

Doctoral Dissertation

博士論文

# Symmetry-Protected Topological Phases of Quantum Particles with Integer Spin

(整数スピンを持つ粒子の対称性に保護されたトポロジカル相)

A Dissertation Submitted for the Degree of Doctor of Philosophy

July 2022

令和4年7月博士(理学)申請

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The University of Tokyo

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(整数スピンを持つ粒子の対称性に保護されたトポロジカル相)

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A Dissertation Submitted for the Degree of  
*Doctor of Philosophy*

in the

Department of Physics, Graduate School of Science,  
The University of Tokyo

JULY 7, 2022





## LIST OF PUBLICATIONS

- [1] Hong Yang, Linhao Li, Kouichi Okunishi, and Hosho Katsura, *Duality, Criticality, Anomaly, and Topology in Quantum Spin-1 Chains*, [arXiv:2203.15791](#).
- [2] Shoichi Tsubota, Hong Yang, Yutaka Akagi, and Hosho Katsura, *Symmetry-protected quantization of complex Berry phases in non-Hermitian systems*, [Phys. Rev. B \*\*105\*\*, L201113 \(2022\)](#).
- [3] Hong Yang, Hayate Nakano, Hosho Katsura, *Symmetry-protected topological phases in spinful bosons with a flat band*, [Phys. Rev. Research \*\*3\*\*, 023210 \(2021\)](#).
- [4] Hong Yang, Hosho Katsura, *Rigorous Results for the Ground States of the Spin-2 Bose-Hubbard Model*, [Phys. Rev. Lett. \*\*122\*\*, 053401 \(2019\)](#).



## ABSTRACT

Symmetry-protected topological (SPT) phases have been gaining much attention. *Gapped* SPT phases refer to the quantum phases of those unique gapped ground states that can never be smoothly connected to trivial product states while preserving certain symmetry. An example is the *Haldane phase*, which is a (1+1)-dimensional (D) gapped SPT phase protected by the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry. In quantum critical systems, it was recently realized that the concept of *gapless* SPT phases can also be developed. In this thesis, I focus on SPT phases in many-body spinful boson systems [1] and spin systems [2]. In fact, boson and spin degrees of freedom (DOF) have no intrinsic difference from each other, because they are both bosonic: In both cases, operators on DOF at different spatial locations commute with each other.

In the first three chapters, I will give an introduction to bosonic SPT phases. Chapter 2 discusses how to understand and classify (1+1)D SPT phases, including both gapped and gapless cases. Chapter 3 is about higher dimensional gapped SPT phases. In particular, weak SPT phases, Lieb-Shultz-Mattis (LSM) anomaly, and crystalline SPT phases will be discussed.

In Chapter 4, we theoretically demonstrate that gapped SPT phases can be realized with ultracold spinful bosonic atoms loaded on the lattices which have a flat band at the bottom of the band structure [1]. Ground states of such systems are not conventional Mott insulators in the sense that the ground states possess not only spin fluctuations but also non-negligible charge fluctuations. The SPT phases in such systems are determined by both spin and charge fluctuations at zero temperature. We find that the many-body ground states of such systems can be exactly obtained in some special cases, and these exact ground states turn out to serve as representative states of the SPT phases. As a concrete example, we demonstrate that spin-1 bosons on a sawtooth chain can be in a Haldane phase and that this SPT phase is a result of spin fluctuations. We also show that spin-3 bosons on a kagome lattice can be in an SPT phase protected by  $D_2$  point group symmetry; however, this SPT phase is a result of charge fluctuations.

Chapter 5 focuses more on the gapless phases [2]. In quantum spin-1 chains, there is a nonlocal unitary transformation known as the Kennedy-Tasaki transformation  $U_{\text{KT}}$ , which defines a duality between the Haldane phase and the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry-breaking phase. We find that  $U_{\text{KT}}$  also defines a duality between an SPT Ising critical phase and a

trivial Ising critical phase, which provides a "hidden symmetry breaking" interpretation for the topological criticality. Moreover, since the duality relates different phases of matter, we argue that a model with self-duality (i.e., invariant under  $U_{\text{KT}}$ ) is natural to be at a critical or multicritical point. We study concrete examples to demonstrate this argument. In particular, when  $H$  is the Hamiltonian of the spin-1 antiferromagnetic Heisenberg chain, we prove that the self-dual model  $H + U_{\text{KT}} H U_{\text{KT}}$  is exactly equivalent to a gapless spin-1/2 XY chain, which also implies an emergent LSM anomaly. On the other hand, we show that the SPT and trivial Ising criticalities that are dual to each other meet at a multicritical point which is indeed self-dual. Our discussions can be generalized to other symmetries beyond the spin-1 chains.

## ACKNOWLEDGMENTS

**T**ime flies like an arrow. Five years have passed since I came to Japan. My deepest appreciation goes to my advisor Professor Hosho Katsura, who is extraordinarily full of wisdom, supportive, responsible, generous, and tolerant. It is my luck to be his student.

During these five years, I also got chances to work with excellent colleagues Linhao Li and Hayate Nakano. Linhao Li is always intelligent and passionate about research, and Hayate Nakano is an ingenious man of action. Professor Kouichi Okunishi also provided meticulous and technical help to my research. I would like to express my gratitude to all of my collaborators.

I would particularly like to thank my parents and all other relatives who have been providing moral support and warm encouragements to me. In particular, I am deeply grateful to my mother for her constant encouragement.

Finally, I appreciate the financial support of JSPS DC1 that made it possible to complete my thesis.



## ABBREVIATIONS AND NOTATIONS

### Abbreviations

AFM	Antiferromagnetic
AKLT	Affleck-Lieb-Kennedy-Tasaki
BHMSC	Bose-Hubbard Model on the Sawtooth Chain
BLBQ	Bilinear-Biquadratic
CFT	Conformal Field Theory
CLS	Compact Localized State
DDI	Dipole-Dipole Interaction
DMRG	Density Matrix Renormalization Group
DOF	Degree(s) Of Freedom
EE	Entanglement Entropy
ES	Entanglement Spectrum
FM	Ferromagnetic
FPS	Fully Packed State
GS	Ground State, Ground States, or Ground-State
KT	Kennedy-Tasaki
LSM	Lieb-Schultz-Mattis
MPS	Matrix Product State
OBC	Open Boundary Condition
PBC	Periodic Boundary Condition
pgSPT	Point-Group-Symmetry-Protected Topological
SPT	Symmetry-Protected Topological
SSB	Spontaneous Symmetry Breaking
TR	Time Reversal
trn	Translation
VUMPS	Variational Uniform Matrix Product State
3DTas	3D Tasaki lattice

## Notations

$\mathcal{B}_X$	the set of bonds on the graph $X$
$D_n$	dihedral group of order $2n$
$H^n[G, \mathbf{U}(1)]$	$n$ th cohomology group of $G$
$\mathcal{O}_{\text{AFM}}^\delta$	AFM correlation in $\delta = x, y, z$ direction
$\mathcal{O}_{\text{FM}}^\delta$	FM correlation in $\delta = x, y, z$ direction
$\mathcal{O}_{\text{str}}^\delta$	string order parameter associated with a group element $\delta$ (or direction $\delta$ )
$P_i^{(S)}$	second-quantized operator that projects atoms at site $i$ onto two-body total spin $S$ .
$P_{i,j}^{(S)}$	projection of two-spin state at two different sites $i, j$ onto total spin $S$ .
$P_{ij}^{(S)}$	projection of two atoms labeled by $i, j$ onto two-body total spin $S$ .
$(\mathbb{Z}^{\text{trn}})^d$	translation symmetry along $d$ linearly independent directions
$\mathbb{Z}_2^{\text{TR}}$	the $\mathbb{Z}_2$ group for time-reversal symmetry
$\mathbb{Z}_2 \times \mathbb{Z}_2$	a general dihedral group of order 4
$\mathbb{Z}_2^y \times \mathbb{Z}_2^z$	the $\mathbb{Z}_2 \times \mathbb{Z}_2$ group generated by of $\pi$ -rotations of spin(s) along two orthogonal axes
$\Lambda_X$	the set of sites (vertices) on the graph $X$
$\Lambda_X^{[k]}$	the subset of $\Lambda_X$ consisting of sites where $k$ CLSs in an FPS overlap
$\hat{\mu}$	nonlocal operator (symmetry flux) in Ising CFT
$\sigma$	mirror reflection
$\hat{\sigma}$	local operator in Ising CFT
$\sigma_j^{x,y,z,+,-}, \sigma_j$	Pauli matrices at position $j$
$\square$	2D Tasaki lattice
$\square$	2D square lattice
$\star$	kagome lattice
$\triangle$	2D triangular lattice
$\square$	3D cubic lattice
$\boxtimes$	Creutz ladder
$\rtimes$	semidirect product



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方以類聚，物以群分，吉凶生矣。

『易經·繫辭上』

## INTRODUCTION

Quantum phases of matter are phases of matter at zero temperature. Therefore, classifying quantum phases really means classifying the ground states (GS) of quantum Hamiltonians. In classical systems, phases are a result of the competition between interactions and thermal fluctuations: While particles tend to develop a certain order to minimize the interaction energy, thermal fluctuations tends to destroy the order. The phase diagram of water (see Fig. 1.1) is one of the most famous examples that demonstrate the competition between interactions and thermal fluctuations. Quantum phases, however, have no thermal fluctuations by definition. Instead, quantum phases are a result of the competition between interactions and *quantum fluctuations*. Quantum fluctuations essentially originate from the impossibility of finding a common ground state of two non-commuting operators. Figure 1.2 shows the conventional classification of quantum phases of matter.

### 1.1 Landau's paradigm

Landau's paradigm, in which the concept of spontaneous symmetry breaking (SSB) plays a central role, has been very successful. Landau's paradigm points out that different phases (orders) actually correspond to different symmetries of the states. For example, particles in liquid and gas have a random but uniform distribution, so that liquid and gas both have continuous translation symmetry, which suggests that liquid and gas should be in the same phase. Indeed, as shown in Fig. 1.1, by properly controlling the parameters, we can smoothly transform liquid into gas without going through a phase transition and vice versa. On the other hand, the continuous translation symmetry is broken down to discrete translation symmetry in a solid crystal, which indicates that crystal and liq-

uid/gas should belong to two different phases. In other words, a phase transition between crystal and liquid/gas is always inevitable.

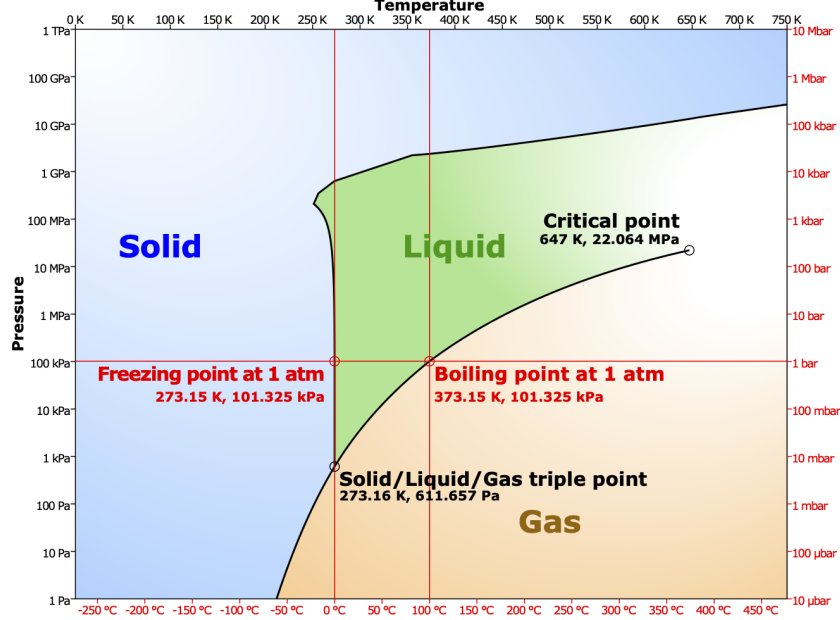


Figure 1.1: Phase diagram of water [3]. Liquid and gas can smoothly become each other without experiencing a phase transition. However, liquid/gas is always separated from the solid phase by a phase transition.

While the above examples about crystal and liquid/gas rather belong to classical physics, Landau's paradigm applies to both classical and quantum systems. As shown in Fig. 1.2, quantum phases are first classified according to Landau's paradigm: existence or absence of SSB. A famous quantum model that demonstrates Landau's theory is the *spin-1/2 transverse-field Ising model* in (1+1)D :

$$H_{\text{Ising}} = - \sum_{j=1}^L (\sigma_j^z \sigma_{j+1}^z + h \sigma_j^x), \quad h \geq 0. \quad (1.1)$$

The model has a  $\mathbb{Z}_2$  spin-flip symmetry  $|\uparrow\rangle \leftrightarrow |\downarrow\rangle$  generated by  $\prod_j \sigma_j^x$ . When  $h = 0$ ,  $H_{\text{Ising}}$  has two degenerate GS which spontaneously break the  $\mathbb{Z}_2$  symmetry:

$$\begin{aligned} |\uparrow\rangle &= |\dots \uparrow\uparrow\uparrow \dots\rangle, \\ |\downarrow\rangle &= |\dots \downarrow\downarrow\downarrow \dots\rangle. \end{aligned} \quad (1.2)$$

On the other hand, when  $h \rightarrow \infty$ , the unique GS is  $\mathbb{Z}_2$ -symmetric:

$$|\Rightarrow\rangle = |\dots \rightarrow\rightarrow\rightarrow \dots\rangle. \quad (1.3)$$

Since  $[\sigma_j^z \sigma_{j+1}^z, \sigma_j^x] \neq 0$ , when  $0 < h < \infty$ , there is quantum fluctuation in the GS.

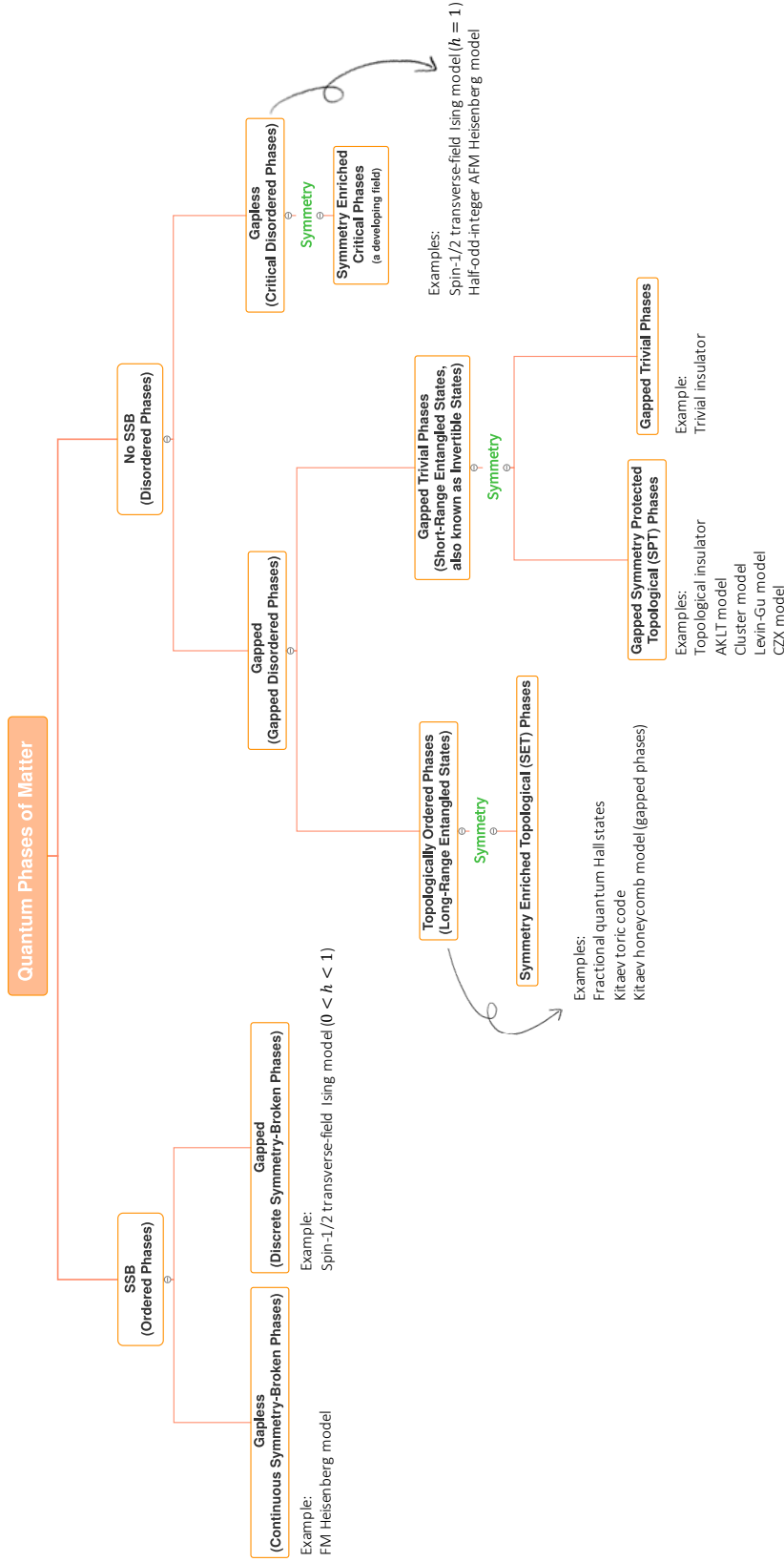


Figure 1.2: Classification of quantum phases of matter. Note that this classification is not complete, as quantum phase classification is still a developing field. In general, to identify a quantum phase, there are several steps. First, the phase is classified by Landau's paradigm. Second, we can ask whether the phase is gapped or gapless (see Definitions 1.2 and 1.3). It is well-known that the gapped disordered phases can be further classified according to the existence or absence of topological order or SPT order. In these years, physicists have started to realize that the critical disordered phases can also be further classified, leading to the concept of, for example, gapless SPT phases.

Let  $|\psi_{\text{GS}}\rangle$  be the GS of  $H_{\text{Ising}}$ . In fact,  $|\psi_{\text{GS}}\rangle$  is in an ordered and gapped phase when  $0 \leq h < 1$ , while it is in a disordered and gapped phase when  $h > 1$ . A state without SSB is said to be disordered, while a state with SSB is said to be ordered. This may be easily seen from the two-point correlation function:

$$\lim_{r \rightarrow \infty} \langle \psi_{\text{GS}} | \sigma_j^z \sigma_{j+r}^z | \psi_{\text{GS}} \rangle = \begin{cases} \text{const.} > 0, & 0 \leq h < 1, \\ 0, & h > 1. \end{cases} \quad (1.4)$$

In particular,  $|\psi_{\text{GS}}\rangle$  is said to have long-range order when  $0 \leq h < 1$ .

Note that when the system size  $L$  is finite and  $h > 0$ , the GS of  $H_{\text{Ising}}$  is *unique*<sup>1</sup>. This is not so surprising, because the  $\mathbb{Z}_2$  symmetry only has 1D irreducible representations and thus cannot give rise to two-fold degeneracy. However, we expect that, when  $0 < h < 1$ , the GS and the first excited state should somewhat look like<sup>2</sup>

$$\begin{aligned} |\psi_{\text{GS}}\rangle &\sim \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle), \\ |\psi_{1\text{st}}\rangle &\sim \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle). \end{aligned} \quad (1.5)$$

We call the states in Eq. (1.5) *cat states*<sup>3</sup>, because they are superposition of macroscopically distinct states. In addition, it is found that the energy separation  $\varepsilon$  between  $|\psi_{\text{GS}}\rangle$  and  $|\psi_{1\text{st}}\rangle$  is given by  $\varepsilon \approx 2h^L$ , which is exponentially small in the system size<sup>4</sup>. In such a case, we say that  $|\psi_{\text{GS}}\rangle$  and  $|\psi_{1\text{st}}\rangle$  are *quasi-degenerate*. For the reason described above, the quasi-degeneracy cannot be an exact degeneracy resulting from the  $\mathbb{Z}_2$  symmetry. Nevertheless, if we add a term  $h_z \sum_j \sigma_j^z$  to  $H_{\text{Ising}}$  that explicitly break the  $\mathbb{Z}_2$  symmetry, the quasi-degeneracy will be destroyed. Therefore, the quasi-degeneracy is indeed protected by the  $\mathbb{Z}_2$  symmetry despite that  $|\psi_{\text{GS}}\rangle$  and  $|\psi_{1\text{st}}\rangle$  do not belong to the same irreducible representation. This suggests that SSB in quantum systems can be defined as follows [5]:

**Definition 1.1 (SSB in quantum systems with a finite symmetry group)** *A quantum system with a finite symmetry group  $G$  is in an SSB phase at zero temperature, iff it has robust quasi-degenerate (or degenerate) GS that belong to at least two different irreducible representations of  $G$ .*

The term "robust" means that the quasi-degeneracy is robust against any perturbations that respect the symmetry  $G$ . Since  $\sigma_j^z$  gives a nontrivial charge of  $\mathbb{Z}_2$ , i.e.,

$$\left( \prod_j \sigma_j^x \right) \sigma_j^z \left( \prod_j \sigma_j^x \right) = -\sigma_j^z, \quad (1.6)$$

---

<sup>1</sup>The uniqueness of the GS can be easily proved by the *Perron-Frobenius theorem* [4].

<sup>2</sup>This can also be easily seen from the perturbation theory.

<sup>3</sup>In quantum information literature, they are often called *GHZ states*.

