P_n(\rho)$ in the reduced density matrix of the given ground state of some condensed matter system such that $\text{Tr}(P_i(\rho))$ is related to $Z(X_i)$.

This thesis aims to make this connection precise. To this end, it proceeds in two steps. First, the candidate partition sums are examined for matrix product states, where they

are related to the known cohomological invariants. Then, the bond dimension – the number of virtual degrees of freedom adjoined to the physical ones – is sent to infinity. The phase of the partition sums is shown to be continuous and quantized in this limit, assuming exponential correlations. The modulus is non-topological in origin.

For convenience, only two partition sums are investigated: those associated with the real projective plane and the Klein bottle. With the exception of class D topological superconductors, these two suffice to diagnose the various commonly discussed topological phases of one-dimensional fermions, i.e., those labeled by pseudo-Cartan labels DIII, CII, CI, AI, BDI, AIII in the periodic table of topological insulators and superconductors [90]. In fact, except for class DIII, all topological phases are diagnosed by the real projective plane invariant $Z(\mathbb{R}P^2)$. The corresponding invariant for the class D case, on the other hand, is already well-known [125]. The labels are used here to facilitate comparison to other approaches and have no connection to symmetric spaces.

In any case, as the calculations are not very specific to the chosen invariants to compute, it is not hard to generalize the argument. In particular, the extension to infinite bond dimension carries over to more complicated polynomials in the density operators.

Chapter 1 starts by introducing graded linear algebra, together with a diagrammatic formalism to ease computations. There is a discussion of peculiarities pertaining to completely positive maps, and to anti-linear operations, in the graded context. Then, chapter 2 sets up the physical models – they are called super quantum spin chains in analogy to quantum spin chains. This class includes spin chains, fermions, and everything in between. The formalism is chosen for its compatibility with matrix product state methods. After these preliminaries, the space of ground states is introduced and the notion of a topological phase is formulated. An overview of both TFT and MPS methods as previously applied in this context is added, which finishes by motivating candidates for many-body topological invariants. In order to advance along these lines, chapter 3 generalizes matrix product states to the graded setting. The real projective plane and the Klein bottle partition sum are computed for matrix product states. The calculation shows that they are topological invariants on the set of matrix product states with finite bond dimension by connecting the partition sums to cohomological objects. The advantage of analytical topological invariants appears most succinctly in the limit of infinite bond dimension, which is the subject of chapter 4. Recall that matrix product states can approximate ground states effectively, but the size of the auxiliary systems increases as the gap of the spectrum diminishes. In particular, critical systems of finite size L can be approximated by MPS only if the bond dimension is chosen polynomial in L [169]. Working in an infinite system, this implies that as the state adiabatically approaches criticality, its bond dimension has to diverge. Starting from this phenomenon, topological phases with symmetry group G have been modeled in the literature as classes of matrix product states of arbitrarily large, but finite, bond dimension, where two MPS are said to be in the same class if their parent Hamiltonians can be deformed into each other within the class of parent Hamiltonians without breaking G nor closing the gap [145]. Hence, instead of looking at gapped states modulo deformations preserving the gap, the setting has shifted to G-symmetric matrix product states modulo structure preserving deformations – phase transitions are identified through the divergence of bond dimension.

However, generic non-critical states, for example free-fermion states with non-flat bands, have infinite bond dimension. It is likely that there is no new physics associated to such problems, as one can argue using entanglement renormalization ideas [171]. Nevertheless, an approach to topological phases that does not depend intrinsically on the choice of formalism helps when combining different methods to deal with the same physical system. Here, this generality is achieved by sending the bond dimension to infinity and maintaining control through the imposition of finite correlation length, thus establishing the aforementioned partition sums as topological invariants on exponentially correlated states.

Super Linear Algebra

This chapter reviews some aspects of the theory of \mathbb{Z}_2 -graded vector spaces, and follow the ramifications of the grading through all the machinery built on top of them, in particular the theory of completely positive maps. Afterwards, some issues relating to G-actions on the previously defined objects are investigated, with a focus on anti-unitary operations. Importantly, the \mathbb{Z}_2 fermion parity operation is not treated as a symmetry.

While there are some original contributions in this chapter, these are to be seen as auxiliary to the discussion of super matrix product states. Those well-acquainted with the ungraded theory might often guess the correct generalization. In appendix A, some of the developments of this section are generalized to \mathbb{Z}_p -graded vector space.

For calculations it is useful to employ a diagrammatic formalism quite common in the tensor network literature, e.g., [24]. The treatment here focuses on the inclusion of: (i) The grading and (ii) The implementation of anti-unitary symmetries. To deal with sign factors appearing by (i), a variety of proposals exists in the literature, e.g., [25] localize the necessary bookkeeping to the tensor lines (here it is the nodes), while [173] uses Grassmann calculus. The presentation here has the advantage that it reduces without further modifications to the bosonic case once all the gradings are chosen trivial. (ii) The inclusion of anti-unitary symmetries is complicated by the fact that tensor diagrams are linear. This can be resolved in two ways. There is the possibility of working over the real numbers, and return to the standard diagrams with the help of complex structures which then commute or anti-commute with the symmetries. The other path chosen here is viable if the vector spaces are Hilbert, for this gives another, canonical, antilinear operation. Then, anti-unitary operations are implemented by bilinear forms. This does not depend on the choice of basis, is more natural in quantum mechanics, and simplifies the algebra.

1.1. Vector Spaces

Definition 1. A super vector space V is a vector space together with a decomposition $V = V^0 \oplus V^1$.

If not further indicated, vector spaces are over the field of complex numbers. Otherwise they are referred to as a vector spaces over \mathbb{K} , where \mathbb{K} is the field used for scalar multiplication.

The set $(V^0 \cup V^1) \setminus \{0\}$ is called the *homogeneous* vectors, and $|\xi| \in \mathbb{Z}_2$ is the *parity* of a homogeneous vector $\xi \in V^{|\xi|}$. The *fermion parity* of V is the operator $P_V(\xi) = (-1)^{|\xi|} \xi$. The tensor product $X = V_1 \otimes V_2$ of super vector spaces is endowed with a grading by declaring $X^{\lambda} = \sum_{\mu_1 + \mu_2 = \lambda} (V_1)^{\mu_1} \otimes (V_2)^{\mu_2}$. The resulting super vector space $X = V_1 \otimes V_2 \otimes V_2 \otimes V_3 \otimes V_4$.

 $X^0 \oplus X^1$ is then denoted by $V_1 \widehat{\otimes} V_2$. For super vector spaces V_1, V_2 introduce the *braiding* isomorphism $\mathscr{B}: V_1 \widehat{\otimes} V_2 \to V_2 \widehat{\otimes} V_1$ by extending linearly from its action on homogeneous product vectors: $\mathscr{B}(\xi_1 \widehat{\otimes} \xi_2) = (-1)^{|\xi_1||\xi_2|} \xi_2 \widehat{\otimes} \xi_1$. Here, $\mathbb{Z}_2 \times \mathbb{Z}_2 \ni (\mu, \nu) \mapsto \mu \nu \in \mathbb{Z}_2$ is the parity pairing.

Given a super vector space V, an element $\xi \in V$ is simply represented by $\longrightarrow \xi$, that is: A node labeled by the vector and an outgoing arrow. The tensor product of n vectors $\xi_1, ..., \xi_n$ with $\xi_i \in V_i$ is then depicted as

It is important orient the arrows since the vector spaces are complex; in particular it allows to take the complex conjugate of a diagram, reversing arrows.

Similarly, an element of the dual space $\varphi \in V^*$ is represented by $\varphi \longrightarrow$, that is: A node labeled by the covector, with an ingoing arrow. This notation is chosen to suggest contractions $V^*\widehat{\otimes}V \to \mathbb{C}, \ \varphi \widehat{\otimes} \xi \mapsto \varphi(\xi)$ by attaching the outgoing line of a vector to the ingoing line of a covector, $\mathscr{C}: \varphi \longrightarrow \xi \mapsto \varphi \longrightarrow \xi$.

Finally, the braiding of tensor factors is implemented by exchanging the endpoints of the arrows (while keeping the nodes fixed). The untying of the resulting crossing, achieved by exchanging the nodes, introduces a Koszul sign:

Note that the crossing is *unsigned*. This is because the super tensor product defines a *symmetric* tensor category. As explained in appendix A, working with more general gradings can change this.

Present the image of $\xi \in V$ under $L \in \mathcal{L}(V,W)$ by $\longrightarrow L(\xi) = \longrightarrow L \longrightarrow \xi$. That is, by a node decorated with that operator, and a box around it, with an ingoing and an outgoing line. $\mathcal{L}(V,W)$ is a super vector space with grading $\mathcal{L}(V,W)^{\lambda} = \sum_{\mu_1 + \lambda = \mu_2} \mathcal{L}(V^{\mu_1}, W^{\mu_2})$.

Definition 2. Let $L: V \to W$ be a linear map between super vector spaces V and W. Then, the dual to L is the linear operator $L': W^* \to V^*$ defined by

$$L'(\varphi) = (-1)^{|L||\varphi|} \varphi \circ L . \tag{1.3}$$

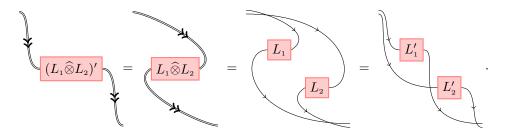
Diagrammatically this corresponds to exchanging the legs of the diagram:

$$L' \rightarrow L$$

The map $L \to L'$ behaves well under tensor products. Indeed, if $L_i : V_i \to W_i$ for i = 1, 2, then

$$(L_1\widehat{\otimes}L_2)'=L_1'\widehat{\otimes}L_2'.$$

This is proven diagrammatically:



Moreover, the definition of the dual map implies that it is a graded anti-homomorphism

$$(L_1L_2)' = (-1)^{|L_1||L_2|} (L_2)'(L_1)'$$
(1.4)

Mapping $L \mapsto L'$ gives a linear graded anti-homomorphism $\mathscr{L}(V) \to \mathscr{L}(V^*)$.

Super Hilbert Spaces. Often, vector spaces carry inner products. In the superworld, standard inner products have the disadvantage of not factoring on super tensor products. This motivates a modification that forces compatibility with the tensor product [166, Section 3.4].

Definition 3. A super vector space V is called super Hilbert space if there is a sesquilinear form h, called a super hermitian form, satisfying:

- (i) $h(\xi_1, \xi_2) = 0$ unless $|\xi_1| = |\xi_2|$,
- (ii) $\xi \mapsto \|\xi\|_h := |h(\xi,\xi)|^{\frac{1}{2}}$ is a norm satisfying the parallelogram identity

$$\frac{1}{2} \|\xi_1 + \xi_2\|_h^2 + \frac{1}{2} \|\xi_1 - \xi_2\|_h^2 = \|\xi_1\|_h^2 + \|\xi_2\|_h^2 , \qquad (1.5)$$

(iii) $h(\cdot,\cdot)$ is super hermitian:

$$\overline{h(\xi_1, \xi_2)} = (-1)^{|\xi_1||\xi_2|} h(\xi_2, \xi_1) . \tag{1.6}$$

On the other hand, V can be endowed with a Hilbert structure. What is their connection? Before this question can be answered first recall that given a bilinear form $\beta: \mathbb{Z}_2 \times \mathbb{Z}_2 \to \mathbb{Z}_2$, a map $q: \mathbb{Z}_2 \to \mathbb{Z}_4$, satisfying

$$q(\mu + \nu) - q(\mu) - q(\nu) = 2 \cdot \beta(\mu, \nu)$$
, (1.7)

is called a *quadratic extension* of β . Equation 1.7 used the embedding $\mathbb{Z}_2 = \{0,1\} \stackrel{2:}{\mapsto} \{0,2\} \subset \mathbb{Z}_4$.

Lemma 1. The following are equivalent, for V a super vector space:

(i) A super hermitian form h on V.

(ii) A tupel $(\langle \cdot, \cdot \rangle, q)$ with $\langle \cdot, \cdot \rangle$ an inner product on V and q a quadratic extension of the parity pairing.

Proof. Start with a super hermitian form. Then, the parallelogram condition 1.5 determines an inner product $\langle \cdot, \cdot \rangle_h$ through polarization:

$$4\langle \xi_1, \xi_2 \rangle_h := \|\xi_1 + \xi_2\|_h^2 - \|\xi_1 - \xi_2\|_h^2 - i\|\xi_1 + i\xi_2\|_h^2 + i\|\xi_1 - i\xi_2\|_h^2 . \tag{1.8}$$

Anticipating the result, write $\frac{1}{4}q_h(\xi) := \frac{1}{2\pi} \arg h(\xi,\xi)$ for homogeneous ξ . By the hermiticity of h, equation 1.6:

$$h(\xi,\xi) = (-1)^{|\xi|} \overline{h(\xi,\xi)} \Rightarrow q_h(\xi) = 2|\xi| - q_h(\xi) \mod 4\mathbb{Z} \Rightarrow 2q_h(\xi) = 2|\xi| \mod 4\mathbb{Z}$$
. (1.9)

It follows that q_h is constant on homogeneous vectors, i.e. $q_h(\xi) = q_h(|\xi|)$. Hence $q_h : \mathbb{Z}_2 \to \mathbb{Z}_4$ takes the form $q_h(\mu) = \pm \mu^2$. It is a quadratic extension of the parity pairing, and well-defined on \mathbb{Z}_2 as $(\mu + 2)^2 = \mu^2 + 4\mathbb{Z}$.

On the other hand, given an inner product $\langle \cdot, \cdot \rangle$ and a quadratic extension q of the parity pairing, $h(\xi_1, \xi_2) := i^{q(|\xi_1|)} \langle \xi_1, \xi_2 \rangle$ is a super hermitian form.

Superalgebras. Consider the ring of endomorphisms $\mathcal{L}(V)$ on some super vector space V. It has a grading-preserving product given by the composition of maps. This is formalized by the following definition:

Definition 4. A superalgebra $A = (V, \cdot)$ is a super vector space V equipped with a bilinear associative pairing $(\xi_1, \xi_2) \mapsto \xi_1 \cdot \xi_2$ satisfying $V^{\mu}V^{\nu} \subset V^{\mu+\nu}$.

Superalgebras fit (by construction) nicely into the super diagrams, mostly owing to the fact that multiplication is an even operation.

The tensor diagram notation makes the multiplication rule on tensor products obvious. Consider the following diagrammatic equality, arising from the Koszul rule of horizontal reordering of tensor nodes:

The left hand side of this tensor diagram amounts to the multiplication $(L_1 \widehat{\otimes} L_2)(M_1 \widehat{\otimes} M_2)$, while the right hand side is $(-1)^{|L_2||M_1|} L_1 M_1 \widehat{\otimes} L_2 M_2$. This shall serve as the motivation to introduce the following multiplication on the tensor product $A_1 \widehat{\otimes} A_2$ of two superalgebras¹

$$(x_1 \widehat{\otimes} x_2) \cdot (y_1 \widehat{\otimes} y_2) := (-1)^{|x_2||y_1|} x_1 x_2 \widehat{\otimes} y_1 y_2 . \tag{1.10}$$

The super tensor product multiplication rule gives by construction the isomorphism of super algebras $\mathscr{L}(V_1 \widehat{\otimes} V_2) \cong \mathscr{L}(V_1) \widehat{\otimes} \mathscr{L}(V_2)$.

¹It will not have gone unnoticed that the notation switched from greek, to large latin, to small latin letters, used for vectors, linear operators, and elements of abstract algebras, respectively.

 C^* -Superalgebras. If V is a Hilbert space, then $A=\mathcal{L}(V)$ carries a natural Banach norm, the operator norm

$$\|L\| := \sup_{\xi \in V} \{\|L(\xi)\| \, : \, \|\xi\| \le 1\} \ ,$$

and an anti-linear involutive antiautomorphism $L \mapsto L^*$ defined by $\langle L(\xi_1), \xi_2 \rangle = \langle \xi_1, L^*(\xi_2) \rangle$. These two structures satisfy the so-called C^* -property

$$||L^*L|| = ||L||^2 . (1.11)$$

This has been axiomatized into the following:

Definition 5. A C^* -superalgebra A is a superalgebra A, which carries a norm $\|\cdot\|$ and an antilinear involutive even antiautomorphism $x \mapsto x^*$ such that $\|x^*x\| = \|x\|^2$.

The notion of a state as a normed element of a Hilbert space is generalized in this context by axiomatizing the expectation value functional furnished by such a vector:

Definition 6. A state ω on a C^* -superalgebra A is an even linear functional $\omega: A \to \mathbb{C}$ that is positive and of unit norm.

The norm is the usual operator norm $\|\omega\| := \sup\{|\omega(x)| : \|x\| \le 1\}$, but by positivity² $\|\omega\| = \omega(1)$.

As argued above, closed sub-superalgebras of $\mathcal{L}(V)$ for a Hilbert space V are C^* -algebras, and one obtains states on such algebras through homogeneous vectors.

If ξ is a homogeneous vector in a super Hilbert space, consider the functional $L \mapsto \langle L \rangle_{\xi} := \|\xi\|^{-2} \langle \xi, L(\xi) \rangle$ with $\langle 1 \rangle_{\xi} = 1$. This is positive:

$$\langle L^*L\rangle_{\xi} = \frac{\|L(\xi)\|^2}{\|\xi\|^2} \ge 0.$$

In fact, given a state on a C^* -algebra, this can be reversed:

Theorem 1. Gel'fand-Naimark-Segal (GNS). If A is a C^* -superalgebra and a state $\omega \in A^*$, then there is a super Hilbert space H_{ω} , a homogeneous vector Ω_{ω} and an even *-homomorphism $\pi_{\omega}: A \to \mathcal{L}(H_{\omega})$ such that

$$\omega(x) = \langle \Omega_{\omega}, \pi_{\omega}(x)\Omega_{\omega} \rangle . \tag{1.12}$$

 $(H_{\omega}, \Omega_{\omega}, \pi_{\omega})$ is called a Gel'fand-triple.

This representation is unique in that if (H, Ω, π) is another triple such that equation 1.12 holds, then there is a unitary $U: H \to H_{\omega}$ such that $\Omega_{\omega} = U\Omega$ and $\pi_{\omega}(x) = (-1)^{|U||\pi(x)|}U\pi(x)U^*$.

²This is a special case of the proof in footnote 5 below. Alternatively check [15, Chapter II.6].

The above theorem shows the importance of states to characterize a given physical system. In this context it is useful to have a *topology* on the set of states, i.e. to have a notion of states being 'close' to each other, or of a sequence converging to a state.

Recall the notion of the graded dual of a map $L: V \to W$ from definition 2. In particular, a vector $\xi \in V$ is dualized to a linear functional $\xi': V^* \to \mathbb{C}$.

The weak*-, or w^* -,topology on V^* is defined by demanding that the ξ' are continuous. That is, the open subsets in V^* – the dual space equipped with this weak*-topology – are those of the form

$$(\xi')^{-1}(S)$$
, $\xi \in V$, $S \subset \mathbb{C}$ open. (1.13)

If $(\varphi_n)_{n\in\mathbb{N}}$ is a sequence, says that $\varphi_n \to \varphi$, if for each neighborhood M of φ there is an N s.t. $\varphi_{n>N} \in M$. Since the neighborhoods take the form indicated in equation 1.13, demand equivalently that for each $\xi \in V$, $\varphi_n(\xi) \to \varphi(\xi)$. Conversely, assume that for a sequence $(\varphi_n)_n \in V^*$ and for any $\xi \in V$ it holds that $\varphi_n(\xi)$ converges. If the φ_n are bounded and linear, the limit depends linearly on ξ and is continuous, that is, there is an element $\varphi \in V^*$ such that $\lim_{n\to\infty} \varphi_n(\xi) = \varphi(\xi)$. But then φ_n converges to φ in the w^* -topology.

Supercentral Superalgebras Superalgebras may have, in general, a complicated structure. For reasons that will become clear while studying maps on superalgebras below, it suffices – for the applications to be considered in this work – to focus on a subclass. If A is a superalgebra and $S \subset A$ a subset, introduce the *commutant* S' and the *supercommutant* $S^{\#}$:

$$S' := \{ x \in A : xs = sx, \forall s \in S \}, \qquad (1.14)$$

$$S^{\#} := \{ x \in A : \ xs = (-1)^{|x||s|} sx \ , \forall s \in S \} \ . \tag{1.15}$$

The center of an algebra A is $Z(A) = A \cap A'$ and its supercenter is $\mathscr{Z}(A) = A \cap A^{\#}$. The (super-)center of a superalgebra is a (super-)commutative superalgebra. If A is a *-algebra, then $\mathscr{Z}(A)^1 = 0$: For $z \in \mathscr{Z}(A)^1$ both $z \pm z^* \in \mathscr{Z}(A)^1$. Moreover, if $(z \pm z^*)^2 = 0$ then z = 0. But $(z \pm z^*)^2 = 0$ as z, z^* anti-commute with each other. An algebra with $Z(A) = \mathbb{C}1$ or $\mathscr{Z}(A) = \mathbb{C}1$ is called central, or supercentral⁴, respectively. A subset $I \subset A$ is called a left ideal if $AI \subset I$, a right ideal if $IA \subset I$ and two-sided if it is a left and a right ideal. It is called proper if $I \neq A$, $\{0\}$ and a (left, right, two-sided) superideal if $I = (I \cap A^0) \oplus (I \cap A^1)$. If a superalgebra A has no proper two-sided (super-)ideals, it is (super-)simple. If A is a direct sum of simple or supersimple algebras, it is called semisimple. Any supersimple algebra is semisimple, but not necessarily simple. A semisimple superalgebra can be decomposed into either its supersimple or its simple

³Unfortunately I use the prime both for the commutant and the dual of a linear map. This is unavoidable since both is quite standard. The dual of a linear map L could also be denoted L^{t} , but this I already use for the transpose w.r.t. a bilinear form. The context will however always unambiguously determine the meaning.

⁴Often A is called supercentral if $Z(A)^0$ is trivial.

components.

Often in this work, there is a connection between the requirement to be (super-) simple and to be (super-)central. Assume A acts non-degenerately on a super Hilbert space V, meaning that if $x\xi = 0$ for all $x \in A$, then $\xi = 0$. To a two-sided ideal $I \subset A$ associate the projection P_I on the complement of the annihilator subspace of I, i.e. the largest subspace such that $x\xi = 0$ for all $x \in I$. Then denote by p_I the central support of P_I , i.e., the smallest projection in the center of A containing P_I . On the other hand, every central projection p gives an ideal in A, the principal ideal generated by p given by I = Ap. Now, if A is a matrix algebra (or more generally if it is a von-Neumann algebra and the ideals are weakly closed [15]), then this is indeed the general case, and there is a one-to-one-correspondence between weakly closed ideals in A and principal ideals generated by central projections.

Theorem 2 ([172],[81]). If A is a finite-dimensional supercentral supersimple superalgebra, then either A is central simple, or A^0 is central simple and there is $\eta \in A^1$ which commutes with all elements of A such that $\eta^2 = 1$ and $A^1 = \eta A^0$.

Introduce an index

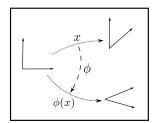
$$\mu_A := \begin{cases} 0 & \text{if } A \text{ central simple ,} \\ 1 & \text{if } A^0 \text{ central simple .} \end{cases}$$
 (1.16)

1.2. Positive and Completely Positive Maps

So far, I introduced vector spaces V and linear maps $\mathcal{L}(V)$ on these vector spaces – which are of course again a special class of vector spaces. – Now the turn has come to consider linear maps on linear maps on vector spaces, or $\mathcal{L}^2(V)$.

Relevant here are structures inherited from the cone of positive elements within $\mathcal{L}(V)$. General references to the theory of the ungraded positive and completely positive maps that are used freely are [126, 47, 161].

Recall that for a C^* -algebra A, a linear map $\phi \in \mathcal{L}(A)$ is called positive if $x \geq 0$ implies $\phi(x) \geq 0$. ϕ is called unital if $\phi(1_A) = 1_A$. For positive maps⁵ $\|\phi\| = \|\phi(1_A)\|$ so that unital positive maps are automatically of unit operator norm.



If A is super, assume that ϕ is homogeneous. Since there are no odd positive maps⁶ this is the same as assuming $\phi_1 = 0$. Here and in the following, assume that A is finite-dimensional.

Definition 7. A positive map ϕ on a C^* -algebra A is reduced by a projection $p \in A$ if

$$\phi(pAp) \subseteq pAp \ . \tag{1.17}$$

⁵To get a lower bound on $\|\phi\|$, consider positive x. Since $1 - \frac{x}{\|x\|} \ge 0$, by positivity $\phi(1) - \frac{\phi(x)}{\|x\|} \ge 0$. ⁶Take positive even $x \in A$, then $\phi(x)$ is odd and positive. Write $\phi(x) = (a_0 + a_1)^2 = (a_0)^2 + (a_1)^2 + a_0 a_1 + a_1 a_0$ for self-adjoint a. The even part vanishes by assumption, hence $a_0 = 0 = a_1$.

If there is no such p, then ϕ is called irreducible. If A is a superalgebra, and there is no homogeneous projection reducing ϕ , then ϕ is superirreducible.

In the super case, homogeneity preserves the superalgebra structure on pAp. However, since odd operators cannot be positive, superirreducibility amounts to excluding the existence of an *even* projection reducing ϕ .

For projections p_1, p_2 onto subspaces V_1, V_2 , let $p_1 \vee p_2$ be the projection onto $V_1 \cup V_2$ and $p_1 \wedge p_2$ the projection on $V_1 \cap V_2$. Furthermore $p_1 < p_2$ if $V_1 \subsetneq V_2$. For $x : V \to V$, let supp(x) be the support projection of x.

Lemma 2. Assume ϕ is even positive and that $p_+ = p_0 + p_1$ reduces ϕ . Then (i) $p_- := p_0 - p_1$ and $q = p_+ \lor p_- = \operatorname{supp}(p_0)$ are projections reducing ϕ , if $q \neq 1_A$. Furthermore, assume that ϕ is superirreducible. Then (ii) $q = 1_A$ and p_\pm are the only projections reducing ϕ .

Proof.

- (i) Apply the fermion parity automorphism P^A to both sides of 1.17 and use that ϕ is even. Thus, ϕ is reduced by $p_0 p_1$. Hence, it is also reduced by q. Write $p_0 + p_1 = (x_0 + x_1)^2 = (x_0^2 + x_1^2) + (x_0x_1 + x_1x_0)$ to see that p_0 is positive and p_1 self-adjoint but not positive. Thus, the support of $p_1, p_0 \pm p_1$ has to be contained in the support of p_0 . On the other hand, suppose ξ is in the support of p_0 . Then, $0 \neq 2p_0\xi = [(p_0 + p_1) + (p_0 p_1)]\xi$ and at least one of the $(p_0 \pm p_1)\xi$ is non-zero, so that ξ is in the support of q.
- (ii) By part (i) p_0 is full rank. Suppose there is another pair of projections $q_{\pm} = q_0 \pm q_1$ reducing ϕ , and let $s_{ab} = p_a \wedge q_b$ for $a, b = \pm$. A non-trivial s_{ab} reduces ϕ . However, if always either $s_{ab} = 0$ or $s_{ab} = p_a = q_b$, then $q_0 = p_0$ and $p_1 = \pm q_1$. Therefore assume that $s_{ab} < p_a$ for some a, b. Then $Ps_{ab}P^{-1} = s_{-a,-b} < p_{-a}$ and hence, $q_{ab} = s_{ab} \vee s_{-a,-b} < p_+ \vee p_- = 1_A$. Thus q_{ab} is an even non-trivial projection reducing ϕ , which contradicts the superirreducibility of ϕ .

If a positive map ϕ is reducible, it is not necessary decomposable into irreducible maps. Since this is a property that is needed later, it is formalized as:

Definition 8. A homogeneous positive map ϕ on a C^* -algebra A is completely reducible if for each projection p reducing ϕ , (1-p) also reduces ϕ and

$$\phi = \phi(p \cdot p) + \phi((1-p) \cdot (1-p)) . \tag{1.18}$$

Moreover, if there is no reducing projection p s.t. $\|\phi(p \cdot p)\| < \|\phi\|$, then ϕ is said to be incontractible.

A completely reducible ϕ can be decomposed into irreducible parts. Pick a projection p_1 such that $\phi_1 = \phi(p_1 \cdot p_1)$ is irreducible. Then proceed with $\tilde{\phi} = \phi((1-p_1) \cdot (1-p_1))$ until there is a set of projections $p_1, ..., p_n$ reducing ϕ such that $\sum_i p_i = 1_A$ and $\phi = \bigoplus_i \phi_i$; where $\phi_i := \phi|_{A_i}$ is irreducible and $A_i = p_i A p_i$.

If A is a superalgebra and ϕ is homogeneous, then the set of projections takes the form

 $p_1, ..., p_n = q_1, ..., q_r, s_{\pm,1}, ..., s_{\pm,\frac{n-r}{2}}$ where the q_i are even and the $s_{\pm,i}$ are parity conjugates. Hence, ϕ can also be decomposed into $r + \frac{n-r}{2}$ superirreducible maps $\bigoplus_i \phi_i$. In both cases, ϕ is incontractible if $\|\phi_i\| = \|\phi_j\|$ for all i, j. This is obviously a fine-tuned demand. However, it arises quite naturally from the applications that is made of positive maps in section 3.2.

Next are spectral considerations. The main tool here is the C^* -version of Perron-Frobenius:

Theorem 3 ([47]). If $\phi: A \to A$ is positive irreducible, then there are unique positive invertible $e, \rho \in A$ such that $\phi(e) = \|\phi\|e$ and $\phi'(\operatorname{tr}(\rho \cdot)) = \operatorname{tr}(\rho\phi(\cdot)) = \|\phi\|\operatorname{tr}(\rho \cdot)$. Moreover, the eigenvalue $\|\phi\|$ is simple.

In the following, usually only the spectrum of ϕ and not its dual ϕ' are discussed, with the understanding that they are exactly parallel, with an explicit isomorphism given by the trace inner product.

Complete reducibility allows to draw conclusions from theorem 3 in the reducible case. Assume for simplicity $\|\phi\| = 1$ and introduce the set of fixed points of ϕ , and the vector space spanned by the reducing projections,

$$\mathrm{FP}(\phi) := \{x \in A \ : \ \phi(x) = x\} \quad \text{and} \quad \mathrm{Red}(\phi) := \mathrm{span}\{p \text{ projection reducing } \phi\} \ . \tag{1.19}$$

Notice that $\operatorname{Red}(\phi)$ is a superalgebra. The projections that reduce to an irreducible ϕ are precisely the extremal points of the cone of positive elements of $\operatorname{Red}(\phi)$.

Corollary 1. Let ϕ be a superirreducible homogeneous positive map. Then, there is an invertible positive even e s.t. $\phi(e) = e$. If ϕ is reducible, it is incontractible and there is an invertible self-adjoint odd z s.t. $\phi(ze) = ze$ and $z^2 = 1$. That is, 1 is a semisimple eigenvalue of degeneracy $\mu_{\phi} + 1 = 1, 2$.

The index $\mu_{\phi} \in 0, 1$ introduced in part (i) of the lemma is used throughout to characterize positive maps. Later on, it will be related to the index introduced below theorem 2. The corollary luminates the fixed points of an incontractible completely reducible homogeneous positive ϕ . Decompose $\phi = \bigoplus_{i=1}^{r} \phi_i$ with the ϕ_i superirreducible. By theorem 3 and incontractability they have unique left, resp. right fixed points $\operatorname{tr}(\rho_i \cdot)$ and e_i . Adopt the standard normalization $||e_i|| = 1$ from which it follows⁷ that $||\rho_i||_1 = 1$. The e_i span the vector space of right fixed points $\operatorname{FP}(\phi)$. It is convenient to use a standard element:

$$e = \bigoplus_{i} e_i \tag{1.20}$$

All other right fixed points have the form $\bigoplus_i c_i e_i = (\sum_i c_i p_i) \cdot e$, with $c_i \in \mathbb{C}$ and p_i the reducing projections, and thus

$$FP(\phi) = Red(\phi) \cdot e . \tag{1.21}$$

⁷Combine the following two inequalities: (i) $|\operatorname{tr}(\rho e)|^2 = |\operatorname{tr}(\sqrt{\rho}\sqrt{\rho}e)|^2 \le \operatorname{tr}(\sqrt{\rho}^2)\operatorname{tr}|\sqrt{\rho}e|^2 \le (\|\rho\|_1\|e\|)^2$, and (ii) $\|\rho\|_1 = \sup\{|\operatorname{tr}(\rho x): \|x\| \le 1\} \le |\operatorname{tr}(\rho e)|$.

For the left fixed points, adopt a standard form in terms of weights w_i :

$$\rho = \bigoplus_{i=1}^{r} w_i \rho_i \; , \quad \sum_{i=1}^{r} w_i = 1 \; ; \tag{1.22}$$

this parameterizes the set of positive left fixed points.

Proof of corollary 1. ϕ is either already irreducible, or there is a unique pair of projections p_{\pm} reducing ϕ as in part (ii) of lemma 2. In the first case, theorem 3 applies directly and gives a simple positive invertible eigenvector e to the eigenvalue 1; by homogeneity, e is even. In the second case, complete reducibility yields $\phi = \phi_{+} \oplus \phi_{-}$, with ϕ_{\pm} irreducible. Since $P^{A} \circ \phi_{+} \circ P^{A} = \phi_{-}$, $\|\phi_{+}\| = \|\phi_{-}\| = \|\phi\|$. Hence, again by theorem 3, there are simple positive invertible e_{\pm} with $\phi_{\pm}(e_{\pm}) = \|\phi\|e_{\pm}$. Then, let $e = e_{+} \oplus e_{-}$ and $e = e_{+} \oplus (-e_{-})$.

Completely Positive Maps. More can be said for a subclass of positive maps which satisfy a stability condition:

Definition 9. For $\phi: A \to A$ and an integer n, introduce maps $\phi_{(n)} \in \mathcal{L}(\mathrm{Mat}_n(\mathbb{C}) \otimes A)$ by: $\phi_{(n)}(M \otimes x) = M \otimes \phi(x)$. Then ϕ is completely positive (c.p.), if all of the $\phi_{(n)}$ are positive.

By Stinespring's dilation theorem ([159]), c.p. maps $\phi: A \to \mathcal{L}(V)$ can be written in terms of a faithful *-representation $\pi: A \to \mathcal{L}(K)$ where w.l.o.g. $\pi(1_A) = \mathrm{id}_K$, and a bounded linear $U: K \to V$, which is isometric if ϕ is unital, as

$$\phi(x) = U^* \pi(x) U . \tag{1.23}$$

Suppose that A is a superalgebra, V a super Hilbert space and ϕ homogeneous. Then, K is a super Hilbert space as well: The parity automorphism of A is represented by a unitary on K.

Furthermore, restrict to the situation where source and target of ϕ are identical, i.e., $A = \mathcal{L}(V)$. Then the representations are of the form $\pi : \mathcal{L}(V) \to \operatorname{Mat}_d(\mathbb{C}) \widehat{\otimes} \mathcal{L}(V)$, $\pi(x) = 1 \widehat{\otimes} x$, where the first factor counts the multiplicity [48, 38]. Such maps are called homogeneous completely positive (h.c.p) maps.

Thus, pick a homogeneous basis $\psi_1,...,\psi_d \subset \mathbb{C}^d$ and operators $E_1,...,E_d \subset \mathcal{L}(V)$ with $|E_s| = |\psi_s|$ to write $U\xi = \sum_s \psi_s \widehat{\otimes} (E_s)^* \xi$. This allows to get the more explicit form

$$\phi(x) \equiv \phi_E(x) \equiv \mathbb{E}(x) = \sum_{s=1}^d (-1)^{|E_s||x|} E_s x(E_s)^* . \tag{1.24}$$

There is some lavishness in using three different symbols for the same map; this is done to interpolate between general statements and the explicit considerations done in the main part of the work, dealing with h.c.p. maps originating in the world of super matrix product states.

In this context, the E_s are called the *Kraus operators* and the closed subsuperalgebra generated by them the *Kraus algebra* A(E).

For h.c.p. maps, there is a connection of the supercommutant $\mathscr{Z}(E) := A(E)^{\#} \subset \mathscr{L}(V)$ and projections reducing said h.c.p. map.