<sup>4</sup> $H_{\text{Ising}}$  is solvable by mapping it to a free fermion system via the *Jordan-Wigner transformation*.

the fact that the two quasi-degenerate states  $|\psi_{\text{GS}}\rangle$  and  $|\psi_{1\text{st}}\rangle$  have long-range order in terms of  $\sigma_j^z$  is equivalent to  $\mathbb{Z}_2$  SSB.<sup>5</sup> However, cat states are considered unphysical. *Physical states* like  $|\uparrow\uparrow\rangle$  and  $|\downarrow\downarrow\rangle$  obey the so-called *clustering* property:

$$\lim_{r \rightarrow \infty} \langle \sigma_j^z \sigma_{j+r}^z \rangle = \lim_{r \rightarrow \infty} \langle \sigma_j^z \rangle \langle \sigma_{j+r}^z \rangle > 0, \quad (1.7)$$

which means  $\langle \sigma_j^z \rangle > 0$ , i.e., the physical GS is not invariant under  $\mathbb{Z}_2$ . This also suggests that within Landau's paradigm, phases can be characterized by *local order parameters*. For more details about the general relation between long-range order and SSB, see Ref. [4].

In general, when the symmetry  $G$  of a quantum system is spontaneously broken, the GS can be gapped or gapless depending on  $G$ . If  $G$  is a continuous group, then *Goldstone's theorem* guarantees the GS to be gapless [6]. A famous example is the ferromagnetic (FM) Heisenberg model, in which the GS breaks the  $\text{SO}(3)$  spin rotation symmetry and the gapless excitations are given by spin waves. On the other hand, when  $G$  is a discrete symmetry (i.e.,  $G$  is a finite symmetry group), the GS is gapped, because the excitations in this case are given by "domain walls".

In the transverse-field Ising chain  $H_{\text{Ising}}$  with the open boundary condition (OBC), the ordered and disordered phases can be exchanged by the *Kramers–Wannier duality* [7, 8], which is a nonlocal transformation that maps the operators as follows:

$$\begin{aligned} H_{\text{Ising}} = - \sum_j (\sigma_j^z \sigma_{j+1}^z + h \sigma_j^x) &\xrightarrow[\text{OBC}]{\text{Kramers–Wannier}} H_{\text{Ising}} = -h \sum_j (\sigma_j^z \sigma_{j+1}^z + h^{-1} \sigma_j^x) \\ \sigma_j^z &\xrightarrow[\text{OBC}]{\text{Kramers–Wannier}} \sigma_j^x \sigma_{j+1}^x \sigma_{j+2}^x \dots \end{aligned} \quad (1.8)$$

Since the duality exchanges the two different phases, one naturally expects that a phase transition occurs when  $H_{\text{Ising}}$  is self-dual. Indeed, when  $h = 1$ , the self-dual model  $H_{\text{Ising}}$  has no SSB and is in a quantum critical point effectively described by the conformal field theory (CFT) with the central charge  $c = 1/2$  (also called the Ising CFT). We say that the GS is in a critical disordered phase. Right at the critical point  $h = 1$ , the Ising universality class yields [9]

$$\langle \psi_{\text{GS}} | \sigma_j^z \sigma_{j+r}^z | \psi_{\text{GS}} \rangle \sim r^{-1/4}. \quad (1.9)$$

## 1.2 Gapped quantum phases and phase transitions between them

We have been using the words "gapped" and "gapless" without a definition. Let us first define a *short-range Hamiltonian* (also called *local Hamiltonian*) to be a Hamiltonian

<sup>5</sup>On the other hand, since  $\sigma_j^x$  carries a trivial charge under  $\mathbb{Z}_2$ , a disordered state can have long-range order measured by  $\sigma_j^x$ , for example,  $\langle \sigma_j^x \sigma_{j+r}^x \rangle > 0$ .

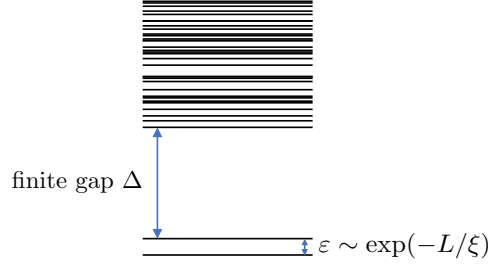


Figure 1.3: Schematic energy spectrum of a gapped quantum system with  $m = 2$ .

that contains only short-range interactions or short-range hopping. I will only consider short-range Hamiltonians in this thesis. A gapped quantum system is then defined as

**Definition 1.2 (gapped quantum system)** *A short-range Hamiltonian  $H$  is gapped iff both of the following two conditions are satisfied.*

1. *When the system size  $L$  is sufficiently large, there are a finite integer  $1 \leq m < \infty$  of lowest energy states which are separated from all the other eigenstates by energy  $\Delta$  and  $\lim_{L \rightarrow \infty} \Delta > 0$ .*
2. *The energy separation  $\varepsilon$  among the lowest energy states is either exactly zero or exponentially small in the system size  $L$ . In other words,  $\lim_{L \rightarrow \infty} \varepsilon = 0$ .*

See also Fig. 1.3. The integer  $m$  is called the degeneracy. However, even if  $H$  is gapped on a space with no boundary, there can be gapless excitations on the boundary when  $H$  is defined on a space with boundary. We do not want the above definition to be depend on the existence or absence of the boundary. Therefore, in Definition 1.2, we always assume that  $H$  is defined on a space with no boundary. Even if we are given a short-range Hamiltonian  $H$  with boundaries, we will always redefine  $H$  such that it is on a space without boundaries before applying Definition 1.2. On the other hand, gapless quantum systems are defined as

**Definition 1.3 (gapless quantum system)** *Quantum systems that are not gapped are said to be gapless.*

A gapped system with degeneracy (i.e.,  $m > 1$ ) and a gapless quantum system have one thing in common: Neither of them has a unique gapped GS.

Quantum phase transitions are zero-temperature transitions between quantum phases. A more precise definition is given by the following.

**Definition 1.4 (quantum phase transition between gapped phases)** *Let  $H(s)$  with  $0 \leq s \leq 1$  be a class of short-range Hamiltonians that smoothly depend on  $s$ . Let  $H(s = 0)$  and  $H(s = 1)$  be the Hamiltonians of gapped systems. In the thermodynamic limit, we say that a quantum phase transition occurs at  $0 < s_c < 1$  iff  $H(s_c)$  is gapless. This can be further divided into two cases.*



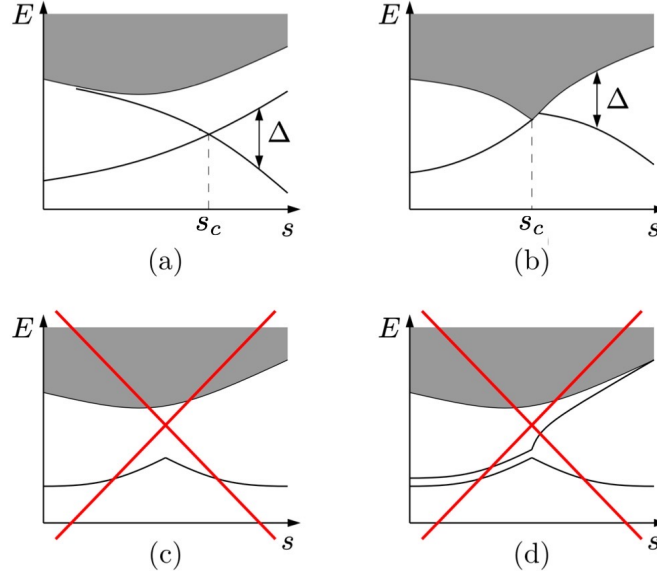


Figure 1.4: Energy spectrum of a gapped quantum system as a function of a parameter  $s$  in the thermodynamic limit. (a) First-order phase transition between gapped phases. A level crossing occurs at  $s = s_c$ . Note that  $H(s_c)$  is considered *gapless* instead of gapped, because we want the gap  $\Delta$  to be defined in a way that changes continuously with respect to  $s$ . (b) Second-order (continuous) phase transition between gapped phases. Gapless elementary excitation has a continuous spectrum at  $s = s_c$ . Scenarios in (c) and (d) cannot happen, because we have assumed that  $H(s)$  smoothly depends on  $s$ . In other words, the expectation value of any physical observable cannot have singularity at  $s = s_c$  in the absence of a quantum phase transition [5]. Figures reproduced with permission from Springer Nature.

1. *First-order phase transition: A level crossing between GS happens at  $s = s_c$ ; See Fig. 1.4(a).*
2. *Second-order (also called continuous) phase transition: Gapless elementary excitation has a continuous spectrum<sup>6</sup>; See Fig. 1.4(b). In this case, we also say that  $H(s_c)$  is critical.*

Roughly speaking, a phase is a collection of physical states with qualitatively the same properties. Within the same phase, the physical properties should change smoothly as we vary parameters smoothly. Similar to the case of liquid and gas of water (see Fig. 1.1), it is natural to say that two states, regardless of classical states or quantum states, are in the same phase if they can be smoothly connected. For gapped quantum ground states, a precise definition of the smooth connection is

<sup>6</sup>There can be cases where  $H(s_c)$  has infinitely many GS, and the gap above the GS is finite, but we expect that the GS degeneracy can be lifted by an infinitesimal perturbation such that the elementary excitation has a continuous spectrum.

**Definition 1.5 (gapped states are smoothly connected)** *Two gapped quantum GS  $|\psi(0)\rangle$  and  $|\psi(1)\rangle$  are smoothly connected iff they are related by a local unitary transformation.*

It is known that a local unitary transformation can be well approximated with a *finite-depth quantum circuit*. See Ref. [5] for details. A graphic representation of a quantum circuit is presented in Fig. 1.5. Instead of focusing on the GS, we can also have an alternative definition for the Hamiltonians.

**Definition 1.6 (gapped Hamiltonians are smoothly connected)** *Let  $H(0)$  and  $H(1)$  be two short-range Hamiltonians of gapped systems. We say that  $H(0)$  and  $H(1)$  are smoothly connected iff both of the following two conditions are satisfied.*

1. *There exists a class of short-range Hamiltonians  $H(s)$  with  $0 \leq s \leq 1$  such that  $H(s)$  smoothly depends on  $s$ .*
2. *There is no quantum phase transition for any  $0 < s < 1$ .*

We are now ready for a very important definition for the same gapped quantum phase:

**Definition 1.7 (the same gapped quantum phase)** *Let  $H(0)$  and  $H(1)$  be the parent Hamiltonians of two gapped GS  $|\psi(0)\rangle$  and  $|\psi(1)\rangle$ , respectively. The two states are  $|\psi(0)\rangle$  and  $|\psi(1)\rangle$  in the same quantum phase, iff at least one of the following statements is found to be true.*

1.  *$|\psi(0)\rangle$  and  $|\psi(1)\rangle$  are smoothly connected.*
2.  *$H(0)$  and  $H(1)$  are smoothly connected.*

The following theorem guarantees Definition 1.7 to be self-consistent.

**Theorem 1.8** *The two statements in Definition 1.7 are equivalent.*

For a proof, see Ref. [5, 10]. An intuitive understanding of the above theorem is that along an adiabatic path that connects  $H(0)$  and  $H(1)$ , the existence of an energy gap prevents the system from exciting to higher energy levels.

With the above definitions, especially Definition 1.7, we are able to classify gapped quantum phases. We consider quantum systems with arbitrary local degrees of freedom (DOF): spins, bosons, fermions, etc. In fact, spins and bosons have no intrinsic difference from each other, because in both cases operators at different spatial locations commute with each other.

**Definition 1.9 (fermionic/bosonic system)** *A quantum system is called fermionic if the fermionic parity  $P_f = (-1)^F$  is considered as an intrinsic  $\mathbb{Z}_2$  symmetry of the system, where  $F$  is the total fermion number operator. Otherwise, it is a bosonic system.*

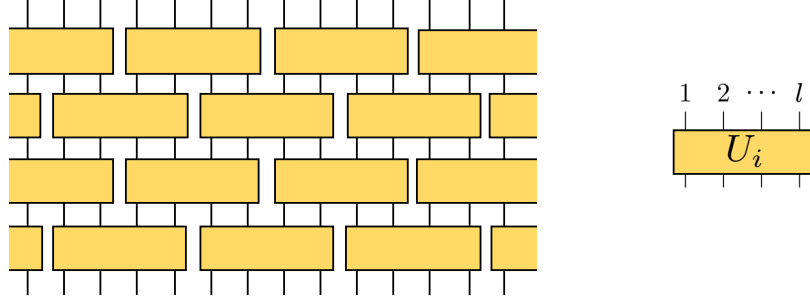


Figure 1.5: A graphic representation of a quantum circuit. Each rectangle is a unitary operators  $U_i$  acting on a finite region. In each layer, the unitary operators acting on non-overlapping regions.

It often happens that a system consisting of fermions can be regarded as a bosonic system when all the eigenstates have the same fermion parity (i.e.,  $P_f$  reduces to a number).

**Theorem 1.10** *All gapped bosonic systems in (1+1)D belong to the same phase if no symmetry is required.*

This theorem has been strongly believed to be true in Refs. [5, 11–13], and it is rigorously proved by means of matrix product states in Refs. [14–16]. As an example, the  $\mathbb{Z}_2$  ordered and disordered phases of  $H_{\text{Ising}}$  in Eq. (1.1) can indeed be smoothly connected if we add a term  $\lambda \sum_j \sigma_j^z$  to the Hamiltonian [4]; See Fig. 1.6. Note that the additional term does not respect the  $\mathbb{Z}_2$  symmetry.

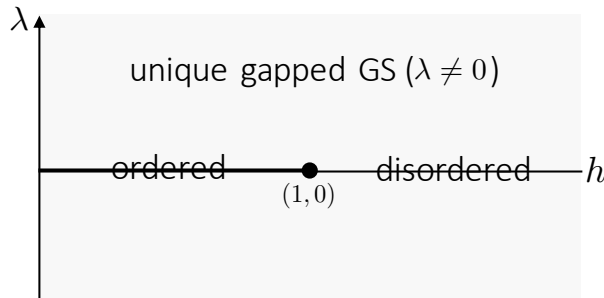


Figure 1.6: Phase diagram of the (1+1)D model  $H_{\text{Ising}} + \lambda \sum_j \sigma_j^z$ . The phase transition point at  $(h, \lambda) = (1, 0)$  can be bypassed with nonzero  $\lambda$ .

### 1.3 Beyond Landau's paradigm

Landau's paradigm has been so successful that physicists used to believe that Landau's paradigm classifies all possible phases of matter. However, this is not the case. Let us

consider a (1+1)D fermionic model with OBC, known as *Kitaev's Majorana chain* [17]:

$$H_{\text{Kitaev}} = - \sum_{j=1}^L (c_j^\dagger c_{j+1} + \text{h.c.}) + \sum_{j=1}^L (c_j c_{j+1} + \text{h.c.}) = i \sum_{j=1}^{L-1} \gamma_{2j} \gamma_{2j+1}, \quad (1.10)$$

where  $c_j = (\gamma_{2j-1} + i\gamma_{2j})/2$  is the spinless fermion operator satisfying  $\{c_i, c_j^\dagger\} = \delta_{ij}$  and  $\gamma_m$  is the Majorana operator satisfying  $\{\gamma_m, \gamma_n\} = \delta_{mn}$ . It is known that  $H_{\text{Kitaev}}$  has two-fold degenerate GS

$$\begin{aligned} |\psi_{\text{GS}}\rangle &= \bigotimes_{j=1}^L |0\rangle_j \\ |\psi'_{\text{GS}}\rangle &= \frac{1}{2} (\gamma_1 - i\gamma_{2L}) \bigotimes_{j=1}^L |0\rangle_j \end{aligned} \quad (1.11)$$

corresponding to Majorana zero modes localized at both ends, where  $(\gamma_{2j} + i\gamma_{2j+1})|0\rangle_j = 0$ . On the other hand, the following model

$$H_{\text{triv}} = - \sum_{j=1}^L \left( c_j^\dagger c_j - \frac{1}{2} \right) = -\frac{i}{2} \sum_{j=1}^L \gamma_{2j-1} \gamma_{2j} \quad (1.12)$$

with OBC has a unique gapped GS:

$$|\psi_{\text{triv}}\rangle = \bigotimes_{j=1}^L (c_j^\dagger |\text{vac}\rangle_j), \quad (1.13)$$

where  $c_j |\text{vac}\rangle_j = 0$ . If a product state is a unique gapped GS, such as Eq. (1.13) and Eq. (1.3), the product state is called a *trivial product state*. All the states in Eq. (1.11) and Eq. (1.13) have the fermion parity symmetry. In fact, in fermion systems, any operator or state that does not obey the fermion parity symmetry is considered unrealistic (unacceptable) in physics. In other words, such operators or states are forbidden. According to Laudau's paradigm, GS in Eq. (1.11) and Eq. (1.13) should be in the same disordered phase. However, this is not the case, because the two-fold degeneracy of  $H_{\text{Kitaev}}$  turns out to be stable against any perturbation (that obey the intrinsic fermion parity symmetry) [18]. This suggests that the GS of  $H_{\text{Kitaev}}$  can never be smoothly deformed into that of  $H_{\text{triv}}$ .<sup>7</sup>

**Definition 1.11 (short/long-range entanglement [5, 10])** *A gapped state is short-range entangled if it is smoothly connected to a trivial product state. Otherwise, it is long-range entangled.*

---

<sup>7</sup>In (1+1)D, a fermionic system and a spin-1/2 system can be mapped into each other via the Jordan-Wigner transformation. In particular, the fermion parity  $P_f = (-1)^F$  is mapped to the  $\mathbb{Z}_2$  spin flip symmetry. In fact, the two-fold degeneracy of  $H_{\text{Kitaev}}$  corresponds to the two SSB states in the transverse-field Ising chain, in which the trivial GS of  $H_{\text{triv}}$  corresponds to the disordered GS of the transverse-field Ising chain. In a spin-1/2 system, the  $\mathbb{Z}_2$  symmetry can be broken by adding a magnetic field. However, breaking the fermion parity symmetry in a fermionic system is never allowed.

According to Definition 1.11, the GS of  $H_{\text{Kitaev}}$  is long-range entangled. The quantum phase represented by the GS of  $H_{\text{Kitaev}}$  is nowadays understood as an *invertible topologically ordered phase* [19–21]. In fact, the  $\nu = 1$  fermionic integer quantum Hall state is also long-range entangled, and it is in an invertible topologically ordered phase. Topological order is in general non-invertible, for example, the fractional quantum Hall states and the GS of Kitaev toric code both have *non-invertible topological order*. A precise definition of topological order can be found in Ref. [5]. Roughly speaking, a quantum system with topological order has robust GS degeneracy on closed spaces, and the GS are long-range entangled. The degeneracy on a given closed space is usually different for different topologies of space. For example, for a  $\mathbb{Z}_2$  topologically ordered state in two (spatial) dimensions, the degeneracy is  $4^g$  on genus  $g$  Riemann surface [5]. Topologically ordered phases are beyond Landau's paradigm.

Theorem 1.10 implies the absence of topological order in (1+1)D bosonic systems. However, let us consider the following model defined on a zigzag chain (see Fig. 1.7), known as the *cluster model*.

$$H_{\text{cluster}} = - \sum_j \sigma_{j-1}^z \sigma_j^x \sigma_{j+1}^z. \quad (1.14)$$

By mapping the model into free fermions, one can find that it is gapped [22]. The model

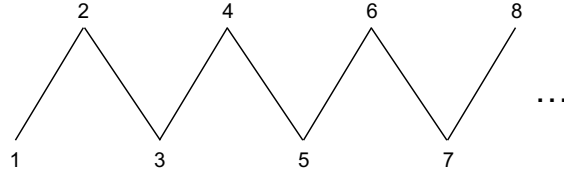


Figure 1.7: Zigzag chain with a spin-1/2 on each vertex. Odd and even sites belong to sublattices  $A$  and  $B$ , respectively.

has  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry, where

$$\begin{aligned} \mathbb{Z}_2 \times \mathbb{Z}_2 &= \{1, X_A, X_B, X_A X_B\}, \\ X_A &= \prod_k \sigma_{2k-1}^x, \\ X_B &= \prod_k \sigma_{2k}^x, \\ X_A X_B &= X_B X_A. \end{aligned} \quad (1.15)$$

Since all the terms in  $H_{\text{cluster}}$  commute with each other and each term squares to one, the GS  $|\psi_{\text{GS}}\rangle$  satisfies  $\sigma_{j-1}^z \sigma_j^x \sigma_{j+1}^z |\psi_{\text{GS}}\rangle = |\psi_{\text{GS}}\rangle$ ,  $\forall j$ . On a chain of length  $L$  with the periodic boundary condition (PBC), the GS is unique because there are  $L$  qubits and  $j = 1, \dots, L$ . On the other hand, on a chain of length  $L$  with OBC, the GS is four-fold degenerate, because  $j = 2, \dots, L-1$ . The four-fold degeneracy is in general not a robust property due to

Theorem 1.10. In other words, it can be smoothly connected to the trivial product state  $|\Rightarrow\rangle$  in Eq. (1.3). However, the degeneracy is indeed robust if the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry is imposed. To see this, consider a half-infinite chain. The generators of  $\mathbb{Z}_2 \times \mathbb{Z}_2$  effectively act on the boundary of the GS:

$$\begin{aligned} X_A |\psi_{\text{GS}}\rangle &= X_A \prod_{k=2}^{\infty} \sigma_{2k-2}^z \sigma_{2k-1}^x \sigma_{2k}^z |\psi_{\text{GS}}\rangle = \sigma_1^x \sigma_2^z |\psi_{\text{GS}}\rangle, \\ X_B |\psi_{\text{GS}}\rangle &= X_B \prod_{k=1}^{\infty} \sigma_{2k-1}^z \sigma_{2k}^x \sigma_{2k+1}^z |\psi_{\text{GS}}\rangle = \sigma_1^z |\psi_{\text{GS}}\rangle. \end{aligned} \quad (1.16)$$

Let

$$\mathcal{U}^A = \sigma_1^x \sigma_2^z, \quad \mathcal{U}^B = \sigma_1^z. \quad (1.17)$$

We see that  $\mathcal{U}^A$  and  $\mathcal{U}^B$  anti-commute with each other, despite that  $X_A$  and  $X_B$  commute with each other. Therefore, the GS degeneracy is protected by the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry. This example suggests that (1+1)D bosonic systems can also be nontrivial if certain symmetry is imposed, giving rise to the concept of *symmetry protected topological (SPT) phases*.

**Definition 1.12 (gapped SPT phase)** *Gapped SPT phases are certain collections of gapped and short-range entangled GS without SSB. A short-range entangled, unique, and gapped GS is in an SPT phase iff it cannot be smoothly connected to a trivial product state while preserving certain symmetry. Otherwise, it is in a trivial phase. (See also Fig. 1.8.)*

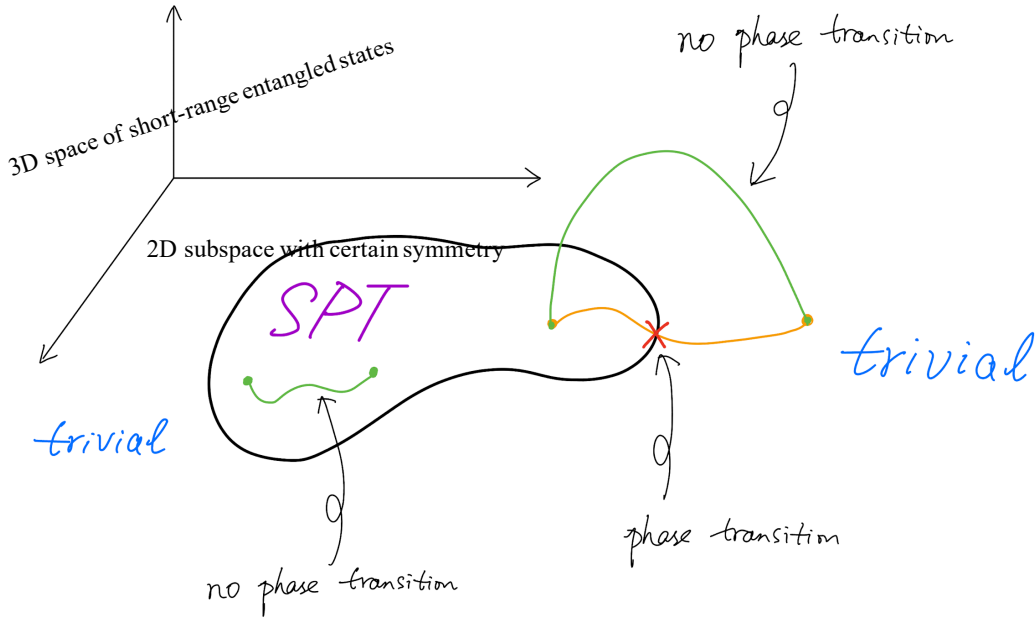


Figure 1.8: A schematic description of Definition 1.12.

In other words, SPT phases are nontrivial only in the presence of certain symmetry. SPT phases protected by *on-site symmetry*<sup>8</sup> can have several interesting properties. For example, the GS of the cluster model in Eq. (1.14) is also characterized by some nonlocal order parameters, known as the *string order parameters*. One of them is

$$\begin{aligned}\mathcal{O}_{\text{str}}^{AB} &= \lim_{r \rightarrow \infty} \langle F_j^{AB} F_{j+r}^{AB} \rangle = \langle \prod_k \sigma_{k-1}^z \sigma_k^x \sigma_{k+1}^z \rangle = 1, \\ F_j^{AB} &= \dots \sigma_{j-1}^x \sigma_j^x \sigma_j^y \sigma_{j+1}^z,\end{aligned}\tag{1.18}$$

where  $F_j^{AB}$  is called a *symmetry flux*.

While we have been focusing on gapped SPT phases in this section, the notion of *gapless SPT phases* has been also proposed [23–30]. Classification of gapless SPT phases is still a developing field. We will see some examples in Sec. 2.2 and 5.6.

Any state in (0+1)D is obviously a trivial product state. In this sense, there are no SPT phases in (0+1)D, but for some reason that will be clear later, we define (0+1)D SPT as follows.

**Definition 1.14 (0D SPT phase)** *Consider a (0+1)D quantum system with symmetry group  $G$  and a unique GS  $|\psi_{\text{GS}}\rangle$ . Under a unitary transformation  $U(g)$  corresponding to the group element  $g \in G$ , there is*

$$U(g) |\psi_{\text{GS}}\rangle = e^{i\theta_g} |\psi_{\text{GS}}\rangle, \quad g \in G.\tag{1.19}$$

*The charge  $\{e^{i\theta_g}\}$  forms a 1D representation of  $G$ . If  $e^{i\theta_g} = 1$  for all  $g$ ,  $|\psi_{\text{GS}}\rangle$  is in a trivial phase. Otherwise,  $|\psi_{\text{GS}}\rangle$  is in an SPT phase protected by  $G$ .*

In general, 1D representation of a group  $G$  is classified by the *first cohomology group*  $H^1[G, \text{U}(1)]$ , which is an abelian group; see Appendix B. For example, if  $G = \text{U}(1)$ , then different 0D SPT phases are labeled by different winding numbers; in other words, we have  $H^1[\text{U}(1), \text{U}(1)] = \mathbb{Z}$  [31]. If  $G$  is a point group, then in Definition 1.14, we further require that there are no microscopic DOF lying precisely at the symmetry center. Otherwise, an SPT/trivial classification is not well-defined; see Sec. 3.3 for details.

Clearly, SPT phases are also beyond Landau's paradigm.

The rest of this thesis is organized as follows. Chapter 2 gives an introduction to (1+1)D SPT phases, including both gapped and gapless cases. Chapter 3 is about higher dimensional gapped SPT phases. In particular, weak SPT phases, LSM anomaly, and crystalline SPT phases will be introduced. My own research projects are presented in Chapter 4 and Chapter 5. In Chapter 4, we will discuss how to realize gapped SPT phases in spinful boson systems with a flat band. In Chapter 5, we will investigate the relationship between the concept of duality and SPT phases.

<sup>8</sup>An on-site symmetry is defined as the following:

**Definition 1.13 (on-site symmetry)** *An on-site symmetry refers to a global symmetry that can be factorized site-by-site, and the symmetry operation on each site is an endomorphism of the on-site Hilbert space.*

The  $\mathbb{Z}_2 \times \mathbb{Z}_2$  spin flip in Eq. (1.15) is an on-site symmetry.





是故一之理，施四海；一之解，際天地。  
 其全也，純兮若樸；其散也，混兮若濁。  
 濁而徐清，沖而徐盈。澹兮其若深淵，泛  
 兮其若浮雲；若無而有，若亡而存。萬物  
 之總，皆闕一孔；百事之根，皆出一門。

『淮南子·原道訓』

## BOSONIC SPT PHASES IN (1+1)D

**B**osonic SPT phases in (1+1)D, including gapped and gapless ones, will be discussed in this chapter. The (1+1)D gapped bosonic SPT phase protected by on-site  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry is also called the *Haldane phase*. A traditional understanding of the Haldane phase will be introduced in Sec. 2.1.1. The complete classification theory of (1+1)D gapped bosonic SPT phases protected by on-site symmetry will be presented in Sec. 2.1.2. In Sec. 2.1.3, I will discuss how the Haldane phase is coupled with a background  $\mathbb{Z}_2 \times \mathbb{Z}_2$ -gauge field. In Sec. 2.2, I will introduce the notion of gapless SPT phases in the simplest universality class: the Ising universality class.

### 2.1 Gapped phases

It is believed that in many cases [not restricted to (1+1)D], a unique gapped GS, exponential decay of correlation functions, and the area law of entanglement entropy (EE) are closely related to each other, although a general mathematical proof is lacking. Nevertheless, there are some rigorous theorems. I briefly introduce them below without providing rigorous statements or proofs.

**Theorem 2.1 (gap implies exponential decay [32, 33])** *In any dimension, (equal-time) two-point correlation functions<sup>1</sup> of a unique gapped GS decays exponentially with respect to the spatial distance.*

**Theorem 2.2 (gap implies area law [34, 35])** *For any (1+1)D system with a unique gapped GS and energy gap  $\Delta$ , the EE  $S$  of the GS satisfies*

$$S \leq \exp(\text{const.}/\Delta). \quad (2.1)$$

<sup>1</sup>Correlation functions of the form  $\text{Corr}(r) := \langle O_j O_{j+r} \rangle - \langle O_j \rangle \langle O_{j+r} \rangle$ .

In other words, the EE obeys the area law <sup>2</sup>.

**Theorem 2.3 (exponential decay implies area law [37, 38])** *The EE of any (1+1)D quantum state with exponential decay of correlations satisfies the area law.*

(Although the above theorems are stated in the form of "A implies B", physicists believe that "A is equivalent to B" in many situations.) Theorem 2.2 further suggests that [39, 40]

**Theorem 2.4 ("faithfulness" of MPS)** *The unique GS of a gapped Hamiltonian in (1+1)D can always be well-approximated by a matrix product state (MPS).*

In fact, the inverse is also true [41]:

**Theorem 2.5 (existence of parent Hamiltonian)** *Given any injective MPS  $|\psi\rangle$ , one can always find a parent Hamiltonian  $H$  such that  $|\psi\rangle$  is the exact, unique, and gapped GS of  $H$ .*

An MPS is a state that looks like [4, 5, 42–44]

$$|\psi\rangle = \sum_{\{\dots, \sigma_{j-1}, \sigma_j, \sigma_{j+1}, \dots\}} \text{Tr} \left( \dots M_{j-1}^{\sigma_{j-1}} M_j^{\sigma_j} M_{j+1}^{\sigma_{j+1}} \dots \right) |\dots, \sigma_{j-1}, \sigma_j, \sigma_{j+1}, \dots\rangle, \quad (2.2)$$

where  $\{M^\sigma\}$  are  $\chi \times \chi$  matrices labeled by the physical index  $\sigma = -S, \dots, S$ , and  $\chi$  is called the bond dimension. The injectivity is defined through the following theorem:

**Theorem 2.6 (injective MPS)** *Consider an MPS defined by a collection of matrices  $\{A^\sigma\}$ . The transfer matrix is defined by the Kronecker product*

$$T = \sum_{\sigma=-S}^S (A^\sigma)^* \otimes A^\sigma. \quad (2.3)$$

*Then the following statements are equivalent to each other (see Appendix A of Ref. [43], Ref. [44], and Sec. 8.2.9 of Ref. [5] together with Sec. IV B of Ref. [12]):*

1. *There exists  $\ell_0$  such that the set of matrices  $A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_{\ell_0}}$  with all possible  $\sigma_1, \dots, \sigma_{\ell_0}$  span the whole space of  $\chi \times \chi$  matrices.*
2. *The largest absolute eigenvalue of  $T$  is non-degenerate.* <sup>3</sup>

*If any of the above statements is found to be true, the MPS is said to be injective.*

The most famous model with a nontrivial MPS as the unique gapped GS is the (1+1)D spin-1 Affleck-Kennedy-Lieb-Tasaki (AKLT) model [4, 45, 46]:

$$H_{\text{AKLT}} = \sum_j P_{j,j+1}^{(2)} = \sum_j \frac{1}{2} \left[ (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \frac{1}{3} (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 + \frac{2}{3} \right], \quad (2.4)$$

<sup>2</sup>In  $(d+1)D$ , the area law means that the EE scales as  $S \sim \text{const.} \times L^{d-1}$ , where  $L$  is the linear size of the subsystem. Details about the area law of gapped systems in  $(2+1)D$  can be found in Ref. [5, 36].

<sup>3</sup>A degenerate largest absolute eigenvalue of  $T$  usually corresponds to cat states such as Eq. (1.5) [5].

where  $P_{j,j+1}^{(2)}$  is a projection operator that projects two spin-1's on neighboring sites onto a two-body state with total spin being 2, and  $S_j = (S_j^x, S_j^y, S_j^z)$  is the spin-1 operator. The model has SO(3) spin rotation symmetry. With PBC,  $H_{\text{AKLT}}$  has a unique, gapped, and exact GS [4, 45, 46]:

$$|\text{AKLT}\rangle = \sum_{\alpha_1, \dots, \alpha_N = -1}^1 \text{Tr}(M^{\alpha_1} M^{\alpha_2} \dots M^{\alpha_N}) |\alpha_1, \dots, \alpha_N\rangle, \quad (2.5)$$

where  $\{|\alpha_1, \dots, \alpha_N\rangle\}$  is the  $S^z$ -basis of the Hilbert space and

$$M^1 = -\sqrt{2}\sigma^+ = -\sqrt{2}\frac{\sigma^x + i\sigma^y}{2} = \begin{pmatrix} 0 & -\sqrt{2} \\ 0 & 0 \end{pmatrix}, \quad M^0 := \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad M^{-1} = \sqrt{2}\sigma^- = \begin{pmatrix} 0 & 0 \\ \sqrt{2} & 0 \end{pmatrix}. \quad (2.6)$$

It can be easily verified that  $|\text{AKLT}\rangle$  is an injective MPS. The structure of this AKLT state can be understood as follows: as shown in Fig. 2.1(a), each spin-1 is viewed as a composite state of two spin-1/2's, and a pair of spin-1/2's on two neighboring sites forms a spin singlet. Similar to the cluster model, on a chain with OBC, the AKLT model has four degenerate GS. From the physical picture of the GS in Fig. 2.1(a), we can see that the GS degeneracy on an open chain comes from an emergent spin-1/2 DOF that is exponentially localized on each edge (see also Fig. 2.2). These localized spin-1/2 DOF are often called *anomalous edge states*.<sup>4</sup> As the unique GS,  $|\text{AKLT}\rangle$  exhibits no long-range order, meaning that

$$\mathcal{O}_{\text{AFM}}^\delta = \lim_{r \rightarrow \infty} (-1)^r \langle S_j^\delta S_{j+r}^\delta \rangle = 0, \quad \delta = x, y, z. \quad (2.8)$$

The GS is actually characterized by string order parameters  $\mathcal{O}_{\text{str}}^\delta$  [47]:

$$\mathcal{O}_{\text{str}}^\delta = -\lim_{r \rightarrow \infty} \langle (F_j^\delta)^\dagger F_{j+r}^\delta \rangle = \langle S_j^\delta \exp\left(i\pi \sum_{k=j+1}^{j+r-1} S_k^\delta\right) S_{j+r}^\delta \rangle = \frac{4}{9}, \quad \delta = x, y, z, \quad (2.9)$$

where

$$F_j^\delta = \exp\left(-i\pi \sum_{k < j} S_k^\delta\right) S_j^\delta, \quad \delta = x, y, z \quad (2.10)$$

is sometimes called the symmetry flux of  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  [see Eq. (2.14)]. The string order  $\mathcal{O}_{\text{str}}^\delta$  measures the so-called *hidden AFM order*: the AFM order of a 1D spin-1 state where all the  $|0\rangle$  states are ignored<sup>5</sup>. For example, the following state

$$|0 + -00 + 0 - +000 - 0000 + - + 0 - 0 + 00 + - + -\rangle \quad (2.11)$$

<sup>4</sup>In the case of OBC, edge states are realized by  $1 \times 2$  or  $2 \times 1$  matrices at the boundary of an MPS:

$$|\text{AKLT}\rangle_{\text{OBC}} = \sum_{\alpha_1, \dots, \alpha_N} L^{\alpha_1} M^{\alpha_2} \dots M^{\alpha_{N-1}} R^{\alpha_N} |\alpha_1, \alpha_2, \dots, \alpha_N\rangle. \quad (2.7)$$

$(L, R)$  can have four different choices, which correspond to four degenerate GS.

<sup>5</sup> $S_j^z |0\rangle_j = 0$ .

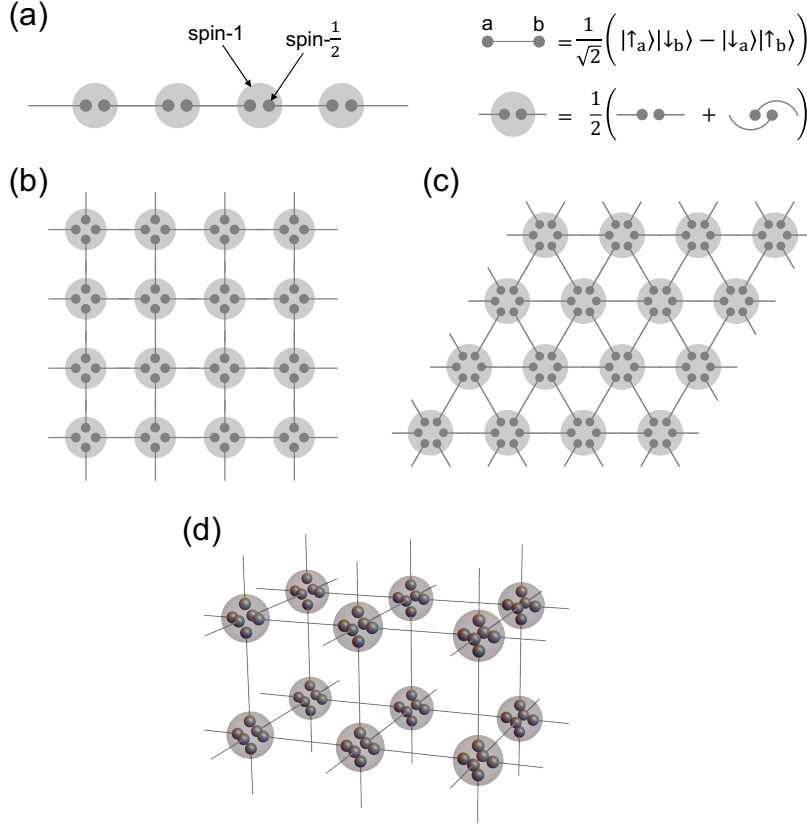


Figure 2.1: Examples of integer-spin AKLT states. Each spin- $f$  is regarded as a composite state of  $2f$  spin- $1/2$ 's, and a spin singlet is formed between two spin- $1/2$ 's on neighboring sites. (a) 1D spin-1 AKLT state, whose expression is given in Eq. (2.5). (b) 2D spin-2 AKLT state on a square lattice, denoted as  $|\text{AKLT}_{2,\square}\rangle$ . (c) 2D spin-3 AKLT state on a triangular lattice, denoted as  $|\text{AKLT}_{3,\triangle}\rangle$ . (d) 3D spin-3 AKLT state on a cubic lattice, denoted as  $|\text{AKLT}_{3,\square}\rangle$ .

has perfect AFM order if we delete all the  $|0\rangle$  states.

Let us summarize the nontrivial properties of the AKLT model:

1. The model with PBC has a unique gapped GS. (The energy gap is often called the *Haldane gap*.)
2. The model with OBC has four gapped and degenerate GS with spin- $1/2$  DOF exponentially localized at the edge.
3. The GS (regardless of PBC or OBC) has no long-range order, but has nonzero string order.

The above three properties can also be found in other spin-1 chains. For example, the spin-1 *bilinear-biquadratic (BLBQ) model* (see also Sec. 4.1.3) with  $|\theta| < \pi/4$ , which

includes the AKLT model and the antiferromagnetic (AFM) Heisenberg model as a special case:

$$H_{\text{BLBQ}}(\theta) = \sum_j \left[ \cos \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 \right], \quad -\frac{\pi}{4} < \theta < \frac{\pi}{4}. \quad (2.12)$$

Another example is the  $\lambda$ - $D$  model

$$H_{\lambda,D} = \sum_j \left( S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \lambda S_j^z S_{j+1}^z \right) + D \sum_j (S_j^z)^2, \quad \lambda, D \geq 0 \quad (2.13)$$

with not so large  $\lambda, D \geq 0$  [4]. The models  $H_{\text{AKLT}}$ ,  $H_{\text{BLBQ}}$ , and  $H_{\lambda,D}$  have three common symmetries

- $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  spin rotation;
- Time reversal (TR);
- Bond-centered mirror reflection.

It turns out that any one of the above symmetries alone can protect the phase represented by  $|\text{AKLT}\rangle$  [48, 49]. In this chapter, I will mainly focus on  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . Time-reversal symmetry will be briefly discussed in Sec. 2.1.2. In fact, as summarized in Table. 2.1, the string order defined in Eqs. (2.9) and (2.10) is always nonzero only when the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry is present, while the anomalous edge states are stable against perturbations that respect either  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  or TR symmetry. The reason will be clear later. The bond-centered reflection symmetry is a little bit special; details will be discussed in the next chapter (see Sec. 3.3).

The abelian group  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  is defined as  $\pi$ -rotations of spins around three orthogonal axes:

$$\begin{aligned} \mathbb{Z}_2^y \times \mathbb{Z}_2^z &= \{1, X_\pi, Y_\pi, Z_\pi\}, \\ \mathbb{Z}_2^y &= \{1, Y_\pi\}, \\ \mathbb{Z}_2^z &= \{1, Z_\pi\}, \\ X_\pi &= \prod_j \exp(-i\pi S_j^x) = Y_\pi Z_\pi = Z_\pi Y_\pi, \\ Y_\pi &= \prod_j \exp(-i\pi S_j^y), \\ Z_\pi &= \prod_j \exp(-i\pi S_j^z). \end{aligned} \quad (2.14)$$

The three nontrivial properties suggest that the GS of  $H_{\text{AKLT}}$ ,  $H_{\text{BLBQ}}$  and  $H_{\lambda,D}$  are all in the SPT phase protected by the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry. In other words, the GS of  $H_{\text{BLBQ}}$  and  $H_{\lambda,D}$  can be smoothly connected to  $|\text{AKLT}\rangle$ . Note that the GS of  $H_{\text{BLBQ}}$  and  $H_{\lambda,D}$  on a finite-length chain with OBC are in general quasi-degenerate, and the exact four-fold degeneracy is realized in the thermodynamic limit. For some historical reason, the SPT phase represented by  $|\text{AKLT}\rangle$  is also called the *Haldane phase*.