Lemma 3. Let $\phi = \phi_E$ be a completely reducible, incontractible, h.c.p. map. Then

- (i) $\operatorname{Red}(\phi_E) = \mathscr{Z}(E)$.
- (ii) $\mathscr{Z}(E)^1 \cap A(E) = \{0\}.$

In combination with part (ii) of corollary 1, this gives

$$FP(\phi_E) = \mathscr{Z}(E) \cdot e \ .$$
 (1.25)

Proof.

(i)" \subseteq ": Any $x \in \text{Red}(\phi)$ can be decomposed as $x = \sum_a c_a p_a$ where p_a is a projection. Therefore, it suffices to show that all of the projections are in the supercommutant. So, pick a projection p reducing ϕ and homogeneous $\xi_1, \xi_2 \in V$. Then:

$$\langle \xi_1, (1-p)\phi(p|\zeta)\langle \zeta|p)(1-p)\xi_2 \rangle =$$

$$= \sum_{|E_s|=0} |\langle \xi_1, (1-p)E_s p \xi_2 \rangle|^2 + \sum_{|E_s|=1} |\langle \xi_1, (1-p)E_s (p_0-p_1)\xi_2 \rangle|^2 .$$

If p reduces ϕ , then the left hand side of this equation is zero, and hence, as the right-hand side is a sum of positive terms, it follows that $pE_s = E_s(p_0 + (-1)^{|E_s|}p_1)$. Then p is in the supercommutant: $px = \sum_{\mu,\nu=0,1} (-1)^{\mu\nu} x_{\mu} p_{\nu}$ for all x in the Kraus algebra.

(i)" \supseteq ": In virtue of being a finite-dimensional C^* -algebra, $\mathscr{Z}(E)$ is generated by its projections. Hence, focus on a projection p in the supercommutant.

A positive map ϕ is reduced by p, if and only if there is a positive real number r s.t. $\phi(p) \leq rp$ ([47]). Now, let $z = z_0 + z_1$ be in the supercommutant. By direct computation, for ϕ in the Kraus form of equation 1.24:

$$\phi(z) = \sum_{s} \left[E_s z_0(E_s)^* + (-1)^{|E_s|} E_s z_1(E_s)^* \right] = z\phi(1) = z . \tag{1.26}$$

So in fact the supercommuting operators are fixed points of ϕ . By taking z to be a projection, the result follows.

(ii) This follows since
$$\mathscr{Z}(E)^1 \cap A(E)$$
 is the supercenter of $A(E)$.

For ϕ positive and $\|\phi\| = 1$, the peripheral spectrum of ϕ is:

$$Per(\phi) := \{x : \phi(x) = \lambda x \text{ for } |\lambda| = 1\} \supseteq FP(\phi) . \tag{1.27}$$

If the inclusion is an equality, ϕ is called *strongly completely reducible*. If ϕ is additionally (super-)irreducible, it is called *strongly (super-)irreducible*.

For completely positive maps, there is the Kadison-Schwarz inequality [126, 31], proven for completeness in the appendix, $\phi(x^*x) \ge \phi(x^*)\phi(x)$. This allows to prove that $\operatorname{Per}(\phi)$ is a group [47]. Then by finite-dimensionality, there is an integer n such that $\operatorname{Per}(\phi^n) = \operatorname{FP}(\phi^n)$. In the physical applications that are considered here, it is always permissible to effectively replace $\phi \to \phi^n$, which corresponds to enlarging the unit cell. A non-trivial peripheral spectrum translates to breaking of translation invariance in spin chains [50].

Furthermore, strongly (super-)irreducible completely positive maps are dense in the set of all completely positive maps [49]. For these reasons, completely positive maps with non-trivial peripheral spectrum are absent from further discussion.

Iterating. After investigating the set of fixed points, turn the attention to the sequence $\{\phi^n\}_n$. As $n \to \infty$, and in finite dimensional algebras, this converges to the projector on the set of fixed points. For later applications it is incumbent to characterize the speed with which this happens.

Recall that the $index \operatorname{ind}_{\lambda}(\phi)$ of an eigenvalue λ of a linear operator ϕ is the dimension of the largest Jordan block corresponding to λ in the decomposition of ϕ along its eigenspaces. Relatedly, let the index of an operator ϕ be the maximum of the indices of the eigenvalues of ϕ ,

$$\operatorname{ind}(\phi) := \max\{\operatorname{ind}_{\lambda}(\phi) : \lambda \text{ in the spectrum of } \phi\}.$$
 (1.28)

Furthermore, for ϕ a contraction introduce the gap δ_{ϕ} :

$$1 - \delta_{\phi} := \sup\{|\lambda| : \lambda \neq 1 \text{ in the spectrum of } \phi\}. \tag{1.29}$$

Proposition 1. Let $\phi: A \to A$ be a positive contraction. Then $\operatorname{ind}_1(\phi) = 1$. If ϕ is strongly completely reducible, then $\phi^{\infty} := \lim_{n \to \infty} \phi^n$ exists and

$$\|\phi^n - \phi^{\infty}\| \le C n^{\operatorname{ind}(\phi) - 1} (1 - \delta_{\phi})^n$$
 for $n > 2$ ind (ϕ) .

Moreover, if $ind(\phi) = 1$, then

$$\|\phi^n - \phi^\infty\| < (1 - \delta_\phi)^n$$
.

Finally, if $\phi = \phi_E$ is h.c.p. and completely reducible, then

$$\phi^{\infty}(x) = \sum_{a} \operatorname{tr}(\rho z_{a} x) \ z_{a} e = \sum_{a} \operatorname{str}(\Lambda z_{a} x) \ z_{a} e \ , \tag{1.30}$$

where $\{z_a\}_a$ are a set of self-adjoint homogeneous elements of $\mathscr{Z}(E)$ such that z_a is a projection if it is even, otherwise $(z_a)^2$ is a projection. Here, $\operatorname{str}(\Lambda \cdot) := \operatorname{tr}(\rho \cdot)$.

Remark 1. Maps with $ind(\phi) = 1$ are important in this work. Recall that such operators are called diagonalizable, and are dense in the set of all operators.

Proof. For the first part, consider ϕ in its Jordan normal form, i.e.,

$$\phi = \sum_{\lambda} (\lambda P_{\lambda} + R_{\lambda}) ,$$

where the sum extends over the spectrum of ϕ . Here, the P_{λ} are disjoint projections, the R_{λ} are nilpotent of order $\operatorname{ind}_{\lambda}(\phi)$. They satisfy the relations $P_{\lambda_1}R_{\lambda_2}=R_{\lambda_2}P_{\lambda_1}=\delta_{\lambda_1\lambda_2}R_{\lambda_1}$. Using the convention $\binom{a}{b}=0$, if b>a:

$$\phi^n = \sum_{\lambda} \sum_{\alpha=0}^{\operatorname{ind}_{\lambda}(\phi)-1} \binom{n}{\alpha} \lambda^{n-\alpha} P_{\lambda}(R_{\lambda})^{\alpha}$$

To show that $1(\phi) = 1$, assume $R_1 \neq 0$. Then pick $x \in \text{im}(P_1)$ s.t. $R_1(x) \neq 0$ but $(R_1)^2(x) = 0$. Then $\phi^n(x) = x + nR_1(x)$, which contradicts ϕ being a contraction. Let n > 2 ind (ϕ) and $x \in A$,

$$\|\phi^{n}(x) - P_{1}(x)\| = \left\| \sum_{\lambda \neq 1} \sum_{\alpha = 0}^{\operatorname{ind}_{\lambda}(\phi) - 1} \binom{n}{\alpha} \lambda^{n - \alpha} P_{\lambda}(R_{\lambda})^{\alpha}(x) \right\| =$$

$$= \sup \left\{ \binom{n}{\alpha} |\lambda|^{n - \alpha} \|P_{\lambda}(R_{\lambda})^{\alpha}(x)\| : \lambda \neq 1 , \alpha < \operatorname{ind}_{\lambda}(\phi) \right\} \leq$$

$$\leq \sup \left\{ \binom{n}{\alpha} |\lambda|^{n - \alpha} : \lambda \neq 1 , \alpha < \operatorname{ind}(\phi) \right\} \|x\| \leq$$

$$\leq \sup \left\{ \binom{n}{\alpha} : \alpha < \operatorname{ind}(\phi) \right\} \sup \left\{ |\lambda|^{n - \alpha} : \lambda \neq 1 , \alpha < \operatorname{ind}(\phi) \right\} \leq$$

$$\leq \binom{n}{\operatorname{ind}(\phi) - 1} (1 - \delta_{\phi})^{n - \operatorname{ind}(\phi) + 1} \|x\| .$$

Using the bound $\binom{n}{k} \leq \left(\frac{ne}{k}\right)^k$:

$$\|\phi^n(x) - P_1(x)\| \le \left(\frac{ne}{\operatorname{ind}(\phi) - 1}\right)^{\operatorname{ind}(\phi) - 1} (1 - \delta_\phi)^{n - \operatorname{ind}(\phi) + 1} \|x\|.$$

If $\operatorname{ind}(\phi) = 1$, the spectral representation is simplified to

$$\|\phi^n(x) - P_1(x)\| = \left\| \sum_{\lambda \neq 1} \lambda^n P_{\lambda} \right\| = \sup\{|\lambda|^n : \lambda \neq 1\} = (1 - \delta_{\phi})^n.$$

For the explicit form of ϕ^{∞} , use equation 1.25.

Completely positive maps are, by Stinespring's dilation theorem cited above, the composition of a representation on some auxiliary space, and an isometry. This auxiliary space

allows to consider variations of the given map.

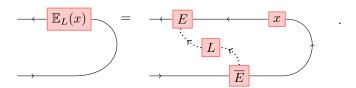
For $\phi = U\left[1_{\mathbb{C}^d}\widehat{\otimes}(\cdot)\right]U^* \in \mathscr{L}^2(V)$ a h.c.p. map and $L \in \operatorname{Mat}_d(\mathbb{C})$, consider:

$$\phi[L](x) \equiv \phi_E[L](x) \equiv \mathbb{E}_L(x) := U\left[L\widehat{\otimes}x\right] U^* =$$

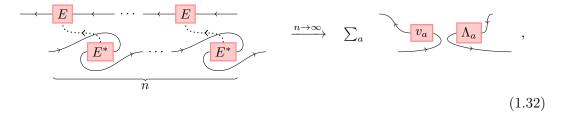
$$= \sum_{s,t=1}^d (-1)^{|E_t||x|} \langle \psi_s, L(\psi_t) \rangle E_s x(E_t)^* . \tag{1.31}$$

There is a convenient way of expressing these maps. Represent E by a tensor diagram as

In fact it is often useful to use also \overline{E} which is obtained from E by reversing all the arrows. For example, the operators \mathbb{E}_L of equation 1.31 are presented diagrammatically as



The limit formula 1.30 for example is expressed diagrammatically as



using the shorthand $v_a = z_a e$ and $\Lambda_a = \Lambda z_a$.

Furthermore, define maps $\mathbb{E}_{\mathcal{O}} \equiv \phi_{E,n}[\mathcal{O}]$ for $\mathcal{O} \in \operatorname{Mat}_d(\mathbb{C})^{\widehat{\otimes}n}$ as the linear extensions of

$$\phi_{E,n}[L_1\widehat{\otimes}\cdots\widehat{\otimes}L_n](x) := \phi_E[L_1]\circ\cdots\circ\phi_E[L_n](x) . \tag{1.33}$$

Lemma 4. Let $\phi = \phi_E$ be h.c.p. Consider for $x \in \mathcal{L}(V)$ and $f \in \mathcal{L}(V)^*$:

$$\phi_{E,x,n}: \operatorname{Mat}_d(\mathbb{C})^{\widehat{\otimes} n} \to \mathcal{L}(V) , \quad \phi_{E,x,n}(\mathcal{O}) = \phi_{E,n}[\mathcal{O}](x) ;$$
 (1.34)

$$\phi_{E,f,n}: \operatorname{Mat}_d(\mathbb{C})^{\widehat{\otimes} n} \to \mathcal{L}(V)^* , \quad \phi_{E,f,n}(\mathcal{O}) = f \circ \phi_{E,n}[\mathcal{O}] .$$
 (1.35)

Then $\phi_{E,x,n}$ or $\phi_{E,f,n}$ are positive and homogeneous if x respectively f are.

Proof. The proof shows the statement only for $\phi_{E,x,n}$, as the other result is strictly analogous.

The first step is to show, by induction in n, that, for $\mathcal{O} \in \operatorname{Mat}_d(\mathbb{C})^{\widehat{\otimes} n}$ and x even:

$$\phi_{E,n,x}(\mathcal{O}) = \sum_{\substack{s_1 \cdots s_n \\ r_1 \cdots r_n}} \langle \psi_{s_1} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_n}, \mathcal{O}(\psi_{r_1} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{r_n}) \rangle E_{s_1} \cdots E_{s_n} x (E_{r_1} \cdots E_{r_n})^* . \quad (1.36)$$

Indeed, the case n=1 is clear so assume the statement to be true for k=1,...,n-1. Consider operators $L\widehat{\otimes}\mathcal{O}_{n-1}\in \mathrm{Mat}_d(\mathbb{C})\widehat{\otimes}\mathrm{Mat}_d(\mathbb{C})^{\widehat{\otimes}(n-1)}$. Then:

$$\phi_{E}[L] \circ \phi_{E,x,n-1}(\mathcal{O}_{n-1}) = \sum_{s,r} (-1)^{|\psi_{r}||\mathcal{O}|} \langle \psi_{s}, L\psi_{r} \rangle \times$$

$$\times \sum_{\substack{s_{1} \cdots s_{n-1} \\ r_{1} \cdots r_{n-1}}} \langle \psi_{s_{1}} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_{n-1}}, \mathcal{O}_{n-1}(\psi_{r_{1}} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{r_{n-1}}) \rangle E_{s} E_{s_{1}} \cdots E_{s_{n-1}} x (E_{r_{1}} \cdots E_{r_{n-1}})^{*} (E_{r})^{*}.$$

The statement follows by observing that

$$(-1)^{|\psi_r||\mathcal{O}|} \langle \psi_s, L\psi_r \rangle \langle \Psi_1, \mathcal{O}\Psi_2 \rangle = (-1)^{|\psi_r||\mathcal{O}|} \langle \psi_s \widehat{\otimes} \Psi_1, L\psi_r \widehat{\otimes} \mathcal{O}\Psi_2 \rangle =$$
$$= \langle \psi_s \widehat{\otimes} \Psi_1, (L \widehat{\otimes} \mathcal{O})(\psi_r \widehat{\otimes} \Psi_r) \rangle .$$

The second step is to become convinced that the expression in equation 1.36 is positive whenever \mathcal{O}, x are positive. Let \mathcal{O}_1, x_1 s.t. $\mathcal{O} = (\mathcal{O}_1)^* \mathcal{O}_1$ and $x = x_1(x_1)^*$. Then:

$$\mathbb{E}_{\mathcal{O}}(1_A) = \sum_{t_1, \dots, t_n} X_{t_1 \dots t_n} (X_{t_1 \dots t_n})^* \ge 0 ;$$
where $X_{t_1 \dots t_n} := \sum_{s_1 \dots s_n} \langle \mathcal{O}_1(\psi_{s_1} \widehat{\otimes} \dots \widehat{\otimes} \psi_{s_n}), \psi_{t_1} \widehat{\otimes} \dots \widehat{\otimes} \psi_{t_n} \rangle E_{s_1} \dots E_{s_n} x_1 .$

The discussion is finished by describing some relations between various cute properties of the objects introduced in this section, all parametrized by one tensor E.

Lemma 5. Suppose $\phi = \phi_E$ is a h.c.p. map. Then t.f.a.e.:

- (i) $A(E) = A(E)^*$.
- (ii) A(E) is a C^* -subsuperalgebra of $\mathcal{L}(V)$.
- (iii) A(E) is semisimple.
- (iv) ϕ is strongly completely reducible.
- (v) For $x \in A(E)$ invertible, the image of the family $(\phi_{E,x,n})_n$ exhausts A(E).
- (vi) For $f \in A(E)^*$ non-degenerate, the image of the family $(\phi_{E,f,n})_n$ exhausts $A(E)^*$.

Furthermore, t.f.a.e.:

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- (vii) ϕ_E is strongly superirreducible.
- (viii) A(E) is supercentral supersimple.

Proof.

- (i) \Rightarrow (ii): Except the closure under the star, A(E) already inherited all properties from $\mathcal{L}(V)$.
- (ii) \Rightarrow (iii): This is as finite-dimensional C^* -algebras are isomorphic to direct sums of matrix algebras [38].
- (iii) \Leftrightarrow (iv): Decompose $E_s = \bigoplus_a E_{a,s}$ into its simple components which gives $\phi = \bigoplus_a \phi_{E_a}$. But $A(E_a)$ is simple and central, so that ϕ_{E_a} is strongly irreducible ([141], also (vii) \Rightarrow (viii) below, after trivializing the grading). The implications can be traced backwards.
- $(iii) \Rightarrow (i)$: A(E), being a direct sum of matrix algebras, is closed under the adjoint.
- (i) \Leftrightarrow (v),(vi): If $A(E)^* = A(E)$ then the span of $E_{s_1} \cdots E_{s_n}$ is the same as

$$E_{s_1}\cdots E_{s_n}(E_{t_n})^*\cdots (E_{t_1})^*$$
.

Conversely if these two spans agree, they are closed under the star since the latter is.

(vii) \Leftrightarrow (viii): Any two-sided superideal I gives a projection p_I reducing ϕ_E , so A(E) has to be supersimple. Furthermore, by lemma 3 there is a 1 : 1 correspondence between the supercenter of A(E) and projections reducing ϕ_E , so supercentrality and superirreducibility are equivalent.

In the case where A(E) is supercentral supersimple but not central simple, the η heralded in theorem 2 can be given in terms of quantities already introduced. Let P be the parity operator in $\mathcal{L}(V)$ and ze the odd fixed point of ϕ . Then $\eta = -iPz$. This implies that the indices introduced below theorem 2 and in corollary 1 agree for a strongly superirreducible h.c.p. map ϕ_E :

$$\mu_{A_E} = \mu_{\phi_E} . \tag{1.37}$$

Since ϕ_E being strongly superirreducible, A(E) supersimple etc. can be read off from the tensors E, they are called the respective property; i.e., E is called supersimple if it generates a supersimple A(E) etc.

1.3. G-Actions

All of the objects introduced in the previous section are endowed with the action of a group G, with the relevant case being some $g \in G$ acting by anti-unitaries. The type of group considered is restricted by

Definition 10. A symmetry group (G, \mathfrak{p}) is a compact group G together with a group homomorphism $\mathfrak{p}: G \to \mathbb{Z}_2$.

Later on, the unitary part will mostly be ignored, and the important part will be whether, and which, anti-unitary symmetries are present.

As mentioned above, fermion parity is always present and not included in G. The group homomorphism \mathfrak{p} is used to keep track of whether a given operation reverses the flow of time, i.e., whether it is represented by anti-unitaries. Since the reversal of time is an involution on observables, this restricts the form.

Relatedly, denote the action of \mathbb{Z}_2 on \mathbb{C} by complex conjugation as

$$\overline{(\cdot)}^r : z \mapsto \begin{cases} z & r = 0 , \\ \overline{z} & r = 1 . \end{cases}$$
(1.38)

Definition 11. For V a vector space, a projective representation of a symmetry group G is a map $\alpha: G \to \operatorname{Aut}(V)$ such that (i) α_g is \mathfrak{p} -linear, meaning $\alpha_g(z\xi) = \overline{z}^{\mathfrak{p}(g)}\alpha_g(\xi)$ for $\xi \in V$ and z a scalar; (ii) $\alpha_1 = \operatorname{id}_V$ and (iii) $\alpha_{g_1}\alpha_{g_2} = v(g_1, g_2)\alpha_{g_1g_2}$ where $v: G \times G \to U(1)$ is a function that satisfies

$$1 = dv(g_1, g_2, g_3) := \frac{v(g_1, g_2 g_3) \overline{v(g_2, g_3)}^{\mathfrak{p}(g_1)}}{v(g_1, g_2) v(g_1 g_2, g_3)} . \tag{1.39}$$

If V is normed, demand that the representation is isometric, $\|\alpha_g(\xi)\| = \|\xi\|$. If V is super, α_g should have a definite fermion parity $\alpha_g(P) =: (-1)^{|\alpha_g|} P$.

The easiest case of a projective representation is when there is a function $\phi: G \to U(1)$ such that

$$v(g_1, g_2) = d\phi(g_1, g_2) := \frac{\phi(g_1)\overline{\phi(g_2)}^{\mathfrak{p}(g_1)}}{\phi(g_1 g_2)}, \qquad (1.40)$$

which solves equation 1.39. Then the function v is eliminated by choosing $\tilde{\alpha}_g := \phi(g)\alpha_g$. A projective representation with trivial or trivializable (by a redefinition) v is called a *(proper) representation* of G, and sometimes the term "projective representation" is reserved the situations where v cannot be eliminated. When $v \neq d\phi$, equation 1.39 ensures associativity, $\alpha_{g_1}(\alpha_{g_2}\alpha_{g_3}) = (\alpha_{g_1}\alpha_{g_2})\alpha_{g_3}$. If $|\alpha_g| = 0$ for all g, the representation is called *even*.

Suppose that A is a C^* superalgebra carrying a proper (G, \mathfrak{p}) -representation α , and ω is a G-invariant state on A. Then by the uniqueness of the Gel'fand construction 1.1 there is a projective representation $\widehat{\alpha}: (G, \mathfrak{p}) \to \operatorname{Aut}(\mathcal{H}_{\omega})$ such that

$$\pi_{\omega} \circ \alpha_g(x) = (-1)^{|\widehat{\alpha}_g||x|} \widehat{\alpha}_g \pi(x) \widehat{\alpha}_g^{-1}$$
.

The study of completely positive maps on $\mathcal{L}(V)$ has revealed that they should be studied in terms of auxiliary (here, in strict inversion of the later dependencies) vector spaces \mathcal{H} .

Definition 12. A tensor $E: \mathcal{H} \to \mathcal{L}(V)$ is G-symmetric if there is an even representation $\alpha^{\mathcal{H}}: G \to \operatorname{Aut}(\mathcal{H})$, and a projective homogeneous representation $\alpha^{V}: G \to \operatorname{Aut}(V)$ satisfying the equivariance condition

$$sAd_{\alpha^{H}} \circ E = E \circ \alpha^{\mathcal{H}}, \quad sAd_{u}(w) := (-1)^{|w||u|} uwu^{-1}; \tag{1.41}$$

For simplicity use the abbreviations $\alpha^{\mathcal{H}} = \alpha$ and $\alpha^{V} = \widehat{\alpha}$.

This definition allows to lift symmetry action between the two spaces, in the following way:

$$\mathbb{E}_{\mathrm{sAd}_{\alpha_q}(L)} = \mathrm{sAd}_{\widehat{\alpha}_q} \circ \mathbb{E}_L \circ (\mathrm{sAd}_{\widehat{\alpha}_q})^{-1} . \tag{1.42}$$

Hence, if z is a fixed point of \mathbb{E} , so is $\operatorname{sAd}_{\widehat{\alpha}_q}(z)$.

Equation 1.41 has also diagrammatic representation, where, however, one strictly has to differentiate between (i) the unitary and (ii) the anti-unitary case. Case (i) is quite easy: for a given unitary operation α and its lift $\hat{\alpha}$, there is the equivariance condition

$$E(\alpha\psi) = (-1)^{|\widehat{\alpha}||\psi|} \widehat{\alpha} E(\psi) \widehat{\alpha}^{-1} , \qquad (1.43)$$

To deal with the second possibility, one first has to introduce a bit more machinery.

Anti-Linear Structrures on Super Vector Spaces. Consider a super Banach space $(V, \|\cdot\|)$ together with a homogeneous anti-linear, isometric $K: V \to V$, i.e. $KV^{\mu} = V^{\mu+k}$, $K(z\xi) = \overline{z}K(\xi)$ and $\|K(\xi)\| = \|\xi\|$. If V is a super Hilbert space, the last condition is $\langle K(\xi_1), K(\xi_2) \rangle = \overline{\langle \xi_1, \xi_2 \rangle}$, that is, K is anti-unitary. Demand that Ad_K is an involution on the even operators.

The first possibility is that Ad_K is already an involution, which allows for $K^2 = z1$ with z a unit complex number. However, it is easy to see that $z = (-1)^{\epsilon_K}$, by using $zK = K^3 = Kz$. In the $\epsilon_K = 0$ case, K is a real structure, while in the $\epsilon_K = 1$ case it is a quaternionic structure, and V is called a real or a quaternionic vector space, respectively. The terminology acquires its justification as K permits to view V as a vector space over the real or quaternionic numbers, respectively:

- \mathbb{R}) Any complex vector space can be seen as a real vector space as $\mathbb{R} \subseteq \mathbb{C}$, but not canonically so. If V is equipped with a real structure, $K^2 = 1$, introduce the real vector space of fixed points of K, $V_{\mathbb{R}} = \operatorname{Fix}(K)$, and a complex structure on $V_{\mathbb{R}} \oplus V_{\mathbb{R}}$ by J(x,y) = (-y,x). Then $V \cong (V_{\mathbb{R}} \oplus V_{\mathbb{R}}, J)$.
- \mathbb{H}) To give V the structure of a quaternionic vector space it is necessary to define an associative and distributive multiplication of quaternions $q \in \mathbb{H}$ with vectors $\xi \in V$. This is possible by an anti-linear K with $K^2 = -1$. Denote the imaginary units as i, j, k. Scalar multiplication with $q = (q_0 + iq_1) + (q_2 + iq_3)j$ is

$$q\xi = (z + wj) \cdot \xi := z\xi + wK(\xi) . \tag{1.44}$$

Associativity $q_1(q_1\xi) = (q_1q_2)\xi$ follows since the imaginary units anticommute.

The second possibility is that $K^2 = zP$. This can be rearranged to show that $(-1)^k = KPK^{-1}P^{-1} = z^2$. There are two roots for z, but they can be exchanged by a redefinition $P \to -P$.

It turns out to be more convenient to group (k, z) into one number as

$$\exp(i\pi q_K/2) := zi^k .$$

If $K^2 = zP$, then $\exp(i\pi q_K/2) = (-1)^k$. The possible values for q_K are tabulated here:

$K^2 = z$			$K^2 = zP$	
$(-1)^{\epsilon}$	$(-1)^{k}$	q	$(-1)^k$	q
1	1	0	1	0
1	-1	1		
-1	1	2	-1	2
-1	-1	3		

Anti-linear operation of the the first kind are referred to as particle-hole transformations and denoted by C, while those of the second kind are called motion-reversal transformations and indicated by the letter T.

These anti-linear operations, together with the Hilbert structure, allow to introduce non-degenerate bilinear forms on V, which play decisive rôles in this work.

An obvious way of obtaining a bilinear form on V is the following: $(\xi_1, \xi_2) \mapsto \langle K(\xi_1), \xi_2 \rangle$. However, this expression is impractical, since it does not behave well under tensor products. To see this, write down the natural tensor product of two bilinear forms (V_1, κ_1) and (V_2, κ_2) :

$$[\kappa_1 \widehat{\otimes} \kappa_2](v_1 \widehat{\otimes} v_2, w_1 \widehat{\otimes} w_2) := (-1)^{|v_2||w_1| + k_2(|v_1| + |w_1|)} \kappa_1(v_1, w_1) \kappa_2(v_2, w_2) , \qquad (1.45)$$

where $k_i = |\kappa_i|$.

Now a short calculation shows that the naïve choice of bilinear form does not satisfy this:

$$\langle [K_1 \widehat{\otimes} K_2](\xi_1 \widehat{\otimes} \zeta_1), \xi_2 \widehat{\otimes} \zeta_2 \rangle = (-1)^{k_2|\xi_1|} \langle K_1(\xi_1) \widehat{\otimes} K_2(\zeta_1), \xi_2 \widehat{\otimes} \zeta_2 \rangle =$$

$$= (-1)^{k_2|\xi_1|} \langle K_1(\xi_1), \xi_2 \rangle \langle K_2(\zeta_1), \zeta_2 \rangle .$$

This non-super factorization produces all kinds of inconveniences on tensor products and, consequently, in diagrams.

Doubling down on the introduction of super hermitian structures of definition 3, define the following canonical bilinear form on a super Hilbert space (V, h) with anti-unitary K:

$$\kappa(\xi_1, \xi_2) := h(K(\xi_1), \xi_2) = i^{q(|K(\xi_1)|)} \langle K(\xi_1), \xi_2 \rangle.$$
(1.46)

Write τ and χ instead of κ to indicate that a bilinear form is induced from a motion-reversal or a particle-hole type transformation, respectively.

With this definition, $\kappa_{12} = \kappa_1 \widehat{\otimes} \kappa_2$: Then using $|K(v_i)| = |w_i|$:

$$\begin{split} \kappa_{12}(\xi_{1}\widehat{\otimes}\zeta_{1},\xi_{2}\widehat{\otimes}\zeta_{2}) &:= i^{|\xi_{2}\widehat{\otimes}\zeta_{2}|} \left\langle [K_{1}\widehat{\otimes}K_{2}](\xi_{1}\widehat{\otimes}\zeta_{1}) , \xi_{2}\widehat{\otimes}\zeta_{2} \right\rangle = \\ &= i^{|\xi_{2}|} i^{|\zeta_{2}|} (-1)^{|\xi_{2}||\xi_{2}|+k_{2}|\xi_{1}|} \left\langle K_{1}(\xi_{1}) , \xi_{2} \right\rangle \left\langle K_{2}(\zeta_{1}) , \zeta_{2} \right\rangle = \\ &=: (-1)^{|\xi_{2}||\zeta_{2}|+k_{2}|\xi_{1}|} \kappa_{1}(\xi_{1},\xi_{2}) \kappa_{2}(\zeta_{1},\zeta_{2}) \;. \end{split}$$

Resting assured that κ behaves well under tensor products, it can be put into the tensor diagram language as $\xi_1 \longrightarrow \kappa \longrightarrow \xi_2 = (-1)^{k|\xi_1|} \kappa(\xi_1, \xi_2)$.

This diagram can be read in all directions; importantly, consider κ as an isomorphism $V \to V^*$:

$$(\kappa \xi_1)(\xi_2) := \kappa(\xi_1, \xi_2) .$$
 (1.47)

The adjoint map $\kappa^*: V^* \to V$ is defined, as usual, as

$$\langle \kappa^* \varphi , \xi \rangle_V := \langle \varphi , \kappa \xi \rangle_{V^*} . \tag{1.48}$$

This is useful as $\kappa \kappa^* = \mathrm{id}_{V^*}$ and $\kappa^* \kappa = \mathrm{id}_{V}$.

Since the anti-linear operations are of a special form, the bilinear forms have symmetry properties. Note first that

$$\kappa(v,w) = i^{|K(v)|} \langle K(v), w \rangle = i^{|K(v)|} \langle K^*(w), v \rangle = i^k (-1)^{|k||v|} \left[i^{|K(w)|} \langle KK^*K^*(w), v \rangle \right] = i^k (-1)^{|k||v|} \kappa((K^*)^2 w, v) , \qquad (1.49)$$

where the anti-unitarity was used. Now, for the two relevant cases:

$$\tau(v,w) = \overline{z_T} i^{k_T} (-1)^{k_T|v|+|w|} \tau(w,v) = \exp(-i\pi q_T/2) (-1)^{|v||w|} \tau(w,v) , \qquad (1.50)$$

$$\chi(v,w) = i^{k_C} (-1)^{k_C|v|} \chi(w,v) = \exp(-i\pi q_C/2) (-1)^{|v||w|} \chi(Pw,v) . \tag{1.51}$$

For diagrams, it is more useful to use the isomorphism $\kappa':V^{**}\to V^*$ obtained by dualizing. Then:

$$\longrightarrow \chi' \longrightarrow = \exp(-i\pi q_C/2) \longrightarrow \chi \longrightarrow P \longrightarrow$$
 (1.53)

The conjugate diagrams are:

$$(-1)^k \leftarrow \tau^{*\prime} \rightarrow = \leftarrow \tau^{\prime*} \rightarrow = (-1)^k \leftarrow \tau^* \rightarrow \cdots$$

$$(1.54)$$

$$(-1)^k \leftarrow \chi^{*\prime} \rightarrow = \leftarrow \chi^{\prime*} \rightarrow = \exp(i\pi q_C/2) \leftarrow P \leftarrow \chi^* \rightarrow \qquad (1.55)$$

Induced Anti-linear Structures on Superalgebras. If $A \subseteq \mathcal{L}(V)$ and V carries a homogeneous antilinear map K, then $\Gamma(x) = \mathrm{sAd}_K(x) = (-1)^{k|x|} KxK^{-1}$ is an antilinear structure on A.

Definition 13. A complex superalgebra A is called real if there is an anti-linear involutive even automorphism Γ . A is called graded real if there is an anti-linear automorphism Γ that squares to the parity on A: $\Gamma^2(x) = (-1)^{|x|}x$.

If A is a C^* -algebra, Γ is demanded to be compatible with the *-structure, and is hence an isometry.

Heed the choice of words here: A real algebra is an algebra over \mathbb{C} with an antilinear involution – an algebra over the reals is called an algebra over \mathbb{R} . There is also the possibility to define the term "real algebra" to refer to an algebra over the reals, and such is the habit in algebra proper. The convention here, on the other hand, is more common among the C^* -community, and is adopted as for physical reasons, complex vector spaces, complex algebras are the primitive objects, from which the vector spaces and algebras over the real numbers emerge in certain contexts. A source on C^* -algebras over the real numbers is [137].

All real central simple algebras are isomorphic to $\operatorname{Mat}_n(\mathbb{R})$ or $\operatorname{Mat}_n(\mathbb{H})$ [33, p. 137ff.]. For a real supercentral supersimple algebra, introduce an index:

$$\varepsilon_A := \begin{cases} 0 & \text{if either } A \text{ or } A^0 \text{ is isomorphic to } \mathrm{Mat}_n(\mathbb{R}) \ , \\ 1 & \text{if either } A \text{ or } A^0 \text{ is isomorphic to } \mathrm{Mat}_n(\mathbb{H}) \ . \end{cases}$$

Finally, for a *-representation of A on a Hilbert space V, the parity on A is induced by a parity operator P on V. Then, define $(-1)^{k_A} := \Gamma(P)$. Thus, there are three \mathbb{Z}_2 indices for real supercentral supersimple algebras, giving $8 = 2^3$ possibilities. That these possibilities are actually realized can be demonstrated by considering Clifford algebras [57, 7].

All graded real supercentral supersimple algebra (A, Γ) are actually already central simple: Suppose A^0 is central simple and let η be the central odd element given by theorem 2. Then η and $\Gamma(\eta)$ are non-zero, linearly independent (by Wigner's theorem) and both central and odd, so that $\Gamma(\eta)\eta$ is a non-trivial even central element.

In the following, the (graded) real structure is used to define a graded linear antiautomorphism on $A = \mathcal{L}(V)$. To that end, recall that an antilinear K on V combines with a super hermitian structure on V to a graded bilinear form κ , as defined in equation 1.46, which in turn gives linear isomorphisms $\kappa: V \to V^*$ and $\kappa^*: V^* \to V$ as in equations 1.47 and 1.48. These define a graded transpose on A, that is, a linear antiautomorphism on A.