Symmetry	String order defined in Eq. (2.9)	Anomalous edge states
$\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ only	Nonzero	Yes
Time reversal (TR) only	Zero	Yes
Bond-centered reflection only	Zero	No

Table 2.1: The Haldane phase can be protected by any one of the three symmetries alone, but the existence of string order (associated to  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ ) or anomalous edge states depends on the symmetry.

On the contrary, GS of the model

$$H_{\text{triv}} = \sum_j (S_j^z)^2 \quad (2.15)$$

is obviously a trivial product state

$$|\text{triv}\rangle = |\dots 0000 \dots\rangle. \quad (2.16)$$

Both  $\langle S_j^\delta \rangle$  and the string order measured by  $F_j^\delta$  in Eq. (2.10) are zero. It is also obvious that  $H_{\text{triv}}$  is gapped. This means that for  $H_{\lambda,D}$ , there must be a phase transition at  $D = D_c > 0$  along the line  $\lambda = 0$  [4], although the SPT phase and the trivial phase cannot be distinguished by local order parameters.

### 2.1.1 Traditional interpretation: Kennedy-Tasaki transformation

Nature of the (1+1)D SPT phase in spin-1 chains protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  was first uncovered by Kennedy and Tasaki in 1992 [50, 51]. They proposed a nonlocal unitary transformation, nowadays known as the *Kennedy-Tasaki (KT) transformation* [50–52]:

$$U_{\text{KT}} = \prod_{1 \leq u < v \leq L} \exp(i\pi S_u^z S_v^x), \quad (2.17)$$

which satisfies  $U_{\text{KT}} = U_{\text{KT}}^\dagger$  and  $U_{\text{KT}}^2 = 1$ . The operator  $U_{\text{KT}}$  obviously has  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry. It transforms spin operators as [4]

$$\begin{aligned} S_j^x &\xrightarrow{U_{\text{KT}}} U_{\text{KT}} S_j^x U_{\text{KT}} = S_j^x \exp\left(i\pi \sum_{k=j+1}^L S_k^x\right), \\ S_j^y &\xrightarrow{U_{\text{KT}}} U_{\text{KT}} S_j^y U_{\text{KT}} = \exp\left(i\pi \sum_{k=1}^{j-1} S_k^z\right) S_j^y \exp\left(i\pi \sum_{k=j+1}^L S_k^x\right), \\ S_j^z &\xrightarrow{U_{\text{KT}}} U_{\text{KT}} S_j^z U_{\text{KT}} = \exp\left(i\pi \sum_{k=1}^{j-1} S_k^z\right) S_j^z. \end{aligned} \quad (2.18)$$

Kennedy and Tasaki pointed out that the two seemingly unrelated properties 2 and 3, i.e., edge states and string orders, can be unified in the framework of *hidden*  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry breaking. To see this, let us note that in  $x$  and  $z$  directions, we have

$$-(F_j^\delta)^\dagger F_{j+r}^\delta = -S_j^\delta \exp\left(i\pi \sum_{k=j+1}^{j+r-1} S_k^\delta\right) S_{j+r}^\delta \xleftrightarrow[\delta=x,z]{U_{\text{KT}}} S_j^\delta S_{j+r}^\delta, \quad (2.19)$$

which means that the string order is KT-dual to the FM order. Local interactions transform under  $U_{\text{KT}}$  as, for example (assume OBC) [4]:

$$\begin{aligned} S_j^x S_{j+1}^x &\xleftrightarrow{U_{\text{KT}}} S_j^x \exp(i\pi S_{j+1}^x) S_{j+1}^x, \\ S_j^y S_{j+1}^y &\xleftrightarrow{U_{\text{KT}}} S_j^y \exp[i\pi(S_j^z + S_{j+1}^x)] S_{j+1}^y, \\ S_j^z S_{j+1}^z &\xleftrightarrow{U_{\text{KT}}} \exp(i\pi S_j^z) S_j^z S_{j+1}^z, \\ (S_j^z)^2 &\xleftrightarrow{U_{\text{KT}}} (S_j^z)^2. \end{aligned} \quad (2.20)$$

Equation (2.20) actually holds for a general integer spin  $S$ . When  $S = 1$ , we have

$$\exp(i\pi S_{j+1}^x) S_{j+1}^x = -S_{j+1}^x, \quad \exp(i\pi S_j^z) S_j^z = -S_j^z. \quad (2.21)$$

In this way, an AFM interaction is transformed into a FM interaction in  $x$  and  $z$  directions. For example, the spin-1 Hamiltonian  $H_{\lambda,D}$  in Eq. (2.13) is transformed into another short-range  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetric Hamiltonian as

$$H_{\lambda,D} \xleftrightarrow[\text{OBC}]{U_{\text{KT}}} \tilde{H}_{\lambda,D} = \sum_j \left[ -S_j^x S_{j+1}^x + S_j^y \exp[i\pi(S_j^z + S_{j+1}^x)] S_{j+1}^y - \lambda S_j^z S_{j+1}^z \right] + D \sum_j (S_j^z)^2. \quad (2.22)$$

Due to the fact that  $U_{\text{KT}}$  is  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetric, one can conclude that

**Theorem 2.7** *In general, if a Hamiltonian  $H$  has the on-site  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry, then the dual Hamiltonian  $\tilde{H} = U_{\text{KT}} H U_{\text{KT}}$  also have the on-site  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry.*

In general, let  $H_{\text{SPT}}$  be a spin-1 chain whose GS is in the Haldane phase. We assume that  $H_{\text{SPT}}$  only contains short-range interactions. With OBC,  $H_{\text{SPT}}$  then has four (quasi-)degenerate GS  $|\text{SPT}_n\rangle$  ( $n = 1, 2, 3, 4$ ) with edge magnetization. If the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry is fully broken in the GS of the dual Hamiltonian  $\tilde{H}_{\text{SPT}} = U_{\text{KT}} H_{\text{SPT}} U_{\text{KT}}$ ,  $\tilde{H}_{\text{SPT}}$  should also have four (quasi-)degenerate GS  $|\text{FM}_n\rangle = U_{\text{KT}} |\text{SPT}_n\rangle$  ( $n = 1, 2, 3, 4$ ) with bulk magnetization [49, 51, 53]; see Fig. 2.2. Indeed, if  $|\text{SPT}_n\rangle$  is in the SPT phase protected by the on-site  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry, then  $|\text{FM}_n\rangle$  must fully break the on-site  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry, and vice versa. This can be seen from Eq. (2.19), the duality of the order parameters. The GS of  $H$  are characterized by nonzero string orders, while the GS of  $\tilde{H}_{\text{SPT}}$  are characterized by FM correlations. Equation (2.19) implies that

$$\mathcal{O}_{\text{str}}^\delta = -\lim_{r \rightarrow \infty} \langle \text{SPT}_n | (F_j^\delta)^\dagger F_{j+r}^\delta | \text{SPT}_n \rangle = \lim_{r \rightarrow \infty} \langle \text{FM}_n | S_j^\delta S_{j+r}^\delta | \text{FM}_n \rangle = \mathcal{O}_{\text{FM}}^\delta, \quad \delta = x, z, \quad n = 1, 2, 3, 4. \quad (2.23)$$

Intuitively speaking, the KT transformation spreads the edge magnetization of  $|\text{SPT}_n\rangle$  to the whole bulk of  $|\text{FM}_n\rangle$ . In the sense of Eqs. (2.19)-(2.23), we say that the GS of  $H_{\text{SPT}}$  has *hidden symmetry breaking*. Moreover, since the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry is fully broken in the GS of  $\tilde{H}_{\text{SPT}}$ , it is clear that  $\tilde{H}_{\text{SPT}}$  is gapped, which also implies that  $H_{\text{SPT}}$  is gapped.

As an example, the four GS of  $\tilde{H}_{\text{AKLT}} = U_{\text{KT}} H_{\text{AKLT}} U_{\text{KT}}$  can be exactly written down. They are product states [50, 51]:

$$\begin{aligned} |\text{FM}_1\rangle &= \bigotimes_j \left( \sqrt{\frac{1}{3}} |0\rangle_j + \sqrt{\frac{2}{3}} |+\rangle_j \right), \\ |\text{FM}_2\rangle &= \bigotimes_j \left( \sqrt{\frac{1}{3}} |0\rangle_j - \sqrt{\frac{2}{3}} |+\rangle_j \right), \\ |\text{FM}_3\rangle &= \bigotimes_j \left( \sqrt{\frac{1}{3}} |0\rangle_j + \sqrt{\frac{2}{3}} |-\rangle_j \right), \\ |\text{FM}_4\rangle &= \bigotimes_j \left( \sqrt{\frac{1}{3}} |0\rangle_j - \sqrt{\frac{2}{3}} |-\rangle_j \right), \end{aligned} \quad (2.24)$$

where  $S_j^z |\pm\rangle_j = \pm |\pm\rangle_j$  and  $S_j^z |0\rangle_j = 0$ . We see that  $\langle \text{FM}_n | S_j^{x,z} | \text{FM}_n \rangle = \pm 2/3$  and  $\langle \text{FM}_n | S_j^y | \text{FM}_n \rangle = 0$ . See Fig. 2.2.

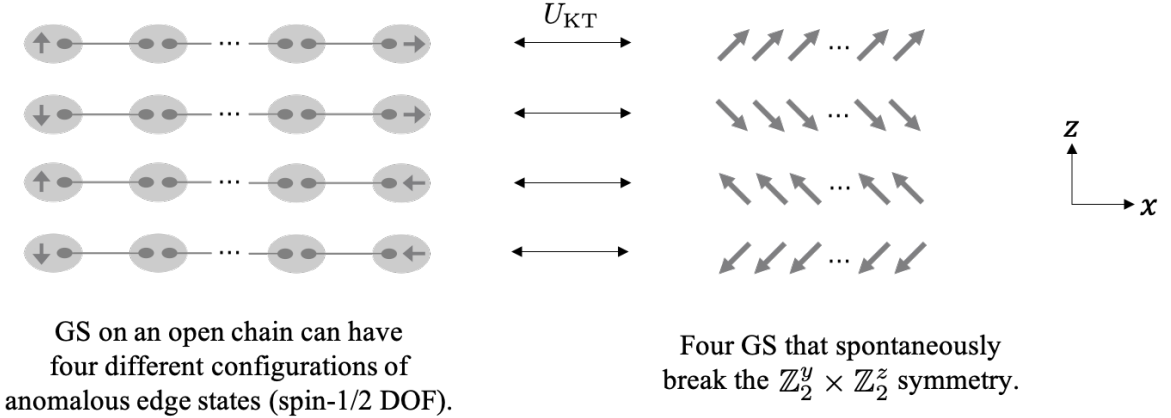


Figure 2.2: Four (quasi-)degenerate GS with edge magnetization are dual to four FM GS. In other words, the KT transformation spreads the edge magnetization to the whole bulk. The FM states on the right-hand side correspond to the four choices of the signs of the expectation values  $\langle S_j^x \rangle = \pm m^x$  and  $\langle S_j^z \rangle = \pm m^z$  [49, 51, 53].

On the contrary,  $H_{\text{triv}} = \sum_j (S_j^z)^2$  is invariant under  $U_{\text{KT}}$ , which suggests that the KT dual of a trivial phase is still trivial. For a general trivial phase protected by the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry,  $\mathcal{O}_{\text{str}}^\delta$  is zero for the trivial phase, and thus so is  $\mathcal{O}_{\text{FM}}^\delta$  for the KT dual of the trivial phase. In other words, a trivial phase is distinct from an SPT phase in that the former has no hidden symmetry breaking.



The KT transformation in Eq. (2.17) and the identities in Eq. (2.18) directly apply to *any integer* spin quantum number  $S \geq 1$ , as long as we take  $S_u^z$  and  $S_v^x$  to be the spin- $S$  operators [52]. The AKLT model in (1+1)D can also be generalized to higher integer spin  $S$  as

$$H_{\text{AKLT}}^S = \sum_j \sum_{F=S+1}^{2S} P_{j,j+1}^{(F)}, \quad (2.25)$$

where the projection operator  $P_{j,j+1}^{(F)}$  can be explicitly expressed by spin operators; see Eq. (4.34). It can be shown that  $H_{\text{AKLT}}^S$  also has a unique and exact GS  $|\text{AKLT}_S\rangle$  [46, 52]. Both  $H_{\text{AKLT}}^S$  and  $U_{\text{KT}} H_{\text{AKLT}}^S U_{\text{KT}}$  have  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry. Surprisingly, it was found by Oshikawa that the string order of  $|\text{AKLT}_S\rangle$  satisfies [52]

$$\mathcal{O}_{\text{str}}^\delta \begin{cases} > 0, & S = 1, 3, 5, \dots \\ = 0, & S = 2, 4, 6, \dots \end{cases} \quad (2.26)$$

According to the arguments above, one can claim that  $|\text{AKLT}_S\rangle$  is in an SPT (Haldane) phase when  $S = \text{odd}$ , while it is in a trivial phase when  $S = \text{even}$ <sup>6</sup>. In other words, the existence or absence of hidden symmetry breaking depends on the parity of  $S$ .

The KT transformation can be generalized to (1+1)D systems with a broad class of symmetries beyond  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , such as  $\mathbb{Z}_n \times \mathbb{Z}_n$  and  $\text{SO}(2n-1)$  [55–58], thus providing the hidden symmetry breaking picture for the SPT phases in such systems. However, the KT transformation may not be almighty: To my best knowledge, whether it can be generalized to anti-unitary symmetries<sup>7</sup> remains an open question. Besides, it cannot be directly generalized to higher dimensions.

### 2.1.2 Modern interpretation: Projective representation

The modern and complete understanding of (1+1)D SPT phases protected by on-site symmetries is based on the MPS [5, 11–13, 31, 48, 49, 59]. Theorem 2.4 and Theorem 2.5 enable us to consider the following MPS as the unique gapped GS of certain parent Hamiltonian  $H$ :

$$|\psi_{\text{GS}}\rangle = \sum_{\sigma_1, \dots, \sigma_L = -S}^S \text{Tr}(A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}) |\sigma_1, \sigma_2, \dots, \sigma_L\rangle. \quad (2.27)$$

We assume that the MPS  $|\psi_{\text{GS}}\rangle$  is *injective*. Also for simplicity, we assume that  $|\psi_{\text{GS}}\rangle$  is translation invariant. Assume  $G$  is an on-site *unitary* symmetry group of  $H$ . In other words, the representation of  $G$  on the Hilbert space is  $\{U^g\}_{g \in G}$ , where

$$U^g = \prod_{j=1}^L u_j^g, \quad g \in G \quad (2.28)$$

<sup>6</sup>It can be shown that  $|\text{AKLT}_S\rangle$  is smoothly connected to a trivial product state when  $S = \text{even}$  [54].

<sup>7</sup>Even if it could be generalized to anti-unitary symmetries, the generalization must be highly nontrivial, because, for example, it is known that there is no simple string order parameter to detect a (1+1)D SPT phase protected by time-reversal symmetry. In such a case the argument provided by Eqs. (2.19) and (2.23) could become meaningless.

We assume that  $\{u_j^g\}$  forms a *linear representation* of  $G$ , i.e.,

$$u_j^g u_j^h = u_j^{gh}, \quad \forall g, h \in G. \quad (2.29)$$

Under a symmetry operation  $U^g$ , the unique GS transforms as

$$\begin{aligned} U^g |\psi_{\text{GS}}\rangle &= e^{i\eta_g} |\psi_{\text{GS}}\rangle = \sum_{\sigma} (A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}) U^g |\sigma_1, \sigma_2, \dots, \sigma_L\rangle \\ &= \sum_{\sigma, \sigma'} (A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}) |\sigma'\rangle \left( \prod_{j=1}^L \langle \sigma'_j | u_j^g | \sigma_j \rangle \right) \\ &= \sum_{\sigma} (B^{\sigma_1} B^{\sigma_2} \dots B^{\sigma_L}) |\sigma_1, \sigma_2, \dots, \sigma_L\rangle, \end{aligned} \quad (2.30)$$

where

$$B^{\sigma} = \sum_{\sigma'=-S}^S \langle \sigma | u^g | \sigma' \rangle A^{\sigma'}. \quad (2.31)$$

It is easily verified that the transfer matrices for the two MPS are identical:

$$T = \sum_{\sigma=-S}^S (B^{\sigma})^* \otimes B^{\sigma} = \sum_{\sigma=-S}^S (A^{\sigma})^* \otimes A^{\sigma}, \quad (2.32)$$

thus the MPS formed by  $\{B^{\sigma}\}$  is also injective. There is an important theorem for injective MPS:

**Theorem 2.8 (uniqueness of MPS [4, 43, 44, 60])** *Suppose that two collections of matrices  $\{A^{\sigma}\}_{\sigma=-S, \dots, S}$  and  $\{B^{\sigma}\}_{\sigma=-S, \dots, S}$  are injective and form the same MPS in the sense that*

$$\sum_{\sigma=-S}^S \text{Tr} (A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}) |\sigma_1 \sigma_2, \dots, \sigma_N\rangle = e^{i\eta} \sum_{\sigma=-S}^S \text{Tr} (B^{\sigma_1} B^{\sigma_2} \dots B^{\sigma_L}) |\sigma_1 \sigma_2, \dots, \sigma_N\rangle, \quad (2.33)$$

*for any  $L$ . Then they have a common bond dimension  $\chi$ , and there exists a  $\chi \times \chi$  unitary matrix  $V$ , which is unique up to a phase factor, such that*

$$B^{\sigma} = e^{i\eta/L} V^{\dagger} A^{\sigma} V, \quad \forall \sigma. \quad (2.34)$$

Equations (2.31) and (2.34) together imply that

$$\sum_{\sigma'=-S}^S \langle \sigma | u^g | \sigma' \rangle A^{\sigma'} = e^{i\eta_g/L} V^{g\dagger} A^{\sigma} V^g, \quad \forall \sigma, \quad (2.35)$$

see also Fig. 2.3.

Now consider two symmetry operations on a matrix:

$$\sum_{\sigma'=-S}^S \langle \sigma | u^g u^h | \sigma' \rangle A^{\sigma'} = e^{i(\eta_g + \eta_h)/L} (V^{h\dagger} V^{g\dagger}) A^{\sigma} (V^g V^h). \quad (2.36)$$

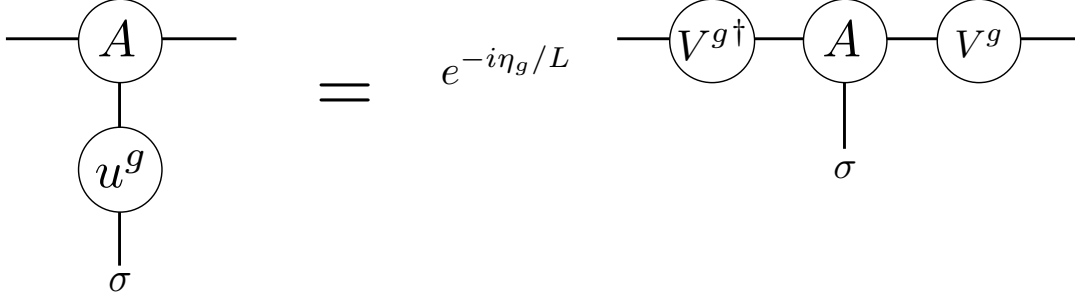


Figure 2.3: Illustration of Eq. (2.35).

On the other hand, since  $u^g u^h = u^{gh}$  by assumption, we have

$$\sum_{\sigma'=-S}^S \langle \sigma | u^g u^h | \sigma' \rangle A^{\sigma'} = \sum_{\sigma'=-S}^S \langle \sigma | u^{gh} | \sigma' \rangle A^{\sigma'} = e^{i\eta_{gh}/L} V^{gh\dagger} A^\sigma V^{gh}. \quad (2.37)$$

The above two equations imply that  $\eta_g + \eta_h = \eta_{gh}$  and

$$(V^{h\dagger} V^{g\dagger}) A^\sigma (V^g V^h) = V^{gh\dagger} A^\sigma V^{gh}. \quad (2.38)$$

Writing  $W = V^g V^h V^{gh\dagger}$ , the above equation implies  $[W, A^\sigma] = 0$  for any  $\sigma$ . By using the relation repeatedly we have

$$[W, A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_{\ell_0}}] = 0, \quad \forall \ell_0 > 0, \forall \sigma. \quad (2.39)$$

The statement 1 in Theorem 2.6 implies that  $W$  commutes with any  $\chi \times \chi$  matrix, and hence  $W$  must be proportional to the identity matrix  $I$ . Note that  $W$  is unitary, so that  $W = e^{i\phi(g,h)} I$ . In other words,

$$V^g V^h = e^{i\phi(g,h)} V^{gh}, \quad \forall g, h \in G. \quad (2.40)$$

We say that  $\{V^g\}_{g \in G}$  forms a *projective representation* of  $G$ . In particular, if the phase factor is always zero, we say that  $\{V^g\}$  forms a *linear representation* of  $G$ . Note that  $\{V^g\}$  has a gauge DOF: Eq. (2.35) is invariant under  $V^g \rightarrow e^{i\theta_g} V^g$ .