Combining the dual of definition 2 with the κ -isomorphisms $V \cong V^*$ therefore produces a linear graded anti-automorphism, a graded transpose:

Definition 14. Suppose L is a linear operator on a super Hilbert space with a graded bilinear form κ . Then the graded transpose is the linear map $L \mapsto L^t$ defined by

$$L^t := (-1)^{|\kappa||L|} \kappa^* \circ L' \circ \kappa , \qquad (1.56)$$

This is conveniently expressed diagrammatically:

$$-\longleftarrow \underline{L^t} \longrightarrow = (-1)^{k|L|} \longrightarrow \kappa^* \longrightarrow \underline{L'} \longrightarrow \kappa \qquad (1.57)$$

Since κ and dualization factors under super tensor products:

$$(a\widehat{\otimes}b)^t = a^t\widehat{\otimes}b^t.$$

To derive an expression for L^t in terms of K, first express equation 1.56 in terms of the bilinear form κ as

$$\kappa(L^t v, w) = (\kappa L^t v)(w) = (-1)^{|\kappa||L|} (L'(\kappa v))(w) = (-1)^{|L||v|} \kappa(v, Lw) . \tag{1.58}$$

Using furthermore the relations between the graded hermitian form, the bilinear form and the inner product on a super Hilbert space:

Hence:

$$L^{t} = (-i)^{|L|} (-1)^{k|L|} K L^{*} K^{-1} . {(1.59)}$$

This formula simplifies to make certain observation about the algebraic nature of this graded transpose:

$$L^{\text{tt}} = (-1)^{|L|} K^2 L K^{-2} . {(1.60)}$$

If V is a super Hilbert space, note the following relation between dualization and taking the Hilbert space adjoint for a map $L: V \to W$:

$$(L^*)' = (-1)^{|L|}(L')^* . (1.61)$$

This equation will be useful later. It is shown by explicit calculation:

$$\begin{split} \left\langle (L')^*\varphi \ , \psi \right\rangle_{W^*} &= (-1)^{|L||\psi|} \left\langle \varphi \ , \psi \circ L \right\rangle_{V^*} = \\ &= (-1)^{|L||\psi|} \left\langle \varphi \circ L^* \ , \psi \right\rangle_{W^*} = (-1)^{|L|} \left\langle (L^*)'\varphi \ , \psi \right\rangle \ . \end{split}$$

The notion of a transpose now allows to return to the quest of finding diagrammatic expressions for the anti-unitary case of 1.41 postponed above. Indeed, assume an anti-linear K and its lift \hat{K} satisfy the equivariance condition,

$$E(K\psi) = (-1)^{\widehat{k}|\psi|} \widehat{K} E(\psi) \widehat{K}^{-1} .$$

In order to allow for diagrammatic expressions, turn to the bilinear forms $\kappa, \hat{\kappa}$ defined by K, \hat{K} respectively and their notion of transposition. Then:

$$E(\kappa^* \varphi) = E^*(\varphi)^{\mathrm{t}} , \qquad (1.62)$$

as is demonstrated by a calculation,

$$E^*(\kappa\psi)^* = (-i)^{|\psi|} E(K\psi) = (-i)^{|\psi|} (-1)^{\hat{k}|\psi|} \widehat{K} E(\psi) \widehat{K}^{-1} = [E(\psi)^*]^{\mathsf{t}} .$$

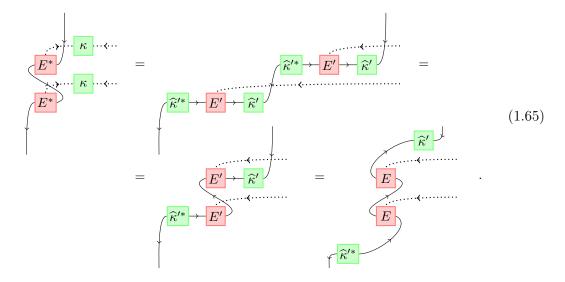
Equation 1.62 is equivalently expressed diagrammatically as

Another form will be useful later on. First study the case of particle-hole symmetry $\kappa = \chi$.

Notice that the identity holds for the time-reversal case $\kappa=\tau$ as well, by simply omitting the fermion parities from the diagrams. By conjugation:

$$= \widehat{\kappa}'^* \longrightarrow \widehat{\kappa}' \qquad (1.64)$$

These diagrams behave well under concatenation.



Similarly:

In the anti-unitary case, when $sAd_{\widehat{K}}$ is an involution, it is useful to choose a basis z_a of the set of fixed points which is fixed by its action,

$$z_a = \mathrm{sAd}_{\widehat{K}}(z_a) \ . \tag{1.67}$$

2. Super Quantum Spin Chains

The question of quantum phases is tackled via states on local algebras. This formalism is introduced. It follows a discussion how that very reduced view - states with certain properties on certain algebras – encapsulate the information necessary to grasp the universal content of topological quantum matter.

2.1. Local Algebras

The goal of this section is to construct an algebra of graded operators on the onedimensional lattice \mathbb{Z} , allowing for the presence of on-site symmetry groups G. In the ungraded case, this is a well-known procedure, for a detailed account of this consult [109]. The exposition is inserted here in order to fix the notation, and also to explain modifications which are appropriate to the graded case.

To each lattice point $x \in \mathbb{Z}$ associate a graded unital finite-dimensional C^* -algebra $\mathcal{A}_{\{x\}}$. For points $x_1 < \cdots < x_n \in \mathbb{Z}$ define

$$\mathcal{A}_{\{x_1,\dots,x_n\}} := \mathcal{A}_{\{x_1\}} \widehat{\otimes} \cdots \widehat{\otimes} \mathcal{A}_{\{x_n\}} . \tag{2.1}$$

Notice that the ordering is crucial since the tensor product is no longer commutative. Quite generally one can find a $\mathcal{H}_{\{x\}}$, termed the *on-site* super Hilbert space, such that $\mathcal{A}_{\{x\}} \subseteq \mathcal{L}(\mathcal{H}_{\{x\}})$, and here the assumption is that this is in fact an equality, so that $\mathcal{A}_{\{x\}}$ is isomorphic to some matrix algebra.

More generally, for any finite subset $X \subset \mathbb{Z}$, \mathcal{A}_X shall denote the algebra which is obtained by first ordering the elements of X and then applying 2.1.

Using the unit $1_{\mathcal{A}_{\{x\}}} \in \mathcal{A}_{\{x\}}$, there is a way of embedding \mathcal{A}_X into \mathcal{A}_Y for $X \subset Y$. Denote by $\mathscr{B}_{Y,X}$ the braiding isomorphism that braids in \mathcal{A}_Y all factors associated to points $x \in X$ to the left of those associated to points $y \in Y \setminus X$. For example if $Y = \{1, 2, 3, 4\}$ and $X = \{1, 3\}$, then $\mathscr{B}_{Y,X}$ permutes Y to $\{1, 3, 2, 4\}$. Then define

$$\iota_{X,Y}: \mathcal{A}_X \to \mathcal{A}_Y , \quad \mathcal{O}_X \mapsto \mathscr{B}_{Y,X}^{-1}(\mathcal{O}_X \widehat{\otimes} 1_{\mathcal{A}_{Y \setminus X}}) .$$
 (2.2)

Since the identity is in the 0-component of A, this braiding does not introduce any signs. For that reason $\iota_{X,Y}$ are injective homomorphisms, and $\iota_{Y,Z} \circ \iota_{X,Y} = \iota_{X,Z}$ for $X \subset Y \subset Z$. Such a collection of algebras A_X and homomorphisms $\iota_{X,Y}$ is called a *direct system* over subsets of \mathbb{Z} .

Given such a direct system, take the direct limit, denoted as

$$\mathcal{A}_X = \overline{\lim_{\to} \mathcal{A}_{\bullet}}^{\|\cdot\|} , \qquad (2.3)$$

for $X \subseteq \mathbb{Z}$ possibly infinite, where a subsequent norm completion is indicated by the customary bar accompanied by the employed norm, not to be confused with complex conjugation, for which the bar is used also.

The direct limit is taken in two steps. First, consider the disjoint union of all A_Y such that Y is a finite subset of X:

$$\bigsqcup_{Y \subset X} \mathcal{A}_Y \ . \tag{2.4}$$

On this set, introduce an equivalence relation R_{ι} between objects $\mathcal{O}_{Y_1} \in \mathcal{A}_{Y_1}$ and $\mathcal{O}_{Y_2} \in \mathcal{A}_{Y_2}$, denoted $\mathcal{O}_{Y_1}R_{\iota}\mathcal{O}_{Y_2}$, if there is a finite $Z \subset X$ such that $Y_1 \subset Z$ and $Y_2 \subset Z$, and:

$$\mathcal{O}_{Y_1} R_{\iota} \mathcal{O}_{Y_2} \iff \iota_{Y_1, Z}(\mathcal{O}_{Y_1}) = \iota_{Y_2, Z}(\mathcal{O}_{Y_2}) . \tag{2.5}$$

The direct limit is then:

$$\mathcal{A}_{X,\text{loc}} := \lim_{\to} \mathcal{A}_{\bullet} := \bigsqcup_{Y \subset X} \mathcal{A}_{Y}/R_{\iota} . \tag{2.6}$$

By the general properties of direct limits¹, this is a graded algebra.

Definition 15. Let \mathcal{A} be a graded finite-dimensional C^* -algebra. Then $\mathcal{A}_{\mathbb{Z},loc}$ is called the algebra of graded local operators. For each graded local operator \mathcal{O} there are finite subsets X such that there are $\mathcal{O}_X \in \mathcal{A}_X$ with $\mathcal{O}_X \in \mathcal{O}$. The smallest such subset is called the support of \mathcal{O} and written as $\operatorname{supp}(\mathcal{O})$. $\mathcal{A}_{\mathbb{Z}}$ is called the algebra of graded quasi-local operators.

The discussion adhered to the definition of $\mathcal{A}_{X,\text{loc}}$ as an algebra of equivalence classes of operators. Commonly, the distinction between an element and its class is blurred, and such is the practice in the following.

The epithet of locality had to be qualified for the following reason: Take local $\mathcal{O}_{1,2}$ with disjoint supports. They act on degrees of freedom separated by a possibly large spatial distance, and therefore should not know of each other – this is exactly what the notion of "locality" was invented to capture. This "not knowing of each other" in terms of operators means of course that they should *commute*.

Now, it is not difficult to see from the structure of these algebras that operators do not do that, but instead *graded commute*:

$$\mathcal{O}_1 \mathcal{O}_2 = (-1)^{|\mathcal{O}_1||\mathcal{O}_2|} \mathcal{O}_2 \mathcal{O}_1 . \tag{2.7}$$

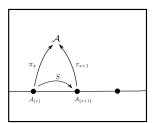
For that reason, the above operators are not "local" in the physical sense. In particular, operators which anti-commute when spatially separated cannot correspond to observables.

This property of the algebra $\mathcal{A}_{\mathbb{Z}}$ is called *graded asymptotic abelianness*.

¹A discussion can be found in [16]. For a modern reformulation – and a change of terminology to *colimit* – check the nlab [115].

2.2. Symmetry Actions

Symmetry actions can be grouped into two types: external and internal operations. Of the former kind, only translations and time-reversals are considered here, although time – or more apt: motion – reversal is, in the non-relativistic Hilbert space formalism, closer to an internal symmetry and is thus dealt with in conjunction to those. The external symmetry operations of reflections or shift-reflections are not treated in this work. A treatment of one-dimensional topological phases with reflection symmetry can be found in [26].



When translation invariant system are to be described, there should be graded isomorphisms $\mathcal{A}_{\{x\}} \cong \mathcal{A}_{\{y\}}$, or, more conveniently, $\pi_x : \mathcal{A}_{\{x\}} \to \mathcal{A}$ for some fixed \mathcal{A} .

Whence the translation action S on operators \mathcal{O} supported at a single site x is $S(\mathcal{O}) := \pi_{x+1}^{-1} \circ \pi_x(\mathcal{O})$. Extend this action to tensor products by

$$S(\mathcal{O}_1 \widehat{\otimes} \cdots \widehat{\otimes} \mathcal{O}_n) = S(\mathcal{O}_1) \widehat{\otimes} \cdots \widehat{\otimes} S(\mathcal{O}_n) , \qquad (2.8)$$

and finally to all of $\mathcal{A}_{\mathbb{Z},loc}$ by continuity and linearity. Thus, there is a \mathbb{Z} -action on the quasi-local algebra by translations.

The discussion of internal symmetry groups supposes translation symmetry. For a group G pick an even representation $\alpha^{\mathcal{H}}: G \to \operatorname{Aut}(\mathcal{H})^0$. Then this induces an even group action $\alpha^{\mathcal{A}}: G \to \operatorname{Aut}(\mathcal{A})$ by

$$\alpha_q(L) = \alpha_q^{\mathcal{H}} \circ L \circ (\alpha_q^{\mathcal{H}})^{-1} . \tag{2.9}$$

This can be lifted to a representation $\alpha^{\mathcal{A}_{\{x\}}}: G^{\Delta} \to \operatorname{Aut}(\mathcal{A}_{\{x\}})$ simply by

$$\alpha_g^{\mathcal{A}_{\{x\}}} := \pi_x \circ \alpha_g^{\mathcal{A}} \circ \pi_x^{-1} . \tag{2.10}$$

On tensor products of the form 2.1, define a representation by

$$\alpha_g^{\mathcal{A}_{\{x_1,\dots,x_n\}}} := \alpha_g^{\mathcal{A}_{\{x_1\}}} \widehat{\otimes} \cdots \widehat{\otimes} \alpha_g^{\mathcal{A}_{\{x_n\}}}. \tag{2.11}$$

If $X \subset Y$, then $\alpha_g^{\mathcal{A}_Y} \circ \iota_{X,Y} = \iota_{X,Y} \circ \alpha_g^{\mathcal{A}_X}$. Hence, this induces a representation $\alpha^{\mathcal{A}_{\mathbb{Z}}}$.

Definition 16. A quasi-local algebra $\mathcal{A}_{\mathbb{Z}}$ together with a G-action as described is termed a graded quasi-local algebra with on-site symmetry group G.

A necessary ingredient for this to work so smoothly is the assumption that all the $\alpha_g^{\mathcal{H}}$ are even. If a symmetry G acts by odd operators on a super Hilbert space, invariant states cannot have definite fermion parity, and hence by the parity super-selection rule, the odd symmetries are in fact broken. Now, in super quantum spin systems it is possible to have, locally, odd symmetry generators, which always combine to even ones in a suitably

chosen thermodynamic limit; i.e., by a convenient choice of unit cell. This guarantees the existence of G-invariant trivial states, i.e., states that have zero correlation length and no entanglement. This is theoretically convenient, but might not always map to a concrete physical lattice system in the presence of crystalline symmetries [19].

What are reasonable choices for G? It is helpful to consider what systems are supposed to be described by the formalism of super quantum spin systems: Systems of electrons. That is, the on-site super Hilbert spaces are typically fermionic Fock space $\mathcal{H} \cong \Lambda(V)$, where V is a (ungraded/trivially graded) N-dimensional Hilbert space describing orbitals, for example of Wannier type, or obtained in tight-binding approximation. To be more explicit, consider some integer N and the super Hilbert space $\mathcal{H} = \Lambda(V)$, the exterior algebra over $V \cong \mathbb{C}^N$ with an ONB $e_1, ..., e_N$ and parity operator $P|_{\Lambda^k} = (-1)^k$. The creation operator of mode e_i , denoted as e_i^* , is:

$$c_i^*(e_{i_1} \wedge \cdots \wedge e_{i_k}) := e_i \wedge e_{i_1} \wedge \cdots \wedge e_{i_k}$$
.

Furthermore, let c_i be its adjoint, the annihilation operator. These satisfy canonical anticommutation relations (CAR):

$$\{c_i^*,c_j^*\} = 0 \ , \quad \{c_i,c_j\} = 0 \ , \quad \{c_i^*,c_j^*\} = \delta_{ij} \ .$$

One way of obtaining symmetry transformations on \mathcal{H} is by tensoring transformations on V. These are called *single-particle* symmetries: Suppose $u:V\to V$ is a unitary, then $u^{\otimes n}$ is a unitary on $V^{\otimes n}$. This is left unchanged by anti-symmetrization, so that $\alpha|_{\Lambda^k}:=u^{\otimes k}$ is a many-body unitary operation. For example, if u is the multiplication by a complex number e^{ix} , then, with $\psi_n\in\Lambda^n(V)$:

$$\alpha_{e^{ix}} \left(\sum_{n} \psi_{n} \right) = \sum_{n} e^{ixn} \psi_{n} . \tag{2.12}$$

This is the $U(1)_Q$ global phase rotation symmetry, whose presence indicates that the system is not in a superconducting state. Similarly, e.g., for the $SU(2)_{\text{spin}}$ group of spin rotations, which is also induced through its action on the single-particle space.

There is also one anti-unitary symmetry of this type, the operation of time- or motion- reversal T. This is the part of fundamental time-reversal that acts on the electrons, and for that reason it inherits from its relativistic counterpart the relation

$$T^2 = P$$

For even N define an anti-linear operation $T|_V$ as

$$T(e_{2i-1}) = e_{2i}$$
, $T(e_{2i}) = -e_{2i-1}$,

so that $T^2|_V = -1$. Then, extend T to $\Lambda(V)$ by

$$T(e_{i_1} \wedge \cdots \wedge e_{i_k}) = [T|_V(e_{i_1})] \wedge \cdots \wedge [T|_V(e_{i_k})],$$

so that indeed $T^2 = P$. This symmetry acts on the creation and annihilation operators

$$Tc_{2i-1}T^{-1} = c_{2i}$$
, $Tc_{2i}T^{-1} = -c_{2i-1}$.

A symmetry which is not obtained in this way is termed a many-body symmetry. It can only arise in many-body systems. Focus on one such operation: The anti-unitary Particle-hole $transformations \Xi$, exchanging creation and annihilation operators:

$$\Xi c_i \Xi^{-1} = c_i^* , \quad \Xi c_i^* \Xi^{-1} = c_i .$$

Because of this property, Ξ has to map Λ^k into Λ^{N-k} .

Following [179], the most convenient way to define Ξ is by using the wedge-product on $\Lambda(V)$:

$$\langle \Xi(\xi_1), \xi_2 \rangle_{\Lambda^k} := \langle \Omega_k, \xi_1 \wedge \xi_2 \rangle ,$$
 (2.13)

where Ω_k is a top-dimensional unit vector with $\Omega_k = (-1)^{N-k} \Omega_{k-1}$. Some manipulations then show that $\Xi^2 = (-1)^{N(N-1)/2} 1$.

An operation of the form Ξ is fine as it is, but it will usually not be a symmetry of realistic Hamiltonians. This is because it forbids all two-body terms. Indeed observe that for $A_{ij} = \overline{A_{ji}}$:

$$\Xi\left(\sum_{ij} A_{ij} c_i^* c_j\right) \Xi^{-1} = -\sum_{ij} A_{ij} c_i^* c_j + \sum_i A_{ii} .$$

This does not rule out that such a transformation appears as a symmetry; it just requires some fine-tuning of the Hamiltonian, as can appear for example in quantum Hall systems at half filling [62, 156, 157, 179]. To allow for one-body terms in a particle-hole symmetric Hamiltonian, twist Ξ with some unitary single-particle involution u. Such transformations are denoted by C. They can appear as symmetries of gapped ground states, for example in Hubbard models at half filling when correlated hopping is negligible [93, 155]. This operation is even if N is even, and $C^2 = \det(u)(-1)^{N(N-1)/2}1$. Since it is convenient to choose the unit cell such that there are symmetric states with no entanglement, assume N even and such that $C^2 = 1$.

Both the single-particle symmetries and C map quasi-particle excitations to other quasi-particle excitations, in the limit where band theory applies. In such a limit, it is hard to motivate other types of symmetries.

Note that both C and T reverse the direction of time. In a space-time picture, reversing time $t \mapsto -t$ is a \mathbb{Z}_2 subgroup. Thus, it has to act as an involution on all observables, i.e., even operators. This allows exactly for the above extensions to odd operators: Either $T^2\mathcal{O}T^{-2} = -\mathcal{O}$ or $C^2\mathcal{O}C^{-2} = +\mathcal{O}$. In this light, the aforementioned constructions are just an explanation of how such symmetries may come about in condensed matter systems.

2.3. States

After introducing the way in which operators are to be modeled in the previous section, this one turns to states on super spin chains. The spatiality and the asymptotic abelianess of the chain algebra reflects on the set of states. Hamiltonians and ground states are introduced. The section finishes with a discussion of states that exhibit superconductivity, and how to model them. The formalism of super matrix product states is committed to the particle-number non-conserving wavefunctions used in this setting and the interpretational problems of the latter are inherited by the former. I argue that such problems loose their edge in the limit of infinite volume, as they become more a question of definition and convenience as of physical phenomena, which are equal in any case. This gives license in handling these mathematical idealization as is deemed most useful.

If ω is a state on a graded quasi-local algebra $\mathcal{A}_{\mathbb{Z}}$ equipped with a translation automorphism S, then ω is translational invariant if $\omega \circ S = \omega$. Throughout assume that ω is an even functional. If \mathcal{A} comes with an on-site G-action, then ω has G-symmetry if $\omega \circ \alpha_g = \omega$ for all $g \in G$. These are the states of concern from now on.

A state ω is said to *strongly cluster* if for any two observables $\mathcal{O}_1, \mathcal{O}_2$:

$$\lim_{r \to \infty} \omega(\mathcal{O}_1 \, S^r(\mathcal{O}_2)) = \omega(\mathcal{O}_1)\omega(\mathcal{O}_2) \ . \tag{2.14}$$

As I do not deal with *weakly* clustering states – which allows for some averaging – the property 2.14 is referred to as *clustering*.

Consider the quantity

$$\operatorname{Corr}_{\omega}(r) := \sup \left\{ \frac{|\omega(\mathcal{O}_{1} \widehat{\otimes} 1^{\widehat{\otimes} r} \widehat{\otimes} \mathcal{O}_{2}) - \omega(\mathcal{O}_{1})\omega(\mathcal{O}_{2})|}{\|\mathcal{O}_{1}\| \|\mathcal{O}_{2}\|} : \mathcal{O}_{1}, \mathcal{O}_{2} \in \mathcal{A}_{\mathbb{Z}, \operatorname{loc}} \right\} , \qquad (2.15)$$

which gives the smallest correlation length in the system. Say that ω has exponential decay with correlation length ℓ_c if there is a constant C such that

$$Corr_{\omega}(r) < C \exp(-r/\ell_c) . \tag{2.16}$$

A state ω is mixed if there are states ω_1, ω_2 and 0 < x < 1 s.t. $\omega = x\omega_1 + (1 - x)\omega_2$. Otherwise ω is pure.

There is a connection between the decomposition of states into pure ones and the clustering of expectation values:

Theorem 4 ([87, 138, 108, 23]). An even translational invariant state ω on $\mathcal{A}_{\mathbb{Z}}$ is pure if and only if it is strongly clustering.

The discussion above focuses on properties of the states, which are supposed to be given, and such is the general approach in this work, as is ubiquitous in the tensor network literature. These states model ground states or low-energy descriptions of matter subject to local gapped dynamics.

Hamiltonians. The first notion is an *interaction*, which is a map Φ from the power set of \mathbb{Z} into $\mathcal{A}_{\mathbb{Z}}$: for $X \subset \mathbb{Z}$, $\Phi(X) \in \mathcal{A}_X$. There are various conditions that can be imposed on Φ in order to allow for analytical control. Here, assume that Φ is *finite range*, i.e., there is a constant R such that $\Phi(X) = 0$ for all |X| > R, and that Φ is translation invariant, i.e., $\Phi(X + r) = S^r \circ \Phi(X)$.

The Hamiltonian is given, formally, in terms of the interaction as $\mathscr{H} = \sum_{X \subset \mathbb{Z}} \Phi(X)$; however this is not in the operator algebra, so it is necessary to be careful. For a finite subset X, let $\mathscr{H}_X = \sum_{Y \subset X} \Phi(Y)$. This is a bounded operator in A_Y and can be used to give more rigorous meaning to \mathscr{H} : Let \mathcal{O} be a local operator then the limit

$$[\mathscr{H},\mathcal{O}] = \lim_{X o\mathbb{Z}} [\mathscr{H}_X,\mathcal{O}]$$

exists by virtue of Φ being finite-range: Only finitely many terms contribute to the limit.

Definition 17. A state ω on $\mathcal{A}_{\mathbb{Z}}$ is a ground state to a Hamiltonian \mathscr{H} if

$$\omega(\mathcal{O}^*[\mathcal{H}, \mathcal{O}]) \ge 0 \tag{2.17}$$

for all local operators \mathcal{O} .

In order to compare this to a more standard notion of ground state, let $(H_{\omega}, \pi_{\omega}, \Omega_{\omega})$ be the GNS-representation of ω , and \mathscr{H}_{ω} be the Hamiltonian implementing the dynamics generated by $\mathcal{O} \mapsto i[\mathscr{H}, \mathcal{O}]$ on \mathcal{O} . Then w.l.o.g. $\mathscr{H}_{\omega}\Omega_{\omega} = 0$ and the condition 2.17 reads (discarding the subscript ω indicating the dependence on the state, and π):

$$0 \le \omega(\mathcal{O}^*[\mathcal{H}, \mathcal{O}]) = \langle \Omega, \mathcal{O}^*(\mathcal{H}\mathcal{O} - \mathcal{O}\mathcal{H})\Omega \rangle = \langle \mathcal{O}\Omega, \mathcal{H}\mathcal{O}\Omega \rangle .$$

Since Ω is cyclic for the representation, the requirement is thus $\langle \Psi, \mathscr{H}_{\omega}(\Psi) \rangle \geq 0$ for all $\Psi \in H$, i.e., \mathscr{H}_{ω} has positive spectrum. The state ω is called *gapped* if there is a $\Delta > 0$ such that the spectrum of \mathscr{H}_{ω} is contained in $\{0\} \cup [\Delta, \infty)$.

To make this explicit, look at some examples.

Heisenberg Model. Suppose the on-site Hilbert space is trivially graded and isomorphic to a spin s representation of SU(2), and let $\{S_{\alpha,x}\}_{\alpha=1,2,3}$ be the spin operators acting on site x. Then the spin-s Heisenberg model in an external magnetic field M_{α} is given by the interaction

$$\Phi(\lbrace x\rbrace) = \sum_{\alpha} M_{\alpha} S_{\alpha,x} ,$$

$$\Phi(\lbrace x,y\rbrace) = J \delta_{y,x+1} \sum_{\alpha=1}^{3} S_{\alpha,x} S_{\alpha,x+1} ,$$

$$\Phi(X) = 0 \text{ for all } |X| \ge 3 .$$

For M=0, if s is chosen even, and J<0, then such a model can be in the *Haldane phase* [70, 2, 1, 162], which is here seen as a special case of fermionic topological phases following [168, 179]. There is some discussion below in section 2.6. Note that if s is chosen odd instead, any translation invariant ground state is gapless [3].

Hubbard Model Consider the situation where the on site Hilbert space describes a single spinful electron, $\mathcal{H} = \Lambda(\mathbb{C}^2)$. Denote the electron creation and annihilation operators of spin $\frac{1}{2}$ at position x by $c_{\sigma,x}^*$ and $c_{\sigma,x}$ respectively. Then, the Hubbard model is obtained by choosing the interaction

$$\begin{split} &\Phi(\{x\}) = U \, c_{+,x}^* c_{+,x} c_{-,x}^* \, c_{-,x} \; , \\ &\Phi(\{x,y\}) = -t \delta_{y,x+1} \sum_{\sigma} (c_{\sigma,x+1}^* c_{\sigma,x} + c_{\sigma,x}^* c_{\sigma,x+1}) \; , \\ &\Phi(X) = 0 \text{ for all } |X| \geq 3 \; . \end{split}$$

If one adds a term $-\frac{U}{2}(c_{+,x}^*c_{+,x}+c_{-,x}^*c_{-,x})$ to $\Phi(\{x\})$, the resulting Hamiltonian is particle-hole symmetric with $u_{\sigma'x'}^{\sigma,x}=\delta_{\sigma'}^{\sigma}\delta_{x'}^{x}(-1)^{x}$.

Of course, to obtain formulas for the ground states of such models is not easy. Even determining whether a given model is gapped is a hard problem [92, 111, 36, 13, 73]. However, assuming a state to be a unique ground state to a local \mathscr{H} allows to draw qualitative conclusions about its correlation functions. The earliest such result were the bounds derived by Lieb and Robinson [97, 112, 109] on the velocity with which perturbations spread. From there Hastings and Koma proved:

Theorem 5 ([74, 73]). If ω is the unique ground state of a finite range Hamiltonian with gap Δ , then there is ℓ_c such that ω has exponential decay with correlation length $\ell_c \propto \Delta^{-1}$.

It should be noted that theorem 5 does not apply directly to physical systems. Consider, e.g., an electron gas with density $\rho(x)$ and Coulomb interactions:

$$\mathscr{H} \supset \frac{1}{4\pi\epsilon_0 e^2} \int \frac{:\rho(x)\rho(y):}{\|x-y\|} d^dx d^dy$$
.

This is not finite range, not even exponentially decaying. However, one expects that the charges are screened, and that the emergent quasiparticles in turn obey some local dynamics with exponentially decaying interactions $||x-y||^{-1} \to \frac{\exp(-||x-y||/\ell_s)}{||x-y||}$.

Superconductivity and BCS Ground States Physically motivated Hamiltonians always preserve global phase rotation symmetry. In contrast to this, in Bogoliubov mean-field theory, quasi-free "Hamiltonians" of the form

$$\sum_{ij} A_{ij} c_i^* c_j + \frac{1}{2} \sum_{ij} \left(B_{ij} c_i^* c_j^* + \overline{B_{ij}} c_i c_j \right)$$
 (2.18)

are used, which give an effective description of low energy excitations in superconductors. However, these are not "Hamiltonians" in the unambigious sense as discussed above. They describe the physical state only after an additional variational procedure (the famous gap equation), as is expected from a mean-field ansatz: Start with a Hamiltonian \mathcal{H}

preserving global phase rotation symmetry. Then, introduce trial wave functions (here for the case of s-wave superconductivity) [11, 67]:

$$\Psi_{\phi}^{\text{BCS}} := \mathcal{N}^{-\frac{1}{2}} \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + e^{2i\phi} v_{\mathbf{k}} \hat{c}_{+,\mathbf{k}}^* \hat{c}_{-,\mathbf{k}}^* \right) |0\rangle$$
 (2.19)

in terms of the wavenumber **k** creation operators $\hat{c}_{\sigma,\mathbf{k}}^*$, the electron vacuum $|0\rangle$ and some variational parameters $u_{\mathbf{k}}, v_{\mathbf{k}}$. Under the U(1) action

$$\alpha_{e^{ix}}(\Psi_{\phi}^{\text{BCS}}) = \Psi_{\phi+x}^{\text{BCS}}$$
,

that is, they do not preserve global phase rotation symmetry. Calculating the energy of this state, or its excitations, with an interacting Hamiltonian with global phase rotation symmetry is equivalent with using operators of the form 2.18, since

$$\left\langle \Psi_{\phi}^{\mathrm{BCS}}, c_{+,x}^* c_{-,x}^* c_{+,x} c_{-,x} \Psi_{\phi}^{\mathrm{BCS}} \right\rangle \approx \left\langle \Psi_{\phi}^{\mathrm{BCS}}, c_{+,x}^* c_{-,x}^* \Psi_{\phi}^{\mathrm{BCS}} \right\rangle \left\langle \Psi_{\phi}^{\mathrm{BCS}}, c_{+,x} c_{-,x} \Psi_{\phi}^{\mathrm{BCS}} \right\rangle \; .$$

This allows the determination of a candidate wavefunction after minimization.

In recent years sub-gap excitations localized to order parameter fluctuations – for example superconductor-metal interfaces – came in experimental and theoretical focus. They are called *Majorana bound states* and of the form

$$a_{\sigma,\mathbf{k}}\hat{c}_{\sigma,\mathbf{k}}^* + b_{\sigma,\mathbf{k}}\hat{c}_{-\sigma,-\mathbf{k}}$$
 (2.20)

They are not to be confused with the solutions to the Dirac equation pioneered by E. Majorana [102] in 1937, in particular they are not fermions proper but rather obey some parastatistics.

The interest in bound states of the form 2.20 is driven by Kitaev's realization that they could be used for quantum computing [91, 101, 123, 53, 144, 143, 134].

The problem with this ansatz is that it is quite unclear whether the resulting particle is observable in principle, and if there is something like a Majorana, whether it is described by an operator of the form 2.20. Indeed [96] argued that instead good Majorana operators to use are

$$\int \sum_{\sigma} (u_{\sigma}(x)\psi_{\sigma}(x) + v_{\sigma}(x)\psi_{\sigma}^{*}(x)X)d^{d}x , \quad \psi_{\sigma}(x) = \sum_{i} \phi_{\sigma,i}(x)c_{\sigma,i} . \qquad (2.21)$$

Here, X is some non-local operator with charge -2 and $\phi_{\sigma,i}(x)$ are some orbitals localized around ion positions x_i .

Moreover, they argued that the exact ground states of superconductors preserve particle number, and that taking generalized coherent states of the BCS type is unphysical.

In mean-field theory, the fluctuations of X are ignored, thereby reducing 2.21 to 2.20. In s-wave superconductivity the damage is negligible, since the order parameter does not have any internal structure. This is different in, and could lead to severe problems for, spinful superconductors. Building up from this work, [99, 98] moved towards a description of Majorana zero modes beyond mean field.

With a similar motivation, [125, 124] demonstrated the existence of Majorana zero modes localized to the edge in a particle-conserving one-dimensional integrable model for superconductivity. While they are skeptical whether their edge modes are experimentally observable due the presence of superselection sectors, they define and calculate a many-body invariant distinguishing trivial from topological superconductors.

It should be mentioned that their model is a bit different in flavor to most suggestions for experimental realization since the superconductivity is not induced by proximity, but arises through spontaneous symmetry breaking ².

Since this work deals with topological superconductors, it is important to clarify how the approach here avoids the aforementioned problems. The most pertinent ambiguities are avoided here simply by not considering finite systems, and hence no Majoranas. Thus, the wavefunctions constructed below in section 3.2 should not be used to describe finite systems, or only with qualifications. It remains to explicate the status of infinite volume states without phase rotation symmetry. This is achieved through a discussion of superconductivity via off-diagonal long-range order (ODLRO) [127, 128, 175]. For comparisons between the BCS and the ODLRO approach, consult [135, 22], and more detailed explanations as presented here can be found in [150, 41].

Off-Diagonal Long-Range Order. Superconductors are aptly described as charged superfluids, that is, they are systems in which the global U(1) phase rotation symmetry is spontaneously broken. Again Goldstone's theorem does not apply since the constituents are charged and Coulomb forces are long-range [63],[160, Part II, Chapter 15].

For simplicity, the discussion restricts to s-wave superconductivity and all complications pertaining to either the continuum (e.g. UV-divergences) or the lattice (e.g. high symmetry points in the Brillouin zone) are ignored. Let ω be the state of a quantum system whose operator algebra is generated by the electron operators $\psi_{\sigma}(x)$ of spin σ at position x. Introduce the pair field $\Phi(X) := \psi_{+}(x_1)\psi_{-}(x_2)$ for $X = (x_1, x_2)$.

The state ω is said to possess off-diagonal long-range order if there is a classical field $\phi(X)$ such that

$$\lim_{|x|\to\infty} \left| \omega(\Phi(X+x)^*\Phi(X')) - \overline{\phi(X+x)}\phi(X') \right| = 0 ,$$

and $\phi(X+x)$ does not tend to zero as $x \to \infty$. It is possible to derive the Meissner and Josephson effect [149] and flux quantization [113] directly from this.

Suppose such a state ω is to be defined as a sequence of states in larger and larger volumes V, with Hamiltonians H_V . For each volume V, and particle number N, let $\mathcal{H}_{V,N}$ be the Hilbert space of N particles in that volume.

Let $|N\rangle$ be the unique ground state of H_V in $\mathcal{H}_{V,N}$. The thermodynamic limit is taken

²Note that Mermin-Wagner type results [105, 77, 34], [56, Chapter 9] do not prohibit this as they use a Coulomb-type interaction which is long-range. The necessity of short-range interactions for the application of this theorem is underscored by *classical* 1d models with symmetry breaking [139, 42, 43]. This is not to say that long-range interactions are a fail-safe recipe for spontaneous symmetry breaking in low dimensions, see [100] for a Mermin-Wagner type for some subclasses of systems.

at constant density N/V.

If $|N\rangle$ indeed converges to a state ω with ODLRO, then for large enough V and ||x||:

$$\langle N|\Phi(X+x)^*\Phi(X')|N\rangle \approx \overline{\phi(X+x)}\phi(X')$$
 (2.22)

On the left side, insert a resolution of $\mathcal{H}_{V,N-2}$ by Hamiltonian eigenstates $|\alpha\rangle$:

$$\overline{\phi(X+x)}\phi(X') \approx \sum_{\alpha} \langle N|\Phi(X+x)^*|\alpha\rangle \langle \alpha|\Phi(X')|N\rangle .$$

Assuming approximate translation symmetry allows to write, with p_{α} the momentum of $|\alpha\rangle$,

$$\langle N|\Phi(X+x)^*|\alpha\rangle = e^{i(p_{\alpha},x)/\hbar}\overline{f_{\alpha}(X)}$$
, $f_{\alpha}(X) = \langle \alpha|\Phi(X)|N\rangle$.

This allows to write both sides of 2.22 as a Fourier series

$$\left[\sum_{q} e^{i(q,x)/\hbar} \overline{\widehat{\phi}_{q}(X)}\right] \phi(X') \approx \sum_{\alpha} e^{i(p_{\alpha},x)/\hbar} \overline{f_{\alpha}(X)} f_{\alpha}(X') .$$

By independence of X and X', the sum on the right collapses to $\alpha = \alpha_0$ and $f_{\alpha_0}(X) = \phi(X)$. Then, by uniqueness of Fourier series, the sum on the left hand side collapses to $q = p_{\alpha_0}$, too, and $\widehat{\phi}_q(X) = f_{\alpha_0}(X) = \phi(X)$. Hence $p_{\alpha_0} = 0$.

Now, assume that the ground state is the only vector with zero momentum – akin to demanding uniqueness of the vacuum state:

$$\langle N - 2|\Phi(X)|N\rangle \approx \phi(X)$$
 (2.23)

Thus the presence of ODLRO forces an infinite degeneracy onto the states $|N+2k\rangle$ in the thermodynamic limit [67]. They are indistinguishable by all observables, but have to be represented by distinct states $\omega_k = \langle \Psi_k, \cdot \Psi_k \rangle$ in the infinite volume Hilbert space. Moreover, these states Ψ_k actually do not represent pure states, in infinite volume. This somewhat paradoxical statement can be seen in the following way: For simplicity assume k=0 and $\langle N|\cdot |N\rangle \to \omega_0$, a pure state. Then, by theorem 4, it has to cluster:

$$\langle N|\Phi(X+x)^*\Phi(X')|N\rangle \sim \langle N|\Phi(X+x)^*|N\rangle \langle N|\Phi(X)|N\rangle = 0, \qquad (2.24)$$

in direct conflict to the assumption of ODLRO.

This is indeed what one would expect when a symmetry is spontaneously broken; namely that while for all finite volumes symmetry-preserving ground states can be found, they become decoherent mixtures in the thermodynamic limit. The difference between a superconductor and, for example, a ferromagnet, is that the exact degeneration of ground states for different particle number only occurs in the thermodynamic limit. However, this holds, e.g., also for antiferromagnets [65].

The discussion also hints at which infinite volume pure states show ODLRO: states that satisfy $\omega(\Phi(X)) = \phi(X)$, i.e., infinite volume limits of BCS states.

This is not too surprising as it is important to realize what it means to say that a state is

pure in infinite volume, a notion that depends heavily on what is the algebra of operators. The discussion above indeed presumed the whole CAR algebra over $L^2(\mathbb{R}^d; \mathbb{C}^2)$, and thus was forced to adopt generalized coherent states of BCS type. Instead, one may restrict the algebra of observable to particle-number preserving operators, i.e., to the subspace $\ker[Q,\cdot]$ within the algebra of electron operators, where Q is the electric charge. Then, while the condition of ODLRO still makes sense to impose on a state, one would not demand a clustering like in equation 2.24 as $\Phi(X)$ is not a local operator in that restricted sense, and hence would not face a contradiction.

While there is no a priori reason to discard such a viewpoint, it should be clear that it complicates considerably the analysis. In particular, $\ker[Q,\cdot]$ has a much more complicated structure than the CAR algebra.

This is in stark contrast to Fermi metals [67]: There, $\psi_+(x_1)\psi_-(x_2)|N\rangle$ resembles more closely two holes in the Fermi sea, ergo an excited state. Its overlap with the vacuum state $|N-2\rangle$ vanishes in the thermodynamic limit. The states $|N+k\rangle$, with k a constant integer, become indistinguishable in the thermodynamic limit. Thus, there is a unique ground state preserving global phase rotation symmetry.

2.4. The Structural Rôle of Gradings

The exact content of declaring an algebra to be graded – and enforcing it on all derived objects – becomes more apparent in comparison to the ungraded case. This is done by fixing an integer N and considering the algebra of operators on the subset $\{1, ..., N\}$. On finite intervals all operators are finite range. Locality is restored as a restriction by considering families of systems, and keeping the allowed range fixed.

Any super algebra A is an ungraded algebra by deleting the grading, which is indicated by a superscript "b" for "bosonic": A^b . In the following, there is the construction of an isomorphism of algebras,

$$\phi_N : \mathcal{A}_{\{1,\dots,N\}} \to (\mathscr{L}(\mathbb{C}^2) \otimes \mathcal{A}^b)^{\otimes N}$$
 (2.25)

To that purpose, introduce Pauli X, Y, Z operators on \mathbb{C}^2 . Then ϕ_N is a homomorphism characterized by

$$1\widehat{\otimes}\cdots\widehat{\otimes}\stackrel{x}{L}\widehat{\otimes}\cdots\widehat{\otimes}1\mapsto (Y\otimes 1)\otimes\cdots\otimes(X\stackrel{x}{\otimes}L)\otimes\cdots\otimes(1\otimes 1). \tag{2.26}$$

To see that this is well-defined, check that it fares well with multiplications. This is precisely ensured by the anti-commutativity of X and Y. Furthermore, ϕ is a *-morphism since X, Y are hermitian.

Construct an algebra of quasi-local operators with on-site algebra $\mathcal{L}(\mathbb{C}^2) \otimes \mathcal{A}^b$. This carries a \mathbb{Z}_2 -action by the Z-operator. However, a operator \mathcal{O} of degree $\mu \neq 0$ is not mapped to a local operator as $N \to \infty$. Indeed, it carries a string of operators which enforce the anticommutation relations. Restricting to the operators of trivial degree:

$$\phi: (\mathcal{A}_{\mathbb{Z}})^0 \to (\mathscr{L}(\mathbb{C}^2) \otimes \mathcal{A}^b)_{\mathbb{Z}}^{\mathbb{Z}/2\mathbb{Z}} ; \qquad (2.27)$$

where the superscript 0 on the left sides indicates that only those objects are to be considered the domain of ϕ which are globally in the trivial component – which does include spatially separated pairs of oppositely graded objects. The superscript \mathbb{Z}_2 on the right side indicates that ϕ only maps to those operators that are uncharged under the action of \mathbb{Z}_2 .

With domain and image restricted as in 2.27, ϕ is an algebra isomorphism; note though that both source and target are not of the type of the algebras constructed earlier.

To be uncharged resembles to be trivially graded, but the charged objects on the right hand side of equation 2.27 do not have a preimage on the left side and the non-trivially graded operators from the left cannot be mapped to the right.

The isomorphism ϕ can be used, in a limited way, for using states obtained on one side for problems on the other. This is the famous Jordan-Wigner transformation. The topic is taken up again to some degree for matrix product states in section 3.2. Pick ω , a state on $\mathcal{A}_{\mathbb{Z}}$. Then $\omega \circ \phi^{-1}$ is a state defined on the uncharged operators in $(\mathcal{L}(\mathbb{C}^2) \otimes \mathcal{A}^b)_{\mathbb{Z}}$. Imposing that only the uncharged operators are observable, i.e., that only their expectation values are to be defined, is the equivalent to imposing a super-selection rule for the \mathbb{Z}_2 -charge.

The advantage of using \mathbb{Z}_2 -graded states is in facilitating certain calculations without introducing spurious parity-changing operators. Chain algebras as constructed in section 2.1 have a much simpler structure compared to the objects considered in this section.

Besides being unwieldy, there is also a further disadvantage, pointed out by [58]. The problem is that these "bosonization" maps are obtained at the level of operator algebras, but they do not lift to the underlying Hilbert spaces. The reason the Gel'fand construction 1.1 does not save us, is, of course, the non-locality of the charged operators. This results in a mischaracterization of entanglement properties of ground states, without impeding the numerical use to obtain, e.g., variational eigenenergies. Given a bosonic model with \mathbb{Z}_2 symmetry, the mapping to a fermionic model can be interpreted as "gauging" the symmetry. This changes the character of possible boundary states [60].

2.5. Symmetry Protected Phases and Topological Field Theory

Thermal states, and, in the limit of low temperatures, ground states of local Hamiltonians, can have manifold and intricate structures. Here, only quite general features of these states are of interest, which are analyzed more easily.

Consider the set $\partial \mathcal{S}^G(\mathcal{A})$ of all G-symmetric pure states with exponential decay on a given chain algebra $\mathcal{A}_{\mathbb{Z}}$. Within this set, consider the mean-field states³ $\partial \mathcal{S}_1^G(\mathcal{A})$ which

³The subscript refers to the fact that they appear as the D=1 case of the yet-to-be-introduced matrix product states with bond dimension D.

are formed, after choosing a vector ψ in the on-site Hilbert space, as:

$$\eta(L_1\widehat{\otimes}\cdots\widehat{\otimes}L_n) := \prod_{i=1}^n \langle \psi, L_i(\psi) \rangle.$$

Notice that for $\omega_{1/2} \in \mathcal{S}^G(\mathcal{A}_{1/2})$, the tensor product state $\omega_1 \widehat{\otimes} \omega_2$ is an element of $\partial \mathcal{S}^G(\mathcal{A}_1 \widehat{\otimes} \mathcal{A}_2)$. Hence, consider the semigroup $\partial \mathcal{S}^G = \bigcup_{\mathcal{A}} \partial \mathcal{S}^G(\mathcal{A})$, where the multiplication is the super tensor product and the union is over all simple finite dimensional superalgebras.

Define an equivalence relation on ∂S^G in the following way: Say $\omega_{1/2} \in S^G(\mathcal{A}_{1/2})$ are equivalent, if there is an on-site algebra \mathcal{A}_3 and a continuous path $[1,2] \ni t \mapsto \nu_t$ in $\partial S^G(\mathcal{A}_3)$ such that

$$u_1 \cong \omega_1 \widehat{\otimes} \eta_1 ; \quad \nu_2 \cong \omega_2 \widehat{\otimes} \eta_2 ,$$

where η_1, η_2 are mean-field states.

Now, typically one would want that the correlation length stays bounded away from infinity along the path, and require some regularity on the path. It is often useful to turn to the Hamiltonians of these ground states, and demand regularity of those [10, 17]. My respective approach in section 4 uses a different assumption about approximability in terms of matrix product states, which is not obviously connected.

Denote the equivalence class of a state ω by $[\omega]$, and define a multiplication by $[\omega_1] \cdot [\omega_2] := [\omega_1 \widehat{\otimes} \omega_2]$. Declare $[\eta]$ to be the trivial class for any mean-field state η . If, for a given ω , there is a ν such that $[\omega] \cdot [\nu] = [\eta]$, denote $[\nu] = [\omega]^{-1}$.

Such a class $[\omega]$ is called a *topological* phase. This resembles the more usual notion of a phase, in some respect. This is because they are all connected to each other by paths of finite correlation length. If two states are separated by a phase transition, the correlation length diverges on the path joining them.

The discussion so far has given a construction of $\pi_0(\partial S^G)$, the zeroth homotopy group of the set of G-symmetric states with exponentially decaying correlation length. This is the first reason to call these phases 'topological', as they are defined up to continuous deformations [54].

There is another important distinction. If $H \subset G$, then $\partial \mathcal{S}^G \subset \partial \mathcal{S}^H$. Take $\omega \in \partial \mathcal{S}^G$. If $[\omega] \neq 0$ in $\partial \mathcal{S}^{\emptyset}$, this phase is said to have topological order, otherwise it is a symmetry protected topological (SPT) phase. If ω_1, ω_2 both map to the same non-trivial element in $\pi_0(\partial \mathcal{S}^{\emptyset})$ but are distinct as elements of $\pi_0(\partial \mathcal{S}^G)$, they are said to be in a symmetry-enriched topological (SET) phase [28]. As this work restricts itself to the one-dimensional case, where SET and SPT phases can be dealt with in an unified approach, there is no further distinction in terminology.

It should be noted that many interesting topological effects cannot be seen in this framework. For example, Verresen et al. showed that states in homotopically trivial phases can have topological phenomena, roughly when there is some low-energy subspace that has symmetries allowing for SPT phases [167].

If ω is a G-symmetric ground state with correlation length ξ , it can be deformed so that $\xi = 0$. Hence, in each class $[\omega]$, there are states of zero correlation length. In particular, the classes cannot be distinguished by the expectation values of local operators. This is the second reason for the description of these states as 'topological': They are locally indistinguishable.

Finally, this freedom of choosing a representative can be used to pick special states, which are more amenable to analysis. For this, note the following. Consider a (1+1)-dimensional quantum field theory of a fermion field $\psi(x)$, say, with canonical anticommutation relations

$$\psi(x)\psi(y)^* + \psi(y)^*\psi(x) = \delta(x-y) , \text{ etc.}$$

and let ω be a state on this continuum QFT. For a field f consider the 'smeared' operators $\psi(f) = \int f(x)\psi(x)dx$. Now divide the real line into intervals of size a. Consider a sequence of on-site algebras at position $x \in a\mathbb{Z}$ as $\mathcal{A}_i \subset \mathcal{A}_{i+1} \subset \cdots \subset \mathcal{A}_{\infty} = \mathcal{L}(L^2([x,x+a)))$. Then ω is a state on the super spin chains $\mathcal{L}(\mathcal{H}_i)\mathbb{Z}$, for all i, and as $i \to \infty$ one obtains the original state. If the original theory has a local G-symmetry, the \mathcal{H}_i can be chosen to have it too, and the state $\omega_i = \omega|_{(\mathcal{A}_i)\mathbb{Z}}$ has exponential decay since ω has it, and is thus pure. If the local basis is chosen in a good way, the expectation is that universal/large-scale phenomena are captured by ω_i even for small i. This justifies analysis of topological phases by relativistic field theories [148, 174].

These comments should serve as a motivation to restrict to a subclass of states in ∂S^G : Those that have zero correlation length and, additionally, continuum limits. Consider expectation values $\omega(\mathcal{O}_1(t_1,x_1)\cdots\mathcal{O}_n(t_n,x_n))$ of local operators $\mathcal{O}_i(t_i,x_i)$. By the assumption of a relativistic continuum limit, and zero correlation length, such expectation values no longer depend on the space-time coordinates (x_i,t_i) , as long as the spacetime points do not coincide. Then the distinction between the continuum and its discretizations has properly disappeared, and ω is a state of a topological field theory (TFT) [54], which for computational reasons might be calculated on a discretization of the space-time manifold [12]. From this perspective, it is incumbent to study the subset of G-symmetric TFT states [83, 54], $\partial S_{\text{TFT}}^G \subset \partial S^G$, expecting

$$\pi_0(\partial S^G) = \pi_0(\partial S^G_{TFT})$$
.

A slightly weaker claim has been established [145]:

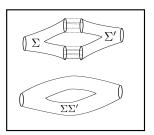
$$\pi_0(\partial S_{\text{MPS}}^G) = \pi_0(\partial S_{\text{TFT}}^G) , \qquad (2.28)$$

where the set of states on the right side is characterized by satisfying an area law for the zeroth entanglement entropy, and are introduced systematically in chapter 3.

Invertible Unitary TFT. Now follows an overview of some classification results achieved within a topological field theory perspective. For this a few mathematical notions are necessary.

Definition 18. A bordism $\Sigma : X_0 \to X_1$ is a d-manifold with $\partial \Sigma = (\partial \Sigma)_0 \sqcup (\partial \Sigma)_1$, and isomorphisms $\varphi_i : (\partial \Sigma)_i \to X_i$, which extend to isomorphism of a neighborhood $\partial \Sigma \subset U_{\epsilon} \subset X$ to $([0, \epsilon) \times X_0) \sqcup ((-\epsilon, 0] \times X_1)$.

For topological purposes, the collars are not strictly necessary; they are crucial however for the operations of differential topology, and if any differentiable structures are to be put on the manifolds.



For two bordisms Σ, Σ' with

$$X_0 \xrightarrow{\Sigma} X_1 \xrightarrow{\Sigma'} X_2$$
, (2.29)

denote by $\Sigma\Sigma'$ the bordism $X_0 \to X_1$ obtained by gluing Σ, Σ' along X_1 using their respective boundary isomorphisms [76, 176]. A 2-dimensional topological field theory is a function Z that associates to one-manifolds X Hilbert spaces $Z(X) := \mathcal{H}_X$ and

to bordisms $\Sigma: X_0 \to X_1$ linear maps $Z(\Sigma): \mathcal{H}_{X_0} \to \mathcal{H}_{X_1}$ [6]. For two bordisms as in 2.29, $Z(\Sigma)$ maps \mathcal{H}_{X_0} to \mathcal{H}_{X_1} , which is mapped to \mathcal{H}_{X_2} by $Z(\Sigma')$. Thus, $Z(\Sigma')$ can be composed with $Z(\Sigma)$. The *gluing* axioms posit that this composition is the value of the TFT on the composed bordism $\Sigma\Sigma'$:

$$Z(\Sigma\Sigma') = Z(\Sigma')Z(\Sigma)$$
.

If $\Sigma: X_0 \to X_1$ is oriented, it induces orientations on X_0, X_1 . Denote by $\overline{\Sigma}: \overline{X_1} \to \overline{X_0}$ the orientation-reversed Σ . Consider a one-manifold X and oriented bordisms $\emptyset \xrightarrow{\Sigma,\Sigma'} X$. Notice that $Z(\Sigma), Z(\Sigma')$ are vectors in \mathcal{H}_X . Hence, there is a form

$$h_X: \mathcal{H}_X \times \mathcal{H}_X \to \mathbb{C} , \quad (Z(\Sigma), Z(\Sigma')) \mapsto Z(\overline{\Sigma}\Sigma') .$$

The TFT Z is called reflection positive or unitary⁴ if h_X is positive definite. Finally, Z is called invertible if dim(\mathcal{H}_X) = 1 for all X [55]. This assumption is designed to capture the uniqueness of the ground state.

In order to describe fermions, the manifolds have to be endowed with Spin structures [95, 57, 89, 117]. The $Spin\ group\ Spin(d) \stackrel{\rho}{\to} SO(d)$ is the simply connected double-cover of the rotation group. A $Spin\ structure$ on an orientable manifold Σ is Spin(d)-principal bundle $P \stackrel{\pi}{\to} \Sigma$ together with an equivariant covering map to the frame bundle $F \to \Sigma$ [95]. If Σ is not orientable, the structure group of the frame bundle is O(d). There are the so-called Pin^{\pm} groups, which are double-covers of the orthogonal group. They are distinguished by the square of the orientation-reversing element. In two space-time dimensions, every manifold has a Pin^- structure [89]. The structure group can be enlarged by tensoring with other unitary groups. $Spin^c$ and Pin^c are related to $Spin\ and$

⁴Trying to formalize (real) time evolution on manifolds encounters the difficulty that the existence of a Minkowski structure on a given manifold imposes strong topological restrictions [122]. In particular, such a rigidity would stall all attempts at characterizing topological phases with anti-unitary symmetries in this way. Instead one uses a 'local' version of this constraint as is done here.

Pin[±] respectively by adding U(1) to the local group. The Pin^{\tilde{c} ,±} groups are defined by letting the orientation-reversing element act on the U(1) group by $z \mapsto z^{-1}$. Similarly, define Spin^h and Pin^{h,±} by adding the unit quaternions $\cong SU(2)$ [4]. In all of these constructions, one has to identify the elements (-1) in both groups, which correspond to the fermion parity operator.

The input, or insight, from physics used here is the spin-charge relation of condensed matter physics [148, Section 2.3]. This is a formalization of the fact that electrons, the fundamental constituents, have electric charge -e and spin $\hbar/2$. This bears fruit if the unit complex numbers and the unit quaternions are identified with the groups of phase and spin rotations respectively, which are gauge symmetries of non-relativistic system of electrons [59]. Once dynamical gauge fields are coupled to their respective currents, and the theory is transported to some arbitrary manifold, all these different structures are allowed to mix. The resulting enlarged space provides greater versatility. This allows to define fermions on manifolds which do not carry any Spin structure. For orientable manifolds, this is important in higher dimensions, since all orientable manifolds of dimensions ≤ 3 are spin⁵. The real projective plane $\mathbb{R}P^2$ does not admit a Pin⁺ structure, but Pin⁻, Pin^c, etc. structures [154, Appendix D].

Table 2.1 summarizes which structure group $G_{\rm TFT}$ should be taken to correspond to which non-relativistic symmetry group G. Note that there is a reversal of sign, $T^2 = P$ maps to ${\rm Pin}^+$ structures, while $C^2 = 1$ to ${\rm Pin}^-$ structures [176, Section 2.3]. The general procedure $G \to G_{\rm TFT}$ is still under discussion, but for those groups appearing in the table there is wide consensus⁶ [83, 84, 82, 176, 55]. One peculiarity is the appearance of a modified U(1)-symmetry that is twisted by particle-hole conjugation. In the literature this is sometimes called a time-reversal symmetry, which, however, squares to the identity. The physical motivation is not entirely clear.

This list has a two-fold justification. (i) The anti-unitary symmetries are chosen like this since these are the only ones appearing in condensed matter systems. The unitary symmetries are those for which there is physical motivation to 'gauge' them, i.e., include them in the structure group. (ii) Any other structure group is Morita-equivalent to one of the G_{TFT} in table 2.1. Morita equivalence between groups G, H is a very weak form of equivalence, demanding only that there is an equivalence of the category of representations of G and H [107]. In the free fermion case, classifications of topological phases in terms of K-theory [90] do depend only on the representations of a symmetry group. In the interacting case however, this is not the case, and there are examples where Morita-equivalent groups have different classifications [158]. It is not clear whether this also happens in (1+1)d. Nevertheless, this gives some motivation to be interested in these

⁵In dimension 4, the complex projective space $\mathbb{C}P^2$ is not spin, while all orientable manifolds of dimension $d \leq 4$ are spin^c [64]. The 5-manifold SU(3)/SO(3) is not spin^c [57, Section 2.4], but every orientable manifold of dimension $d \leq 7$ is spin^h [4]. The introduction of bordism groups below will make it clear that the (non-)existence of spin structures on certain 5-manifolds is important for the classification of SPTs in (3+1) space-time dimensions. However, that is beyond the scope of this thesis, which is confined to one-dimensional physics.

⁶It should be mentioned that the matching was to some degree done by comparing the cobordism classification to results for interacting SPTs obtained by other means.

Cartan	G	G_{TFT}	$\Omega_2^{G_{ m TFT}}$	Generator
\overline{D}	Ø	Spin	\mathbb{Z}_2	T^2
DIII	\mathbb{Z}_4^T	Pin^+	\mathbb{Z}_2	K
AII	$\mathbb{Z}_4^T \ltimes U(1)_Q$	$\mathrm{Pin}^{ ilde{c},+}$	$\mathbb Z$	$\mathbb{R}P^2$
CII	$\mathbb{Z}_2^C \times SU(2)_{\text{spin}}$	$Pin^{h,-}$	\mathbb{Z}_2	$\mathbb{R}P^2$
C	$SU(2)_{\rm spin}$	Spin^h	0	Ø
CI	$\mathbb{Z}_4^T \times SU(2)_{\rm spin}$	$Pin^{h,+}$	\mathbb{Z}_2	$\mathbb{R}P^2$
AI	$\mathbb{Z}_2^C \ltimes U(1)_{\widetilde{O}}$	$\operatorname{Pin}^{\tilde{c},-}$	$\mathbb{Z}\oplus\mathbb{Z}_2$	$T^2, \mathbb{R}P^2$
BDI	\mathbb{Z}_2^C	Pin ⁻	\mathbb{Z}_8	$\mathbb{R}P^2$
\overline{A}	$U(1)_Q$	Spin^c	\mathbb{Z}	T^2
AIII	$\mathbb{Z}_2^{\stackrel{\circ}{C}} \times U(1)_Q$	Pin^c	\mathbb{Z}_4	$\mathbb{R}P^2$

Table 2.1.: The first column refers to the labels used in the periodic table of topological insulators and superconductors [90, 140]. The names in principle refer to Cartan's classification of symmetric spaces, however here they are conventional labels. Both C and T commute with the group of non-relativistic rotations $SU(2)_{\rm spin}$. The charge Q commutes with T and anti-commutes with C, the opposite for \widetilde{Q} . Concerning the fifth column, the spin structures are not indicated here. For example, the torus T^2 has to be endowed with its non-bounding spin structure in order to generate $\Omega_2^{\rm Spin}$, and for ${\rm Spin}^c$ one has to put a non-trivial line bundle on the Torus. K is the Klein bottle and $\mathbb{R}P^2$ the real projective plane. The table is adapted from [55, 89, 154].

groups in particular.

In this thesis, the precise choices of symmetry groups and their labels is not too important. What is essential is the presence of anti-unitary symmetries, which allow to define partition functions on non-orientable manifolds, and, finally, that the value of this partition function on these non-orientable generators determines – for some symmetry groups – the class a given state is in. From this perspective, the symmetry groups labeled BDI and DIII in table 2.1 can be seen as 'fundamental', and all that additional symmetries can do is to restrict the values of the partition function, which happens in section 3.4. There is one exception, which is that in the presence of an SU(2)-symmetry, the state can factor, as is explained later. From table 2.1 it can be inferred, that this classifies the symmetry groups labeled DIII, CII, CI, AI, AIII. Note that AII does not allow for a SPT phase since a factor $\mathbb Z$ is trivial in homotopy, as is explained below.

Classification of Invertible Unitary TFT. Invertible unitary TFTs are particularly simple, since they are classified by their partition function. To quote the precise statement, the following definition is lacking:

Definition 19. The d-dimensional bordism group with structure group H is the set of

equivalence classes

$$\Omega_d^H := \frac{\left\{ \substack{\text{closed }d\text{-manifolds}\\ \text{with }H\text{ structure}} \right\}}{\left\{ \substack{(d+1)\text{-bordisms}\\ \text{with }H\text{ structure}} \right\}} \ ,$$

with the group operation given by the disjoint sum $(\Sigma, \Sigma') \to \Sigma \sqcup \Sigma'$.

For example, the torus is in the same equivalence class as the empty set in Ω_d^{SO} , since the solid torus is a bordism $T^2 \to \emptyset$.

Theorem 6 ([176]).

$$\frac{\left\{\begin{array}{l}\text{invertible unitary TFTs}\\\text{with } H \text{ structure}\\\text{and } Z(S^2) = 1\end{array}\right\}}{\left\{\text{Isomorphisms}\right\}} \cong \text{Hom}(\Omega_2^H, U(1)) \ . \tag{2.30}$$

This is not quite the answer yet, since for SPT phases one needs deformation classes not isomorphism classes. This is not too dramatic, however. For suitable structure groups H, the bordism group is (non-canonically) isomorphic to [176]:

$$\Omega_H^d \cong \mathbb{Z}^n \oplus \mathbb{Z}_{k_1}^{n_1} \oplus \cdots \mathbb{Z}_{k_r}^{n_r}$$
.

Some examples are listed in table 2.1. The \mathbb{Z} summands are not relevant for topological phases in d dimensions, since they can be deformed away: Let Σ_0 be the generator of such a subgroup. Then $Z(\Sigma_0^n) = z^n$ for some unit complex number z. Once deformations are allowed, this can be continued to z = 1, therefore giving a trivial theory. This is not the case for \mathbb{Z}_k -factors, since the allowed values for z are kth roots of unity, which cannot be continuously connected.

Z-summands do play a rôle in one dimension lower. They give rise to a Chern-Simons theory. In this way, e.g., the thermal quantum Hall effect can be understood to descend from the Z-classification given by the gravitational Chern-invariant on 4-manifolds with Spin structure [83, Appendix].

Hence, taking deformation classes of TFTs and theorem 6, combine to the following classification of SPT phases:

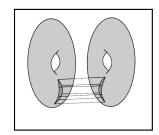
$$\pi_0(\partial S_{\mathrm{TFT}}^G) \cong \mathrm{Hom}((\Omega_2^{G_{\mathrm{TFT}}})_{\mathrm{torsion}}, U(1))$$
,

where the subscript indicates that only the torsion part of the bordism group is included. The task is then the following: For a given symmetry group G, determine the generating manifolds $\Sigma_1, ..., \Sigma_n$ of the torsion subgroup of $\Omega^{G_{\text{TFT}}}$, and compute the partition function on them. For basic G, there might be but one generator, but for sufficiently complicated G one could think of intricate non-bounding manifolds, on which the partition sum has to be computed. This gives many-body indices that determine in which deformation class a given state is.

Partition Functions generalized beyond TFT. Considering a not purely topological, but continuum quantum field theory with a given symmetry group G, the partition function contains information on its topological sectors. The partition function on a closed surface Σ has the form (in euclidean signature) $Z(\Sigma) = \exp(-\Delta + i\eta)$, with η the topological contribution [121, 106]. Since the topological part cannot be sensitive to short-range regulators, this opens the possibility to calculate partition functions on discretized space-times

Manipulations of the spatial manifold are not very difficult to envision [20, 39], and are physically realizable by compactifying the system on a ring and threading some magnetic flux through the system, or endowing it in some other way with some non-trivial holonomy. This was exploited for example by [125], who used such a method to obtain an invariant for Kitaev-type models. A more classic example is the Chern invariant for the quantum Hall phases in two spatial dimensions [114, 8].

A less restricted manipulation of the space-time manifolds appeared in the study of entanglement in conformal field theories, where it was useful to interpret gth powers of the reduced density matrix σ_X of a given state ω as the partition sum on a genus g Riemann surface Σ^g [27]:



$$\operatorname{Tr}((\sigma_X)^g) = Z(\Sigma^g)$$
.

This is derived using the path integral, where σ_X has a representation as a 2-torus, with a slit along X. The surface Σ^g is then obtained by gluing g tori along these slits.

The spatial slices of such manifolds are disconnected circles, so that all the interesting features appear only through the (imaginary) time direction.

By using similar path integral methods, [154] realized that applying a partial transpose to the reduced density operator has the effect of inducing an orientation-reversing operation along the cut. It thus can be used to manufacture non-orientability.

Doing this properly requires the development of quite some machinery of differential topology – and even then this would only address topological phases in relativistic quantum field theories. As an exposition of these techniques would be rather tangent to the main line of thought, I feel justified to exclaim: *Vita brevis, ars longa!* and instead just give a glimpse of how one would proceed, and otherwise refer to the works of Shiozaki et al. [153, 151, 154, 152].

The coherent state representation of the density operator on the discretized ring $S^1 = \{1, ..., N\}$, with periodic boundary conditions, has the following (schematic) form

$$\sigma_{S^1} = \int D_{S^1}(\xi^-) D_{S^1}(\xi^+) Z_{\xi^+,\xi^-}(S^1 \times I) |\xi^+; S^1\rangle \langle \xi^-; S^1| . \tag{2.31}$$

The terms appearing in this formula need explanation. For $X \subset S^1$, $|\xi; X\rangle = \exp(\sum_i \gamma_i \xi_i)|0\rangle_X$ is a fermionic coherent state on \mathcal{H}_X parametrized by the Grassmann variables ξ_i , the Majorana operators γ_i and the Fock vacuum $|0\rangle$. The "integral" $\int D_X(\xi)$ refers to Grassmann "integration" on X. Finally, the term Z has the interpretation as

the partition function of a Grassmann field ψ on the discretized cylinder $S^1 \times I$, with the boundary values

$$\psi|_{S^1 \times \{0\}} = \xi^- , \quad \psi|_{S^1 \times \{1\}} = \xi^+ .$$

Starting from equation 2.31, form the reduced density matrix on $X \subset S^1$:

$$\sigma_X = \int D_X(\xi^-) D_X(\xi^+) Z_{\xi^+,\xi^-}(\Sigma) |\xi^+; X\rangle \langle \xi^-; X|.$$

In this expression, the partition sum is now over the discretized manifold Σ , which is $S^1 \times I$, where the ends of the interval have been identified along X^c , and anti-periodic boundary conditions on ψ have been imposed on the Grassmann field ψ . The anti-periodic boundary condition marks the necessity of a Spin structure to define a spinor field on a manifold, which is ignored in the following. Note that $\partial \Sigma = X^+ \cup X^-$. The splitting of X in X^+ and X^- should indicate that indeed X has doubled, as S^1 had before; one for the ket and one for the bra. Topologically, Σ is thus a torus with a hole. For the first check, consider $\text{Tr}((\sigma_X)^g)$. This corresponds to g tori with holes which are glued to each other; thus a genus-g surface.

In the following the objects corresponding to the partition function on the real projective plane $\mathbb{R}P^2$, and the Klein bottle K, are explained in more detail for a quantum super spin system.

Therefore, suppose a super quantum spin system with local Hilbert space \mathcal{H} has an onsite anti-linear symmetry K. Denote by $L \mapsto L^{t}$ the graded transposition introduced in definition 14 in terms of the bilinear form κ induced by K as in equation 1.46.

Definition 20. If A_1 , A_2 are superalgebras with graded transposition,

$$x_1 \widehat{\otimes} x_2 \mapsto (x_1 \widehat{\otimes} x_2)^{\mathsf{t}} = (-1)^{k(|x_2| + |x_1|)} (x_1)^{\mathsf{t}} \widehat{\otimes} (x_2)^{\mathsf{t}} ,$$
 (2.32)

introduce the partial graded transposes by transposing just one factor:

$$(x_1 \widehat{\otimes} x_2)^{\mathbf{t}_1} := (-1)^{k|x_2|} (x_1)^{\mathbf{t}} \widehat{\otimes} x_2 , \quad (x_1 \widehat{\otimes} x_2)^{\mathbf{t}_2} := (-1)^{k|x_1|} x_1 \widehat{\otimes} (x_2)^{\mathbf{t}} . \tag{2.33}$$

The notion of (bosonic) partial transpositions is ancient in the field of quantum information theory [129, 78], where it is used for detection of entanglement. Indeed, take a density matrix σ on a bipartite system, $\mathcal{H}_1 \widehat{\otimes} \mathcal{H}_2$. Now, suppose σ is a product state, $\sigma = \sigma_1 \widehat{\otimes} \sigma_2$, in particular both σ_1, σ_2 are even and positive. Then $\sigma^{t_1} = (\sigma_1)^t \widehat{\otimes} \sigma_2 = (K\sigma_1 K^{-1}) \widehat{\otimes} \sigma_2$ is positive. Thus, if $\text{Tr}(\sigma^{t_1}\sigma)$ is not positive, then σ cannot be a product state. As is shown later, the argument of this object is quantized.

One of the earlier attempts to define such objects consistently on fermionic objects is [46]. However, this definition does not work very nicely with tensor products, which was remedied by Shapourian et al. [151, 154, 152]. They introduced the graded transpose and graded partial transpose as described above, working out the transformations of CAR-operators⁷.

⁷To convince yourself that I indeed use the same notion as them, comparison with equation 1.59 will be useful.

The same authors also proposed to use such partial transposes to detect topological phases, inspired by topological quantum field theory [153]. In the bosonic case, this had already been done using a different language drawing more from the analogy to string operators [133].

Denote the partial graded transpose on X as \mathcal{O}^{t_X} . If the subset X is of the form $\{1,...,n\}$ then the partial transpose is abbreviated as $\mathcal{O}^{t_{\{1,...,n\}}} \equiv \mathcal{O}^{t_n}$. Next, for ω a translation invariant state on said super quantum spin system, let $\sigma_n = \sigma_n(\omega)$ be the n-site reduced density matrix, i.e., $\omega|_{\mathcal{A}_{\{1,...,n\}}}(\mathcal{O}) = \operatorname{Tr}_{\mathcal{H}^{\widehat{\otimes}n}}(\sigma_n\mathcal{O})$. For

$$Y = \{1, ..., k_1, \} \cup \{d + k_1 + 1, ..., d + k_1 + k_2\}$$

denote the reduced density matrix as $\sigma_X = \sigma_{k_1,k_2|d}(\omega)$. Then, let

$$Z_{k,\ell}^C(\omega) := \operatorname{Tr}(\sigma_{k+\ell} \left[\sigma_{k+\ell}\right]^{\mathsf{t}_k}) , \qquad (2.34)$$

$$Z_{k_1,k_2|d}^T(\omega) := \text{Tr}(\sigma_{k_1,k_2|d}[\sigma_{k_1,k_2|d}]^{t_{k_1}}).$$
(2.35)

[154] argued that Z^C is a partition function on the discretized real projective plane $\mathbb{R}P^2$, and Z^T is a partition function on the discretized Klein bottle K. For the latter, observe that $\sigma_{k_1,k_2|d}$ approximately corresponds to a two-holed torus. The partial transpose reverses the boundary orientation on one of them, after which the two tori are glued back together [35, 79].