Sometimes, by properly choosing the gauge, we can make  $e^{i\phi(g,h)} = 1$  for all  $g, h \in G$ . For example, consider  $G = \mathbb{Z}_n$  and let  $a_k = \exp[\frac{2\pi i}{n}(k-1)]$ . Clearly  $\{a_k\}_{k=1,\dots,n}$  is not a linear representation of  $\mathbb{Z}_n$ , because  $a_k a_\ell = e^{-2\pi i/n} a_{k\ell}$ . Nevertheless, if we define  $a'_k = e^{2\pi i/n} a_k$ , there will be

$$a'_k a'_\ell = a'_{k\ell}, \quad \forall k, \ell \in \mathbb{Z}_n. \quad (2.41)$$

In general, under the gauge transformation  $V^g \rightarrow e^{i\theta_g} V^g$ , the phase factor in Eq. (2.40) transforms as

$$e^{i\phi(g,h)} \rightarrow e^{i\phi(g,h)} \beta(g, h), \quad \forall g, h \in G, \quad (2.42)$$

where  $\beta$  is called a *2-coboundary* and defined as

$$\beta(g, h) = e^{i\theta_{gh}} e^{-i\theta_g} e^{-i\theta_h} \quad \forall g, h \in G. \quad (2.43)$$

Note that all the 2-coboundaries form a group. Two projective representations are said to be *equivalent* to each other if they are related to each other through Eqs. (2.42) and (2.43). If  $e^{i\phi(g,h)} = e^{i\theta_{gh}} e^{-i\theta_g} e^{-i\theta_h}$  for all  $g, h \in G$ , then the phase factor  $e^{i\phi(g,h)}$  can always be eliminated for all  $g, h \in G$ , i.e., the projective representation is equivalent to a linear representation.

**Definition 2.9 (trivial/nontrivial projective representation)** *A projective representation is trivial iff it is equivalent to a linear representation. Otherwise, it is nontrivial.*

Observe that the associativity  $(u^{g_1} u^{g_2}) u^{g_3} = u^{g_1} (u^{g_2} u^{g_3})$  implies  $(V^{g_1} V^{g_2}) V^{g_3} = V^{g_1} (V^{g_2} V^{g_3})$ , which further implies the condition:

$$e^{i\phi(g_1, g_2)} e^{i\phi(g_1 g_2, g_3)} = e^{i\phi(g_2, g_3)} e^{i\phi(g_1, g_2 g_3)}, \quad \forall g_1, g_2, g_3 \in G. \quad (2.44)$$

A phase factor  $e^{i\phi(\cdot, \cdot)}$  satisfying Eq. (2.44) is called a *2-cocycle*. Note that all the 2-cocycles also form a group. The classification of projective representations of  $G$  then boils down to finding 2-cocycles with the equivalence relation defined by Eq. (2.42). In other words, the quotient group

$$H^2[G, \text{U}(1)] := \frac{\{2\text{-cocycles}\}}{\{2\text{-coboundaries}\}} \quad (2.45)$$

completely classifies the projective representations of  $G$ . The group  $H^2[G, \text{U}(1)]$  is called the *second cohomology group* of  $G$ ; see Appendix B for more details. The SPT phases protected the on-site unitary group  $G$  is then completely classified by  $H^2[G, \text{U}(1)]$ .

**Definition 2.10 ([5, 11, 12, 31, 59])** *Let  $|\psi_{\text{GS}}\rangle$  be a unique gapped GS with an on-site unitary symmetry  $G$ . The phase of  $|\psi_{\text{GS}}\rangle$  is labeled by an element in  $H^2[G, \text{U}(1)]$ . The GS is in a trivial phase protected by  $G$  if  $\{V^g\}_{g \in G}$  forms a trivial projective representation of  $G$ . In other words, the trivial phase corresponds to the trivial element (identity) of  $H^2[G, \text{U}(1)]$ . Otherwise,  $|\psi_{\text{GS}}\rangle$  is in an SPT phase protected by  $G$ .*

The above definition is natural because it is obvious that  $\{V^g\}$  in a trivial product state gives a trivial projective representation of  $G$ . Since  $H^2[G, \text{U}(1)]$  is a discrete group<sup>8</sup>, the phase, i.e., an element  $\omega \in H^2[G, \text{U}(1)]$  cannot change smoothly. Exceptions happen at the quantum phase transition points, where the GS is no longer an injective MPS, or cannot even be well-approximated by an MPS. In such cases the above classification theory breaks down, and a change of element  $\omega \in H^2[G, \text{U}(1)]$  can happen.

It is known that  $H^2[G, \text{U}(1)] = \{1\}$  when  $G = \mathbb{Z}_n, \text{U}(1), \text{SU}(2)$  [31]. However, for the group  $\mathbb{Z}_2 \times \mathbb{Z}_2 \in \text{SO}(3)$ , it is known that [31]

$$H^2[\text{SO}(3), \text{U}(1)] = H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2. \quad (2.46)$$

<sup>8</sup>I do not know if there is any theorem that guarantees the discreteness of  $H^2[G, \text{U}(1)]$ , but at least  $H^2[G, \text{U}(1)]$  is discrete for the known cases [31].

In particular, since  $\mathbb{Z}_2 \times \mathbb{Z}_2$  is an abelian group,

$$V^g V^h = V^h V^g, \quad \forall g, h \in \mathbb{Z}_2 \times \mathbb{Z}_2 \quad (2.47)$$

corresponds to the trivial element in  $H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)]$ . On the other hand, it can be shown that

$$V^g V^h = -V^h V^g \quad \text{with } g \neq h \quad (2.48)$$

corresponds to the nontrivial element in  $H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)]$ ; see Example B.13. If we regard  $\mathbb{Z}_2 \times \mathbb{Z}_2$  as  $\pi$ -rotations of a spin around three orthogonal axes, then rotations of an integer spin give the trivial projective representation, while rotations of a half-odd-integer spin give the nontrivial projective representation. For example, in the  $S^z$  basis, rotations of spin-1 are:

$$e^{-i\pi S^x} = \begin{pmatrix} & -1 \\ & \\ -1 & \end{pmatrix}, \quad e^{-i\pi S^y} = \begin{pmatrix} & 1 \\ -1 & \\ 1 & \end{pmatrix}, \quad e^{-i\pi S^z} = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}. \quad (2.49)$$

On the other hand, for spin-1/2,

$$e^{-i\sigma^x/2} = -i\sigma^x, \quad e^{-i\sigma^y/2} = i\sigma^y, \quad e^{-i\sigma^z/2} = -i\sigma^z. \quad (2.50)$$

Let us now classify the phase of the AKLT state in Eq. (2.5). Let  $u^\delta = e^{-i\pi S^\delta}$  ( $\delta = x, y, z$ ). According to Eqs. (2.6) and (2.49), one can choose  $\eta_\delta = 0$  for all  $\delta$  and

$$V^\delta = \sigma^\delta, \quad \delta = x, y, z \quad (2.51)$$

such that Eq. (2.35) is satisfied. It is now clear that the spin-1 AKLT ground state is in an SPT protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ .

The string order can also be understood within the framework of MPS. Here instead of discussing the rigorous approach [60, 61], I will introduce an approach below that might not be completely rigorous yet provides an intuitive picture.

**Proposition 2.11 (symmetry fractionalization)** *Given an injective MPS  $|\psi_{\text{GS}}\rangle$  as a GS, we let  $U = \prod_j u_j$  be an on-site unitary symmetry of  $|\psi_{\text{GS}}\rangle$ . Then for a sufficiently large  $r$ , we have*

$$\prod_{j=k}^{k+r} u_j |\psi_{\text{GS}}\rangle = \mathcal{U}_L \mathcal{U}_R |\psi_{\text{GS}}\rangle, \quad (2.52)$$

where  $\mathcal{U}_L$  ( $\mathcal{U}_R$ ) is a unitary operator which is exponentially localized at the left (right) of the segment of sites  $j = k, k+1, \dots, k+r$ . See Fig. 2.4. If there is GS degeneracy on an open chain, then the operators  $\mathcal{U}_L$  ( $\mathcal{U}_R$ ) do not depend on which of the degenerate GS they are acting upon.

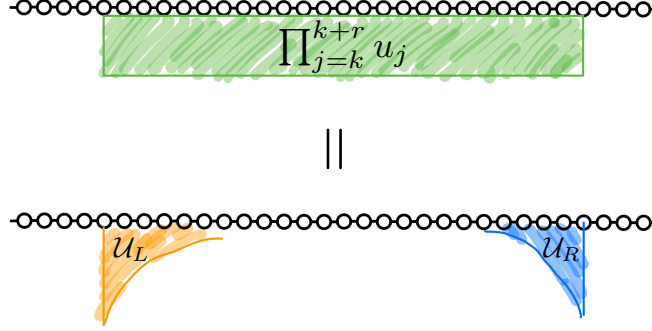


Figure 2.4: Illustration of Eq. (2.52).

For a proof of the above proposition, see Appendix A of Ref. [62]. For an on-site unitary group  $G$ , it is obvious that

$$\langle \mathcal{U}_L^g \mathcal{U}_R^g \mathcal{U}_L^h \mathcal{U}_R^h \rangle = \langle \mathcal{U}_L^{gh} \mathcal{U}_R^{gh} \rangle, \quad \forall g, h \in G, \quad (2.53)$$

where  $\langle \cdot \rangle$  stands for  $\langle \psi_{\text{GS}} | \cdot | \psi_{\text{GS}} \rangle$ . Since  $\mathcal{U}_L$  and  $\mathcal{U}_R$  have little overlap and we assume that they are bosonic operators, Eq. (2.53) implies that

$$\begin{aligned} \mathcal{U}_L^g \mathcal{U}_L^h | \psi_{\text{GS}} \rangle &= e^{i\phi(g,h)} \mathcal{U}_L^{gh} | \psi_{\text{GS}} \rangle, \\ \mathcal{U}_R^g \mathcal{U}_R^h | \psi_{\text{GS}} \rangle &= e^{-i\phi(g,h)} \mathcal{U}_R^{gh} | \psi_{\text{GS}} \rangle. \end{aligned} \quad (2.54)$$

Again Eq. (2.52) allows  $\mathcal{U}_L$  and  $\mathcal{U}_R$  to have gauge DOF. Therefore, Eq. (2.54) suggests that  $\{\mathcal{U}_L^g\}_{g \in G}$  can be classified by the second cohomology group  $H^2[G, \text{U}(1)]$ . As an example, for the cluster model in Eq. (1.14),  $\mathcal{U}_L$  and  $\mathcal{U}_R$  are exactly localized at the boundary, and they form a nontrivial projective representation of  $\mathbb{Z}_2 \times \mathbb{Z}_2$ ; see Eqs. (1.17) and (1.16). A nontrivial projective representation  $\{\mathcal{U}_L^g\}$  guarantees the GS degeneracy on an open chain.

Now let us investigate the string order parameters. Let us start with the definition of symmetry fluxes:

**Definition 2.12 (symmetry fluxes for unique gapped GS)** Let  $U^g = \prod_j u_j^g$  be the on-site linear representation of  $g \in G$  on the Hilbert space, the symmetry flux of  $g$  is defined as

$$F_j^g = \dots u_{j-3}^g u_{j-2}^g u_{j-1}^g B_j^g, \quad (2.55)$$

where  $B_j^g$  is an operator at site  $j$  chosen such that the correlation of two symmetry fluxes, known as the string order, has long-range order, i.e.,  $\mathcal{O}_{\text{str}}^g = \lim_{r \rightarrow \infty} \langle F_j^{g\dagger} F_{j+r}^g \rangle > 0$ .

Note that

$$\begin{aligned} \mathcal{O}_{\text{str}}^g &= \lim_{r \rightarrow \infty} \langle F_j^{g\dagger} F_{j+r}^g \rangle \\ &= \lim_{r \rightarrow \infty} \langle B_j^{g\dagger} u_{j+1}^g \dots u_{j+r-1}^g B_{j+r}^g \rangle \\ &= \lim_{r \rightarrow \infty} \langle B_j^{g\dagger} \mathcal{U}_L^g \rangle \langle \mathcal{U}_R^g B_{j+r}^g \rangle \neq 0. \end{aligned} \quad (2.56)$$

I have used Eq. (2.52) and the clustering property in the above equation. The condition  $\mathcal{O}_{\text{str}}^g \neq 0$  then reduces to  $\langle B_j^{g\dagger} \mathcal{U}_L^g \rangle \neq 0$  and  $\langle \mathcal{U}_R^g B_{j+r}^g \rangle \neq 0$ . As an example, let us determine the symmetry flux associated to  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . In the case of the Haldane phase, there must be  $\mathcal{U}_L^x \mathcal{U}_L^z |\psi_{\text{GS}}\rangle = -\mathcal{U}_L^z \mathcal{U}_L^x |\psi_{\text{GS}}\rangle$ , where  $x, z$  refers to the elements  $X_\pi$  and  $Z_\pi$ , respectively [see Eq. (2.14)]. Consider a  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ -symmetric state  $|\psi_{\text{GS}}\rangle$  with OBC. Then we have  $\langle B_j^{z\dagger} \mathcal{U}_L^z \rangle = \langle X_\pi B_j^{z\dagger} X_\pi X_\pi \mathcal{U}_L^z X_\pi \rangle = \langle X_\pi B_j^{z\dagger} X_\pi \mathcal{U}_L^x \mathcal{U}_L^z \mathcal{U}_L^x \rangle = -\langle (X_\pi B_j^{z\dagger} X_\pi) \mathcal{U}_L^z \rangle$ , where we have assumed that  $\mathcal{U}_L^z |\psi_{\text{GS}}\rangle \propto |\psi_{\text{GS}}\rangle$ . If we choose  $B_j^z$  such that

$$X_\pi B_j^z X_\pi = -B_j^z, \quad (2.57)$$

then the string order can have long-range order. This explains the symmetry flux in Eq. (2.10). Similarly, the string order of the cluster model in Eq. (1.18) can also be explained. In fact, a nonzero string order can also be defined for the trivial phase: In such case  $\mathcal{U}_L^x \mathcal{U}_L^z |\psi_{\text{GS}}\rangle = \mathcal{U}_L^z \mathcal{U}_L^x |\psi_{\text{GS}}\rangle$ , so we can simply choose  $B_j^z = 1$  such that  $X_\pi^\dagger B_j^z X_\pi = B_j^z$ . See also Appendix B of Ref. [30]. In general, can we tell the phase by observing the symmetry flux?

**Proposition 2.13 (uniqueness of symmetry flux)** *Given a symmetry  $G$  and a symmetry-protected phase (either SPT or trivial), two symmetry fluxes  $F_j^g$  and  $F_j'^g$  are said to be equivalent to each other if their difference is not a symmetry flux, i.e.,  $\langle (F_j^{g\dagger} - F_j'^{g\dagger})(F_{j+r}^g - F_{j+r}'^g) \rangle$  has no long-range order. Up to the equivalence relation,  $F_j^g$ , the symmetry flux associated with a group element  $g$  is unique.*

For a proof of the above proposition, see Appendix A.3.b of Ref. [23]. Let  $\{F_j^g\}_{g \in G}$  be a set of symmetry flux associated with  $G$ . Proposition 2.13 suggests that under  $G$ , a symmetry flux should transform as

$$U^h F_j^g U^{h\dagger} = \dots u_{j-2}^{hgh^{-1}} u_{j-1}^{hgh^{-1}} (u_j^h B_j^g u_j^{h\dagger}) = e^{i\chi(g,h)} F_j^{hgh^{-1}} + F_{\text{sub}}^{hgh^{-1}}, \quad g, h \in G, \quad (2.58)$$

where  $F_{\text{sub}}$  is some decaying term<sup>9</sup> that does not affect the long-range order. Note that the phase  $e^{i\chi(g,h)}$  is well-defined due to Proposition 2.13. The phase of the GS is then encoded in the phase factor  $e^{i\chi(g,h)}$ . In particular, if we choose  $h$  to be the stabilizer of  $g$ , i.e.,  $h \in \{k \in G | kg = gk\}$ , then [23]

$$e^{i\chi(g,h)} = e^{-i[\phi(h,g) + \phi(hg, h^{-1})]}. \quad (2.59)$$

For example, for the Haldane phase, each of the three string order parameters  $F_j^\delta$  ( $\delta = x, y, z$ ) in Eq. (2.10) forms a nontrivial 1D representation of  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ , while for the trivial phase, the symmetry flux  $\dots u_{j-2}^\delta u_{j-1}^\delta$  transforms trivially under  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . In general, if  $G$  is an abelian group like  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , then the cocycle can be reconstructed from  $\{e^{i\chi(g,h)}\}$  [23]. This is not true for an arbitrary group  $G$  (see Appendix A of [61]). Nevertheless, in practice, knowing  $\{e^{i\chi(g,h)}\}$  is often equivalent to knowing the projective representations [23].

<sup>9</sup>Sometimes by properly choosing  $\{F_j^g\}_{g \in G}$ ,  $F_{\text{sub}}$  can be exactly zero. Note that Eq. (2.58) is an operator identity, but in general,  $F_{\text{sub}}$  is a "decaying term" only in the sense of a unique gapped ground state.

Finally, let us consider the general case in which  $G$  is not necessarily a unitary symmetry. In other words, some group elements in  $G$  may be *anti-unitary*. The representation theory of such a group  $G$  can be found in Ref. [63] and Appendix B of Ref. [31]. For an anti-unitary group element  $m \in G$ , it acts on the Hilbert space as

$$U^m = \left( \prod_{j=1}^L u_j^m \right) K, \quad (2.60)$$

where  $u_j^g$  is a *unitary* operator and  $K$  is the complex conjugation. For a general  $G$ , Eq. (2.36) should be modified as

$$\sum_{\sigma'=-S}^S \sum_{\alpha} u_{\sigma,\alpha}^g C_g(u_{\alpha,\sigma'}^h) C_{gh}(A^{\sigma'}) = e^{i\eta_g/L} C_g(e^{i\eta_h/L}) C_g(V^{h\dagger}) V^{g\dagger} A^{\sigma} V^g C_g(V^h), \quad (2.61)$$

where  $u_{\sigma,\alpha}^g = \langle \sigma | u^g | \alpha \rangle$  and the map  $C_g$  is defined as a nontrivial group action<sup>10</sup>:

$$C_g(u) = \begin{cases} u^* \text{ (complex conjugation of } u), & \text{if } g \text{ contains complex conjugation} \\ u, & \text{elsewise} \end{cases}, g \in G. \quad (2.62)$$

Equation (2.40) should thus be modified to

$$V^g C_g(V^h) = e^{i\phi(g,h)} V^{gh}. \quad (2.63)$$

We say that  $\{V^g\}_{g \in G}$  forms a projective representation of  $G$ . The 2-coboundary now becomes

$$\beta(g, h) = e^{i\theta_{gh}} e^{-i\theta_g} C_g(e^{-i\theta_h}) \quad \forall g, h \in G. \quad (2.64)$$

Observe that the associativity  $(u^{g_1} u^{g_2}) u^{g_3} = u^{g_1} (u^{g_2} u^{g_3})$  implies

$$[V^{g_1} C_{g_1}(V^{g_2})] C_{g_1 g_2}(V^{g_3}) = V^{g_1} C_{g_1}[V^{g_2} C_{g_2}(V^{g_3})], \quad (2.65)$$

thus the 2-cocycle becomes

$$e^{i\phi(g_1, g_2)} e^{i\phi(g_1 g_2, g_3)} = C_{g_1}[e^{i\phi(g_2, g_3)}] e^{i\phi(g_1, g_2 g_3)}, \quad \forall g_1, g_2, g_3 \in G. \quad (2.66)$$

Again, the second cohomology group  $H^2[G, \text{U}(1)] = \{2\text{-cocycles}\} / \{2\text{-coboundaries}\}$  completely classifies the projective representations of  $G$ ; note that  $G$  now has a nontrivial action on  $\text{U}(1)$  according to Eq. (2.62); see Appendix B for more details. Proposition 2.11 can also be generalized to anti-unitary symmetry; see Appendix B of Ref. [62] for details.

Let us consider the time-reversal symmetry group  $\mathbb{Z}_2^{\text{TR}} = \{1, \text{TR}\}$  as an example. We assume  $\text{TR}^2 = 1$  on each site. Let us choose a gauge such that  $V^1 = I$ . According to Eq. (2.63),

$$V^{\text{TR}}(V^{\text{TR}})^* = e^{i\phi} I, \quad (2.67)$$

<sup>10</sup>If  $G$  is a unitary symmetry group, then  $\{C_g\}_{g \in G}$  reduces to a trivial group action.



or equivalently,  $V^{\text{TR}} = e^{i\phi}(V^{\text{TR}})^T$ . Repeating this relation again, we get  $e^{i\phi} = \pm 1$ . This tells us that

$$H^2[\mathbb{Z}_2^{\text{TR}}, \text{U}_T(1)] = \mathbb{Z}_2, \quad (2.68)$$

where  $\text{U}_T(1)$  is simply the group  $\text{U}(1)$  and we use the subscript T to emphasize the non-trivial action<sup>11</sup> of  $\mathbb{Z}_2^{\text{TR}}$  on  $\text{U}(1)$ . It is now clear that for (1+1)D bosonic systems with time-reversal symmetry only, there are two phases: the nontrivial projective representation  $V^{\text{TR}}V^{\text{TR}*} = -I$  corresponds to the SPT phase and  $V^{\text{TR}}V^{\text{TR}*} = I$  corresponds to the trivial one [48, 49]. For example, for the AKLT MPS in Eq. (2.6), we have  $V^{\text{TR}} = \sigma^y$ . In fact, if we replace the matrices in Eq. (2.6) to  $\tilde{M}^{\pm 1} = M^{\pm 1}$  and  $\tilde{M}^0 = iM^0$ , one can show that the MPS formed by  $\{\tilde{M}^1, \tilde{M}^0, \tilde{M}^{-1}\}$  is in a trivial phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ , but it is in an SPT phase protected by time-reversal symmetry.

It is known that there is no simple string order parameter to detect a (1+1)D SPT phase protected by time-reversal symmetry [61].<sup>12</sup> Nevertheless, the SPT phase is still distinct from the trivial one in that the SPT phase has anomalous edge states. For the spin- $S$  AKLT chain in Eq. (2.25), with OBC the GS has a spin- $S/2$  DOF localized at each edge. If  $S$  is an odd number, then the two-fold degeneracy at each edge is guaranteed by the *Kramers theorem*. In this sense, the edge states are protected by time-reversal symmetry [49].