2.6. Cohomology Classifications

The TFT perspective can be generalized to higher space dimensions. In one space dimension however, there is another approach to the classification and characterization of SPT phases, which is explained in this section.

It relies strongly, in its formulation, on a setting which is akin to matrix product representations. While this does not confine them to those states, as is to be explained below, this leads to the invariants effectively characterizing boundaries, may they be virtual or real. This is no restriction to their usefulness, however their computation is convoluted.

Since SPT phases do not differ in any local expectation value, the pertinent question is what distinguishes such states. The answer is: The entanglement structure, or equivalently, the structure of edge states.

One of the earliest examples, in hindsight, of a SPT phases was the Haldane phase [70, 2] of SO(3)-symmetric spin-1 chains. It exhibits the entanglement structure typical for SPT states. If the chain is cut at any bond, a degeneracy in the entanglement spectrum appears. This degeneracy is protected, since the edge carries a projective representation of SO(3), which combines with the representation on the other edge to a proper one. Within the framework of bosonic matrix product states, this was generalized to obtain the group cohomology classification of bosonic SPT phases [145, 30, 29]. To that end,

consider a G-symmetric matrix product state on a ring, in terms of $D \times D$ -matrices $E_1, ..., E_d$:

$$\Psi = \sum_{s_1, \dots, s_n} \operatorname{tr}(E_{s_1} \cdots E_{s_n}) |s_1 \cdots s_n\rangle .$$

Cutting the ring at any bond, gives the following set of unnormalized vectors, all yielding equivalent states in the bulk:

$$\Psi(v,w) = \sum_{s_1,\dots,s_n} (v, E_{s_1} \cdots E_{s_n} w) |s_1 \cdots s_n\rangle ,$$

where v,w are in the bond space. Since they are equivalent in the bulk, these are all ground states, with some exponential corrections in system size. As is explained below, the G-representation on the on-site Hilbert space $g|s\rangle = |g \cdot s\rangle$ splits into two projective representations $\widehat{\alpha}_g$, or equivalently a proper representation of a centrally extended symmetry group \widehat{G} , such that $\widehat{\alpha}_g E_{g \cdot s} \widehat{\alpha}_g^{-1} = E_s$. The G-action on Ψ then localizes and fractionalizes to the edge:

$$\alpha_q \Psi(v, w) = \Psi(\widehat{\alpha}_q(v), \widehat{\alpha}_q(w))$$
.

Introducing additional G-invariant local interactions may reduce or enhance, but never lift, the edge degeneracy, if the extended symmetry group \widehat{G} does not sport one-dimensional representations. Of course, non-G-symmetric boundary terms can lift the multiplicity, and so do G-symmetric terms that couple the two edges, which are, however, non-local. As projective representations of a group G are in one-to-one-correspondence with the second group cohomology group $H^2(G,U(1)_{\mathfrak{p}})$, so are the distinct SPT phases described by uniform matrix product states for a given group G. Here, the subscript \mathfrak{p} indicates the conjugation action of anti-unitary g on the U(1) factor. That the chosen cycle in $H^2(G,U(1)_{\mathfrak{p}})$ is indeed stable within the realm of matrix product states can proven by constructing, for any two matrix product states within the same class, a path of matrix product states connecting the two [145]. Hence at least within the set of bosonic matrix product states, the classification by $H^2(G,U(1)_{\mathfrak{p}})$ characterizes the set of homotopy classes:

$$\pi_0(\partial S_{\text{MPS}}^G) \cong H^2(G, U(1)_{\mathfrak{p}})$$
.

A crucial element in this construction was the so-called *entanglement renormalization* [171], which yields *fixed-point*-wave functions in a limiting procedure [146]. They are characterized by a vanishing correlation length and are thus connected to topological field theory [85, 153].

Since the work of Kitaev [91], it had been known that fermionic chains in one dimension sport one example of topological order, hallmarked by the appearance of non-abelian quasi-particles, the celebrated Majorana fermions. While in higher dimensions, these anyons force a radical split between the treatment of topological ordered phases, and the more tame SPT phases, in one dimensions this was realized to be unnecessary on

account of the topographic restrictions of these excitations. This is a fundamental fact of one-dimensional physics, that the import of exchange statistics, so crucial in higher dimensions, is diminished by the inability to actually implement any adiabatic exchange protocol [68, Chapter IV.5], unless they are allowed to cross through each other [66]. This has forced those desiring to harvest the computing power of Kitaev's Majoranas to elaborate geometries [143].

More systematically, [164] developed the connection between TFT and fixed-point MPS to a connection between spin TFT and fixed-point super MPS, thereby attaining a classification of G-symmetric super matrix product states by

$$\pi_0(\partial S_{\text{sMPS}}^G) \cong \mathbb{Z}_2 \times H^1(G, \mathbb{Z}_2) \times H^2(G, U(1)_{\mathfrak{p}}) , \qquad (2.36)$$

as a set.

The meaning of these factors can be elucidated again by cutting. The first factor counts whether there is a Hilbert space localized to either edge, or to both together. The second factor, whether the symmetry action can be chosen in terms of even operators. The last is the group cohomology known from the bosonic case.

To spell out two examples that are used later, for superconductors with particle-hole symmetry, $G = \mathbb{Z}_2^C$, the cohomology groups are $H^1(G, \mathbb{Z}_2) \cong \mathbb{Z}_2$ and $H^2(\mathbb{Z}_2, U(1)_{\mathfrak{p}}) = \mathbb{Z}_2$. Therefore such phases are classified by $(\mu, k, \epsilon) \in \mathbb{Z}_2^3$, which correspond to the indices of real supersimple superalgebras defined in section 1.3. Cohomology cycles may also be used as data to construct TFTs, through *state-sum constructions* [28], to obtain a TFT state corresponding to that cycle. In these constructions, a given manifold is triangulater and dressed with a copy of G at each vertex. The action functional is a function on $G \times G$. In order for the partition function not to depend on the choice of triangulation – any two of which are connected by the so-called *Pachner moves* – this function has to be a cocycle. This can be extended to construct spin TFTs [117, 14, 163]. This is important to show equation 2.28.

These cohomology programs still bore the stigma that they strictly speaking only applied to (super) matrix product states. Since matrix product states are believed to approximate ground states well, it was known to be complete, i.e., for each SPT phase there are sMPS representing it. However, at this point it was unclear whether it was separating, i.e., whether distinct sMPS-SPT phases always corresponded to distinct SPT phases, or whether distinct $[\omega]$, $[\omega']$ could be mapped to the same SPT phase.

This remained possible, since continuous deformations within sMPS do not allow for the possibility to join two such classes by a path of states with diverging bond dimension, but finite correlation length. Such states are not very exotic, all free-fermion models that do not have flat bands are of this type.

Besides this, it is theoretically a bit unsatisfactory to define an invariant of a given state by some property of an approximating state.

In this context [103, 104] showed that states that satisfy an area law for the von-Neumann entanglement entropy satisfy the split property⁸, which is the following statement:

⁸A state being split should be interpreted as the statement that it has no long-range entanglement; being trivially true in 1d, the split property in 2 spatial dimensions implies the absence of topological order [110].

Definition 21. Suppose ω is a state on the chain algebra $\mathcal{A}_{\mathbb{Z}}$. Denote by $\pi_{\omega_{\mathbb{N}}}$ the GNS representation of ω restricted to the half-space algebra $\mathcal{A}_{\mathbb{N}}$. Then ω is said to be split if $\pi_{\omega_{\mathbb{N}}}(\mathcal{A}_{\mathbb{N}})''$ is a type I von-Neumann algebra.

Recall that any such double commutant is a von-Neumann algebra, i.e. a weakly, and strongly, closed *-subalgebra of $\mathcal{L}(H_{\omega_{\mathbb{N}}})$, but that it is type I is a strong restriction [15]. This allowed to introduce an index with values in the Cohomology group on the r.h.s. of 2.36 for such half-space algebras, and so *mutatis mutandis* for area law states on quantum spin chains. In a second step the *stability* of this index under deformations was proven, thus demonstrating homotopy invariance [17, 18, 120].

In one space dimension, the quest of classifying SPT phases with G-symmetry has therefore been achieved rigorously. The invariants which detect a given phase are primarily defined in terms of observables on a virtual or real cut through the chain. As unproblematic as this is from a classificatory perspective, it leaves the determination of a state's class difficult practically. Suppose given is a gapped and G-symmetric state ω . Pick an integer n and a positive ϵ , and find a G-symmetric MPS with bond dimension D, $\omega_{D,n}$ which approximates ω on observables of support at most n:

$$|\omega(\mathcal{O}) - \omega_{D,n}(\mathcal{O})| < \epsilon ||\mathcal{O}||$$
.

The cohomology class of $\omega_{D,n}$ can be computed by investigating the transformation properties of its generating tensor under the G-symmetry. If ϵ is chosen sufficiently small, and n sufficiently large, then this should characterize the given state ω .

The classification using von-Neumann algebras encounters practical problems as well. It guarantees that the index is well-defined for ω . But exact expressions for ground state are rare. So again it might be necessary to turn to approximations, e.g., if it has been determined numerically. So here, too, the problem of algebraically characterizing an object of only approximate quality would appear.

This is not impossible. It shows however the usefulness of many-body invariants which are defined directly in terms of the ground state, and which allow for a notion of convergence, such as to have a tool to measure the quality of approximations when using them. For unitary symmetries, this can be done in terms of string order parameters [131, 133, 132]. The invariants used below in section 3.3 have a similar function, but differ by indicating a topological phase through a quantized argument.

3. Super Matrix Product States

This chapter shall deal with a set of construction methods for states on a chain algebra $\mathcal{A}_{\mathbb{Z}}$, with on-site Hilbert space \mathcal{H} .

I begin by generalizing the approach of [50, 49] to the case of graded algebras, i.e., constructing states on $\mathcal{A}_{\mathbb{Z}}$ directly in the infinite volume limit. There is a discussion of some crucial properties of the states thus obtained: Where they differ from the well-known properties of finitely correlated states (FCS) on quantum spin chains, and where they agree. An emphasis is laid here on expectation values and their clustering; this clarifies some ambiguities pertaining to an approach that focuses on wavefunctions.

Afterwards, the focus is shifted to a complementary point of departure. Starting from matrix product vectors (MPVs), i.e., families of vector states defined on $\mathcal{H}^{\widehat{\otimes}n}$ for all n given by a tensor network, the thermodynamic limit is taken, generalizing some known results to the graded case. This is done here for twofold reasons; on the one hand, some things are easier to conceptualize or even to prove starting from more standard vector states; on the other hand, the community usually discusses matrix product states in this way [26, 130, 24, 146, 32].

Furthermore, it clarifies the rôle of the grading in super matrix product states. In approaches which are centered on discussing decomposition properties of wave-functions only, the grading appears as some additional \mathbb{Z}_2 -symmetry. The discussion of expectation values and decomposition of states corrects such a view.

Auch a detailed exposition also allows to unambiguously use the diagrammatic formalism for graded linear algebra developed in chapter 1 for computations. This stays as true to the simpler bosonic formalism as possible, in particular there is no use of Grassmann variables [173] or modified contractions [25]. This in turn allows for the existence of a forgetful functor which takes a super matrix product state on $\mathcal{A}_{\mathbb{Z}}$, and turns it into a matrix product state on $(\mathcal{A}^0)_{\mathbb{Z}}$, i.e., on the quantum spin system whose on-site algebra are just the even elements of $\mathcal{A} = \mathcal{L}(\mathcal{H})$.

Before diving into the (rather technical) constructions, a final warning is to be heeded: It is not advisable to interpret the (super) matrix product vectors Ψ_n (sMPVs) defined on some finite interval $\{1,...,n\}$ as to correspond to the ground state of some system on that very interval. If the wave-function preserves global phase rotation symmetry this is rather unproblematic, but if superconductors are to be described, the intricacies discussed in section 2.3 should be considered. It might be asvisable to project such a family onto a subspace of fixed particle number.

3.1. Super Matrix Product States

The states on $\mathscr{L}(\mathcal{H})_{\mathbb{Z}}$ that are to be constructed directly in the infinite volume limit are parametrized by the following data: A D-dimensional super Hilbert space H, a map $E: \mathcal{H} \to \mathscr{L}(H)$, and a special element $\rho \in \mathscr{L}(H)$. Indeed, introduce an even map, in terms of operators $E_1, ..., E_d \subset \mathscr{L}(H)$, and an orthonormal basis $\psi_1, ..., \psi_d \in \mathcal{H}$:

$$U_E: H \to \mathcal{H} \widehat{\otimes} H , \quad \xi \mapsto \sum_{s=1}^d \psi_s \widehat{\otimes} (E_s)^* \xi .$$
 (3.1)

As explained in section 1.1, these are in one-to-one-correspondence with h.c.p. maps $\mathbb{E} \in \mathcal{L}^2(H)$ as given in equation 1.24.

At first sight, the definition 3.1 depends on the choice of basis. This appearance can be dispelled by introducing a linear map $E: \mathcal{H} \to \mathcal{L}(H)$ such that $E(\psi_s) = E_s$. This has the right transformation properties. Assume w.l.o.g. that the Kraus algebra A(E) acts non-degenerately – otherwise replace H with $p_{A(E)}H$ where $p_{A(E)}$ is the largest projection in A(E). Finally, for $\mathcal{O}_n \in \mathcal{L}(\mathcal{H})^{\widehat{\otimes} n}$, let $\mathbb{E}_{\mathcal{O}_n}$ be the map of equation 1.33.

Proposition 2. For H, E as above, assume that (i) $||\mathbb{E}|| = 1$ and (ii) that \mathbb{E} is completely reducible and incontractible as defined in definition 8. Let e be the standard right fixed point of equation 1.20 and pick a positive left fixed point ρ parametrized by weights w_i as in equation 1.22. Then define the sequence of functionals

$$\omega_{(n)E,\rho}: \mathscr{L}(\mathcal{H})^{\widehat{\otimes}n} \to \mathbb{C} , \quad \mathcal{O}_n \mapsto \operatorname{tr}(\rho \mathbb{E}_{\mathcal{O}_n}(e)) .$$
 (3.2)

Then:

- (i) The sequence $(\omega_{(n)E,\rho})_n$ combines to a state $\omega_{E,\rho}$ on the chain algebra $\mathcal{A}_{\mathbb{Z}}$.
- (ii) $\mathbb{E}_{\mathcal{O}}$ and $\mathbb{E}'_{\mathcal{O}}$ satisfy the inequalities:

$$|\omega_{E,\rho}(\mathcal{O})| \le ||\mathbb{E}_{\mathcal{O}}(e)|| \le ||\mathcal{O}||, \qquad (3.3)$$

$$|\omega_{E,\rho}(\mathcal{O})| \le ||\mathbb{E}_{\mathcal{O}}'(\operatorname{tr}(\rho \cdot))|| \le ||\mathcal{O}||,$$
 (3.4)

(iii) The correlations of this state are determined by the transfer operator in that there is a constant C>0 such that

$$C \| \mathbb{E}^k - e \widehat{\otimes} \operatorname{tr}(\rho \cdot) \|_{A(E)} \le \operatorname{Corr}_{\omega_{E,\rho}}(k) \le \| \mathbb{E}^k - e \widehat{\otimes} \operatorname{tr}(\rho \cdot) \|_{A(E)}$$
 (3.5)

- (iv) The state $\omega_E = \omega_{E,\rho}$ is pure if and only if \mathbb{E} is strongly superirreducible.
- (v) ω_E has correlation length $\ell_c = -\frac{1}{\log(1-\delta)}$ if and only if \mathbb{E} is strongly superirreducible and has gap δ .

A state $\omega_{E,\rho}$ defined as in part (i) of the proposition in terms of a tensor E and a fixed point ρ is here called a *super matrix product state*. In the situation of part (iv) of this theorem, when \mathbb{E} is superirreducible, there is a unique fixed point. Thus in that case $\omega_E \equiv \omega_{E,\rho}$ is determined by E alone.

By the assumed complete reducibility of \mathbb{E} , any given $\omega_{E,\rho}$ can always be decomposed as

$$\omega_{E,\rho} = \sum_{i} w_i \ \omega_{E^{(i)}}$$

Where $\omega_{E^{(i)}}$ is pure and the weights w_i are those appearing in the decomposition of ρ as in equation 1.22. This is a *barycentric subdivision* of the original state into extremal states, which is therefore mixed.

Observe that the state clusters, according to part (iv) even when \mathbb{E} is not irreducible; it allows for a second fixed point [26]. This is possible because this second fixed point never appears in expectation values, thus not interfering with the clustering. However, the many-body invariants discussed below in section 3.3 are able to extract some dependence on this hidden structure.

Finally, if \mathbb{E} is diagonalizable, the constant C in part (iii) can be taken to be unity by part (v).

Proof of proposition 2.

(i) To see that the $\omega_{(n)E,o}$ combine to a functional on $\mathcal{A}_{\mathbb{Z}}$, check that

$$\omega_{(n+1)E,\rho}(1\widehat{\otimes}\mathcal{O}_n) = \omega_{(n)E,\rho}(\mathcal{O}_n) = \omega_{(n+1)E,\rho}(\mathcal{O}_n\widehat{\otimes}1)$$

i.e., that equivalent elements of $\mathcal{A}_{\mathbb{Z}}$ have the same value. Indeed, this follows by using that e and ρ are right, respectively left, fixed points of \mathbb{E} :

$$\mathbb{E}_{\mathcal{O}_n \widehat{\otimes} 1}(e) = \mathbb{E}_{\mathcal{O}_n} \circ \mathbb{E}(e) = \mathbb{E}_{\mathcal{O}_n}(e) , \quad \operatorname{tr}(\rho \mathbb{E}_{1 \widehat{\otimes} \mathcal{O}_n}(\cdot)) = \operatorname{tr}(\rho \mathbb{E} \circ \mathbb{E}_{\mathcal{O}_n}(\cdot)) = \operatorname{tr}(\rho \mathbb{E}_{\mathcal{O}_n}(\cdot)) .$$

Thus define a linear functional $\omega_{E,e} \in (\mathcal{A}_{\mathbb{Z},loc})^*$ by

$$\omega_{E,\rho}(\mathcal{O}) = \omega_{(\text{supp}(\mathcal{O}))E,\rho}(\mathcal{O}) . \tag{3.6}$$

Note that the $\omega_{(n),E,\rho}$ are positive by lemma 4, and so is $\omega_{E,\rho}$. So to check that it is continuous and normalized it suffices to evaluate it on the identity: $\omega_{E,\rho}(1) = \operatorname{tr}(\rho e) = 1$. By continuity $\omega_{E,\rho}$ can be extended to $\mathcal{A}_{\mathbb{Z}}$.

(ii) The second inequality of the proposition follows by the fact that the operator norm of a positive map between C^* -algebras is determined by its value at the identity. The first one is proven by:

$$|\omega_{E,\rho}(\mathcal{O})| = |\operatorname{tr}(\rho \mathbb{E}_{\mathcal{O}}(e))| \leq \operatorname{tr}|\rho| \|\mathbb{E}_{\mathcal{O}}(e)\|,$$

whence the statement.

(iii) Consider operators $\mathcal{O}_1, \mathcal{O}_2$ of finite support. Then

$$\begin{aligned} |\omega(\mathcal{O}_{1}\widehat{\otimes}1^{\widehat{\otimes}k}\widehat{\otimes}\mathcal{O}_{2}) - \omega(\mathcal{O}_{1})\omega(\mathcal{O}_{2})| &= |\mathrm{tr}(\rho\mathbb{E}_{\mathcal{O}_{1}}\circ(\mathbb{E}^{k} - e\widehat{\otimes}\mathrm{tr}(\rho \cdot))\circ\mathbb{E}_{\mathcal{O}_{2}}(e))| \leq \\ &\leq \|\mathbb{E}^{k} - e\widehat{\otimes}\mathrm{tr}(\rho \cdot)\|_{A}\|\mathbb{E}_{\mathcal{O}_{2}}(e)\|\|(\mathbb{E}_{\mathcal{O}_{1}})'(\mathrm{tr}(\rho \cdot))\| \leq \\ &\leq \|\mathbb{E}^{k} - e\widehat{\otimes}\mathrm{tr}(\rho \cdot)\|_{A}\|\mathcal{O}_{1}\|\|\mathcal{O}_{2}\|; \end{aligned}$$

where part (ii) was used. Hence

$$\operatorname{Corr}_{\omega}(k) \leq \|\mathbb{E}^k - e\widehat{\otimes}\operatorname{tr}(\rho \cdot)\|_A$$
.

On the other hand:

$$\|\mathbb{E}^k - e\widehat{\otimes} \operatorname{tr}(\rho \cdot)\|_A = \sup_{a,b \in A} \{|\operatorname{tr}(b(\mathbb{E}^k - \mathbb{E}^\infty)(a))| \mid \|a\| = 1, \|\operatorname{tr}(b \cdot)\| = \|b\|_1 = 1\}, \quad (3.7)$$

where $||x||_1 := \operatorname{tr}|x|$ is the 1-norm on A. Since both $\mathcal{O} \mapsto \mathbb{E}_{\mathcal{O}}(1_A)$ and $\mathcal{O} \mapsto (\mathbb{E}_{\mathcal{O}})'(\operatorname{tr}(\rho \cdot))$ are surjective by lemma 5, find $\mathcal{O}_a, \mathcal{O}_b$ s.t. $a = \mathbb{E}_{\mathcal{O}_a}(1_A)$ and $\operatorname{tr}(b \cdot) = \operatorname{tr}(\rho \mathbb{E}_{\mathcal{O}_b}(\cdot))$. Then:

$$\frac{|\operatorname{tr}(b\mathbb{E}_{\circ}(a))|}{\|a\|\|b\|_{1}} = \frac{\|\mathcal{O}_{a}\|\|\mathcal{O}_{b}\|}{\|a\|\|b\|_{1}} \frac{|\omega(\mathcal{O}_{b}\widehat{\otimes}1^{\widehat{\otimes}k}\widehat{\otimes}\mathcal{O}_{a}) - \omega(\mathcal{O}_{b})\omega(\mathcal{O}_{a})|}{\|\mathcal{O}_{a}\|\|\mathcal{O}_{b}\|}.$$

Note that the association of \mathcal{O}_a to a is by no means unique. What seems appropriate, to obtain the smallest upper bound, is to take the infimum over all possible choices for $\mathcal{O}_a, \mathcal{O}_b$:

$$M(a) := \inf_{\mathcal{O}_a} \frac{\|\mathcal{O}_a\|}{\|a\|} = \inf \left\{ \frac{\|\mathcal{O}\|}{\|\mathbb{E}_{\mathcal{O}}(1_A)\|} : \mathbb{E}_{\mathcal{O}}(1_A) = a \right\} =$$

$$= \left[\sup \left\{ \frac{\|\mathbb{E}_{\mathcal{O}}(1_A)\|}{\|\mathcal{O}\|} : \mathbb{E}_{\mathcal{O}}(1_A) = a \right\} \right]^{-1} \le \left[\sup \left\{ \frac{|\omega(\mathcal{O})|}{\|\mathcal{O}\|} : \mathbb{E}_{\mathcal{O}}(1_A) = a \right\} \right]^{-1},$$

where again part (ii) gave the inequality. Similarly define N(b), with the operator norm on a replaced by the 1-norm. Taking the supremum over a, b as required in equation 3.7 can be split into taking the supremum over a, b and $\mathcal{O}_a, \mathcal{O}_b$ separately, which gives

$$\sup_{a,b \in A} \left\{ |\operatorname{tr}(b(\mathbb{E}^k - \mathbb{E}^{\infty})(a))| \mid ||a|| = 1, ||b||_1 = 1 \right\} \leq \\
\leq \underbrace{\left[\sup_{\|a\| < 1} M(a) \right]}_{C_1} \underbrace{\left[\sup_{\|b\|_1 \le 1} N(b) \right]}_{C_2} \sup_{\mathcal{O}_1 \ne 0 \ne \mathcal{O}_2} \left\{ \frac{|\omega(\mathcal{O}_1 \widehat{\otimes} 1^{\widehat{\otimes} k} \widehat{\otimes} \mathcal{O}_2) - \omega(\mathcal{O}_1)\omega(\mathcal{O}_2)|}{\|\mathcal{O}_1\| \|\mathcal{O}_2\|} \right\} .$$

Both C_1 and C_2 are non-zero by finite-dimensionality of the bond algebra. Thus, with $C = (C_1 C_2)^{-1}$:

$$C \| \mathbb{E}^k - e \widehat{\otimes} \operatorname{tr}(\rho \cdot) \|_A \le \operatorname{Corr}_{\omega}(k)$$
.

(iv) By theorem 4, a state is pure if and only if it is clustering. Observe that lemma 5 establishes that the Kraus algebra of a superirreducible \mathbb{E} is supercentral. By lemma 3 this implies that $\mathbb{E}^{\infty}|_{A} = e \widehat{\otimes} \operatorname{tr}(\rho \cdot)$. Then proposition 1 yields that $\|\mathbb{E}^{k} - e \widehat{\otimes} \operatorname{tr}(\rho \cdot)\|$ decays exponentially. By part (iii), ω clusters exponentially, and thus it is pure.

For \Rightarrow , suppose A was not supercentral. Then $\|\mathbb{E}^{\infty} - e \widehat{\otimes} \operatorname{tr}(\rho \cdot)\|_{A} = 1$. By the inverse triangle inequality,

$$\|\mathbb{E}^k - e\widehat{\otimes} \operatorname{tr}(\rho \cdot)\|_A \ge \left| \|\mathbb{E}^k - \mathbb{E}^\infty\|_A - \|\mathbb{E}^\infty - e\widehat{\otimes} \operatorname{tr}(\rho \cdot)\|_A \right| , \qquad (3.8)$$

and the right side approaches 1 exponentially fast by proposition 1. For completely irreducible h.c.p. maps supercentrality and supersimplicity are equivalent.

(v): Assume \mathbb{E} has gap δ . Then proposition 1 and part (iv) of this proof give $C \geq 0$ and $\alpha \in \mathbb{N}$ such that

$$\operatorname{Corr}_{\omega}(k) \le \|\mathbb{E}^k - \mathbb{E}^{\infty}\| \le Ck^{\alpha}(1-\delta)^k$$
 (3.9)

On the other hand, assume that ω has exponential decay of correlations, with correlation length ℓ_c . Gelfand's formula expresses the spectral radius of an operator x as $||x^k||^{1/k}$. Consequently:

$$1 - \delta_{\mathbb{E}} = \lim_{k \to \infty} \|\mathbb{E}^k - \mathbb{E}^\infty\|^{1/k} \le \lim_{k \to \infty} \left[C^{-1} \operatorname{Corr}_\omega(k) \right]^{1/k} \le \exp(-1/\ell_c) . \tag{3.10}$$

Suppose the tensor E is G-symmetric with on-site representation $g \mapsto \alpha_g$ and virtual representation $\widehat{\alpha}_g$ as explained in definition 12. Then by using equation 1.42, it follows that $\omega_{E,\rho} \circ \alpha_g^{\mathcal{A}_{\mathbb{Z}}} = \omega_{E,\rho}$, where $\alpha_g^{\mathcal{A}_{\mathbb{Z}}}$ is the G-representation of equation 2.11. Hence, ω is G-symmetric.

Denote the set of G-symmetric super matrix product states on $\mathcal{A}_{\mathbb{Z}}$ of bond dimension D by $\mathcal{S}_{D}^{G}(\mathcal{A})$, and the pure states within this set as $\partial \mathcal{S}_{D}^{G}(\mathcal{A})$. The notation with the boundary symbol should indicate that any $\omega \in \mathcal{S}_{D}(\mathcal{A})$ has a convex decomposition in terms of $\omega_{i} \in \partial \mathcal{S}_{D_{i}}^{G}(\mathcal{A})$ with $\sum_{i} D_{i} = D$.

After this ad-hoc construction of $\partial \mathcal{S}_D^G(\mathcal{A})$, whose elements are characterized by a finitedimensional Hilbert space H and a map $E: \mathcal{H} \to \mathcal{L}(H)$, it is natural to ask whether there can be given some characterization to the set of all such states. The answer is positive, but first recall the definition of Renyi entanglement entropies, where $\sigma_n(\omega)$ is the reduced density matrix of ω on $\{1, ..., n\}$ and $\alpha \geq 0$:

$$R_{\alpha}(\omega, n) = \frac{1}{1 - \alpha} \log \operatorname{Tr}(\sigma_n(\omega)^{\alpha}) . \tag{3.11}$$

There are some special cases: $R_0(\omega, n) = \operatorname{rank}(\sigma_n)$ and $R_1(\omega, n) = S(\sigma_n)$ with $S(\sigma) = -\operatorname{Tr}(\sigma \log \sigma)$ the von Neumann entropy.

Theorem 7 ([17]). Let ω be a pure, translation invariant and G-symmetric state satisfying an area law for R_0 , i.e., the rank of its reduced density matrices is bounded. Then there is a finite-dimensional super Hilbert space H and a G-symmetric pure tensor $E: \mathcal{H} \to \mathcal{L}(H)$ such that $\omega = \omega_E$.

While this is explicit, the physical relevance is obscure. Compare to the discussion in section 4.2 below; there it is argued that from physical grounds there are area laws for R_s , with the parameter s strictly greater than zero. For example all gapped free fermion ground states with non-trivial dispersion do not satisfy this bound.

For later use, the constructions explained above are put into diagrams. To make everything super, switch from ρ to $\Lambda = \widehat{P}\rho$:

$$\lambda(a) = \operatorname{str}(\Lambda a) = \underbrace{\Lambda - a}_{\bullet} .$$

It should be noted that while ρ is in the Kraus algebra, Λ does not need to be. The expectation value of an operator $L_1 \widehat{\otimes} \cdots \widehat{\otimes} L_n$ is then simply

$$\omega(L_1\widehat{\otimes}\cdots\widehat{\otimes}L_n) = \underbrace{\begin{array}{c} \Lambda & \longleftarrow E \\ \vdots \\ \vdots \\ \hline F \cdot \cdot \cdot L_1 \cdot F \cdot \vdots \\ \hline E \end{array}} \cdots \underbrace{\begin{array}{c} E \\ \vdots \\ \hline F \cdot \cdot \cdot L_n \cdot F \cdot \vdots \\ \hline E \end{array}} . \quad (3.12)$$

The reduced density operator σ_n is awkward to use in the fermionic tensor diagrams, since it is partnered with the "unnatural" (in the superworld) operation of taking a trace. Thence a graded density operator $\Sigma_n := P_n \sigma_n$, where P_n is the fermion parity, is more convenient:

$$\operatorname{sTr}(\Sigma_n \mathcal{O}_n) = \operatorname{Tr}(\sigma_n \mathcal{O}_n) = \omega(\mathcal{O}_n)$$
.

In such calculations it is helpful to let the lines of the physical Hilbert space run vertically, i.e., rotate the diagram of equation 3.12 by $\pi/2$. As E is an even tensor, this poses no problems and yields

Here it is understood that the physical in- and outgoing lines have some common ordering.

3.2. Matrix Product Vectors and Thermodynamic limits

As advertised, this section takes a step back and discuss vector states on sites $\{1, ..., n\}$. Let \mathcal{H}, H be super Hilbert spaces. Consider pairs $\{\psi_s \equiv |s\rangle\}_{s=1,...,d} \subset \mathcal{H}$ and $\{E_s\}_{s=1,...,d} \subset \mathcal{L}(H)$, both of which are assumed to be homogeneous. Let $x \in \mathcal{L}(H)$. This defines a family of matrix product vectors (MPV):

$$\Psi_n^{E|x} := \sum_{s_1, \dots, s_n} \overline{\operatorname{str}(xE_{s_1} \cdots E_{s_n})} \, \psi_{s_1} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_n} \in \mathcal{H}^{\widehat{\otimes} n} \,. \tag{3.14}$$

If $|E_s| = |\psi_s|$, then $\Psi_n^{E,x}$ is called a *super matrix product vector* (sMPV) or fermionic matrix product vector (fMPV). Since the parity operations P and \widehat{P} on \mathcal{H} and H respectively are allowed to be trivial, the class of super matrix product states contains the class of matrix product vectors in the more conventional sense [146]. More explicitly, observe that if the sMPV constraint is satisfied, it allows to introduce a map $E: \mathcal{H} \to \mathcal{L}(H)$ as a linear extension of $\psi_s \mapsto E_s$ satisfying the \mathbb{Z}_2 -equivariance condition

$$\widehat{P}E(\psi)\widehat{P}^{-1} = E \circ P(\psi) . \tag{3.15}$$

More non-trivially, the above definition without the constraint $|E_s| = |\psi_s|$ describes the possibility of using ungraded MPVs for graded quantum spin systems, and the other way around.

The set $\{E_s\}_s$ allows the introduction of a h.c.p. map \mathbb{E} as in equation 1.24. Denote the Kraus algebra generated by the E_s as A(E).

Two-sided ideals in A(E) translate to a decomposition of Ψ^E into a superposition of matrix product vectors with more elementary tensors: Suppose E to be semisimple and unital. Then there is a decomposition of super Hilbert spaces $H = \bigoplus_i H_i$ such that

$$\Psi_n^{E|x} = \sum_i (d_i)^{n/2} \Psi_n^{E^{(i)}|x_i} , \qquad (3.16)$$

where $\mathbb{E}^{(i)} \in \mathcal{L}^2(H_i)$ is supersimple and unital and $d_i \leq 1$.

To that purpose, decompose A(E) into its supersimple components A_i with support projections p_i . Then $H_i = p_i H$ and $E_s^{(i)} = (d_i)^{-1/2} p_i E_s$ where $d_i \leq 1$ is chosen such that $\|\mathbb{E}^{(i)}\| = 1$. Moreover, write $x_i = p_i x p_i$.