Note that the  $n$ th cohomology group  $H^n[G, \text{U}(1)]$  is a group, so the phases protected by  $G$  have a group structure. In particular, if we stack two different SPT phases, such a stack is actually equivalent to a third different phase. This is why SPT phases are sometimes called *invertible phases*. For example, as shown in Fig. 2.5, since  $H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2$ , a stack of two spin-1 AKLT states  $|\text{AKLT}\rangle \otimes |\text{AKLT}\rangle$  can be smoothly connected to a trivial product state  $|\text{triv}\rangle \otimes |\text{triv}\rangle$ ; see Ref. [64] or Appendix D of Ref. [65].



Figure 2.5: Stacking of two AKLT states (left) is equivalent to a trivial product state (right).

### 2.1.3 Haldane phase coupled with a gauge field

Let  $M_d$  be a  $d$ -dimensional manifold in the real space and  $S^1$  be a circle standing for the imaginary time  $\tau$  with PBC. On  $M_d$ , consider a Hamiltonian  $H$  with  $G$  as its symmetry

<sup>11</sup>Note that if  $\mathbb{Z}_n$  acts trivially on  $\text{U}(1)$ , then  $H^2[\mathbb{Z}_n, \text{U}(1)] = \{1\}$  as we have shown in Page 25.

<sup>12</sup>The simplest string order for time-reversal symmetry is rather involved: It requires two copies of the system and a partial swap [61].

group. We focus on the cases in which  $G$  is an on-site unitary symmetry. The GS partition function is defined on  $M_d \times S^1$  as

$$Z[0] = \lim_{\beta \rightarrow \infty} \text{Tr} e^{-\beta H}. \quad (2.69)$$

Next let us introduce a background gauge field  $A$  associated with  $G$  to  $M_d \times S^1$ . Let  $Z[A]$  be the partition function in the presence of the  $G$ -gauge field. It turns out that if  $|\text{GS}\rangle$  (the GS of  $H$  without gauge field) is in an SPT phase protected by  $G$  (in the bulk of  $M_d$ ), then under a gauge transformation  $A \rightarrow A + d\alpha$ , the partition function  $Z[A]$  should transform as

$$Z[A] \rightarrow Z[A + d\alpha] = \begin{cases} Z[A], & \text{if } M_d \text{ is closed,} \\ Z[A] \exp(i\phi), & \text{if } M_d \text{ has a boundary,} \end{cases} \quad (2.70)$$

and in particular, it is impossible to eliminate the phase factor  $\exp(i\phi)$  by introducing a *local* gauge transformation. When  $M_d$  has a  $(d-1)$ -dimensional boundary  $\partial M_d$  and  $|\text{GS}\rangle$  is in an SPT phase (protected by  $G$ ) in the bulk of  $M_d$ , we say that there is a *quantum anomaly* on  $\partial M_d$ .

Let us begin by a simple example: the (1+1)D Haldane phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . Let  $M_1 = [0, \infty)$  be a half-infinite chain. Since the Haldane phase is an SPT phase, the partition function under the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ -gauge field is given by [66]

$$Z[A^y, A^z] = Z[0, 0] \exp\left(i\pi \int_{M_1 \times S^1} A^y \wedge A^z\right), \quad (2.71)$$

where  $A^y$  and  $A^z$  are a  $\mathbb{Z}_2^y$ -gauge field and a  $\mathbb{Z}_2^z$ -gauge field, respectively. By definition, a  $\mathbb{Z}_2$  gauge field should satisfy the restriction (taking  $A^y$  as an example) [66]:

$$\begin{aligned} \int_0^\infty A_\mu^y d\mu &= 0, 1 \pmod{2}, \\ \oint_{S^1} A_\tau^y d\tau &= 0, 1 \pmod{2}, \\ dA^y &= 0 \quad (\text{almost everywhere}), \\ dA^y &\neq 0 \quad (\text{at monodromy defects}), \\ \int_{M_1 \times S^1} dA^y &= 0 \pmod{2}, \end{aligned} \quad (2.72)$$

where

$$A^y = A_\mu^y d\mu + A_\tau^y d\tau. \quad (2.73)$$

Now consider the gauge transformation<sup>13</sup>  $A^y \rightarrow A^y + d\alpha^y$ . The partition function trans-

<sup>13</sup>A more precise definition of  $\mathbb{Z}_2$  gauge field is built on triangulating the 2D spacetime manifold into 2-simplices. The 1-form gauge field  $A^y$  is defined on each edge of the 2-simplices, while  $dA^y$  is defined on each 2-simplex. The 0-form field  $\alpha^y$  is defined on the vertices, and  $\alpha^y \pmod{2} = 0, 1$  is satisfied on each vertex. Strictly speaking, the gauge field of a discrete group is a cochain rather than a differential form [67, 68].

forms as <sup>14</sup>

$$Z[A^y + d\alpha^y, A^z] = Z[A^y, A^z] \exp\left(i\pi \int_{M_1 \times S^1} d\alpha^y \wedge A^z\right) = Z[A^y, A^z] \exp\left(i\pi \int_{\partial M_1 \times S^1} \alpha^y \wedge A^z\right), \quad (2.74)$$

where the second equal sign holds due to the Stokes theorem, and we have applied the identity <sup>15</sup>  $\exp\left(i\pi \int_{M_1 \times S^1} \alpha^y \wedge dA^z\right) = 1$ . We see that the partition function indeed gains an additional phase after the gauge transformation. Moreover, since the additional phase only depends on  $\partial M_1 \times S^1$ , we say that the (1+1)D Haldane phase corresponds to a (0+1)D anomaly protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ .

## 2.2 Gapless phases: Ising criticality as an example

While it has been a well-known fact that gapped phases can be further classified with certain symmetries imposed, it is recently realized that for critical systems, a universality class can also split into distinct subclasses when certain symmetries are imposed, yielding the concept of *symmetry-enriched quantum criticality* [23–30]. In particular, when two subclasses can be distinguished by symmetry properties of certain nonlocal operators, an *SPT/trivial* classification of quantum criticalities becomes possible [23].

In a critical system, there is no long-range order measured by operators associated with gapless DOF: All the correlations (associated with gapless DOF) decay algebraically with respect to spatial distance. Nevertheless, we can generalize the concept of long-range order in gapped systems to *slowest possible algebraic decay* in gapless systems [23]. Let us now generalize the concept of symmetry flux (Definition 2.12) to critical systems:

**Definition 2.14 (symmetry fluxes for critical systems)** Let  $U^g = \prod_j u_j^g$  be the on-site linear representation of  $g \in G$  on the Hilbert space; the symmetry flux of  $g$  is defined as

$$F_j^g = \dots u_{j-3}^g u_{j-2}^g u_{j-1}^g B_j^g, \quad (2.75)$$

where  $B_j^g$  is an operator at site  $j$  chosen such that the correlation of two symmetry fluxes has slowest possible algebraic decay. In other words,  $\langle F_j^{g\dagger} F_{j+r}^g \rangle \sim r^{-2\Delta}$  with the smallest possible  $\Delta$ . (If  $g$  is associated with gapped DOF, then  $\Delta = 0$  and the correlation has long-range order. Otherwise,  $\Delta > 0$ .)

The classification of symmetry-enriched quantum criticality is still a developing field. In this section, I will focus on the simplest quantum criticality: the Ising criticality. For the Ising CFT, it is known that [9]

<sup>14</sup>Strictly speaking, we should use the cup product  $\smile$  instead of the wedge product  $\wedge$  because a  $\mathbb{Z}_2$  gauge field is a cochain rather than a differential form. See Appendix B of Ref. [68], Appendix J.4.e of Ref. [31], and Refs. [67, 69] for details.

<sup>15</sup>After triangulation, it will be clear that  $\alpha^y \wedge dA^z$  (strictly speaking,  $\alpha^y \smile dA^z$ ) is always an even number.

- The smallest nonzero scaling dimension is  $\Delta = 1/8$ , meaning that the slowest possible algebraic decay of certain operator  $\hat{O}(x)$  is given by  $\langle \hat{O}(x)\hat{O}(0) \rangle \sim x^{-2\Delta}$ .
- The CFT has a *unique local operator* <sup>16</sup>  $\hat{\sigma}(x)$  with scaling dimension  $\Delta = 1/8$ . (Note that in the lattice level, the choice of such a local operator is not unique.)

Moreover, similar to the gapped cases (Proposition 2.13), for the symmetry fluxes of critical cases, it can be argued that

**Proposition 2.15 (uniqueness of symmetry flux for Ising universality class)** *Two symmetry fluxes for critical systems are equivalent to each other if their difference is not a symmetry flux. Given a  $G$ -symmetric lattice model in which some DOF are described by the Ising universality class and other DOF (if present) are gapped, then up to the equivalence relation, any  $g \in G$  has a unique symmetry flux.*

For an argument of the above proposition based on Ising CFT, see Sec. III A.3 of Ref. [23]. Let  $\{F_j^g\}_{g \in G}$  be a set of symmetry flux associated with  $G$ . Proposition 2.15 suggests that under  $G$ , a symmetry flux should transform as

$$U^h F_j^g U^{h\dagger} = \dots u_{j-2}^{hgh^{-1}} u_{j-1}^{hgh^{-1}} (u_j^h B_j^g u_j^{h\dagger}) = e^{i\chi(g,h)} F_j^{hgh^{-1}} + F_{\text{sub}}^{hgh^{-1}}, \quad g, h \in G, \quad (2.76)$$

where  $F_{\text{sub}}$  is some faster-decaying term <sup>17</sup> that does not affect the scaling dimension  $\Delta = 1/8$ . Note that the phase  $e^{i\chi(g,h)}$  is well-defined due to Proposition 2.15.

We can thus use the local operators or the nonlocal operators (symmetry fluxes) to classify the symmetry-enriched Ising universality class. Two simplest examples with a local operator are given by the two critical Ising chains [23]:

$$H_0 = - \sum_j (\sigma_j^z \sigma_{j+1}^z + \sigma_j^x), \quad (2.77a)$$

$$H_1 = - \sum_j (\sigma_j^y \sigma_{j+1}^y + \sigma_j^x). \quad (2.77b)$$

Besides the Ising  $\mathbb{Z}_2$  symmetry, the two models both have the  $\mathbb{Z}_2^K := \{1, K\}$  symmetry, where  $K$  is the complex conjugation. In the lattice level, we can naturally choose the local operator to be  $\hat{\sigma}(x) \sim \sigma_j^z$  for  $H_0$  and  $\hat{\sigma}(x) \sim \sigma_j^y$  for  $H_1$ . In fact, these two Ising CFTs are enriched by the  $\mathbb{Z}_2^K$  symmetry. This can be seen by noting that  $K\hat{\sigma}K = \hat{\sigma}$  for  $H_0$  while  $K\hat{\sigma}K = -\hat{\sigma}$  for  $H_1$ . This means that the interpolation  $\lambda H_0 + (1-\lambda)H_1$  with  $0 \leq \lambda \leq 1$  must at some point go through a different universality class. Indeed, at  $\lambda = 1/2$ , the system is at a multicritical point with a dynamical critical exponent  $z_{\text{dyn}} = 2$ , which is *not* described by a CFT. While  $H_0$  and  $H_1$  can be distinguished by the symmetry properties of local operators, a more interesting case is when two symmetry-enriched CFTs can only be distinguished

<sup>16</sup> $\hat{\sigma}(x)$  is an operator at the CFT level depending on the coordinate  $x$ , not to be confused with Pauli matrix  $\sigma_j^x$  at the lattice level.

<sup>17</sup>Sometimes by properly choosing  $\{F_j^g\}_{g \in G}$ ,  $F_{\text{sub}}$  can be exactly zero.

by the symmetry properties of nonlocal operators. For example, consider the following model [23]:

$$H_2 = \sum_j \left( -\sigma_j^z \sigma_{j+1}^z - \sigma_{j-1}^z \sigma_j^x \sigma_{j+1}^z \right), \quad (2.78)$$

where the second term is given by the cluster model in Eq. (1.14). The models  $H_0$  and  $H_2$  cannot be distinguished by local operators because both are described by the Ising universality class with  $\hat{\sigma}(x) \sim \sigma_j^z$ . What about nonlocal operators? For  $H_0$ , we can choose  $\hat{\mu}(x) \sim \dots \sigma_{j-2}^x \sigma_{j-1}^x \sigma_j^x$ , which is the Kramers-Wannier duality of  $\sigma_j^z$  [see Eq. (1.8)]. For  $H_2$ , however, we can choose  $\hat{\mu}(x) \sim \dots \sigma_{j-1}^x \sigma_j^x \sigma_j^y \sigma_{j+1}^z$  [28]. Note that in both cases, the adjacent symmetric phase has long-range order  $\lim_{r \rightarrow \infty} \langle \hat{\mu}(x) \hat{\mu}(x+r) \rangle \neq 0$  [see Eq. (1.18)]. Since  $K \hat{\mu} K = \hat{\mu}$  for  $H_0$  and  $K \hat{\mu} K = -\hat{\mu}$  for  $H_2$ , the two models belong to two different symmetry-enriched Ising CFTs. Moreover, since this is based on charges of nonlocal operators, we say that they are topologically distinct. In particular, since the gapped SPT phase is an adjacent phase of  $H_2$ , we say that the GS of  $H_2$  is in an SPT Ising critical phase.<sup>18</sup>

The two models  $H_0$  and  $H_2$  also have the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry defined in Eq. (1.15). Let  $X_A = \prod_k \sigma_{2k-1}^x$ . We can see that

$$X_A \hat{\mu} X_A = \begin{cases} \hat{\mu}, & \text{for } H_0 \\ -\hat{\mu}, & \text{for } H_2 \end{cases}. \quad (2.79)$$

In other words, the GS of  $H_2$  is in a gapless SPT phase protected by  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , while  $H_0$  is trivial. As we have seen in Sec. 2.1.2, for the gapped phases, a symmetry flux carrying nontrivial charge implies a nontrivial projective representation, which further implies the GS degeneracy in the presence of OBC. In fact, this extends to the gapless case [23]. For the gapped SPT phase protected by  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , there are four (quasi-)degenerate GS on an open chain which correspond to spin-1/2 DOF localized at the edges. We denote the four GS as

$$\begin{aligned} |\text{FM}\rangle_{\pm} &= |\uparrow_L \uparrow_R\rangle \pm |\downarrow_L \downarrow_R\rangle, \\ |\text{AFM}\rangle_{\pm} &= |\uparrow_L \downarrow_R\rangle \pm |\downarrow_L \uparrow_R\rangle. \end{aligned} \quad (2.80)$$

The energy difference between these four GS is exponentially small for the gapped case. However, in a gapless system,  $|\text{AFM}\rangle_{\pm}$  are split from  $|\text{FM}\rangle_{\pm}$  at the scale of  $1/L$ , the same as the finite-size bulk gap [70, 71]. In other words, edges can sense their (mis)alignment through the critical bulk.<sup>19</sup> We thus have only two GS  $|\text{FM}\rangle_{\pm}$ . Since a CFT has no length scales by definition, the only quantity with units of energy is  $1/L$ . Therefore, in a finite-size system, the energy split of  $|\text{FM}\rangle_{\pm}$  could be given by scales of order  $\xi^\alpha / L^{1+\alpha}$  or

<sup>18</sup>More precisely, since  $\hat{\mu}(x) \sim \dots \sigma_{j-1}^x \sigma_j^x \sigma_j^y \sigma_{j+1}^z$  is also a symmetry flux for the gapped SPT phase [see Eq. (1.18)], it is natural to say that the GS of  $H_2$  is in an gapless SPT phase.

<sup>19</sup>The model  $H_2$  with OBC has four exactly degenerate GS because  $[H_2, \sigma_1^z] = [H_2, \sigma_L^z] = 0$ , but the degeneracy can be lifted by adding perturbations, and the energy split of two GS scales algebraically [23].

$\exp(-L/\xi)$ , where  $\xi$  is a constant with units of length [23]. See Fig. 2.6. In particular, if the symmetry flux  $\hat{\mu}$  carries a nontrivial charge under a symmetry which is associated with gapped DOF, then the energy split of  $|\text{FM}\rangle_{\pm}$  is at most of order  $\exp(-L/\xi)$  [23]; examples will be presented in Eq. (2.81) and Sec. 5.6.

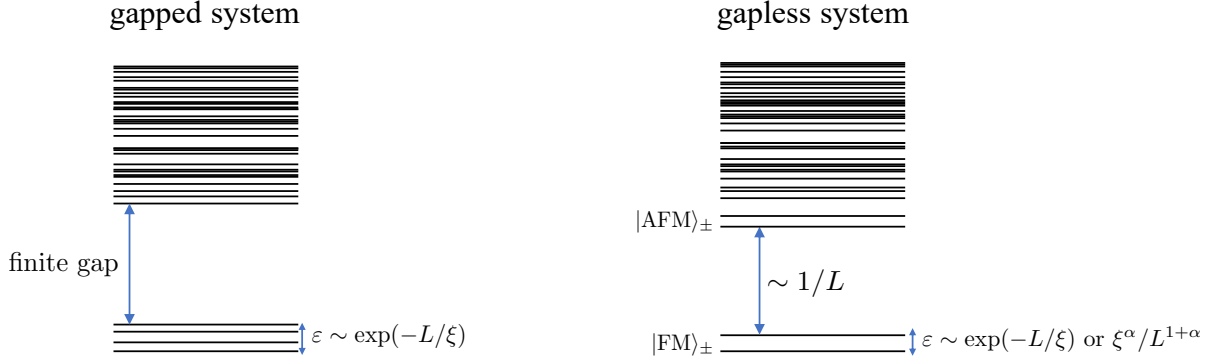


Figure 2.6: Finite-size energy splitting of low-energy states in gapped and gapless systems. In the right figure, we have presumed that the model has an FM sign (like  $H_2$ ).

Let us take a look at an example which exhibits an SPT Ising criticality with both gapless and gapped DOF. Consider the spin-1 XXZ chain:

$$H_3 = \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + J S_j^z S_{j+1}^z), \quad J > 0. \quad (2.81)$$

The model obviously has the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry. The Haldane phase and the  $\mathbb{Z}_2$  SSB phase are separated by an Ising critical point at  $J_c \approx 1.1856$  [72], at which the symmetry fluxes in Eq. (2.10) carries nontrivial charges under  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . Indeed, both  $\langle F_j^x F_{j+r}^x \rangle$  and  $\langle F_j^y F_{j+r}^y \rangle$  decay algebraically. However, as  $J$  increases, the hidden AFM order gradually becomes the explicit AFM order in  $z$  direction. More precisely,

$$\lim_{J \rightarrow \infty} \left[ -\langle F_j^z F_{j+r}^z \rangle - (-1)^r \langle S_j^z S_{j+r}^z \rangle \right] = 0. \quad (2.82)$$

In other words, the string order  $\mathcal{O}_{\text{str}}^z = -\lim_{r \rightarrow \infty} \langle F_j^z F_{j+r}^z \rangle$  is nonzero not only for the Haldane phase ( $J < J_c$ ) but also for the SSB phase ( $J > J_c$ ). This suggests that even at the critical point  $J_c$ ,  $F_j^z$  has long-range order, i.e.,  $\mathcal{O}_{\text{str}}^z \neq 0$ . Since  $F_j^z$  is associated with the group element  $Z_\pi$ , we call  $\mathbb{Z}_2^z$  a symmetry associated with gapped DOF, or a *gapped symmetry* for short. It can be shown that with OBC, the two GS  $|\text{AFM}\rangle_{\pm}$  have an exponentially small energy splitting, and there are edge modes exponentially localized at the edges [23].

In the presence of  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry, how many symmetry-enriched Ising criticalities (with codimension one<sup>20</sup>) can we have in (1+1)D? There are six gapped phases for  $\mathbb{Z}_2 \times \mathbb{Z}_2$ -

<sup>20</sup>If only one parameter needs to be tuned to achieve criticality, such CFTs are said to have codimension one. Ising CFTs with higher codimension can occur but physically correspond to accidental criticalities in a phase diagram.

symmetric Hamiltonians: Three Ising SSB phases represented by  $H_x = -\sum_j \sigma_j^x \sigma_{j+1}^x$ ,  $H_y = -\sum_j \sigma_j^y \sigma_{j+1}^y$ , and  $H_z = -\sum_j \sigma_j^z \sigma_{j+1}^z$ ; A fully symmetry-breaking phase  $H_{xy} = -\sum_j (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y)$ ; A Haldane phase  $H_{\text{cluster}} = -\sum_j \sigma_{j-1}^z \sigma_j^x \sigma_{j+1}^z$  and a trivial phase  $H_{\text{triv}} = -\sum_j \sigma_j^x$ . There are thus nine symmetry-enriched Ising CFTs; see Fig. 2.7. Given a general symmetry group  $G$ , how can we classify the  $G$ -enriched Ising CFTs? Assume that an Ising criticality appears between two gapped phases  $A$  and  $B$ , and the symmetry group of each phase is denoted as  $G_A$  and  $G_B$ , respectively. Assume that the phase  $B$  has lower symmetry<sup>21</sup>. Then we have  $G_B \subset G_A \subset G$  and  $G_A/G_B = \mathbb{Z}_2$ , where the latter is because an additional  $\mathbb{Z}_2$  symmetry is broken when we go from phase  $A$  to  $B$  (otherwise it is not Ising CFT). We can thus have a complete classification:

**Proposition 2.16 (complete classification of symmetry-enriched Ising CFTs [23])**

*For a unitary group  $G$ , symmetry-enriched Ising CFTs of codimension one are labeled by two subgroups and an element  $(G_A, G_B, \omega)$  such that*

$$G_B \subset G_A \subset G, \quad G_A/G_B = \mathbb{Z}_2, \quad \omega \in H^2[G_A, \text{U}(1)]. \quad (2.83)$$

Note that an additional label  $\omega' \in H^2[G_B, \text{U}(1)]$  is unnecessary, because there has to be  $\omega|_{G_B} = \omega'$  for consistency. In practice,  $\omega$  can be read out from the charges of symmetry fluxes; see Eq. (2.76). As an example of the above classification theory, in the case of  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , we can choose  $(G_A, G_B) = (\mathbb{Z}_2, \{1\})$  or  $(\mathbb{Z}_2 \times \mathbb{Z}_2, \mathbb{Z}_2)$ . Note that  $\mathbb{Z}_2 \times \mathbb{Z}_2$  has three different  $\mathbb{Z}_2$  subgroups. Since  $H^2[\mathbb{Z}_2, \text{U}(1)] = \{1\}$ ,  $(G_A, G_B) = (\mathbb{Z}_2, \{1\})$  gives three Ising CFTs. On the other hand,  $(G_A, G_B) = (\mathbb{Z}_2 \times \mathbb{Z}_2, \mathbb{Z}_2)$  gives  $3 \times 2 = 6$  Ising CFTs. Hence there are nine in total.

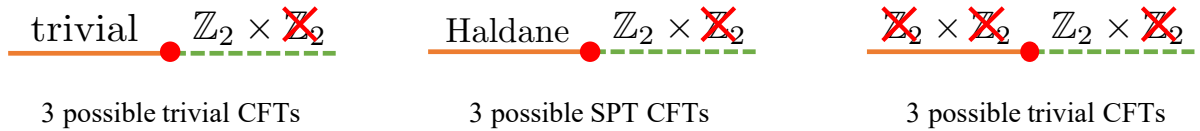


Figure 2.7: There are nine possible symmetry-enriched Ising criticalities [23]. A crossing denotes a broken symmetry.

As described in Sec. 2.1.1, a broad class of gapped SPT phases can be understood in the framework of hidden symmetry breaking. A natural question is that if certain SPT criticalities can also be understood from the picture of hidden symmetry breaking. Our answer is yes: the KT transformation also defines a duality between an SPT Ising criticality and a trivial Ising criticality; see Sec. 5.6 for details.

<sup>21</sup>If the phase  $B$  has no symmetry, then  $G_B = \{1\}$ .





道生一，一生二，二生三，三生萬物。

『道德經·四十二章』

## GAPPED BOSONIC SPT PHASES IN HIGHER DIMENSIONS

**C**an we understand higher dimensional gapped SPT phases from lower dimensional ones? In particular, is it possible to construct higher dimensional gapped SPT phases using lower dimensional ones? What kind of symmetries can protect gapped phases in general? The answers to these two questions are yes provided that we focus on two kinds of SPT phases: weak SPT phases and crystalline SPT phases, which will be introduced in Sec. 3.1 and Sec. 3.3, respectively. Strong SPT phases, on the other hand, cannot be directly constructed from lower dimensional SPT phases; see Sec. 3.2.

### 3.1 Weak SPT phases and LSM theorems

The most naive approach to construct gapped SPT phases in higher dimensions is by stacking lower dimensional gapped SPT phases. For example, one can stack spin-1 AKLT states to form a 2D state; see Fig. 3.1. However, as mentioned at the end of Sec. 2.1.2, the stacking of two spin-1 AKLT states is in fact a trivial state. Therefore, if we group the spin-1 AKLT states in Fig. 3.1 two-by-two, the 2D state can be smoothly connected to a trivial product state while preserving the global  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry. A more intuitive way to see this is by looking at the boundary. As shown in Fig. 3.1, the boundary is effectively a spin-1/2 chain, so that the degeneracy can be lifted by adding perturbations to these spin-1/2 DOF. For example, one can add AFM Heisenberg interaction  $\sum_j \sigma_{2j}^x \sigma_{2j+1}^x$  respecting the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry, where  $\sigma_k = (\sigma_k^x, \sigma_k^y, \sigma_k^z)$  acts on the spin-1/2 anomalous DOF on the  $k$ th AKLT state. This means the edge states are unstable with the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry. Therefore, the 2D state in Fig. 3.1 is in a trivial phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ . Instead of stacking lower dimensional states, how about generalizing the AKLT model to higher dimensions? It is known that AKLT states can be constructed on any lattice in

any dimensions [46, 73, 74]. For example, the spin-2 AKLT model on a square lattice is defined as

$$H_{\text{AKLT}}^{2,\square} := \sum_{\langle j,j' \rangle} P_{j,j'}^{(4)}, \quad (3.1)$$

where  $P_{j,j'}^{(4)}$  projects the two nearest-neighbor spin-2 onto a state with total spin 4. The exact and unique GS of  $H_{\text{AKLT}}^{2,\square}$ , denoted as  $|\text{AKLT}_{2,\square}\rangle$ , is illustrated in Fig. 2.1(b). Similarly, the spin-3 AKLT model on a cubic lattice can also be constructed:

$$H_{\text{AKLT}}^{3,\boxplus} := \sum_{\langle j,j' \rangle} P_{j,j'}^{(6)}, \quad (3.2)$$

where  $P_{j,j'}^{(6)}$  projects the two nearest-neighbor spin-3 onto a state with total spin 6. The exact and unique GS of  $H_{\text{AKLT}}^{3,\boxplus}$ , denoted as  $|\text{AKLT}_{3,\boxplus}\rangle$ , is illustrated in Fig. 2.1(d). Are  $|\text{AKLT}_{2,\square}\rangle$  and  $|\text{AKLT}_{3,\boxplus}\rangle$  in a (2+1)D SPT phase protected by  $\mathbb{Z}_2 \times \mathbb{Z}_2$ ? Let us again look at the boundary. As shown in Fig. 3.2, their boundaries are also spin-1/2 systems, which can be gapped out by adding  $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetric perturbations. This means that  $|\text{AKLT}_{2,\square}\rangle$  and  $|\text{AKLT}_{3,\boxplus}\rangle$  are also trivial states even under  $\mathbb{Z}_2 \times \mathbb{Z}_2$ .

However, there are a series of powerful theorems which state that with certain symmetry, a half-odd-integer spin system can *never* have a unique gapped GS. These theorems are known as the *Lieb-Shultz-Mattis (LSM) theorems* [11, 32, 75–88]. A typical modern statement reads

**Theorem 3.1 (LSM)** *Consider a  $(d+1)D$  system with a symmetry  $\mathcal{G} = G \times (\mathbb{Z}^{\text{trn}})^d$ , where  $G$  is an (either unitary or anti-unitary) on-site symmetry group and  $(\mathbb{Z}^{\text{trn}})^d$  is the translation symmetry in  $d$  linearly independent spatial axes. The translation symmetry  $(\mathbb{Z}^{\text{trn}})^d$  defines the unit cells. If  $G$  acts as a nontrivial projective representation on each unit cell, then the system can never have a unique gapped GS. In other words, the GS must have any one of the following:*

1. A continuum of low energy excitations (gapless);
2. SSB (degenerate and gapped);
3. Topological order (degenerate and gapped).

*In this case, we say that the system has an LSM anomaly protected by  $\mathcal{G}$ .*

**Corollary 3.2** *A  $\mathcal{G}$ -symmetric system with a half-odd-integer spin per unit cell cannot have a unique gapped GS if  $\mathcal{G}$  is any of the following:*

1.  $\text{SO}(3) \times (\mathbb{Z}^{\text{trn}})^d$ ;
2.  $\mathbb{Z}_2 \times \mathbb{Z}_2 \times (\mathbb{Z}^{\text{trn}})^d$ ;
3.  $\mathbb{Z}_2^{\text{TR}} \times (\mathbb{Z}^{\text{trn}})^d$ .

This suggests that the edge states of aforementioned models are stable against perturbations that respect any of the three symmetries in Corollary 3.2. When an on-site symmetry alone is not enough to protect an SPT phase, such phase is called a *weak SPT phase*. We can therefore claim that the stacking of spin-1 AKLT states,  $|\text{AKLT}_{2,\square}\rangle$ , and  $|\text{AKLT}_{3,\boxplus}\rangle$  are in weak SPT phases protected by any of the three symmetries in Corollary 3.2 [5, 89, 90]. The correctness of this claim is guaranteed by the *bulk-boundary correspondence*. More precisely, there is a so-called *SPT-LSM theorem* [91, 92]:

**Theorem 3.3 (SPT-LSM)** *Consider a  $(d+1)D$  system with the symmetry  $\mathcal{G} = G \times (\mathbb{Z}^{\text{trn}})^d$  defined in Theorem 3.1. If the system is in a weak SPT phase protected by  $\mathcal{G}$ , then its  $(d-1)$  dimensional spatial boundary must have an LSM anomaly protected by  $\mathcal{G}$ . The converse is also true: If a  $[(d-1)+1]D$  system has an LSM anomaly protected by  $\mathcal{G}$ , then it can always be regarded as the boundary of a  $(d+1)D$  weak SPT phase protected by  $\mathcal{G}$ .*

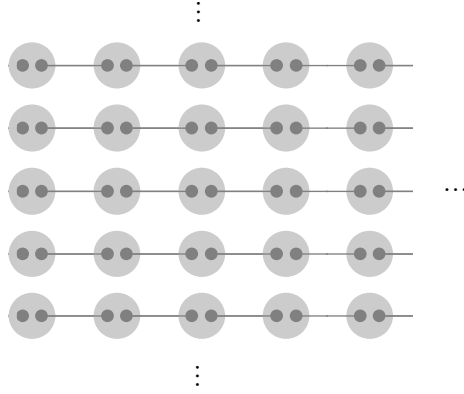



Figure 3.1: A 2D state formed by stacking spin-1 AKLT states. The boundary is effectively a spin-1/2 chain.

On the other hand, consider the spin-3 AKLT model on a triangular lattice

$$H_{\text{AKLT}}^{3,\Delta} := \sum_{\langle j,j' \rangle} P_{j,j'}^{(6)}, \quad (3.3)$$

where  $P_{j,j'}^{(6)}$  projects the two nearest-neighbor spin-3 onto a state with total spin 6. The exact and unique GS of  $H_{\text{AKLT}}^{3,\Delta}$ , denoted as  $|\text{AKLT}_{3,\Delta}\rangle$ , is illustrated in Fig. 2.1(c). On a half-infinite plane, every site on the 1D boundary of  $|\text{AKLT}_{3,\Delta}\rangle$  hosts two "dangling" spin-1/2's, as shown in the figure: . Since the six spin-1/2's on the same site form a totally symmetric spin-3 degree of freedom, the two "dangling" spin-1/2's have to form a symmetric spin-1 degree of freedom. One can add perturbations at the boundary that couple these spin-1's through, for example, the translation invariant spin-1 AKLT Hamiltonian. This perturbation thus results in a gapped edge state without breaking the three

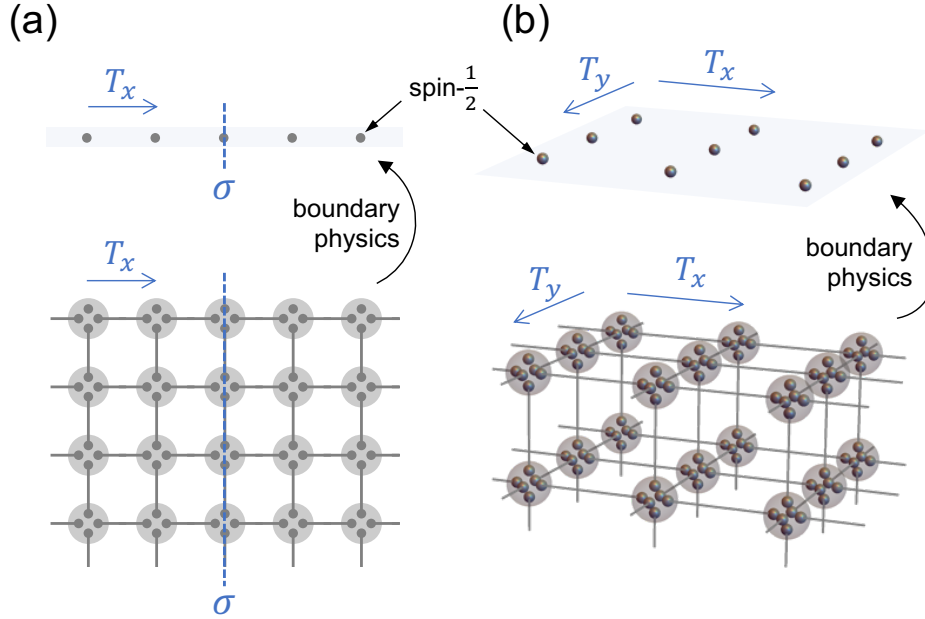


Figure 3.2: LSM theorems as a special case of constraints at the boundaries of SPT phases: gapless or degenerate edge states ensured by certain symmetry in the boundary implies a weak SPT phase protected by the same symmetry in the bulk. The translation group is generated by  $T_x$  and  $T_y$ , while the group  $D_1 = \{1, \sigma\}$  is generated by the site-centered reflection  $\sigma$ . (a) A spin-1/2 simple linear chain can be regarded as the edge of  $|\text{AKLT}_{2,\square}\rangle$ . (b) A spin-1/2 system on a square lattice can be regarded as the surface of  $|\text{AKLT}_{3,\boxplus}\rangle$ .

symmetries in Corollary 3.2, and hence  $|\text{AKLT}_{3,\Delta}\rangle$  is in a trivial phase protected by these symmetries.

In fact, in Corollary 3.2,  $(\mathbb{Z}^{\text{trn}})^d$  can be generalized to some other crystalline symmetries. For example, in (1+1)D half-odd-integer spin systems,  $\mathbb{Z}_2 \times \mathbb{Z}_2 \times D_1$  and  $\mathbb{Z}_2^{\text{TR}} \times D_1$  also guarantee the absence of a unique gapped GS [79, 82, 86], where the point group  $D_1$  is a *site-centered* reflection symmetry; see Fig. 3.2(a). A summary of the phases of AKLT states in terms of different symmetries is presented in Table 4.5.

## 3.2 Strong SPT phases

Is it possible that an on-site symmetry alone can stabilize an SPT phase? The answer is yes, and such phases are called *strong SPT phases*. Strong SPT phases in higher than (1+1)D dimensions are beyond the scope of this thesis, so I will only give a very brief introduction. So far, it is known that many strong SPT phases in  $(d+1)$ D can be classified by the  $(d+1)$ th cohomology group  $H^{d+1}[G, \text{U}(1)]$  [31, 59], which is related to the *Dijkgraaf-Witten theory* [93]. [Mathematical details of the  $(d+1)$ th cohomology group can be found in

Appendix B.] Examples of (2+1)D models whose GS exhibit strong SPT phases classified by the second cohomology group include the *CZX model* [5, 89, 94] and the *Levin-Gu model* [95], both of which are protected by an on-site  $\mathbb{Z}_2$  symmetry. However, there are some strong SPT phases whose classifications are given by *cobordism groups*, which are beyond group cohomology [96].

### 3.3 Crystalline SPT phases

Is it possible that an SPT phase can be protected by a certain crystalline symmetry alone? The answer is yes. In this section, I will mainly focus on the SPT phases protected by point group symmetries, dubbed *point-group-symmetry protected topological (pgSPT) phases*. Crystalline symmetries are not on-site. However, it turns out that any pgSPT phases in spatial dimension  $d$  can be adiabatically connected, preserving symmetry, to a system composed of lower-dimensional strong SPT states protected by on-site symmetry.

Let us start with the simplest point group  $D_1 = \{1, \sigma\}$ , where  $\sigma$  stands for a mirror reflection. Suppose the GS  $|\psi_{\text{GS}}\rangle$  in spatial dimension  $d$  is in an SPT phase. By definition (see Chapter 1),  $|\psi_{\text{GS}}\rangle$  is smoothly connected to a trivial product state  $|\text{triv}\rangle$  via a local unitary transformation (or finite-depth quantum circuit):

$$U^{\text{loc}} |\psi_{\text{GS}}\rangle = |\text{triv}\rangle, \quad (3.4)$$

where  $U^{\text{loc}}$  is illustrated in Fig. 1.5. Note that  $U^{\text{loc}}$  has to break the  $D_1$  symmetry. Let us now divide the system into three regions  $r_1$ ,  $r_0$ , and  $\sigma r_1$  as shown in Fig. 3.3. The two regions  $r_1$  and  $\sigma r_1$  are related to each other by the mirror reflection  $\sigma$ , and  $r_0$  is  $D_1$ -symmetric. Besides, the width  $w$  of  $r_0$  is held fixed in the thermodynamic limit and is chosen to be much bigger than the correlation length  $\xi$ , which means that  $r_0$  is effectively a  $(d-1)$ -dimensional region. We now show that, there exists a  $D_1$ -symmetric local unitary  $\tilde{U}^{\text{loc}}$  such that  $|\psi_{\text{GS}}\rangle$  can be extensively trivialized (but not completely trivialized), meaning that [97]

$$\tilde{U}^{\text{loc}} |\psi_{\text{GS}}\rangle = |\text{triv}\rangle_{r_1} \otimes |\psi\rangle_{r_0} \otimes |\text{triv}\rangle_{\sigma r_1}, \quad (3.5)$$

where  $D_1$  acts like an on-site symmetry for  $|\psi\rangle_{r_0}$ . The approach to find  $\tilde{U}^{\text{loc}}$  in Eq. (3.5) is called a *dimensional reduction*. We note that a finite-depth quantum circuit can be restricted to act in a smaller region [98]; see Fig. 3.4 as an example. Let  $U_{r_1}^{\text{loc}}$  be the restriction of  $U^{\text{loc}}$  to  $r_1$  and extending slightly to  $r_0$  [97]. A few correlation lengths away from the boundary of  $r_1$ , the action of  $U_{r_1}^{\text{loc}}$  on  $|\psi_{\text{GS}}\rangle$  should be indistinguishable from that of  $U^{\text{loc}}$ . Thus we have  $U_{r_1}^{\text{loc}} |\psi_{\text{GS}}\rangle = |\text{triv}\rangle_{r_1}$ . Due to the  $D_1$  symmetry of  $|\psi_{\text{GS}}\rangle$ , it is clear that  $U_{\sigma r_1}^{\text{loc}} = U_{\sigma} U_{r_1}^{\text{loc}} U_{\sigma}$  trivializes the region  $\sigma r_1$ , where  $U_{\sigma}$  represents the action of mirror reflection on the Hilbert space. We can thus define

$$\tilde{U}^{\text{loc}} = U_{r_1}^{\text{loc}} U_{\sigma r_1}^{\text{loc}}, \quad (3.6)$$

which trivializes  $r_1 \cup \sigma r_1$ , leaving only the  $(d-1)$ -dimensional region  $r_0$  nontrivial. Note that  $\tilde{U}^{\text{loc}}$  preserves the  $D_1$  symmetry, i.e.,  $U_\sigma \tilde{U}^{\text{loc}} U_\sigma = \tilde{U}^{\text{loc}}$ . It is now clear that  $D_1$  acts like an on-site  $\mathbb{Z}_2$  symmetry in  $r_0$ . For example, a (3+1)D SPT phase protected by  $D_1$  symmetry may be smoothly connected to  $|\text{triv}\rangle_{r_1} \otimes |\psi\rangle_{r_0} \otimes |\text{triv}\rangle_{\sigma r_1}$  with  $|\psi\rangle_{r_0}$  being the GS of the CZX model [5, 89]<sup>1</sup>. On the other hand, all the (2+1)D short-range entangled states (see Definition 1.11) with  $D_1$  symmetry only are trivial, because  $H^2[D_1 \cong \mathbb{Z}_2, \text{U}(1)] = \{1\}$ . (Note that the symmetry-protected phase of  $|\text{triv}\rangle_{r_1} \otimes |\psi\rangle_{r_0} \otimes |\text{triv}\rangle_{\sigma r_1}$  is always the same as that of  $|\psi\rangle_{r_0}$ , because stacking a trivial state  $|\text{triv}\rangle_{r_1} \otimes |\text{triv}\rangle_{\sigma r_1}$  should not change the phase of  $|\psi\rangle_{r_0}$ .)

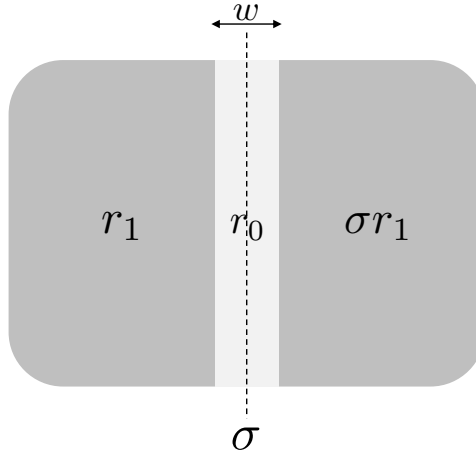


Figure 3.3: The GS  $|\psi_{\text{GS}}\rangle$  in spatial dimension  $d$  with  $D_1$  symmetry is divided into three regions  $r_1$ ,  $r_0$ , and  $\sigma r_1$ , where  $\sigma$  is the mirror reflection. The width  $w$  of  $r_0$  is held fixed in the thermodynamic limit and is chosen to be much bigger than the correlation length  $\xi$ .

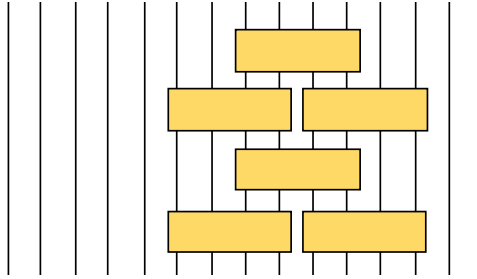


Figure 3.4: Restriction of the 1D quantum circuit in Fig. 1.5 to a certain region.