After these preliminary, algebraic concerns, the task is to take the limit $n \to \infty$ in some way, and recover the infinite volume state $\omega_{E,\rho}$ introduced in the previous section. Begin the discussion by computing matrix elements of factorized operators $\mathcal{O} = L_1 \widehat{\otimes} \cdots \widehat{\otimes} L_n$ between sMPVs generated by $\{E_s^{(i)}\}_s \subset \mathcal{L}(H_i)$. First observe:

$$\left\langle \Psi_n^{E^{(1)}|x_1}, \mathcal{O}\Psi_n^{E^{(2)}|x_2} \right\rangle =$$

$$= \sum_{\substack{s_1...s_n \\ r_1...r_n}} \underbrace{\operatorname{str}\left(x_1 E_{s_1}^{(1)} \cdots E_{s_n}^{(1)}\right)}_{(1)} \underbrace{\operatorname{str}\left(x_2 E_{r_1}^{(2)} \cdots E_{r_n}^{(2)}\right)}_{(2)} \underbrace{\left\langle s_1 \cdots s_n | L_1 \widehat{\otimes} \cdots \widehat{\otimes} L_n | r_1 \cdots r_n \right\rangle}_{(2)} .$$

Let's first compute (2):

$$\langle s_1 \cdots s_n | L_1 \widehat{\otimes} \cdots \widehat{\otimes} L_n | r_1 \cdots r_n \rangle = \left[\prod_{k > \ell} (-1)^{|L_k| ||r_\ell\rangle|} \right] \left[\prod_k \langle s_k | L_k | r_k \rangle \right] . \tag{3.17}$$

For (1) use $\overline{\operatorname{str}(x)} = \operatorname{str}(x^*)$ and the notation $\overline{x} = (x^*)'$, where the graded dual of definition 2 is deployed:

$$\operatorname{str}\left(x_{1}E_{s_{1}}^{(1)}\cdots E_{s_{n}}^{(1)}\right) \operatorname{\overline{str}}\left(x_{2}E_{r_{1}}^{(2)}\cdots E_{r_{n}}^{(2)}\right) =$$

$$= \underbrace{x_{1} + \underbrace{E_{s_{1}}^{(1)} + \cdots + \underbrace{E_{s_{n}}^{(1)}}_{E_{s_{n}}} + \cdots + \underbrace{E_{s_{n}}^{(2)} + \cdots + \underbrace{E_{r_{n}}^{(1)}}_{E_{r_{n}}^{(1)}} + \underbrace{E_{s_{1}}^{(1)} + \underbrace{E_{s_{1}}^{(1)}}_{E_{s_{n}}^{(1)}} + \underbrace{E_{s_{n}}^{(1)}}_{E_{s_{n}}^{(1)}} + \underbrace{E_{s_{n}}^{(1)}}_{E_{s_{n}}^{(1)}} + \underbrace{E_{s_{n}}^{(1)} + \underbrace{E_{s_{n}}^{(1)}}_{E_{s_{n}}^{(1)}} + \underbrace{E_{s$$

In general, the combined sign factor

$$\prod_{k>\ell} (-1)^{|E_{r_{\ell}}^{(2)}|(|E_{s_{k}}^{(1)}|+|E_{r_{k}}^{(2)}|)+|L_{k}|||r_{\ell}\rangle|}$$
(3.19)

forbids simplification. There are two scenarios which allow to proceed. (i) If the sMPV constraint $|E_s| = |\psi_s|$ is satisfied, the two factors in 3.19 exactly cancel. (ii) Somewhat more artificially: If $|L_k| = 0$ and $|E_r^{(2)}| = 0$, both terms vanish individually. Then, $A(E^{(2)})$ consists only of even operators and is called bosonic. In either case:

$$\left\langle \Psi_n^{E^{(1)}|x_1}, \left[L_1 \widehat{\otimes} \cdots \widehat{\otimes} L_n \right] \Psi_n^{E^{(2)}|x_2} \right\rangle = \operatorname{str}_{H_1 \widehat{\otimes} H_2^*} \left(\left[x_1 \widehat{\otimes} 1 \right] \circ \mathbb{E}_{L_1}^{(1,2)} \circ \cdots \circ \mathbb{E}_{L_n}^{(1,2)} \circ \left[1 \widehat{\otimes} \overline{x_2} \right] \right) , \tag{3.20}$$

with a newly defined family of operators $\mathbb{E}_L^{(1,2)} \in \mathscr{L}^2(H_2, H_1)$:

$$\mathbb{E}_{L}^{(1,2)}(x) = \sum_{s,r} (-1)^{|x||E_{r}^{(2)}|} \langle \psi_{s}, L\psi_{r} \rangle E_{s}^{(1)} \circ x \circ (E_{r}^{(2)})^{*}.$$

Proposition 3. Suppose E is supersimple and satisfying the sMPV constraint. Then for $\mathcal{O} \in \mathcal{A}_{\mathbb{Z},loc}$:

$$\lim_{n \to \infty} \|\mathbb{E}\|^{-n} \left\langle \Psi_n^{E|x}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E|x} \right\rangle = f(x) \omega_E(\mathcal{O}) , \quad f(x) = \sum_{a=0}^{\mu} (-1)^{a|x|} \operatorname{str}(x v_a x^* \Lambda_a) ;$$
(3.21)

where ω_E is the state defined in proposition 2, S is the shift operator of equation 2.8, and v_a , $\operatorname{str}(\Lambda_a \cdot)$ are the unique right, respectively left, eigenvectors of $\mathbb E$ to the eigenvalue $\|\mathbb E\|$. This is written as $\Psi_n^{E|x} \to \omega_E$.

The proposition shows that for a supersimple E the choice of x does not matter, as the state does not depend on it. For that reason it is suppressed in the notation $\Psi_n^{E,x} = \Psi_n^E$ with the understanding that some x is chosen such that f(x) = 1. The following choice is convenient: x = 1 if $\mu = 0$ and $x = 2^{-1/2}z$ if $\mu = 1$. Note the factum that if $\mu = 1$, one should choose x to not belong to A(E). Indeed, for $x \in A(E)$ and $\mu = 1$:

$$f(x) = \operatorname{str}(xex\Lambda) + (-1)^{|x|} \operatorname{str}(xzex^*\Lambda z) = \operatorname{str}(xex\Lambda) - \operatorname{str}(xex\Lambda) = 0.$$

A discussion of this can be found in [26].

Proposition 4. Suppose E supersimple and bosonic (i.e., simple). Then, for $\mathcal{O} \in (\mathcal{A}^0)_{\mathbb{Z},loc}$:

$$\lim_{n \to \infty} \|\mathbb{E}\|^{-n} \left\langle \Psi_n^{E|x}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E|x} \right\rangle = f(x) \omega_E(\mathcal{O}) , \quad f(x) = \operatorname{tr}(\rho x e x^*) ; \qquad (3.22)$$

where ω_E is the state defined in proposition 2 and $e, \operatorname{tr}(\rho \cdot)$ are the unique right, respectively left, eigenvectors of \mathbb{E} to the eigenvalue $\|\mathbb{E}\|$.

Within the formalism developed so far, it seems unnatural to consider such objects. However, note that often the interest lies in calculating observables like the energy density. In this situation there is no reason to burden yourself with gradings on your auxiliary Hilbert spaces. The proof is omitted here, as it is sufficiently analogous to the proof of proposition 3, and can be found in the literature [146].

Proof of proposition 3. The limit is understood in the following way: It suffices to consider \mathcal{O} with support contained in some finite subset of size 2k + 1. Hence, for large enough n:

$$\left\langle \Psi_n^{E|x}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E|x} \right\rangle = \operatorname{str}_{H \widehat{\otimes} H^*} \left([x \widehat{\otimes} 1] \circ \mathbb{E}^{\lfloor n/2 \rfloor - k} \circ \mathbb{E}_{\mathcal{O}} \circ \mathbb{E}^{\lceil n/2 \rceil - k} \circ [1 \widehat{\otimes} \overline{x}] \right) \ .$$

If A(E) is supersimple, by lemma 5 the h.c.p. map \mathbb{E} is strongly superirreducible. Hence,

$$\lim_{n \to \infty} \left\langle \Psi_n^{E|x}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E|x} \right\rangle = \sum_{a,b=0}^{\mu} \underbrace{x + v_a}_{x + v_a} \underbrace{\Lambda_a + v_b}_{x + v_b} \underbrace{\Lambda_b}_{x + v_b} = \sum_{a,b=0}^{\mu} (-1)^{b|x|} \operatorname{str}(x v_a x^* \Lambda_b) \underbrace{\operatorname{str}(\Lambda_a \mathbb{E}_{\mathcal{O}}(v_b))}_{=\delta_{ab} \omega_E(\mathcal{O})}.$$

For simplicity this assumed that $\|\mathbb{E}\| = 1$.

After constructing states in the thermodynamic limit, it is natural to ask what can be said about overlaps between different such sMPVs. The answer is surprisingly simple: They all vanish in the thermodynamic limit. This is the fundamental theorem of matrix

product states, due to its extensive ramifications, and is proven here in its graded version; the ungraded statement can be found in [130, 142, 146].

It is a consequence of the uniqueness of the GNS constructions explained in theorem 1.1, and indeed that is how the authors of [17] proved the related theorem 7.

Afterwards, three consequences are explored. First of all, suppose a matrix product vector representation Φ_n is given for a family of vector states on graded Hilbert spaces, which are parity eigenstates. Then part (i) of corollary 2 shows that it is possible to construct a grading on the virtual space such that Φ_n is a family of super matrix product vectors. This is a useful result since while the grading on the physical space is given and fixed, this does not hold for the virtual grading. In particular a grading has to be distinguished from a \mathbb{Z}_2 -symmetry. The latter would make sMPS a special case of G-symmetric MPS. Such differences are not visible if the structure of expectation values remains outside the discussion [26]. Here, I show the reversed inclusion. Notably, part (ii) of corollary 2 shows that the proper notion of lifting an on-site symmetry involves the grading. Finally, corollary 3 shows how to form the tensor product of sMPVs: By taking the graded tensor product. This again drives home the point that fermion parity is not a symmetry, on account of being interwoven into the structures. Breaking it renders the expressions ill-defined.

Theorem 8. Suppose $E^{(1)}$, $E^{(2)}$ supersimple, unital, and satisfying the sMPV constraint. Then either there is a homogeneous isometry $u: H_2 \to H_1$ and a phase $e^{i\phi}$ such that

$$E_s^{(1)} = (-1)^{|u||E^{(2)}|} e^{i\phi} u E_s^{(2)} u^{-1} ; (3.23)$$

or there is r < 1 such that for all $\mathcal{O} \in \mathcal{A}_{\mathbb{Z},loc}$, $n > \operatorname{supp}(\mathcal{O})$:

$$\left| \left\langle \Psi_n^{E^{(1)}}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E^{(2)}} \right\rangle \right| \lesssim r^{n - \text{supp}(\mathcal{O})} \|\mathcal{O}\| . \tag{3.24}$$

Furthermore, suppose E is supersimple, unital, and bosonic. Then, either there is a isometry $u: H_2 \to H_1$ and a phase $e^{i\phi}$ such that 3.23 holds (with trivial grading), or 3.24 is true for all $\mathcal{O} \in (\mathcal{A}^0)_{\mathbb{Z},loc}$.

Before proving this statement, observe that it implies that two supersimple sMPS are either identical or in different superselection sectors of $\mathcal{A}_{\mathbb{Z}}$ or $(\mathcal{A}^0)_{\mathbb{Z}}$ respectively. Indeed, suppose $E^{(1)}$ is not isomorphic to $E^{(2)}$. Then in the thermodynamic limit superpositions become decoherent:

$$c_1 \Psi_n^{E^{(1)}} + c_2 \Psi_n^{E^{(2)}} \longrightarrow |c_1|^2 \omega_{E^{(1)}} + |c_2|^2 \omega_{E^{(2)}},$$
 (3.25)

which indicates they live in different superselection sectors.

Importantly, the phenomenon of equation 3.25 also allows for the appearance of spontaneous symmetry breaking. Observe what happens when there are two distinct sM-PVs Ψ_n , Φ_n together with a \mathbb{Z}_2 symmetry action $g \cdot \Psi_n = \Phi_n$ and $g \cdot \Phi_n = \Psi_n$. Then for all finite n, there is a basis of singlet states $(\Phi_n \pm \Psi_n)/\sqrt{2}$. Importantly though, by the above argument, these become decoherent in the thermodynamic limit

 $(\Phi_n \pm \Psi_n)/\sqrt{2} \to (\omega_{\Psi} + \omega_{\Phi})/2$, and the symmetry is broken¹. The usage of a \mathbb{Z}_2 symmetry was for convenience, the analysis can be repeated to yield that only one-dimensional representations on sMPVs remain unbroken.

Indeed, this allows to take the thermodynamic limit of quite general matrix product vectors of the form 3.16:

$$\Psi_n^{E|x} \longrightarrow \sum_{i:d_i=1} f(x_i)\omega_{E^{(i)}} . \tag{3.26}$$

In lieu of the alternative between isomorphy and orthogonality stated in theorem 8, call a MPV reduced if all of the d_i in equation 3.16 are unity; in other words: if \mathbb{E} is incontractible in the sense of definition 8. Recall from that this ensures that \mathbb{E} has positive invertible left and right fixed points, which in turn guarantees that E can be used to build a super matrix product state in the sense of proposition 2.

Proof of theorem 8. Assume w.l.o.g. $\|\mathbb{E}^{(1)}\| = 1 = \|\mathbb{E}^{(2)}\|$. Then, by lemma 6 proven in appendix B, $\|\mathbb{E}^{(1,2)}\| \leq 1$. Assume first equality, i.e., there is $u: H_2 \to H_1$ normalized by $\|u\| = 1$ such that $\mathbb{E}^{(1,2)}(u) = e^{i\phi}u$. Then, by the Kadison-Schwarz inequality from aforementioned lemma 6:

$$\mathbb{E}^{(2)}(u^*u) \ge \mathbb{E}^{(1,2)}(u)^* \mathbb{E}^{(1,2)}(u) = u^*u , \quad \mathbb{E}^{(1)}(uu^*) \ge \mathbb{E}^{(1,2)}(u) \mathbb{E}^{(1,2)}(u)^* = uu^* .$$

Now by Theorem 2.3 of [47], this implies that u^*u and uu^* are fixed points of $\mathbb{E}^{(2)}$ and $\mathbb{E}^{(1)}$ respectively. Hence, by strong irreducibility, u is an isometry. Finally, consider, for $\xi \in H_1$:

$$\sum_{s} \| (E_{s}^{(1)} - (-1)^{|u||E_{s}^{(2)}|} e^{i\phi} u E_{s}^{(2)} u^{*})^{*} \xi \|^{2} =$$

$$= \sum_{s} \langle \xi, \left[E_{s}^{(1)} - (-1)^{|u||E_{s}^{(2)}|} e^{i\phi} u E_{s}^{(2)} u^{*} \right] \left[E_{s}^{(1)} - (-1)^{|u||E_{s}^{(2)}|} e^{i\phi} u E_{s}^{(2)} u^{*} \right]^{*} \xi \rangle =$$

$$= \langle \xi, (\mathbb{E}^{(1)}(1_{H_{1}}) + u \mathbb{E}^{(2)}(u^{*}u) u^{*} - e^{i\phi} u \mathbb{E}^{(1,2)}(u)^{*} - e^{-i\phi} \mathbb{E}^{(1,2)}(u) u^{*}) \xi \rangle = 0 .$$

Equation 3.23 follows as each summand of a vanishing sum of non-negative terms has to vanish individually, and the arbitrariness of ξ .

Now for the second alternative $\|\mathbb{E}^{(1,2)}\| = r < 1$, use equation 3.20 for any local observable with connected support:

$$\left| \left\langle \Psi_n^{E^{(1)}}, S^{\lfloor n/2 \rfloor}(\mathcal{O}) \Psi_n^{E^{(2)}} \right\rangle \right| \lesssim r^{n-\operatorname{supp}(\mathcal{O})} \|\mathcal{O}\| . \tag{3.27}$$

As before, there is no proof of the bosonic version as it is strictly analogous. \Box

¹A connection to the more usual accounts in the difference: symmetric Hamiltonian – symmetry broken ground state can be taken by the construction of so-called *parent Hamiltonians* [50, 130] which are not featured here.

Now in general this fundamental theorem can be used to lift symmetries from the physical to the virtual Hilbert space. In this, the \mathbb{Z}_2 -parity transformation plays a structural rôle. Indeed, start with a MPV tensor $E:\mathcal{H}\to\mathscr{L}(\tilde{H})$, where \tilde{H} is here endowed with the trivial grading. Suppose that $\Psi_n^{E,x}$ is eigenvector of the n-site parity operation P_n . Then by the second part of the theorem 8, there is a unitary \hat{P} such that the sMPV constraint 3.15 is fulfilled. By a redefinition, $\hat{P}^2=1$, and hence $H=(\tilde{H},\hat{P})$ is a super Hilbert space.

Corollary 2. Let $\Psi_n^{E|x}$ be a matrix product vector given in terms of a semisimple reduced unital $E: \mathcal{H} \to \mathcal{L}(H)$. Suppose $\alpha: (G, \mathfrak{p}) \to \operatorname{Aut}(H)$ is an even representation.

- (i) If the $\Psi_n^{E|x}$ are eigenvectors of P_n , then there is a unitary involution \widehat{P} on H such that E satisfies the sMPV constraint for P, \widehat{P} .
- (ii) If the $\Psi_n^{E|x}$ are eigenvectors of all the $(\alpha_g)^{\widehat{\otimes} n}$, satisfy the sMPV constraint, and there is no symmetry breaking in the thermodynamic limit, then there is a projective homogeneous representation $\widehat{\alpha}:(G,\mathfrak{p})\to \operatorname{Aut}(H)$ such that for all $g\in G$:

$$E \circ \alpha_g = \mathrm{sAd}_{\widehat{\alpha}_g} \circ E \ . \tag{3.28}$$

As this proposition shows, the virtual grading modifies how symmetries are lifted to the virtual level.

Proof.

(i) Denote by Q the parity operator of H, and H^b the Hilbert space obtained by trivializing the grading. Since $\Psi_n^{E|x} = \Psi_n^{E|Qx}$, where on the right hand side the virtual gradings have been trivialized, reduce to the situation of trivial virtual grading.

Decompose E into its (super-)simple elements as in equation 3.16. Then, by assumption:

$$P_n\left(\sum_{i=1}^r \Psi^{E^{(i)}}\right) = \pm \sum_{i=1}^r \Psi^{E^{(i)}}.$$

Since $P_n^2 = 1$, there is an involution π on $\{1, ..., r\}$ with $P_n \Psi^{E^{(i)}} = \pm \Psi^{E^{(\pi^{(i)})}}$. If a given i is a fixed point of π , use the second part of theorem 8 to obtain a unitary \widehat{P} such that the sMPV constraint 3.15 is fulfilled. If $i \neq \pi(i)$, define a parity operator $\widehat{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ on $H_i \oplus H_{\pi(i)}$. Then, $E^{(i)} \oplus E^{(\pi(i))}$ satisfies the sMPV constraint.

(ii) By excluding spontaneous symmetry breaking, assume that each of the supersimple components of $\Psi_n^{E|x}$ is mapped onto itself by the action of G. Therefore assume that A(E) is supersimple.

The following identity for $f \in H^*$, u a unitary, and an ONB $\{\psi_s\}_s$ is useful:

$$\sum_{s} \overline{f(\psi_s)}^{1-\mathfrak{p}(g)} \alpha_g(\psi_s) = \sum_{s} \overline{f((\alpha_g)^* \psi_s)}^{1-\mathfrak{p}(g)} \psi_s . \tag{3.29}$$

Acting with α_g on the sMPV:

$$\alpha_g^{\widehat{\otimes} n} \Psi_n^E = \sum_{s_1, \dots, s_n} \overline{\operatorname{str}(xE(\psi_{s_1}) \cdots E(\psi_n))}^{1-\mathfrak{p}(g)} (\alpha_g \psi_{s_1}) \widehat{\otimes} \cdots \widehat{\otimes} (\alpha_g \psi_{s_n}) . \tag{3.30}$$

Note that for each tensor factor, $\psi \mapsto \text{str}(xE(\psi_{s_1})\cdots E(\psi)\cdots E(\psi_n))$ is a linear functional. Use identity 3.29 to shift the α_g -action:

$$\alpha_g^{\widehat{\otimes} n} \Psi_n^E = \sum_{s_1, \dots, s_n} \overline{\operatorname{str}(xE(\alpha_g^* \psi_{s_1}) \cdots E(\alpha_g^* \psi_n))}^{1-\mathfrak{p}(g)} |s_1 \cdots s_n\rangle . \tag{3.31}$$

If α_g is unitary, the r.h.s. has already the form of a sMPV $\Psi_n^{E\circ(\alpha_g)^*}$, and the assumption that the sMPVs are fixed by the symmetry gives $\Psi_n^E = \Psi_n^{E\circ(\alpha_g)^*}$. Hence, by the first part of theorem 8, there is a unitary homogeneous $\widehat{\alpha}_g$ such that equation 3.28 is satisfied. If α_g is anti-unitary, this is not so obvious and indeed there is some massaging necessary to get a similar result. Recall that anti-unitary operations K give rise to bilinear forms κ .

It is furthermore convenient to introduce the super Hilbert adjoint L^* defined by

$$h(L^{\star}\xi_1, \xi_2) = (-1)^{|L||\xi_1|} h(\xi_1, L\xi_2) . \tag{3.32}$$

This is useful as it gives rise to an anti-linear homomorphism $\mathcal{L}(V, W) \to \mathcal{L}(V^*, W^*)$, $L \mapsto L^c = (L^*)'$, with the property

$$\operatorname{str}_{V}(x) = \overline{\operatorname{str}_{V^{*}}(x^{c})} . \tag{3.33}$$

This identity allows to rewrite equation 3.31 in standard form:

$$\alpha_g^{\widehat{\otimes} n} \Psi_n^{E|x} = \sum_{s_1, \dots, s_n} \overline{\operatorname{str}_{H^*}(x^c E(\alpha_g^* \psi_{s_1})^c \cdots E(\alpha_g^* \psi_n)^c)} |s_1 \cdots s_n\rangle = \Psi_n^{(E \circ \alpha_g^*)^c |x^c|}.$$

The first part of theorem 8 gives a homogeneous unitary $\tilde{\alpha}_g: H \to H^*$ such that

$$[E \circ \alpha_g(\psi)]^c = (-1)^{|\tilde{\alpha}_g||\psi|} \tilde{\alpha}_g E(\psi) \tilde{\alpha}_g^{-1} . \tag{3.34}$$

That is, there is an anti-linear, anti-unitary lift $\widehat{\alpha}_q: H \to H$ defined by

$$h_H(\widehat{\alpha}_q(\psi_1), \psi_2) = \widetilde{\alpha}_q(\psi_1)(\psi_2) . \tag{3.35}$$

Having thus obtained a set $\{\widehat{\alpha}_g\}_{g\in G}$, dive into the task of characterizing the structure of this set.

The condition $E = E \circ \alpha_{g_1} \circ \alpha_{g_2} \circ \alpha_{(g_1g_2)^{-1}}$ leads to the constraint:

$$v(g_1, g_2) \ x = x \ v(g_1, g_2) \ , \quad v(g_1, g_2) := \widehat{\alpha}_{g_1} \widehat{\alpha}_{g_2} \widehat{\alpha}_{(g_1 g_2)^{-1}}$$

for all $x \in A(E)$. Thus $v(g_1, g_2)$ is in the even center of A(E), hence proportional to the identity. This furnishes a projective representations in the sense of definition 11.

The corollary allows to give the following cute construction:

Forgetful Map. As advertised above, one can introduce a map

$$\mathcal{F}: \mathcal{S}_D^G(\mathcal{A}) \to \mathcal{S}_D^G(\mathcal{A}^0)$$

in the following way. Pick a $\omega_{E,\rho} \in \mathcal{S}_D^G(\mathcal{A})$ with $E: \mathcal{H} \to \mathcal{L}(H)$. For a super Hilbert space V, denote by V^b the Hilbert space which is V with trivial grading. Let $E^b: \mathcal{H}^b \to \mathcal{L}(H^b)$ be the map E, but with all gradings trivialized. Then $\mathcal{F}(\omega_{E,\rho}) = \omega_{E^b,\rho}$. Note that $(\mathcal{A}^0)_{\mathbb{Z}} \subset \mathcal{A}_{\mathbb{Z}}$, and \mathcal{F} has the property that

$$\mathcal{F}(\omega_{E,\rho}) = \omega_{E,\rho}|_{(\mathcal{A}^0)_{\mathbb{Z}}}$$
.

This is most easily seen by comparing the wavefunctions. Moreover, corollary 2 implies that \mathcal{F} is invertible: Suppose there is given a state $\omega_{E,\rho} \in (\mathcal{A}^0)_{\mathbb{Z}}$. Then the bond space can be endowed with a grading such that $\mathcal{F}^{-1}(\omega_{E,\rho}) := \omega_{E^f,\rho} \in \mathcal{A}_{\mathbb{Z}}$ is an extension to the complete chain algebra, where for a Hilbert space V and a unitary involution P, V^f refers to V as a super Hilbert space with parity P.

The grading enters in one more structural aspect; and this is in tensor products of states.

Corollary 3. The tensor product of two sMPVs $\Psi_n^{E^{(1/2)}}$ with on-site Hilbert spaces $\mathcal{H}_{1/2}$ is

$$\mathcal{B}_{\text{mix}}\left(\Psi_{n}^{E^{(1)}|x_{1}}\widehat{\otimes}\Psi_{n}^{E^{(2)}|x_{2}}\right) = (-1)^{|x_{1}||x_{2}|}\Psi_{n}^{E^{(1)}\widehat{\otimes}E^{(2)}|x_{1}\widehat{\otimes}x_{2}},$$

$$\left[E^{(1)}\widehat{\otimes}E^{(2)}\right](\psi_{1}\widehat{\otimes}\psi_{2}) = E^{(1)}(\psi_{1})\widehat{\otimes}E^{(2)}(\psi_{2}).$$
(3.36)

Here, \mathscr{B}_{mix} is the braiding operation that maps the Hilbert spaces

$$\mathscr{B}_{\text{mix}}: (\mathcal{H}_1)^{\widehat{\otimes} n} \widehat{\otimes} (\mathcal{H}_2)^{\widehat{\otimes} n} \to (\mathcal{H}_1 \widehat{\otimes} \mathcal{H}_2)^{\widehat{\otimes} n} .$$
 (3.37)

Proof. Given two graded quantum spin systems with on-site Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ and MPVs $\Phi_i = \Psi_n(\varphi_i, E_i) \in \mathcal{H}_{i,n}$, the tensor product $\Phi_1 \widehat{\otimes} \Phi_2$ is a family of vectors with on-site Hilbert space $\mathcal{H}_1 \widehat{\otimes} \mathcal{H}_2$. Note that as the algebras are graded, expectation values do not factor. Also, writing $\Phi_1 \widehat{\otimes} \Phi_2$ as a tensor product over sites introduces braiding factors.

Denote by $\{\psi_s^{(i)}\}_{s=1,\dots,d_i}$ a orthonormal basis of \mathcal{H}_i . Then:

$$\begin{split} & \left\langle \Psi_{n}^{E^{(1)}} \widehat{\otimes} \Psi_{n}^{E^{(2)}}, [\psi_{s_{1}}^{(1)} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_{n}}^{(1)}] \widehat{\otimes} [\psi_{r_{1}}^{(2)} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{r_{n}}^{(2)}] \right\rangle = \\ & = \left\langle \Psi_{n}^{E^{(1)}}, \psi_{s_{1}}^{(1)} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_{n}}^{(1)} \right\rangle \left\langle \Psi_{n}^{E^{(2)}}, \psi_{s_{1}}^{(2)} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_{n}}^{(2)} \right\rangle = \\ & = \operatorname{str} \left(x_{1} E^{(1)} (\psi_{s_{1}}^{(1)}) \cdots E^{(1)} (\psi_{s_{n}}^{(1)}) \right) \operatorname{str} \left(x_{2} E^{(2)} (\psi_{r_{1}}^{(2)}) \cdots E^{(2)} (\psi_{r_{n}}^{(2)}) \right) = \\ & = (-1)^{|x_{1}||x_{2}|} \operatorname{str} \left([x_{1} \widehat{\otimes} x_{2}] \left[E^{(1)} (\psi_{s_{1}}^{(1)}) \cdots E^{(1)} (\psi_{s_{n}}^{(1)}) \widehat{\otimes} E^{(2)} (\psi_{r_{1}}^{(2)}) \cdots E^{(1)} (\psi_{r_{n}}^{(2)}) \right] \right) \; . \end{split}$$

Braiding on both sides with \mathscr{B}_{mix} gives, in terms of $\psi_{sr}^{(12)} = \psi_s^{(1)} \widehat{\otimes} \psi_r^{(2)}$:

$$\left\langle \mathscr{B}_{\text{mix}} \left(\Psi_n^{E^{(1)}} \widehat{\otimes} \Psi_n^{E^{(2)}} \right), \psi_{s_1 r_1}^{(12)} \widehat{\otimes} \cdots \widehat{\otimes} \psi_{s_n r_n}^{(12)} \right\rangle =$$

$$= (-1)^{|x_1||x_2|} \text{str} \left([x_1 \widehat{\otimes} x_2] \left[E^{(1)} (\psi_{s_1}^{(1)}) \widehat{\otimes} E^{(2)} (\psi_{r_1}^{(2)}) \right] \cdots \left[E^{(1)} (\psi_{s_n}^{(1)}) \widehat{\otimes} E^{(2)} (\psi_{r_n}^{(2)}) \right] \right) ,$$
which proves the claim.

3.3. Many-Body Invariants of Super Matrix Product States

Recall the density matrix bilinears defined in terms of the partial transpose 20:

$$Z_{k,\ell}^C(\omega) := \operatorname{Tr}(\sigma_{k+\ell} [\sigma_{k+\ell}]^{\mathbf{t}_k}) ,$$

$$Z_{k_1,k_2|d}^T(\omega) := \operatorname{Tr}(\sigma_{k_1,k_2|d} [\sigma_{k_1,k_2|d}]^{\mathbf{t}_{k_1}}) ,$$

$$\Delta_n(\omega) := -\log \operatorname{Tr}([\sigma_n]^2) .$$

The last line is the second Renyi entropy, which plays a distinguished rôle.

In this section, I compute $Z^{C/T}$ in the thermodynamic limit for super matrix product states. This establishes them as homotopy invariants of super matrix product states with particle-hole, respectively motion-reversal, symmetry.

Proposition 5. Let ω be a pure super matrix product state with bond algebra A and virtual parity operator \widehat{P} . Then $\Delta(\omega) := \lim_{n \to \infty} \Delta_n(\omega)$ exists and

$$|e^{-\Delta_n(\omega)} - e^{-\Delta(\omega)}| \le 2||\mathbb{E}^n - \mathbb{E}^\infty||. \tag{3.38}$$

Moreover:

(i) Suppose ω is invariant under a particle-hole symmetry C. Denote by \widehat{C} the lift of C on the bond space, and recall the three indices $\mu = \mu_A$, $(-1)^{\widehat{c}} = \widehat{C}\widehat{P}\widehat{C}^{-1}\widehat{P}$ and $(-1)^{\epsilon} = \widehat{C}^2$. Then $Z^C(\omega) := \lim_{k,\ell \to \infty} Z^C_{k,\ell}(\omega)$ exists and

$$Z^{C} = \exp\left(-\frac{3}{2}\Delta - 2\pi i \frac{\eta_{C}}{8}\right) , \quad \eta_{C}(\omega) = 4\epsilon + 2\hat{c} - \mu \in \mathbb{Z}/8\mathbb{Z} . \tag{3.39}$$

The convergence is estimated by

$$|Z_{k,\ell}^C(\omega) - Z^C(\omega)| \le 2\left(\|\mathbb{E}^k - \mathbb{E}^\infty\| + \|\mathbb{E}^\ell - \mathbb{E}^\infty\|\right). \tag{3.40}$$

(ii) Suppose ω is invariant under a time-reversal symmetry T with lift \widehat{T} . Let $(-1)^{\widehat{t}} = \widehat{T}\widehat{P}\widehat{T}^{-1}\widehat{P}$. Then $Z^T(\omega) := \lim_{k_1,k_2,d\to\infty} Z_{k_1,k_2,d}^T(\omega)$ exists and

$$Z^T = \exp\left(-2\Delta + 2\pi i \frac{\eta_T}{2}\right) , \quad \eta_T(\omega) = \hat{t} \in \mathbb{Z}/2\mathbb{Z} ,$$
 (3.41)

The convergence is estimated by

$$|Z_{k_1,k_2|d}^T(\omega) - Z^T(\omega)| \le 2\left(\|\mathbb{E}^{k_1} - \mathbb{E}^{\infty}\| + \|\mathbb{E}^d - \mathbb{E}^{\infty}\| + \|\mathbb{E}^{k_2} - \mathbb{E}^{\infty}\| \right) . \quad (3.42)$$

In [133], the authors obtained a similar result for Z^C on (bosonic) matrix product states, in which case the motion-reversal and the particle-hole case are not distinct. The authors of [151, 154, 152], which proposed to calculate $Z_{k,\ell}^C(\omega)$ and $Z_{k_1,k_2|d}^T(\omega)$, were able to compute them for certain fixed-point states. They motivated that it would indeed apply to general states, and would be a topological invariant by numerics on a quasi-free translation invariant Hamiltonian, and arguments from topological quantum field theory. Proposition 5 summarizes what can be said about $Z_{k,\ell}^C(\omega)$ and $Z_{k_1,k_2|d}^T(\omega)$ for the larger class of super matrix product states. Moreover, by connecting the values of these objects to topological invariants on the set of super matrix product states, it establishes that Z^T and Z^C , or rather their arguments, indeed do give invariants of super matrix product states.

The stress which is laid on the convergence is important in lieu of section 4, which pushes beyond super matrix product states.

Before jumping to the proof, a few comments as to how the continuity of these quantities can be estimated, as a function of the state ω . For simplicity, focus on $Z_{k,\ell}^C = Z_{k,\ell}$:

$$|Z_{k,\ell}(\omega_1) - Z_{k,\ell}(\omega_2)| = = |\text{Tr}(\sigma_{k+\ell}(\omega_1)^{t_k} [\sigma_{k+\ell}(\omega_1) - \sigma_{k+\ell}(\omega_2)] + \sigma_{k+\ell}(\omega_2) [\sigma_{k+\ell}(\omega_1) - \sigma_{k+\ell}(\omega_2)]^{t_k})|.$$

Using identity 3.44 below, the partial transpose in the second term can be shifted to yield

$$|Z_{k,n-k}(\omega_1) - Z_{k,n-k}(\omega_2)| = |(\omega_1 - \omega_2)([\sigma_n(\omega_1) + \sigma_n(\omega_2)]^{t_k})| =$$

$$\leq 2||\sigma_n(\omega_1) - \sigma_n(\omega_2)||_1.$$
(3.43)

Where the inequalities $|\operatorname{Tr}(X)| \leq \operatorname{Tr}|X|$ and $\operatorname{Tr}|XY| \leq ||X||_{\infty} ||Y||_{1}$ found application.

The partial transpositions commute and combine to full transpositions, $(x^{t_1})^{t_2} = (x^{t_2})^{t_1} = x^t$. Moreover, similar to the usual transpose, it holds that $\operatorname{tr}(x^{t_1}) = \operatorname{tr}(x)$, where tr is the trace on $A_1 \widehat{\otimes} A_2$. This is most easily proven in the case that $A_1 \widehat{\otimes} A_2 \cong \operatorname{Mat}_n(\mathbb{C})$, or some subset thereof, in which case x may be decomposed as $x = n^{-1}\operatorname{tr}(x)1 + (x - n^{-1}\operatorname{tr}(x)1)$. This can then be used to show that

$$\operatorname{tr}(x^{t_1}y) = \operatorname{tr}(xy^{t_1})$$
 (3.44)

The first step is $\operatorname{tr}(x^{t_1}y) = \operatorname{tr}((x^{t_1}y)^{t_1})$. As the partial transpose is not an anti-automorphism, the product reads somewhat complicated

$$\left[(x_1 \widehat{\otimes} x_2)^{t_1} (y_1 \widehat{\otimes} y_2) \right]^{t_1} = (-1)^{k|y_2| + |x_2||y_1| + |x_1||y_1|} (y_1)^t (x_1)^{tt} \widehat{\otimes} x_2 y_2 .$$

But once this is traced over:

$$(-1)^{k|y_2|+|x_2||y_1|+|x_1||y_1|}\mathrm{tr}((x_1)^{\mathrm{tt}}(y_1)^{\mathrm{t}})\mathrm{tr}(x_2y_2) = (-1)^{|x_1|+|x_1||y_1|}\mathrm{tr}(xy^{\mathrm{t}_1}) \ ,$$

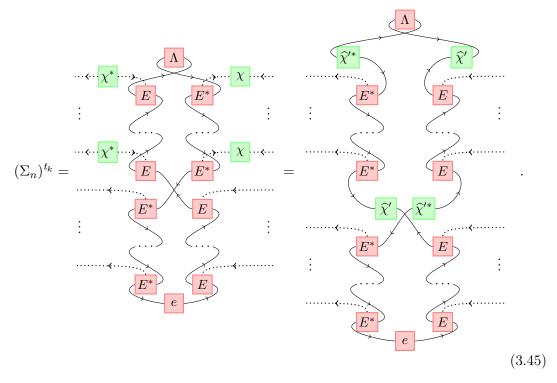
where the last sign is seen to disappear as the trace is nonzero only for $|x_1| = |y_1|$.

Proof of part (i) of proposition 5. Qua assumption, there is an anti-linear on-site involutive transformation C. As developed in section 1.3, this may be combined with the super-hermitian form introduced in definition 3 to give a bilinear form $\chi: \mathcal{H} \widehat{\otimes} \mathcal{H} \to \mathbb{C}$. Then equation 1.58 gives the graded transpose of an operator in terms of the bilinear form.

Since C is assumed to be even:

$$(\Sigma_n)^{t_k} = P_n(\sigma_n)^{t_k} .$$

Simplification is most easily done diagrammatically. By equation 1.57, the transpose is implemented by exchanging incoming with outgoing legs of the graded density operator of equation 3.13, and to add tensors χ, χ^* on both sides. This explains the first step:

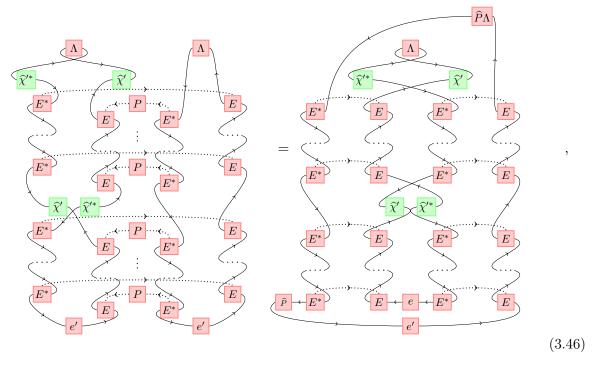


Again, the fact that χ is even has been used to discard all precautions about tensor ordering. By assumption there is a lift \widehat{C} on H, of the form explained in section 1.3. It allows to push the χ s to the virtual level, as in equations 1.63 and 1.64. This, together with the composition identities 1.66 and 1.65 gives an expression for the partially transposed density operator with just four $\widehat{\chi}$ tensors. If this is performed, the second equality in 3.45 arises.

The object that is to be calculated is

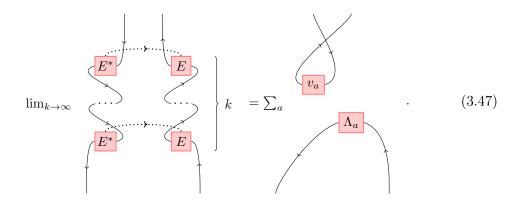
$$Z_{k,\ell}^C \equiv Z_{k,\ell} = \text{Tr}(\sigma_{k+\ell}[\sigma_{k+\ell}]^{t_k}) = \text{sTr}(P_{k+\ell}\Sigma_{k+\ell}[\Sigma_{k+\ell}]^{t_k}) .$$

Gluing together diagrams 3.45 and 3.13 gives



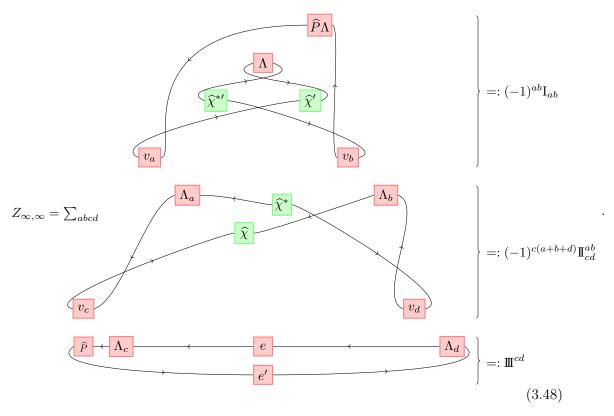
where the fermion parities are pushed to the virtual level and the vertical strands are exchanged such that physical contractions are adjacent.

If the state ω is pure, by proposition 2 the transfer operator is strongly irreducible. By proposition 1:



Inserting equation 3.47 for the limiting behavious of \mathbb{E}^k into equation 3.46 for $Z_{k,\ell}$ yields

the following:



Before turning to the computation of the indicated subdiagrams, note that the speed with which the limit is attained can be estimated in terms of the approximation of \mathbb{E}^k to its limit. Indeed, $Z_{k,\ell} - Z_{\infty,\infty}$ can be written as a sum of four terms, each of which have an insertion of $\mathbb{E}^n - \mathbb{E}^\infty$ in one of the four subdiagrams of equation 3.46 containing strings of transfer operators. This already implies equation 3.40, by applying the Cauchy-Schwarz inequality for the trace pairing on $\mathcal{A}_{k+\ell}$ since $|Z_{k,\ell}| \leq 1$.

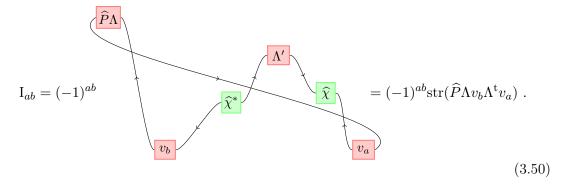
The definitions of the subdiagrams I, II and III should be read with caution. To properly disassemble the diagram into its factors one first has to separate its parts horizontally, accumulating signs in the process.

The signs included in the right side are such that

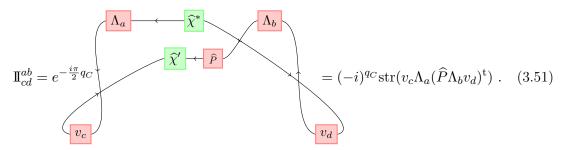
$$Z_{\infty,\infty} = \sum_{abcd} \mathbf{I}_{ab} \mathbf{I}_{cd}^{ab} \mathbf{I}_{cd}^{cd} , \qquad (3.49)$$

where each of the factors in the sum is given by the diagram is obtained by removing the other subdiagrams, with signs. Thence, the remaining task is the computation of these subdiagrams.

Begin with I_{ab} :



For the second diagram, use the symmetry properties of χ^* . Then:



The third subdiagram is disentangled to:

$$\mathbb{I}^{cd} = \underbrace{\widehat{P} \wedge \Lambda_c \wedge e \wedge \Lambda_d}_{e'} = \operatorname{str}(\widehat{P}\Lambda_c e \Lambda_d e) .$$

The penultimate step is to compute the above supertraces. As an entrée

$$\mathbb{I}^{cd} = sTr(\widehat{P}\Lambda_c e \Lambda_d e) = \delta_{cd} tr(\Lambda e)^2 . \tag{3.52}$$

The next course, I_{ab} , is not too difficult either. Use $\Lambda^t = (-1)^{\hat{c}} \Lambda$ and, with $v_a = z_a e$ and $\Lambda_a = \Lambda z_a$, that $\Lambda z_a = (-1)^a z_a \Lambda$ and $z_a z_b = z_{a+b}$. Whence:

$$I_{ab} = (-1)^{ab} \operatorname{str}(\widehat{P}\Lambda v_b \Lambda^{t} v_a) = (-1)^{ab+\hat{c}+a} \delta_{ab} \operatorname{tr}(\Lambda e \Lambda e z_{a+b}) = (-1)^{\hat{c}} \delta_{ab} \operatorname{tr}(\Lambda e)^2 . \quad (3.53)$$

Finally, the pièce de résistance, \mathbb{I}_{cd}^{ab} . Use $v_a^{\rm t}=i^av_a$ and $\Lambda_a^{\rm t}=(-1)^{\hat c}(-i)^a\Lambda_a$

$$\mathbf{II}_{aa}^{bb} = (-i)^{q_C} \operatorname{str}(v_b \Lambda_a(\widehat{P}\Lambda_a v_b)^{t}) = (-i)^{q_C} (-1)^{ab} i^{a-b} (-1)^{\hat{c}} \operatorname{tr}(z_{a+b}^2 e \Lambda e \Lambda) =
= (-i)^{q_C} (-1)^{\hat{c}} i^{(a-b)^2} \operatorname{tr}(\Lambda e)^2.$$
(3.54)

Inserting equations 3.53, 3.54 and 3.52 into 3.49 gives, for $\mu_A = 0$:

$$Z^C = \left[(-1)^{\hat{c}} \mathrm{tr}(\Lambda e)^2 \right] \left[(-i)^{q_C} (-1)^{\hat{c}} \mathrm{tr}(\Lambda e)^2 \right] \left[\mathrm{tr}(\Lambda e)^2 \right] = (-i)^{q_C} \left[\mathrm{tr}(\Lambda e)^2 \right]^3 \ .$$

For $\mu_A = 1$ instead:

$$Z^{C} = \sum_{ab=1}^{\mu} \left[(-1)^{\hat{c}} \operatorname{tr}(\Lambda e)^{2} \right] \left[(-i)^{q_{C}} (-1)^{\hat{c}} i^{(a-b)^{2}} \operatorname{tr}(\Lambda e)^{2} \right] \left[\operatorname{tr}(\Lambda e)^{2} \right] =$$

$$= \left[\operatorname{tr}(\Lambda e)^{2} \right]^{3} (-i)^{q_{C}} \sum_{ab} i^{(a-b)^{2}} = \left[(-i)^{q_{C}} \frac{1+i}{\sqrt{2}} \right] \left[\sqrt{2} \operatorname{tr}(\Lambda e)^{2} \right]^{3} .$$

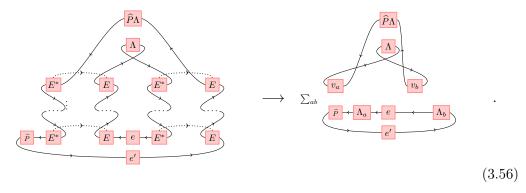
The combined expression is for $\mu = \mu_A$ and $q_C = \hat{c} + 2\epsilon$:

$$Z^{C}(\omega) = \left[2^{\mu} \left(\text{tr}(\Lambda e)^{2} \right)^{2} \right]^{\frac{3}{2}} \exp\left(-\frac{2\pi i}{8} (4\epsilon + 2\hat{c} - \mu)\right) . \tag{3.55}$$

To interpret this expression, compute $\Delta(\omega)$. The definition is:

$$e^{-\Delta(\omega)} = \lim_{n \to \infty} \operatorname{Tr}(\sigma_n)^2 = \lim_{n \to \infty} \operatorname{sTr}(P_n(\Sigma_n)^2)$$
.

The limit is again conveniently done diagrammatically:



By similar reasoning as for the approach of Z to its limit, this also shows 3.38. The right hand side of equation 3.56 is translated into equations as

$$e^{-\Delta(\omega)} = \sum_{ab=0}^{\mu} \operatorname{tr}(\Lambda v_b \Lambda v_a) \operatorname{tr}(e\Lambda_a e\Lambda_b) = \sum_{ab=0}^{\mu} \left[(-1)^{|v_a|} \delta_{ab} \operatorname{tr}(\Lambda e)^2 \right]^2 = 2^{\mu} \left[\operatorname{tr}(\Lambda e)^2 \right]^2 . \tag{3.57}$$

Remark 2. If, instead of a particle-hole type symmetry a time-reversal symmetry is used, the parity factor in the second diagram 3.51 is deleted. Thus, for e = 1:

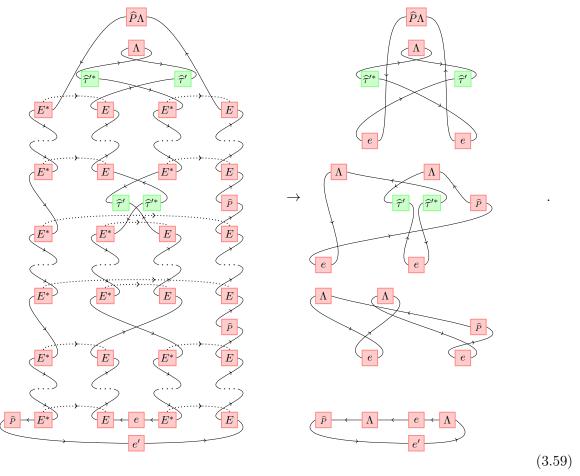
$$\mathbf{I}^T = (-1)^{\hat{t}} \operatorname{str}(\Lambda \Lambda^{t}) = \operatorname{str}(\rho^2) .$$

This, too, can be expressed in terms of the density matrix, $sTr(\sigma_n)^2 \longrightarrow str(\rho^2)$. However, this does not satisfy any area law; so while it is some real number, there is no reason why it should be bounded away from zero. Thus, calculating the adjacent transpose with a time-reversal symmetry does not give a homotopy invariant.

Proof of part (ii) of proposition 5. This is done a bit hastier than before, since the methods are the same. The expression is

$$\operatorname{Tr}(\sigma_{k_1,k_2|d}(\sigma_{k_1,k_2|d})^{t_{k_1}}) = \operatorname{sTr}(P_{k_1,k_2|d}\Sigma_{k_1,k_2|d}(\Sigma_{k_1,k_2|d})^{t_{k_1}}), \qquad (3.58)$$

As that the state ω is T-symmetric, and in the limit where k_1, k_2, d are all taken to infinity:



The details are not included here. The uppermost and the lowermost subdiagrams correspond to subdiagrams I and III, respectively, of 3.48. The other two are new, but both just give another factor of $tr(\Lambda e)^2$. Hence:

$$Z^{T}(\omega) = (-1)^{\hat{t}} \left[\operatorname{tr}(\Lambda e)^{2} \right]^{4} = (-1)^{\hat{t}} e^{-2\Delta(\omega)} . \tag{3.60}$$

The speed of convergence can be similarly estimated through the number of transfer operator limit subdiagrams. \Box

Remark 3. Similar to the discussion in remark 2, using a particle-hole symmetry here instead of a time-reversal symmetry does not produce a homotopy invariant: Again, a factor of $str(\rho^2)$ appears, which can be smoothly continued through zero within matrix product states, generically.

3.4. Calculation of $\pi_0(\partial S^G)$ for some G

The partition functions Z^T and Z^C can be used to determine $\pi_0(\partial S^G)$ for some particularly simple G, namely those mentioned in table 2.1.

Particle-Hole Symmetry. Recall from table 2.1, that the entries labeled by BDI, AIII, CII and AI are completely classified by their value on $\mathbb{R}P^2$, and the presence of a particle hole symmetry allows to define Z^C .

- BDI. For the label BDI, all eight possibilities can be realized, which reproduces the \mathbb{Z}_8 classification for superconductors with particle-hole symmetry in the presence of interactions [51].
- AIII. The label AIII here indicates an insulator with particle-hole symmetry, i.e., on top of the lifted particle hole symmetry \widehat{C} , there is also a $U(1)_Q$ charge symmetry, with lifted representation $e^{i\phi} \mapsto e^{i\phi\widehat{Q}}$. Then $\widehat{C}\widehat{Q}\widehat{C}^{-1} = -\widehat{Q}$, as can be seen by differentiating the action of both symmetries on an element x of $\mathcal{L}(H)$:

$$\begin{split} \frac{d}{d\phi}\bigg|_{\phi=0} \left[\operatorname{Ad}_{e^{i\phi\widehat{Q}}} \circ \operatorname{Ad}_{\widehat{C}}(x) \right] &\stackrel{!}{=} \frac{d}{d\phi}\bigg|_{\phi=0} \left[\operatorname{Ad}_{\widehat{C}} \circ \operatorname{Ad}_{e^{i\phi\widehat{Q}}}(x) \right] \\ \Rightarrow \left[\widehat{Q}, \widehat{C}x\widehat{C}^{-1} \right] &= -\widehat{C}[\widehat{Q}, x]\widehat{C}^{-1} \ . \end{split}$$

A continuous connected symmetry group is necessarily represented by even operators, i.e., $\widehat{Q} \in \mathcal{L}(\mathcal{H})^0$. If $\mu = 1$, there is an element ν in the odd center. If $\nu_{\phi} = \exp(i\phi[\widehat{Q},\cdot])(\nu)$ is not proportional to ν , then there would be another linearly independent element in the center. However, if ν is \widehat{C} -invariant, so is ν_{ϕ} , and hence $\nu_{\phi} = \nu$. Finally, the parity of ν is given by

$$-\nu = P\nu P^{-1} = \exp(i\pi[\hat{Q},\cdot])(\nu) = \nu_{\pi} = \nu$$
,

a contradiction! Hence, $\mu=0$. That both k and ϵ can be non-zero is most easily seen by constructing particle-hole conjugations on Fock spaces $\Lambda(\mathbb{C}^N)$ for N=1,2,3,4. Thus, $\eta_C(\omega)\in\mathbb{Z}_4$, which reproduces the \mathbb{Z}_4 classification of one-dimensional insulators with particle-hole symmetry.

- AI. Differentiate the symmetry action as in case AIII. Thus on virtual Hilbert space, $\widehat{C}\widehat{\widehat{Q}}\widehat{C}^{-1} = \widehat{\widehat{Q}}$. Suppose $\mu = 1$, with ν the odd real central element, then $\nu_{\phi \neq 0,\pi}$, defined as in case AIII, is linearly independent from ν and hence A(E) cannot be supercentral. Thus, $\mu = 0$. Then, since \widehat{C} preserves the eigenspaces of $\widehat{\widehat{Q}}$, by the spin-charge relation it preserves eigenspaces of the parity operator and k = 0. The common eigenspaces of both have no further structure. Hence, they admit $\epsilon = 0, 1$ and $\eta_C(\omega) \in \mathbb{Z}_2$.
- CII. If, instead of a charge symmetry, a spin rotation symmetry is present, similar arguments give that $\widehat{C}\widehat{S}_i\widehat{C}^{-1} = -\widehat{S}_i$, where \widehat{S}_i are the generators of the spin rotation

group. This allows to conclude as before that $\mu=0$. Since \widehat{C} commutes with the Casimir operator of $SU(2)_{\rm spin}$, it can only mix representation of the same spin quantum number, which have the same parity by the spin-charge relation of $SU(2)_{\rm spin}$. Hence, \widehat{C} is even. As in the AI case, $\epsilon=0,1$ is possible since the common eigenspace have no further structure. Thus $\eta_C(\omega) \in \mathbb{Z}_2$.

Motion-Reversal Symmetry. The presence of a motion-reversal symmetry T allows to define the "Klein bottle" partition function Z^T . According to table 2.1 this allows to classify the SPT phases labeled therein as DIII, CI and AII. The last two are special as they have a time-reversal symmetry, but their bordism group is generated by $\mathbb{R}P^2$.

DIII. As remarked above, the lifted time-reversal symmetry can be even or odd. \widehat{T} even is the standard case and corresponds to the trivial phase, \widehat{T} odd is a bit more exotic. It can be realized on a Fock space over an odd-dimensional single particle space V, by a modified particle-hole conjugation $\widehat{T} := \Xi_Q := \Xi \exp(i\pi Q/2)$, where $Q|_{\Lambda^k} = k - \frac{\dim V}{2}$. This is odd, and:

$$(\Xi_Q)^2 = \pm e^{\frac{i\pi}{2}\dim V} P \ .$$

Hence, $\eta_T = 0, 1$, which recovers the \mathbb{Z}_2 -classification for time-reversal symmetric superconductors.

- AII. The lifted time-reversal symmetry and the lifted phase rotation symmetry have to satisfy $\widehat{T}\widehat{Q}\widehat{T}^{-1}=\widehat{Q}$. Hence, \widehat{T} is even and $\eta_T=0$. In this symmetry group, table 2.1 reveals an oddity, namely that the bordism group is \mathbb{Z} , and generated by $\mathbb{R}P^2$. As was explained above, \mathbb{Z} -summands in bordism groups do not correspond to SPT phases since they do not yield non-trivial deformation classes. This is reflected in the fact noted in remark 2: Using the adjacent partial transpose with a T-symmetry gives a finite result, with a non-trivial phase; but there is no constraint that prohibits deformations. As an example that gives $\operatorname{str}(\rho^2)=0$ consider $H=\Lambda(\mathbb{C}^2)$, with $\rho=\frac{1}{4}\operatorname{id}_H$ and \widehat{T} acting on \mathbb{C}^2 irreducibly. Then $\operatorname{str}(\rho^2)=\frac{1}{16}(1+(-2)+1)=0$. Therefore, this is no candidate for a homotopy invariant.
- CI. Similar to case CII above, the spin-charge relation forces \widehat{T} to be even, so $\eta_T=0$. However, the SU(2) symmetry has a peculiar effect [178]. As explained in appendix C, one may deform the state to one which is non-trivial only on local SU(2)-singlets. This corresponds to a reduction of the symmetry group to \mathbb{Z}_2^T , which then is implemented in a bosonic MPS. Bosonic MPS with time-reversal symmetries are subsumed, in this work under particle-hole symmetric insulators with trivial grading, and hence fall into the series classified by the partition function Z^C . Since $\mu=k=0$, only a \mathbb{Z}_2 -classification remains, by the sign of \widehat{T}^2 , the lift of the time-reversal symmetry to the virtual Hilbert space. Essential ingredient here was the spin-charge relation, which allows to reduce to a bosonic MPS.

Since the invariants (μ, \hat{c}, ϵ) and \hat{t} characterize a given cohomology class for $G = \mathbb{Z}_2^C$ and $G = \mathbb{Z}_4^T$ respectively [52, 168], proposition 5 gives a link between the classifications

in terms of bordisms and cohomology, respectively. Thereby, these algebraic invariants, which are connected to the virtual boundaries, attain a purely bulk character.

Here, the labels used to refer to specific symmetry groups are purely conventional. They refer to the periodic table of free-fermion topological superconductors and insulators. In the free fermion classification, which uses K-theory, the usage of these labels is vindicated by connections to Cartan's classifications of symmetric spaces. In particular, there is some freedom in which symmetries are chosen to represent a given symmetric space. For example, class BDI is sometimes represented as a system with $C, T, U(1)_Q$ and $SU(2)_{\text{spin}}$ symmetry [88, 5]. This freedom is lost in the approach here. Indeed, a state with these symmetries is forced, by the argument put forward concerning the label CII, to have $\eta_C(\omega) \in \mathbb{Z}_2$. This does not imply that the SPT phases with this symmetry has only a \mathbb{Z}_2 classification, since for this more complicated structure group the bordism group is more complicated as well. In higher dimensions, this equivalence seems to be lost [158].

This indicates that the many-body invariants introduced above, which may be used in principle to classify the set of SPT phases for a given symmetry group G, are not the best tool to do so. In particular in one space dimension, the most effective such tool is the classification by group cohomology alluded to in section 2.6. Their use is therefore more to *extract* the topological indices from a given state, when the symmetry classification, and the generators of the bordism group, are already known.

4. Beyond Finite Bond Dimension

So far, invariants have been defined and calculated for super matrix product states with arbitrary but finite bond dimension D. The next development is to consider sequences $(\omega_{\alpha})_{\alpha}$ of such states, with bond dimensions D_{α} , with $D_{\alpha} \to \infty$ but $\omega_{\alpha} \to \omega$. Which set of states is reached in such a manner?

4.1. Approximation by Matrix Product States

First of all, it is important to notice that the more prevalent approximation results for ground states of local Hamiltonians, both those for approximations of vector states on finite chains [170, 169, 71] and those for uniform approximations of density matrices in the thermodynamic limit [37, 147] are not helpful in this respect despite appearance and their usefulness in numerical simulations [94]. The reason for this is that these results deal with matrix product states in a generalized sense compared to this work, namely those where to each lattice point a different tensor is associated. For finite chains, such a state can be written as a manifestly translation invariant matrix product state – those that were considered in this work – whose bond dimension however can diverge in the thermodynamic limit [130, 141]. For these generalized matrix product states, much of the machinery essential to compute the above invariants is not available. In particular, it is unclear how to lift symmetries or take limits of large separations.

In light of these difficulties, a set of more rough approximation results turns out to be more helpful. Fannes et al. proved that any translation-invariant state ω on a quantum spin chain can be approximated by a sequence ω_{α} of mixed matrix product states [50, 49]. The states ω_{α} are obtained from ω by restricting them to finite subsets, and translating them along the chain. From this procedure it is clear that if ω is a state on a super spin chain and invariant under the action of an on-site symmetry group G, so will be the approximating series ω_{α} . In a second step, they proved that the series could be purified, i.e., ω_{α} could be taken to be pure even if ω was mixed. This is quite similar to the approximation of matrices by diagonalizable ones, in that here too the mixedness of ω_{α} is related to some geometric degeneracy condition within the space $\mathscr V$ of matrix product tensors which is untypical in the sense that infinitesimal perturbations suffice to lift it. Similarly, if some of the ω_{α} have non-diagonalizable transfer operators, they can be perturbed infinitesimally to lift the degeneracies. Any present symmetries or gradings are not touched by this argument, assuming them to remain unbroken in the limit. To see this, the theorem 7 of Bourne-Ogata cited above is helpful.

This argument is summarized as:

Theorem 9 ([50, 49]). Let ω be a translation-invariant state on the super chain algebra

 $\mathcal{A}_{\mathbb{Z}}$ with G-symmetry. Then there is a sequence of pure G-symmetric super matrix product states $(\omega_{\alpha})_{\alpha \in \mathbb{Z}}$ with diagonalizable transfer operators approximating ω in the w^* -topology.

In general, the bond dimension D_{α} diverges, i.e., the limiting state is not a super matrix product state. In particular, while the partial transpose and $Z_{k\ell}^C(\omega)$ as defined in equation 2.34 are well-defined, proposition 5 does not apply and hence, it is unclear whether the limits of proposition 5 exists.

4.2. Exponentially Clustering States

The failure to define an invariant for general $\omega \in \mathcal{T}$ hints at a certain over-ambitiousness of the program, as this allows for systems at a second order phase transition or other gapless states. Therefore, the set of states should be restricted to gapped ground states of local Hamiltonians:

$$\mathcal{T}_{GS} := \{ \omega \in \mathcal{T} : \exists \text{ local Hamiltonian } H \text{ s.t. } \omega \text{ unique G.S. to } H \} .$$
 (4.1)

This definition is sensible, but difficult to work with from the formalism chosen here, as it lies heavy focus on the Hamiltonians. An easier subset are states that have exponentially decaying correlations:

$$\mathcal{T}_{\exp} := \bigcup_{C,\ell_c \in \mathbb{R}_+} \mathcal{T}_{C,\ell_c} , \qquad (4.2)$$

$$\mathcal{T}_{C,\ell_c} := \{ \omega \in \mathcal{T} : \operatorname{Corr}_{\omega}(\ell) \le C \exp(-\ell/\ell_c) \} . \tag{4.3}$$

Note that if $\ell_1 < \ell_2$ then $\mathcal{T}_{C,\ell_1} \subset \mathcal{T}_{C,\ell_2}$, and similarly for C. Thus $(\mathcal{T}_{C,\ell_c})_{C,\ell_c}$ is a filtration of \mathcal{T}_{\exp} . Also, in the following C is not discussed explicitly and it should be just assumed that it is treated analogously.

By theorem 5:

$$\mathcal{T}_{GS} \subseteq \mathcal{T}_{exp}$$
 (4.4)

Thus, proving a quantization of η on \mathcal{T}_{exp} would render the classification task complete. The proof that is used below requires one more information on the state considered: it needs an upper bound on the Rényi entropy, an area law. This is a property generic states do not have [75]. Another theorem by Hastings [72] however proves that, in one dimension, ground states of local Hamiltonians indeed satisfy such an area law. Consult [44, 45, 61] for a more general review.

At this point it is not yet clear what the connection between the area-law and the exponential-decay states is, i.e., if it is necessary to impose the area-law condition independently from the exponential-decay condition to model ground states without having to explicitly reference their local Hamiltonians. In fact, [21] proved that if ω has (C_*, ℓ_*) decay, then there is a bound Δ_* on the von-Neumann entropy S. The authors of that paper have a slightly different way of defining exponential decay of correlations which is particular convenient in their quantum information setup. They say a state ω has

 (ℓ_0, ℓ_c') -exponential decay if $\operatorname{Corr}_{\omega}(\ell) \leq 2^{-\ell/\ell_c'}$ for all $\ell \geq \ell_0$. Here is how to translate between the two: If ω has (C, ℓ_c) -decay as used in this work, then for all $\ell_0 > \ell_c \log C$ it has (ℓ_0, ℓ_c') -decay as used by Brandão et al. where $\frac{1}{\ell_c} = \frac{\log(2)}{\ell_c'} + \frac{\log C}{\ell_0}$. In terms of these new quantities

$$S(\sigma_n(\omega)) \le \Delta_* = A_1 \ell_0 \exp(A_2 \ell_c' \log(\ell_c')) , \qquad (4.5)$$

where A_1, A_2 are universal constants. Since the Rényi entropies are monotonously decreasing with the order, this automatically gives a bound

$$\Delta_n(\omega) \le \Delta_* \ . \tag{4.6}$$

Thus, \mathcal{T}_{\exp} seems to be the right space to look for a quantization of η . I show first a weaker result. Consider the subset $\overline{\text{sMPS} \cap \mathcal{T}_{C_*,\ell_*}}$; i.e., those states ω that are w^* -limits of sequences of sMPS $(\omega_{\alpha})_{\alpha} \subset \mathcal{T}_{C_*,\ell_*}$. For such states:

Proposition 6. For all C_*, ℓ_* : Let $\omega \in \overline{\text{sMPS} \cap \mathcal{T}_{C_*, \ell_*}}$

(i) If ω is invariant under particle-hole symmetry C, then

$$\exp\left(\frac{2\pi i}{8}\eta_C(\omega)\right) := \lim_{k,\ell\to\infty} e^{\frac{3}{2}\Delta_{k+\ell}(\omega)} Z_{k,\ell}^C(\omega) \tag{4.7}$$

is well-defined and $\eta_C(\omega) \in \mathbb{Z}/8\mathbb{Z}$.

(ii) If ω is invariant under time-reversal symmetry T, then

$$\exp\left(\frac{2\pi i}{2}\eta_T(\omega)\right) := \lim_{k_1, k_2, d \to \infty} e^{2\Delta_{k_1 + k_2 + d}(\omega)} Z_{k_1, k_2 \mid d}^C(\omega) \tag{4.8}$$

is well-defined and $\eta_C(\omega) \in \mathbb{Z}/2\mathbb{Z}$.

Proof of proposition 6. The proof restricts to $\eta = \eta_C$, but the proof for η_T is similar. Pick an G-symmetric pure approximation series $(\omega_{\alpha})_{\alpha} \in \text{sMPS} \cap \mathcal{T}_{C_*,\ell_*}$ with diagonalizable transfer operators for ω . The proof proceeds in four steps:

(i) Let $n=(k,\ell)$. For convenience, the limit $n\to\infty$ is used to denote the limit when both k and ℓ are taken to infinity. Sometimes the notation is abused in that a quantity is written as if it only depended on n when it depends on k,ℓ separately. Thus, let $Q_n(\omega_\alpha) := e^{\frac{3}{2}\Delta_n(\omega_\alpha)} Z_{k,\ell}(\omega_\alpha)$. Then, there is $x_\alpha \in \mathbb{Z}/8\mathbb{Z}$ such that

$$\left| Q_n(\omega_\alpha) - e^{\frac{2\pi i}{8}x_\alpha} \right| \le 7C_* e^{\frac{5}{2}\Delta_*} e^{-n/\ell_*} , \qquad (4.9)$$

in particular the limit is uniform in α .

- (ii) The limit 4.7 exists.
- (iii) $x_{\alpha} \to x \in \mathbb{Z}/8\mathbb{Z}$.

(iv)
$$\eta(\omega) = x$$
.

(i) The ω_{α} are super matrix product states. Hence, by proposition 5, there is $x_{\alpha} \in \mathbb{Z}/8\mathbb{Z}$ such that $Q_n(\omega_{\alpha}) \xrightarrow{n \to \infty} \exp(2\pi i x_{\alpha}/8)$.

Quite generally for states $\nu_1, \nu_2 \in \mathcal{T}_{C_*, \ell_*}$:

$$\begin{aligned} |Q_{n_1}(\nu_1) - Q_{n_2}(\nu_2)| &= \left| e^{\frac{3}{2}\Delta_{n_1}(\nu_1)} Z_{k_1\ell_1}(\nu_1) - e^{\frac{3}{2}\Delta_{n_2}(\nu_2)} Z_{k_2\ell_2}(\nu_2) \right| = \\ &\leq \left| e^{\frac{3}{2}\Delta_{n_1}(\nu_1)} - e^{\frac{3}{2}\Delta_{n_2}(\nu_2)} \right| |Z_{k_1\ell_1}(\nu_1)| + e^{\frac{3}{2}\Delta_{n_2}(\nu_2)} |Z_{k_1\ell_1}(\nu_2) - Z_{n_2}(\nu_2)| \ . \end{aligned}$$

For the first term, the middle-value theorem yields $|x^{-3/2} - y^{-3/2}| \leq \frac{3}{2}|z|^{-5/2}|x - y|$, if z is an upper bound of both x and y. This can be combined with the upper bound $\Delta_{n_{1/2}(\nu_{1/2})} \leq \Delta_*$ to

$$|Q_{n_1}(\nu_1) - Q_{n_2}(\nu_2)| \le \frac{3e^{\frac{5\Delta_*}{2}}}{2} \left| e^{-\Delta_{n_1}(\nu_1)} - e^{-\Delta_{n_2}(\nu_2)} \right| + e^{\frac{3\Delta_*}{2}} |Z_{k_1\ell_1}(\nu_1) - Z_{k_2\ell_2}(\nu_2)| .$$

$$(4.10)$$

Thus, using equations 3.38 and 3.40:

$$\left| Q_n(\omega_\alpha) - e^{\frac{2\pi i}{8}x_\alpha} \right| \le \frac{3e^{\frac{5}{2}\Delta_*}}{2} 2\|\mathbb{E}^n - \mathbb{E}^\infty\| + 2e^{\frac{3}{2}\Delta_*} \left(\|\mathbb{E}^k - \mathbb{E}^\infty\| + \|\mathbb{E}^\ell - \mathbb{E}^\infty\| \right) \le \left(3e^{\frac{5}{2}\Delta_*} + 4e^{\frac{3}{2}\Delta_*} \right) C_* e^{-n/\ell_*} ,$$

thus the claim.

(ii): First combine equations 3.43, a similar result for Δ_n , and 4.10 to conclude

$$|Q_n(\nu_1) - Q_n(\nu_2)| \le 5e^{\frac{5\Delta_*}{2}} \|\sigma_n(\nu_1) - \sigma_n(\nu_2)\|_1 . \tag{4.11}$$

The next step is to prove that $(Q_n(\omega))_n$ is Cauchy. Pick $\epsilon > 0$ and write

$$|Q_n(\omega) - Q_m(\omega)| < |Q_n(\omega) - Q_n(\omega_0)| + |Q_m(\omega) - Q_m(\omega_0)| + |Q_n(\omega_0) - Q_m(\omega_0)|.$$

By part (i) $(Q_n(\omega_\alpha)_n)$ converges uniformly in α . Thus, pick n and m large enough such that the last term is smaller than $\epsilon/3$. With the integers n and m fixed to some values, the first two terms are bounded with the help of equation 4.11 by the 1-distance of the density operators of ω and ω_α on \mathcal{H}_n and \mathcal{H}_m . But since all operator norms are equivalent on finite-dimensional Hilbert spaces, the 1-distances converge both to zero as $\alpha \to \infty$. Hence, pick α large enough s.t. either of the terms is smaller than $\epsilon/3$. Thus, $(Q_n(\omega))_n$ is Cauchy and the limit exists.

(iii): Note that the 8th roots of unity have a distance from each other of $\sqrt{2-\sqrt{2}}$. Hence, pick $\epsilon < \sqrt{2-\sqrt{2}}/2$. Write:

$$\left| e^{\frac{2\pi i}{8}x_{\alpha}} - e^{\frac{2\pi i}{8}x_{\beta}} \right| \leq \left| Q_n(\omega_{\alpha}) - e^{\frac{2\pi i}{8}x_{\alpha}} \right| + \left| Q_n(\omega_{\beta}) - e^{\frac{2\pi i}{8}x_{\beta}} \right| + \left| Q_n(\omega_{\alpha}) - Q_n(\omega_{\beta}) \right|.$$

Pick n large enough such that either of the first two terms is smaller than $\epsilon/3$. Then, pick α and β big enough such that the last term is smaller than $\epsilon/3$. But, since $\exp(2\pi i x_{\alpha}/8)$ is pinned to the 8th roots of unity, and ϵ is smaller than half the smallest distance between any of them, the sequence actually has to be constant for large enough α .

(iv): The only thing left to show is that $\eta(\omega) = x$, that is, that the limits of $\alpha \to \infty$ and $n \to \infty$ of the sequence $(Q_n(\omega_\alpha))_{n,\alpha}$ commute. A $\epsilon/4$ argument confirms this:

$$\left| e^{2\pi i x/8} - e^{2\pi i \eta(\omega)/8} \right| \le \left| e^{2\pi i x/8} - e^{2\pi i x_{\alpha}/8} \right| + \left| e^{2\pi i x_{\alpha}/8} - Q_n(\omega_{\alpha}) \right| +$$

$$+ \left| Q_n(\omega_{\alpha}) - Q_n(\omega) \right| + \left| Q_n(\omega) - e^{2\pi i \eta(\omega)/8} \right|.$$

By parts (i) and (ii), the second and the fourth term can each be made smaller than $\epsilon/4$ by choosing n large enough, and by parts (ii) and (iii), the first and the third term can each be made smaller than $\epsilon/4$ by choosing α large enough. thus proving the claim. \square

This chapter finishes with a discussion in which way proposition 6 defines a homotopy invariant for gapped ground states, or possibly fails to do so.

A given ground state ω describing a topological phase is exponentially correlated, i.e., there are $(C, \ell_c) < \infty$ s.t. $\omega \in \mathcal{T}_{C,\ell_c}$. Consider a pure super matrix product state approximating series, $(\omega_{\alpha})_{\alpha}$. Since these are pure states and have finite bond dimension, they are exponentially clustering with constants $(C_{\alpha}, \ell_{\alpha})$, i.e., $\omega_{\alpha} \in \overline{\text{sMPS}} \cap \mathcal{T}_{C_{\alpha},\ell_{\alpha}}$. Now if, after deleting finitely many elements from this sequence, there is an upper bound (C_*, ℓ_*) of $(C_{\alpha}, \ell_{\alpha})$, then $\omega \in \overline{\text{sMPS}} \cap \mathcal{T}_{C_*,\ell_*}$ and the above proposition applies. Hence, the difficulty is whether it is possible to give an upper bound of the correlations of the approximating sequence of super matrix product states given a bound on the correlations of the approximated state.

There are several difficulties in obtaining such a bound. Their nature is explained in the following. They seem to be connected to the approximability of the low-energy spectrum of gapped ground states.

The prime obstacle in advancing is that w^* -convergence is very weak. In particular, it is not necessary, or at least it is noy clear whether it is necessary, that $\operatorname{Corr}_{\omega_{\alpha}}(\ell) \to \operatorname{Corr}_{\omega}(\ell)$. Denote by $\operatorname{Corr}_{\nu}(n_1:n_2|\ell)$ the correlations of a state ν between patches of size n_1, n_2 separated by a distance ℓ . In finite dimensions, all notions of convergence are identical¹. Therefore, for fixed n_1, n_2, ℓ , the w^* -convergence of ω_{α} implies that $\operatorname{Corr}_{\omega_{\alpha}}(n_1:n_2|\ell) \to \operatorname{Corr}_{\omega}(n_1:n_2|\ell)$. Furthermore, $\operatorname{Corr}_{\nu}(n_1:n_2|\ell) \leq \operatorname{Corr}_{\nu}(\ell)$.

It holds that $\operatorname{Corr}_{\nu}(n_1:n_2|\ell) \leq \operatorname{Corr}_{\nu}(\ell)$, and of course it converges for $n_1, n_2 \to \infty$. Define an integer-valued function $N(\omega)$ by

$$\operatorname{Corr}_{\omega}(N(\omega):N(\omega)|\ell) = \operatorname{Corr}_{\omega}(\ell) \quad \forall \ \ell \in \mathbb{N} \ .$$

¹More details on the relationship between the different topologies on the set of states can be found for example in [136].

If there is a uniform bound $N(\omega_{\alpha}) \leq N_*$, the correlation length of ω_{α} is uniformly bounded by the correlation length of the limit state ω :

$$\operatorname{Corr}_{\omega_{\alpha}}(\ell) = \operatorname{Corr}_{\omega_{\alpha}}(N_* : N_* | \ell) \to \operatorname{Corr}_{\omega}(N_* : N_* | \ell) \le \operatorname{Corr}_{\omega}(\ell) \le Ce^{-\ell/\ell_c}$$
;

that is, $\operatorname{Corr}_{\omega_{\alpha}}(\ell)$ Cauchy-converges to an uniformly bounded sequence. Hence, for any C' > C, by deleting finitely many elements of the sequence:

$$Corr_{\omega_{\alpha}}(\ell) \leq C' e^{-\ell/\ell_c}$$
,

and $\overline{\text{sMPS} \cap \mathcal{T}_{C,\ell_c}} = \mathcal{T}_{C',\ell_c}$. Thus, proposition 6 would define a homotopy invariant on all gapped ground states.

However, it is not quite clear how to obtain such a bound N_* . For finite bond dimension, introduce the *injectivity index* $\iota(\omega)$. This is the smallest integer such that $\mathbb{E}_{\mathcal{O}}(e)$ generates the whole bond algebra, where the support of \mathcal{O} is $\iota(\omega)$. Obviously $N(\omega) \leq \iota(\omega)$. The latter can be bounded by a polynomial in the bond dimension [141]. This bound therefore diverges as $D_{\alpha} \to \infty$, and there is furthermore no reason to believe that $\iota(\omega_{\alpha})$ would not share its fate. It is possible that $N(\omega_{\alpha})$ follows suit. This would correspond to the scenario that while the correlation length of the approximating matrix product states diverges, the strongly correlated operators need larger and larger patches to manifest in the bond algebra, and proposition 6 does not define a homotopy invariant on the set of gapped ground states.

On the other hand, there are reasons for hope. The objection to the above scenario sustains that there is no need to generate the full bond algebra to obtain the necessary bound. What should happen is that the eigenvectors of the transfer operator to eigenvalues very close to the unit disc are generated on small patches. This could be quite a general feature of gapped ground states, assuming that ω has particle-like excitations. This is expressed more technically as the statement that the low-lying energy-momentum spectrum consists of isolated energy shells [109, Section 6.1.2]. Then the low-lying excitations, i.e., those operators that maximize the correlation bound, can be approximated exponentially fast in the support size by the action of local operators on the ground state [69]. Numerical and analytical studies indicate furthermore that the highest magnitude eigenvalues of approximating MPS approximate the dispersion relations of low-lying excitations [177, 165]. This seems to indicate that $\operatorname{Corr}_{\omega}(n:n|\ell)$ converges to $\operatorname{Corr}_{\omega}(\ell)$ with exponential speed, and the spectrum of the transfer operator could be controlled through knowing the low-energy spectrum of the approximated state.

In line of such inquiries, it is tempting to model sufficiently well-behaved state directly as a kind of matrix product state, albeit with infinite dimensional bond space [103, 118, 119, 17, 120, 104, 103]. Algebraic methods are unproblematic, and if the difficulties sketched above could be overcome, a fair deal could be said furthermore about the analytic structure of these matrix product presentations.

Summary and Outlook

The long-range physics of gapped ground states is described in terms of topological quantum field theory. Advances in the latter, which were to some extent driven by the challenge from physics, give a characterization of symmetry protected phases in terms of cobordisms. Re-importing this knowledge into the environment of interacting fermions in one dimension leads to proposals for many-body invariants, analogous to partition functions of field theories on non-orientable manifolds, for topological phases protected by anti-unitary symmetries.

In this thesis, this connection has is made more precise. It is proven that Z^C and Z^T are indeed topological invariants in the set of states approximable by super matrix product states with an upper bound on their correlation length. This defines purely bulk invariants of topological phases with anti-unitary symmetries, which can be connected, for super matrix product states, with invariants defined on the boundary, or entanglement, Hilbert spaces.

To calculate these invariants, the theory of super matrix product states is developed. While the theory of *ungraded* matrix product states is quite comprehensive, the *graded* one has important gaps in the literature. This includes certain facts about completely positive maps on superalgebras, which are the bread-and-butter of all calculations in the matrix product world. Furthermore, to properly lift anti-unitary symmetries to graded bond spaces, and to define graded transposes, in a basis-independent way, bilinear forms appropriate to super vector spaces are introduced. In this context it also became possible to elucidate the necessity to use *graded* bond algebras for fermionic systems.

Equipped with this machinery, the calculation of the proposed many-body invariants for particle-hole or motion-reversal symmetric super matrix product states poses no further challenge. This proves them to be homotopy invariants on the set of super matrix product states. Since their definition is neither algebraic nor dependent on any particular formalism to describe ground states, they can be extended to limits of super matrix product states. In order to restrict to gapped ground states as limits, a uniform bound on the correlation length of the states in the sequence is imposed. While this is not yet necessarily the set of all gapped ground states, arguments are given why it should capture the relevant set. With this assumption, the proposed quantities are shown to be homotopy invariants on this set.

The many-body invariants calculated in this work allow to reproduce the known classifications of one-dimensional symmetry protected phases for particularly simple symmetry groups. To gain many-body invariants for more general phases is not difficult in light of this work; what is necessary is to know the bordism group corresponding to that symmetry, and how to obtain the generating manifolds by the cutting and gluing operation possible in condensed matter systems. The expressions can then be evaluated using the

formalism of super matrix product states as is done here. However, the primary usage of the invariants is to extract information about the class of a given state.

The gap between the two assumptions – of the limit of a sequence of matrix product states being gapped, and the sequence itself having a uniform bound – is connected to questions about the excitations of general gapped ground states, and their entanglement structures. In particular, it is incumbent to turn the numerical and heuristic results of [177] more comprehensive.

Generalizations to higher dimensions, with similar methods, mostly face the challenge that such a powerful tool is not available to compute in the thermodynamic limit, as is the transfer operator in one spatial dimension. The strictures imposed against chiral tensor networks [40] are tangent here since d-dimensional chiral states are to be understood as connected to (d+1)-dimensional bordism groups and have to be dealt with in other ways anyhow, e.g., [9].

A. \mathbb{Z}_p -graded Linear Algebra

Graded Vector Spaces A vector space V is graded with type Δ if $V = \bigoplus_{\lambda \in \Delta} V^{\lambda}$. It is not required that the V^{λ} are non-trivial vector spaces, in particular $V^{\lambda} = \{0\}$ for all λ is included. Any vector space V can be considered as a graded vector space by declaring $V^0 = V$ and $V^{\lambda \neq 0} = \{0\}$. The union (of sets) $\bigcup_{\lambda} V^{\lambda} \setminus \{0\}$ are the homogeneous vectors. On homogeneous vectors introduce a map $|\cdot|$ such that $|\xi| = \lambda$ if $\lambda \in V^{\lambda}$, called the degree or parity of ξ . Any vector can be decomposed as $\xi = \sum_{\lambda} \xi^{\lambda}$.

Examples of Graded Vector Spaces. For F a vector space, the *exterior algebra* over F, denoted by $\Lambda(F)$, is a \mathbb{N} -graded vector space: $\Lambda(F) = \bigoplus_{n \in \mathbb{N}} \Lambda^n(F)$. If F is finite-dimensional of dimension k, then $\Lambda^n(F) = \{0\}$ for n > k. Similarly, one may form the symmetric algebra S(F), which is also \mathbb{N} -graded, but with $S^n(F) \neq \{0\}$ for all $n \geq 0$, unless $F = \{0\}$. Both $\Lambda(F)$ and S(F) can be considered as \mathbb{Z} -graded vector spaces by taking all negative-graded spaces to be trivial. Furthermore, to obtain a \mathbb{Z}_2 -graded vector space, group $\Lambda(F) = \Lambda^{\text{even}}(F) \oplus \Lambda^{\text{odd}}(F)$.

Graded Tensor Products Consider graded vector spaces V_1, V_2 . Their tensor product $V_1 \otimes V_2$ can be endowed with a Δ -grading by

$$(V_1 \otimes V_2)^{\lambda} := \bigoplus_{\mu + \nu = \lambda} V_1^{\mu} \otimes V_2^{\nu} . \tag{A.1}$$

The resulting Δ -graded vector space is denoted as $V_1 \otimes_{\Delta} V_2$.

Observe that there are isomorphisms, for $z \in \mathbb{C}$, $\xi \in V$: $\xi \otimes_{\Delta} z \mapsto z \xi$ and $z \otimes_{\Delta} \xi \mapsto z \xi$, so that one can consider \mathbb{C} with its trivial grading as a unit w.r.t. the graded tensor product:

$$V \otimes_{\Delta} \mathbb{C} \cong V \cong \mathbb{C} \otimes_{\Delta} V . \tag{A.2}$$

The tensor product, as a bilinear operator, can be concatenated. However, the associator $a: (V_1 \otimes_{\Delta} V_2) \otimes_{\Delta} V_3 \to V_1 \otimes_{\Delta} (V_2 \otimes_{\Delta} V_3)$, defined simply by

$$(\xi_1 \otimes_{\Delta} \xi_2) \otimes_{\Delta} \xi_3 \mapsto \xi_1 \otimes_{\Delta} (\xi_2 \otimes_{\Delta} \xi_3) , \qquad (A.3)$$

determines an isomorphism of theses concatenations. The brackets indicating the order of tensor products are hence omitted.

This allows to endow the category of Δ -graded vector spaces Δ Vect with a monoidal¹ structure. The pair $(\Delta \text{Vect}, \otimes_{\Delta})$ is called a monoidal category.

¹For more details check the n-lab [116]. The associator and the unit need to satisfy some coherence axioms, called the *triangle* and the *pentagon* equation. They are not listed here because they are trivially satisfied in the abelian case considered here.

Braiding. For vector spaces V_1, V_2 the tensor products $V_1 \otimes_{\Delta} V_2$ and $V_2 \otimes_{\Delta} V_1$ are vector spaces of the same dimension, hence isomorphic. Pick an $\varepsilon : \Delta \times \Delta \to \mathbb{C}$, and define one such isomorphism, called a *braiding*, as

$$\mathcal{B}_{V_1,V_2}: V_1 \otimes_{\Delta} V_2 \to V_2 \otimes_{\Delta} V_1 ,$$

$$\xi_1 \otimes_{\Delta} \xi_2 \mapsto \varepsilon(|\xi_1|, |\xi_2|) \quad \xi_2 \otimes_{\Delta} \xi_1 .$$
 (A.4)

The above defined Δ Vect together with the braiding \mathcal{B} defines a *braided* monoidal category [80], if a coherence condition – the *hexagon equations* – holds. Due to the trivial associator, these coherence conditions further boil down to demanding that the following diagrams commute (suppressing the reference to the grading on the tensor products):



Both these diagrams express that for braiding purposes one can lump tensor factors together in an arbitrary fashion. In terms of ε , they read:

$$\varepsilon(\mu + \mu', \nu) = \varepsilon(\mu, \nu)\varepsilon(\mu', \nu) , \quad \varepsilon(\mu, \nu + \nu') = \varepsilon(\mu, \nu)\varepsilon(\mu, \nu') .$$
 (A.5)

Consider $\mu' = 0 = \nu'$ in the above equations:

$$\varepsilon(\mu,\nu)\varepsilon(0,\nu) = \varepsilon(\mu,\mu) = \varepsilon(\mu,\nu)\varepsilon(\mu,0)$$
 (A.6)

Hence, $\varepsilon(\mu, 0) = 1 = \varepsilon(0, \nu)$. The special case $\mu = -\mu'$ gives:

$$\varepsilon(0,\nu) = 1 = \varepsilon(\mu,\nu)\varepsilon(-\mu,\nu) \iff \varepsilon(-\mu,\nu) = \varepsilon(\mu,\nu)^{-1} ,$$

$$\varepsilon(\mu,0) = 1 = \varepsilon(\mu,\nu)\varepsilon(\mu,-\nu) \iff \varepsilon(\mu,-\nu) = \varepsilon(\mu,\nu)^{-1} ,$$
(A.7)

A simplifying assumption is that braiding back and forth gives the identity, or in terms of ε :

$$\varepsilon(\mu,\nu)\varepsilon(\nu,\mu) = 1$$
 (A.8)

A tensor category with an ε satisfying A.8 is called a $symmetric^2$ monoidal category. For now, however, the categories are not necessarily symmetric.

For example, let $\Delta = \mathbb{Z}_p$ for $p \in \mathbb{N}$. Then for each r = 0, 1, ..., p - 1 there is a possible choices of ε :

$$\varepsilon_{p,r}(\mu,\nu) = \exp\left(\frac{2\pi i r}{p}\mu\nu\right) .$$
 (A.9)

If p = 2r, $\varepsilon(\mu, \nu) = (-1)^{\mu\nu}$ induces a symmetric monoidal structure. This leads back to the super vector spaces of chapter 1.

²In tensor diagrams, this manifests itself that for *symmetric* monoidal categories it is not necessary to distinguish between the different ways two lines can cross.

Example: The Clock and Shift Operators. Pick an integer p. Let $z = \exp(2\pi i/p)$ be a p-th root of unity. Define an operator \mathscr{P} on $V = \mathbb{C}^p$ by $\mathscr{P}(e_\mu) = z^\mu e_\mu$, where $\{e_\mu\}_{\mu=1,\dots,p}$ is the standard basis of \mathbb{C}^p which defines the standard inner product. This \mathscr{P} operator grades V: $\mathbb{C}^p = \bigoplus_{\mu} \mathbb{C}e_{\mu}$, so that \mathscr{P} appears as a parity operator for the group homomorphism

$$\gamma: \mathbb{Z}_p \ni \ell \mapsto z^{\ell} \in \{z^r : r = 0, 1, ..., p - 1\}$$
 (A.10)

Let X be the operator defined by $\langle e_i, Xe_i \rangle = \delta_{i+1,j}$. By direct calculation

$$\mathscr{P}X\mathscr{P}^{-1} = zX \ . \tag{A.11}$$

Denote by A the C^* -algebra generated by X. Furthermore, define $Y := \mathscr{P}X$. Then (a) $Y^{\mu} \in \mathscr{L}(V)^{\mu}$, (b) $Y^{\mu} \notin A$ for $\mu \neq 0 \mod p$, and (c) $xY^{\mu} = z^{\mu|x|}Y^{\mu}x$ for $x \in A$. Hence, the graded commutant of A in $\mathscr{L}(V)$ is the algebra generated by the Y^{μ} .

 Δ -Graded Local Algebras Very Similar to the construction of \mathbb{Z}_2 -graded local algebras in section 2.1, associate a Δ -graded Hilbert space $\mathcal{H}_{\{x\}}$, a Δ -graded closed subalgebra $\mathcal{A}_{\{x\}} \subset \mathcal{L}(\mathcal{H}_{\{x\}})$, where as before the easiest choice is in the presence of isomorphisms $\mathcal{H}_{\{x\}} \cong \mathcal{H}_{\{y\}}$. As before, introduce algebras associated to subsets by picking points $x_1 < \cdots < x_n \in \mathbb{Z}$ and defining

$$\mathcal{A}_{\{x_1,\dots,x_n\}} := \mathcal{A}_{\{x_1\}} \otimes_{\Delta} \dots \otimes_{\Delta} \mathcal{A}_{\{x_n\}} . \tag{A.12}$$

Finally, $\mathcal{A}_{\mathbb{Z}}$ is the Δ -graded chain algebra.

 $\mathcal{A}_{\mathbb{Z}}$ is Δ -asymptotically abelian. Take local $\mathcal{O}_{1,2}$ with disjoint supports. From the structure of these algebras that generic operators do not do that, but instead *graded commute*:

$$\mathcal{O}_1 \mathcal{O}_2 = \varepsilon(|\mathcal{O}_1|, |\mathcal{O}_2|) \mathcal{O}_2 \mathcal{O}_1 . \tag{A.13}$$

Why Δ -Graded Algebras? The bosonization map of section 2.4 can be generalized to the setting of $\Delta = \mathbb{Z}_p$, for which task the clock and shift operators introduced above come in handy. The isomorphism of algebras that is constructed as, for $L \in \mathcal{A}^{\mu}$:

$$\phi_N: A_{\{1,\ldots,N\}} \to (\mathscr{L}(\mathbb{C}^p) \otimes \tilde{\mathcal{A}})^{\otimes N}$$
.

This is characterized by

$$1 \otimes_{\Delta} \cdots \otimes_{\Delta} \overset{x}{L} \otimes_{\Delta} \cdots \otimes_{\Delta} 1 \mapsto (Y^{\mu} \otimes 1) \otimes \cdots \otimes (Y^{\mu} \otimes 1) \otimes (X^{\mu} \overset{x}{\otimes} L) \otimes 1 \otimes 1 \cdots \otimes 1.$$

As in the bosonization case, the correct Δ -graded commutation relations are guaranteed by the clock- and shift operators.

One can construct an algebra of quasi-local operators with $\mathscr{L}(\mathbb{C}^p) \otimes \tilde{\mathcal{A}}$. However, fixing some operator \mathcal{O} , of degree μ , $\phi_N(\mathcal{O})$ does not correspond to a local operator as $N \to \infty$.

Indeed, it carries a string of operators which enforce the graded commutation relation. Restricting to the operators of trivial degree, one may indeed construct a mapping

$$\phi: (\mathcal{A}_{\mathbb{Z}})^0 \to (\mathscr{L}(\mathbb{C}^p) \otimes \tilde{\mathcal{A}})_{\mathbb{Z}}^{\mathbb{Z}_p} ;$$

where the superscript 0 on the left sides indicates that only objects those are to be considered the domain of ϕ which are globally in the trivial component – which does not include spatially separated pairs of oppositely graded objects – while the superscript \mathbb{Z}_p on the right side indicates that ϕ only maps to those operators that are uncharged under the action of \mathbb{Z}_p .

 Δ -Graded Matrix Product States It is not difficult to continue further the construction to Δ -graded matrix product state. For this, consider tensors $E: \mathcal{H} \to \mathcal{L}(H)$ and introduce $\mathbb{E}_L \in \mathcal{L}^2(H)$ for $L \in \mathcal{L}(\mathcal{H})$,

$$\mathbb{E}_L(x) := \sum_{s,r} \varepsilon(|\psi_s|,|x|) \langle \psi_s, L(\psi_r) \rangle E(\psi_s) x E(\psi_r)^*.$$

Again, $\mathbb{E} = \mathbb{E}_1$ is the transfer operator, and if $\operatorname{tr}(\rho \cdot)$ and e are left resp. right eigenvalues this allows to define as before a state

$$\omega_{E,\rho}(L_1 \otimes_{\Delta} \cdots \otimes_{\Delta} L_n) := \operatorname{tr}(\rho \mathbb{E}_{L_1} \cdots \mathbb{E}_{L_n}(e))$$
.

One can proceed again through the decomposition theory of such states, and of the transfer operators, and will obtain structurally analogous results; in particular the bond algebra A(E) of a pure Δ -graded MPS is Δ -graded central; and

$$\lim_{n\to\infty} \mathbb{E}^n(x) = \sum_a v_a \operatorname{tr}(\rho_a x) ,$$

where v_a is in the Δ -commutant of A(E) in $\mathcal{L}(H)$, which is at most p-dimensional as for the clock and shift operators.

 \mathbb{Z}_p -graded super matrix product states could be used to calculate expectation values and partition functions for \mathbb{Z}_p -gauge theories. The charged operators correspond to matter fields with gauge strings attached. As indicated above in the discussion of the braiding, the diagrams are more involved as two lines can wind around each other.

It could also be used in order to define matrix product states for parafermionic systems, for example spinons with p = 4 [66].

B. Kadison-Schwarz Inequality for h.c.p. Maps

Homogeneorus completely positive maps satisfy a generalization of the Cauchy-Schwarz inequality, proven first by Kadison:

Lemma 6 (Generalized Kadison-Schwarz). Assume $E^{(\alpha)}: \mathcal{H} \to \mathcal{L}(H_{\alpha})$ generate strongly irreducible unital transfer operators $\mathbb{E}^{(\alpha)}$. Introduce the "mixed" operator $\mathbb{E}^{(1,2)} \in \mathcal{L}^2(H_2, H_1)$:

$$x \mapsto \sum_{s} (-1)^{|x||E_s^{(2)}|} E_s^{(1)} x (E_s^{(2)})^*$$
.

Then $\mathbb{E}^{(1,2)}$ and $\mathbb{E}^{(2,2)} = \mathbb{E}^{(2)}$ satisfy a Kadison-Schwarz like inequality

$$\mathbb{E}^{(2)}(x^*x) \ge \mathbb{E}^{(1,2)}(x)^*\mathbb{E}^{(1,2)}(x)$$
.

Furthermore $\|\mathbb{E}^{(1,2)}\| \leq 1$.

As this is a bit more general than the usual version, discussing super vector spaces and allowing for different spaces to mediate a short proof. For the ungraded case check [146]. The proof of this statement needs the following technical result [126]:

Lemma 7. Let $x: H_2 \to H_1$, then:

$$\begin{pmatrix} 1_{H_1} & x \\ x^* & 1_{H_2} \end{pmatrix} \ge 0 \quad \Leftrightarrow \quad ||x|| \le 1 \ .$$

Proof of lemma 6. For the first statement consider the positive map $\phi = \mathbb{E}^{(1)} \oplus \mathbb{E}^{(2)}$ on $\mathcal{L}(H_1 \oplus H_2)$. Pick some $y: H_2 \mapsto H_1$. Pick a positive element:

$$\begin{pmatrix} 1 & y \\ y^* & y^*y \end{pmatrix} = \begin{pmatrix} 1_{H_1} & y \\ 0 & 0 \end{pmatrix}^* \begin{pmatrix} 1_{H_1} & y \\ 0 & 0 \end{pmatrix} \ge 0 \quad ;$$

As ϕ is positive:

$$0 \le \phi \begin{pmatrix} 1 & y \\ y^* & y^* y \end{pmatrix} = \begin{pmatrix} 1_{H_1} & \mathbb{E}^{(1,2)}(y) \\ \mathbb{E}^{(1,2)}(y)^* & \mathbb{E}^{(1,2)}(y^* y) \end{pmatrix}.$$

Pick $\xi \in H_2$ arbitrary. Then

$$0 \le \left\langle \begin{pmatrix} -\mathbb{E}^{(1,2)}(y)\xi \\ \xi \end{pmatrix}, \begin{pmatrix} 1_{H_1} & \mathbb{E}^{(1,2)}(y) \\ \mathbb{E}^{(1,2)}(y)^* & \mathbb{E}^{(2)}(y^*y) \end{pmatrix} \begin{pmatrix} -\mathbb{E}_{12}(y)\xi \\ \xi \end{pmatrix} \right\rangle =$$

$$= \left\langle \xi, [\mathbb{E}^{(2)}(y^*y) - \mathbb{E}^{(1,2)}(y)^*\mathbb{E}^{(1,2)}(y)]\xi \right\rangle,$$

and the statement follows.

To the second claim, consider

$$\phi \begin{pmatrix} 1_{H_1} & x \\ x^* & 1_{H_2} \end{pmatrix} = \begin{pmatrix} 1_{H_1} & \mathbb{E}^{(1,2)}(x) \\ \mathbb{E}^{(1,2)}(x)^* & 1_{H_2} \end{pmatrix} .$$

By lemma 7, $\|\mathbb{E}^{(1,2)}(x)\| \le 1$ if $\|x\| \le 1$.

C. Reduction of Symmetry Group

Consider a (G, \mathfrak{p}) -symmetric pure super matrix product tensor $E: H \to \mathcal{L}(H)$ and denote by ω the state generated by E. Let $G_0 := \mathfrak{p}^{-1}(0)$ be the compact subgroup of unitarily represented symmetries. Both the on-site algebra \mathcal{A} and the bond algebra A decompose, as vector spaces, under the unitary G_0 :

$$\mathcal{A} = \bigoplus_{\Delta \in S} \mathcal{A}_{\Delta} , \quad A = \bigoplus_{\Delta \in \widehat{S}} A_{\Delta} ; \qquad (C.1)$$

here S respectively \widehat{S} is the set of isomorphism classes of representations of G_0 appearing in the decomposition. Fix a standard representation R_{Δ} for each type Δ . Then following [178]

$$\mathcal{A}_{\Delta} \cong \underbrace{\operatorname{Hom}_{G_0}^{\operatorname{Vect}}(R_{\Delta}, \mathcal{A})}_{=:\mathcal{B}_{\Delta}} \widehat{\otimes} R_{\Delta} , \quad A_{\Delta} \cong \underbrace{\operatorname{Hom}_{G_0}^{\operatorname{Vect}}(R_{\Delta}, A)}_{=:B_{\Delta}} \widehat{\otimes} R_{\Delta} ,$$

by using the homomorphism to map a standard representation element into the algebra, $X \widehat{\otimes} r \mapsto X(r)$. The superscript Vect should remind that these are vector space homomorphisms.

Consider the special case that the anti-unitaries in G commute with the action of G_0 . This is for example the case for $G_0 = SU(2)$ and with the anti-unitaries K = T, C of time-reversal and motion-reversal respectively. In this case, K preserves the type Δ of a representation, and thus it has to factor. In the following, the virtual algebra is discussed, but the on-site algebra behaves strictly analogous:

$$K = \bigoplus_{\Delta} K_{\Delta} , \quad K_{\Delta} \cong K_{B_{\Delta}} \widehat{\otimes} K_{R_{\Delta}} .$$

Restricting to one definite type Δ and henceforth supressing its reference, there can occur modifications of the algebraic properties of the factor K_B . For example, for K=T and $G_0=SU(2)$, it holds that $K^2=P$. But on an irreducible SU(2)-module R with spin $\Delta=j\in\frac{1}{2}\mathbb{Z}$, time-reversal squares to $(T_R)^2=(-1)^{2j}$. Furthermore, by the spin-charge relation of SU(2), the parity operator factors as $P=1\widehat{\otimes}(-1)^{2j}$. Hence, $(T_B)^2=1$. Thus, there appears a change from a graded real structure on A to a real structure on B, which is trivially graded by the generalized spin-charge relation.

Turning to the super matrix product state transfer operator, recall the lift \mathbb{E} . : $L \to \mathcal{L}^2(H)$ and denote $\phi(L \widehat{\otimes} x) := \mathbb{E}_L(x)$. For $L \in \mathcal{A}_{\Delta}$ and $x \in A_{\Delta'}$, find $r, r' \in R_{\Delta, \Delta'}$ and $\ell \in \mathcal{B}_{\Delta}$ and $X \in \mathcal{B}_{\Delta'}$ such that $L = \ell(r)$ and x = X(r'). Consequently:

$$\phi(L\widehat{\otimes}x) =: \phi_{\Delta,\Delta'}(\ell\widehat{\otimes}X\widehat{\otimes}r\widehat{\otimes}r') \ .$$

Since representations tensor,

$$R_{\Delta} \widehat{\otimes} R_{\Delta'} \cong \bigoplus_{\Delta'' \in S(\Delta, \Delta')} R_{\Delta''} , \quad |\Delta, k\rangle \widehat{\otimes} |\Delta', k'\rangle = \sum_{\Delta''} \sum_{k''} c_{\Delta, \Delta'}^{\Delta''}(k, k', k'') |\Delta'', k''\rangle ,$$

with $S(\Delta, \Delta')$ the set of isomorphism classes of representations of G_0 appearing in the decomposition into irreducibles, and $|\Delta, k\rangle$ some basis of R_{Δ} . Thus, the above map decomposes

$$\phi_{\Delta,\Delta'}(\ell \widehat{\otimes} X \widehat{\otimes} | \Delta, k) \widehat{\otimes} | \Delta', k' \rangle) = \sum_{\Delta''} \sum_{k''} c_{\Delta,\Delta'}^{\Delta''}(k, k', k'') \phi_{\Delta,\Delta'}^{\Delta''}(\ell \widehat{\otimes} X \widehat{\otimes} | \Delta'', k'' \rangle) \ .$$

Use that ϕ is G_0 equivariant. This forces

$$\phi_{\Delta,\Delta'}^{\Delta''}(\ell \widehat{\otimes} X \widehat{\otimes} r) = \psi_{\Delta,\Delta'}^{\Delta''}(\ell \widehat{\otimes} X) \widehat{\otimes} r =: [\Psi_{\Delta,\Delta'}^{\Delta''}]_{\ell}(X) \widehat{\otimes} r \ .$$

The developments are summarized as

$$\mathbb{E}_{\ell(|\Delta_1,k_1\rangle)}(X(|\Delta_2,k_2\rangle)) = \sum_{\Delta_3} \sum_k c_{\Delta_1\Delta_2}^{\Delta_3}(k_1,k_2,k_3) \left[\Psi_{\Delta_1,\Delta_2}^{\Delta_3}\right]_{\ell}(X) \widehat{\otimes} |\Delta_3,k\rangle . \tag{C.2}$$

Taking again the example of $G_0 = SU(2)$, these coefficients have a particular simple form, namely

$$c_{j_1j_2}^{j_3}(m_1, m_2, m_3) = \langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle$$
,

with the Clebsch-Gordan matrix elements.

So far, the analysis has produced not much more than cumbersome notation. To obtain license for some drastic steps, it is necessary to switch gears and ponder for a moment the super matrix product state ω defined by the expectation values

$$\omega(\ell_1(r_1)\widehat{\otimes}\cdots\widehat{\otimes}\ell_n(r_n)) = \operatorname{tr}(\rho(1)\mathbb{E}_{\ell_1(r_1)}\circ\cdots\circ\mathbb{E}_{\ell_n(r_n)}(e(1)) ,$$

where the left, resp. right fixed points of the transfer operator have been represented by maps $\rho, e: R_0 \to A$, and with operators from isomorphism classes $\Delta_1, ..., \Delta_n$. I want to argue that it is permissible to *locally* average over G_0 , without leaving the SPT class $[\omega]$. Local averaging, here, refers to defining a state as

$$\overline{\omega}(L_1\widehat{\otimes}\cdots\widehat{\otimes}L_n) = \int_{G_0^n} \left[\prod_{i=1}^n d\mu(g_i) \right] \omega\left(\alpha_{g_1}(L_1)\widehat{\otimes}\cdots\widehat{\otimes}\alpha_{g_n}(L_n)\right) .$$

 $\overline{\omega}$ is positive as a sum of positive terms; it is normalized as

$$\overline{\omega}(1_{\mathcal{A}_n}) = \int_{G_0^n} \left[\prod_{i=1}^n d\mu(g_i) \right] \omega \circ \left(\alpha_{g_1} \widehat{\otimes} \cdots \widehat{\otimes} \alpha_{g_n} \right) (1_{\mathcal{A}_n}) = \left[\int_{G_0} d\mu(g) \right]^n \omega(1_{\mathcal{A}_n}) = 1 ,$$

and it clusters since

$$\left| \overline{\omega}(\mathcal{O}_1 \widehat{\otimes} \underbrace{1 \widehat{\otimes} \cdots \widehat{\otimes} 1}_{n \text{ times}} \widehat{\otimes} \mathcal{O}_2) - \overline{\omega}(\mathcal{O}_1) \overline{\omega}(\mathcal{O}_2) \right| = \left| \omega(\overline{\mathcal{O}_1} \widehat{\otimes} \underbrace{1 \widehat{\otimes} \cdots \widehat{\otimes} 1}_{n \text{ times}} \widehat{\otimes} \overline{\mathcal{O}_2}) - \overline{\omega}(\overline{\mathcal{O}_1}) \overline{\omega}(\overline{\mathcal{O}_2}) \right| \le \operatorname{Corr}_{\omega}(n) \left\| \overline{\mathcal{O}_1} \right\| \left\| \overline{\mathcal{O}_2} \right\|.$$

This also neatly shows that what is done here effectively is to add a projection on the G_0 -invariant subspace at each lattice site.

To see that it is in the same SPT class as ω , modify the Haar measure to a normalized $d\mu_t(g)$, which satisfies $\int d\mu_0(g)f(g) = f(1)$ and $d\mu_1(g)d\mu(g)$. This gives a continuous path of G-symmetric clustering states, hence a homotopy. For example, if $G_0 = SU(2)$, a possible choice is

$$d\mu_t(g) = \frac{\det(1-g)^{\frac{1}{t}-1}d\mu(g)}{\int_{G_0} \det(1-g')^{\frac{1}{t}-1}d\mu(g')} .$$

Bolstered by these arguments, the task is to average equation C.2. This produces immediate simplification. Indeed, the averaging forces $\Delta_1 = 0$, the trivial representation. But then the coefficients simplify,

$$c_{0\Delta_2}^{\Delta_3}(0, k_2, k_3) = \delta_{\Delta_2}^{\Delta_3} \delta_{k_3}^{k_2}$$
.

Since the right-most transfer operator starts with $\Delta = 0$, the averaged state has the following representation on operators $L_i = \ell_i(1)$ from the trivial representation:

$$\overline{\omega}(\ell_1(1)\widehat{\otimes}\cdots\widehat{\otimes}\ell_n(1)) = \operatorname{tr}(\rho\Psi_{\ell_1}\circ\cdots\circ\Psi_{\ell_n}(e)) , \quad \Psi_{\ell} = [\Psi^0_{0,0}]_{\ell} .$$

Since $\overline{\omega}$ has finite entanglement spectrum across any link, it is a super matrix product state. The next step is to study the symmetry action on this state.

To that effect recall the decomposition of the physical and virtual algebras C.1. The local averaging had the effect to restrict to the singlet subalgebras. Note that B_0 and \mathcal{B}_0 carry an algebra structure by $(X_1 \cdot X_2)(1) = X_1(1)X_2(1)$. Since the X are G_0 -equivariant, the only non-trivial remaining symmetries are the anti-unitary ones, which can be lifted to B_0 . In this context a sMPS with $\mathbb{Z}_2^T \times SU(2)_{\text{spin}}$ symmetry can transform effectively to a MPS with \mathbb{Z}_4^T -symmetry.

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