For (1+1)D short-range entangled states with  $D_1$  symmetry only, there are two symmetry-protected phases, because  $H^1[D_1 \cong \mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2$ , which simply means that the eigenvalues of  $U_\sigma$  are  $\pm 1$ . It is obvious that in Eq. (3.5), the two states  $\tilde{U}^{\text{loc}} |\psi_{\text{GS}}\rangle$  and  $|\psi\rangle_{r_0}$  carry the

<sup>1</sup>Although  $H^3[\mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2$ , the classification of (3+1)D SPT phases protected by  $D_1$  symmetry is in fact (at least)  $\mathbb{Z}_2 \times \mathbb{Z}_2$  instead of  $\mathbb{Z}_2$ ; see Ref. [97] for details.

same  $U_\sigma$  eigenvalue. Therefore, in (1+1)D, classifying a short-range entangled state  $|\psi_{\text{GS}}\rangle$  with  $D_1$  symmetry only<sup>2</sup> is equivalent to classifying the  $\mathbb{Z}_2$  charge carries by  $|\psi_{\text{GS}}\rangle$ . Let us use the spin-1 AKLT state  $|\text{AKLT}\rangle$  in Eq. (2.5) as an example. In the graph representation of AKLT states, we can assign an arbitrary direction to each spin-1/2 singlet bond, because a singlet state is antisymmetric. Reversing the direction of a singlet bond is equivalent to adding a minus sign; see Fig. 3.5. If  $D_1$  is a *bond-centered* symmetry, then there are always odd number of singlet bonds being reversed<sup>3</sup>, and thus  $U_\sigma |\text{AKLT}\rangle = -|\text{AKLT}\rangle$ . According to Definition 1.14, we conclude that the spin-1 AKLT state is in an SPT phase protected by bond-centered  $D_1$ , which is consistent with the conclusion given by the MPS [48, 49]. Indeed, the SPT phase is stable under the Zeeman term  $B \sum_j S_j^x$  that preserves  $D_1$  symmetry [48, 99].

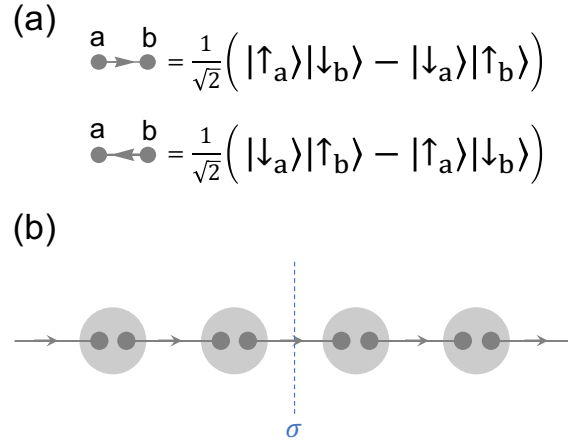


Figure 3.5: (a) In every AKLT state (not restricted to 1D spin-1 case), a direction can be assigned to each singlet bond. Two opposite directions differ by a minus sign. (b) The spin-1 AKLT state carries a nontrivial charge of  $D_1 = \{1, \sigma\}$ .

When studying pgSPT phases, one needs to pay attention to where the symmetry center is. For example, if  $D_1$  is a *site-centered* symmetry in 1D, that is, there is microscopic DOF lying precisely at the symmetry center of  $D_1$ , then an SPT/trivial classification cannot be well-defined. The reason is as follows. Let  $\bigotimes_{j=-L}^L |\alpha_j\rangle_j$  be a basis vector of the Hilbert space, and let the site  $j = 0$  be the symmetry center. The mirror reflection can be decomposed as  $U_\sigma = \bigotimes_j u_j$ . Usually  $u_j$  is defined as  $u_j |\alpha_j\rangle_j = |\alpha_j\rangle_{-j}$ . However, one

<sup>2</sup>In 1D,  $D_1$  is the only point group.

<sup>3</sup>In the thermodynamic limit, it may be subtle to ask if the number is even or odd. Nevertheless, it is always possible to identify the phase of a finite-size system. The fact is that, the symmetry-protected phase of a finite-size system should be identical to that of an infinite system. The reason is as follows. All the SPT phases are about local properties of the system, since there is only short-range entanglement in the bulk. In fact, as we have seen, most pgSPT phases in 1D or 2D are determined by the properties of a 0D local region around the symmetry center. Local properties are obviously not affected by the those degrees of freedom that are infinitely far away.



2D point group $G$	Classification
$C_n$ ( $n = 2, 3, 4, 6$ )	$\mathbb{Z}_n$
$D_1, D_3$	trivial
$D_n$ ( $n = 2, 4, 6$ )	$\mathbb{Z}_2 \times \mathbb{Z}_2$

Table 3.1: Classifications of (2+1)D pgSPT phases for all nine crystallographic point groups [65].  $C_n$  stands for the  $n$ -fold rotation.  $D_n$  is the *dihedral group* of order  $2n$ , which is the symmetry group of a regular  $n$ -sided polygon (when  $n > 1$ ). The classification of  $D_n$  pgSPT phases is based on Eq. (3.7) except for  $D_1$  and  $D_3$ . For (2+1)D pgSPT phases to be well-defined, the symmetry centers should not be put on any microscopic DOF.

is also free to define  $u_j |\alpha_j\rangle_j = -|\alpha_j\rangle_{-j}$ , in which case the sign of the eigenvalue of  $U_\sigma$  is altered (since there are odd number of sites in total). This means that there are still two distinct phases in the presence of the site-centered  $D_1$  [100], but it is meaningless to say which one is SPT, because the trivial and nontrivial representations in Definition 1.14 are indistinguishable [65, 97]. In such a case, we say that the phase is not well-defined. On the other hand, for a bond-centered  $D_1$ , the trivial/nontrivial 1D representation is always well-defined.

Although we have been focusing on  $D_1$ , it is easy to see that the dimensional reduction approach applies to any point group symmetry. For example, consider the point group  $D_2 = \{1, \sigma_1, \sigma_2, \sigma_1\sigma_2\}$ , which are generated by two perpendicular mirror planes  $\sigma_1$  and  $\sigma_2$ . In 2D, after arriving at the 1D region  $r_0$  in Fig. 3.3 using  $\sigma_1$ , we can always further reduce  $r_0$  to a 0D region using  $\sigma_2$ , because a 1D region  $r_0$  with an on-site  $\mathbb{Z}_2$  symmetry is always trivial (i.e.,  $H^2[\mathbb{Z}_2, \text{U}(1)] = \{1\}$ ). In fact, there is the following proposition [65]:

**Proposition 3.4 (pgSPT in 2D)** *Except for the point group  $D_1$ , all the pgSPT phases in (2+1)D can be reduced to (0+1)D SPT phases by the dimensional reduction approach.*

This means that classifying a 2D short-range entangled state  $|\psi_{\text{GS}}\rangle$  protected by the point group  $G$  is essentially equivalent to classifying the 1D representation of  $G$  on  $|\psi_{\text{GS}}\rangle$ . However, there is one exception: the point group  $D_3$ . In general, the dihedral group  $D_n$  is isomorphic to the semidirect product group  $\mathbb{Z}_n \rtimes \mathbb{Z}_2$ , and [31]

$$H^1[\mathbb{Z}_n \rtimes \mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2 \times \mathbb{Z}_{[3+(-1)^n]/2}. \quad (3.7)$$

Hence  $D_3$  seems to result in a  $\mathbb{Z}_2$  classification, which is in fact not true:  $D_3$  only gives a trivial phase; see Sec. II.B in Ref. [65] for details. Table 3.1 gives the classification for the nine crystallographic point groups in 2D.

Similar to  $D_1$  in 1D, it is easily believed that for any pgSPT phases that can be reduced to (0+1)D SPT phases, the symmetry center matters. For such pgSPT phases to be well-defined, the symmetry centers should *not* be put on any microscopic DOF [65]. Be-



sides, for the same point group, different legal symmetry centers can result in different pgSPT phases. Let us use the state  $|\text{AKLT}_{2,\square}\rangle$  as an example; see Fig. 3.6. For  $|\text{AKLT}_{2,\square}\rangle$  with a plaquette-centered  $D_2$  symmetry, there are an even number of singlet bonds being reversed by a mirror reflection. However, for a bond-centered  $D_2$  symmetry, with respect to the mirror plane perpendicular to the central bond, there are an odd number of singlet bonds being reversed<sup>4</sup>, which results in a nontrivial representation of  $D_2$ . We thus see that in this example, the phase depends on the (legal) position of the symmetry center.<sup>5</sup> On the other hand, for the state  $|\text{AKLT}_{3,\triangle}\rangle$ , the bond-centered symmetry happens to be the only legal choice. As shown in Fig. 3.7,  $|\text{AKLT}_{3,\triangle}\rangle$  is in an SPT phase protected by  $D_2$ .

Note that  $D_1$  pgSPT phases in  $d \geq 2$  dimensions cannot be reduced to (0+1)D SPT phases, so the pgSPT phases are not classified by  $H^1[D_1 \cong \mathbb{Z}_2, \text{U}(1)]$ . In such cases, there is no restriction on the symmetry center of  $D_1$ .

From the above discussions, we arrive at the following corollary:

**Corollary 3.5 (absence of anomalous edge states)** *All the pgSPT phases in (1+1)D and (2+1)D have no anomalous edge states nor stable<sup>6</sup> string orders.*

This is because 0D SPT phases clearly has no anomalous edge states nor string orders. This also explains Table. 2.1.

In spatial dimension  $d \geq 3$ , the classification of pgSPT phases is more involved, because not all pgSPT phases can be reduced to 0D<sup>7</sup>. One can also generalize the idea of pgSPT phases to SPT phases protected by wallpaper groups or space groups, see Refs. [65, 101] for details.

<sup>4</sup>One might naively think that one single mirror plane alone (point group  $D_1$ ) is sufficient to distinguish the SPT from the trivial phase, which is indeed true in  $d = 1, 3$  spatial dimensions [49, 97]. However, let me emphasize that in the  $d = 2$  dimension,  $D_1$  symmetry alone can only give a trivial phase, because  $H^2[\mathbb{Z}_2, \text{U}(1)] = \{1\}$ .

<sup>5</sup>How can the same point group in the same system results in two distinct phases by only choosing a different symmetry center? The reason is that the plaquette-centered symmetry and the bond-centered symmetry are inequivalent in the sense that one symmetry alone does not imply the other. In the presence of translation symmetry, point groups centered in inequivalent positions are included in a larger space group (or wallpaper group). It is reasonable to say that the state  $|\text{AKLT}_{2,\square}\rangle$  is in an SPT phase protected by the wallpaper group  $p4m$ , since bond-centered  $D_2$  is a subgroup of  $p4m$ . See Ref [65] for the theory of wallpaper-group-protected phases.

<sup>6</sup>The state  $|\text{AKLT}\rangle$  has nonzero string order, but this string order is unstable under perturbations that do not have the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry.

<sup>7</sup>In  $d = 3$  dimension, we can allow symmetry centers sitting on microscopic DOF, because, for example, for  $D_1$ , there is  $H^2[\mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2$ .

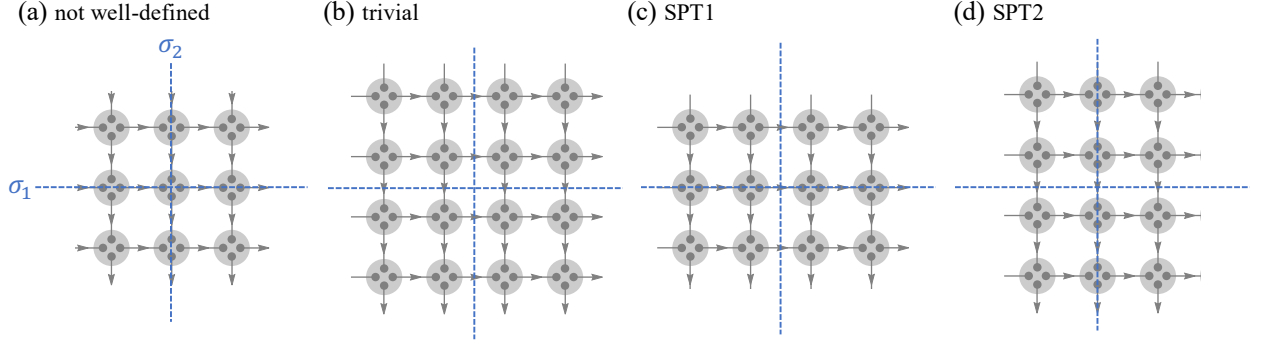


Figure 3.6: Spin-2 AKLT state on a square lattice  $|\text{AKLT}_{2,\square}\rangle$ . Meaning of the arrows is illustrated in Fig. 3.5(a). The state  $|\text{AKLT}_{2,\square}\rangle$  has  $D_2 = \{1, \sigma_1, \sigma_2, \sigma_1\sigma_2\}$  symmetry, but the phase depends on the symmetry center. (a) The SPT/trivial phase is not well defined for a site-centered symmetry. (b)  $|\text{AKLT}_{2,\square}\rangle$  results in a trivial 1D representation of a plaquette-centered  $D_2$ , so it is in a trivial phase. (c)  $|\text{AKLT}_{2,\square}\rangle$  is in an SPT phase protected by a vertical-bond-centered  $D_2$ , because it carries a nontrivial charge of  $U_{\sigma_2}$ . (d)  $|\text{AKLT}_{2,\square}\rangle$  is in an SPT phase protected by a horizontal-bond-centered  $D_2$ , because it carries a nontrivial charge of  $U_{\sigma_1}$ . The two SPT phases in (c) and (d) are different because their 1D representations are different.

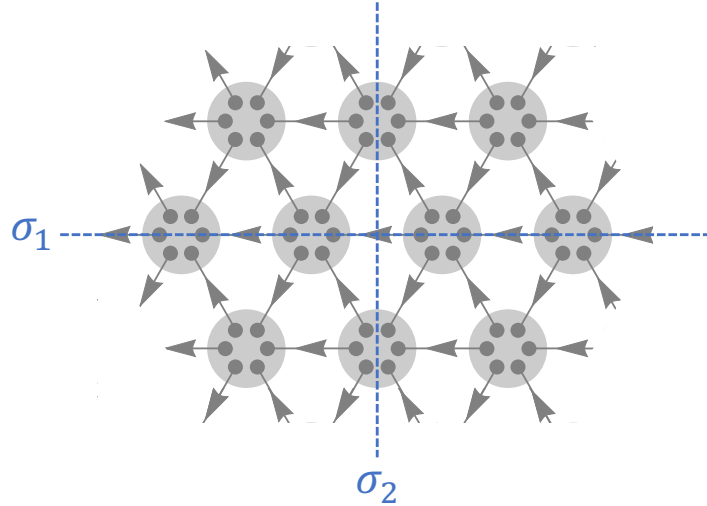


Figure 3.7: Spin-3 AKLT state on a triangular lattice  $|\text{AKLT}_{3,\triangle}\rangle$ . Meaning of the arrows is illustrated in Fig. 3.5(a).  $|\text{AKLT}_{3,\triangle}\rangle$  is in an SPT phase protected by a bond-centered  $D_2$ , because it carries a nontrivial charge of  $U_{\sigma_2}$ .

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## SPT PHASES IN SPINFUL BOSONS WITH A FLAT BAND

Ultracold atoms/molecules in optical lattices serve as an ideal platform for realizing topological quantum phases due to the high tunability of interactions, the viability of building various lattice structures, and the feasibility of directly measuring nonlocal order parameters [102, 103]. Motivated by recent experimental progress, many theoretical predictions about the existence of the Haldane phase in lattice systems of bosons [104–115] and fermions [116–125] have been made.

Alkali-metal atoms carry integer spins and are thus often treated as spinful bosons in experiments [126, 127]. Spinful bosons in optical lattices typically have both spin and charge<sup>1</sup> degrees of freedom (DOF). Free from the Pauli exclusion principle, one major difficulty of theoretically studying the systems of many-body spinful bosons lies in their immense Hilbert spaces (i.e., a huge number of DOF). Therefore, except for very few rigorous results [128, 129], various approximations or constraints have been employed to simplify the problem (i.e., to reduce the Hilbert-space dimension by freezing some DOF). In particular, to theoretically investigate the Haldane phase of bosonic atoms in 1D, there have been two main approaches. One is to study the effective spin Hamiltonians by focusing on the conventional Mott insulating limit where the charge DOF are frozen [115]; see also Sec. 4.1.3. For example, the system of Mott insulating spin-1 bosons is effectively described by the bilinear-biquadratic (BLBQ) model, whose ground state in 1D has been known to exhibit the Haldane phase in a wide parameter region [130]. The other approach is to study models that describe itinerant but spinless bosons. (A system is said to be itinerant if it has charge DOF.) In the itinerant case, it is generally believed that a sufficiently strong long-range (repulsive) interaction is indispensable for triggering the SPT

<sup>1</sup>"Charge" in this chapter refers to the particle number instead of the electric charge.

phase [104–112, 114]. The mechanism is as follows. At the filling of one spinless boson per site on average, if we truncate the particle number on each site to  $n = 0, 1, 2$ , one can define pseudo-spin as  $S^z := n - 1$ , thus resulting in an effective spin-1 model, where the long-range repulsion acts as an anisotropic spin exchange interaction [48, 105]. However, among bosonic alkali-metal atoms, although a relatively strong dipole-dipole interaction plays the role of long-range interaction in certain situations [126, 127], the dipole-dipole interaction is usually much weaker than the short-range  $s$ -wave collision, and thus the long-range interaction is typically negligible in many experiments [126, 127].

In short, despite the fact that itinerant, spinful, and short-range interacting bosonic atoms are very common in experiments, due to the difficulty of theoretically dealing with the huge amount of DOF, it remains an open question whether the SPT phases can be realized in such systems. Moreover, if the answer is yes, what kinds of SPT phases can we get? We address these issues and argue that, when there is a flat band at the bottom of the band structure (which we dub a *bottom flat band*), SPT phases can be realized with short-range interacting bosons that possess both unfrozen spin and charge DOF. As a result, the SPT phases in such systems are characterized by nontrivial spin or charge entanglement.

A flat band refers to an energy band that is independent of the quasimomentum. Usually, a flat band in an optical lattice is the highest band. However, by shaking the optical lattices, one can invert the sign of hopping [131–136], and the flat band thus becomes the lowest band. Such lattice shaking techniques have been realized experimentally [137–141].

Single-body eigenstates of a flat band can usually be chosen to be strictly localized on a finite number of lattice sites. Such eigenstates are termed as *compact localized states* (CLSs) [142, 143]. Different CLSs reside in different patches (regions) of the lattice. Short-range interaction ( $s$ -wave collision) between two bosons can happen only when their wave functions have a finite overlap. (This is natural, because the short-range interaction does not occur unless two particles are very close to each other.) At low temperatures, boson wave functions tend to avoid overlapping each other in order to lower the system's energy. Let  $X$  be a  $d$ -dimensional lattice with a bottom flat band and  $N$  unit cells. When  $N$  spin- $f$  bosons are loaded on  $X$ , the wave function overlaps can be minimized if each of the  $N$  CLSs hosts a boson. In other words,  $N$  bosons are distributed into  $N$  different patches. A boson is free to move around within a patch, which gives rise to charge fluctuations in the ground state. On the other hand, since all the patches (CLSs) are occupied by bosons (i.e., the whole lattice is fully "packed" with bosons), partial overlaps between neighboring wave functions are inevitable. We notice an analogy between the Hamiltonian that describes the short-range  $s$ -wave collision among spin- $f$  bosons and the spin- $f$  AKLT Hamiltonian. This analogy implies that the wave function overlaps will not cost

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energy, if the spins of bosons entangle in a clever way similar to a spin- $f$  AKLT state. (Intuitively, since the  $s$ -wave collision is spin-dependent by its nature, when the bosons are in a certain spin state, the collision between them can be avoided even if the bosons are very close to each other.) When certain parameters in the Hamiltonian are fine-tuned, the above configuration (lattice fully packed with CLSs) becomes the exact and unique ground state, and the state turns out to serve as a representative state of the symmetry-protected phases of the system. (In this chapter, the term "symmetry-protected phase" refers to either SPT or trivial phase.) We find that the phases are determined by the spin or charge fluctuations in the ground state. In this chapter, we find a large class of models whose ground states can be exactly written down when certain parameters are properly chosen. Each model has several on-site and crystalline symmetries. Depending on the symmetry, these exact ground states can be in either SPT or trivial phases. In particular, in terms of crystalline symmetries, charge fluctuations can play a nontrivial role.

This chapter will gradually build up a general framework on the SPT phases of spinful bosons with a flat band, starting from a simple 1D spin-1 model before progressing towards general dimensions and general spins. The remainder of this chapter is divided into three parts: Sec. 4.1, Sec. 4.2, and Sec. 4.3. Section 4.1 gives a background introduction to spinful bosons in optical lattice.

In Sec. 4.2, we use spin-1 bosons on the 1D sawtooth chain as a concrete example to demonstrate our argument. The sawtooth chain has two energy bands, and the bottom one is flat. We prove that when the interaction between spin-1 bosons is fine-tuned, the ground state is unique and can be exactly written down. The proof is based on the fact that the ground state can be exactly mapped to the 1D spin-1 AKLT state. This exact ground state turns out to be in a Haldane phase. Beyond the fine-tuned case, based on perturbation theory and numerical calculations, we confirmed that the Haldane phase exists in a rather broad parameter region.

In Sec. 4.3, we discuss the SPT phases with a general setup: short-range interacting spin- $f$  bosons on a bottom-flat-band lattice  $X$  in  $d$  dimensions. Let  $|\text{GS}_{f,X}\rangle$  be the many-body ground state. Let  $|\text{AKLT}_{f,X'}\rangle$  be the spin- $f$  AKLT state defined on a lattice  $X'$  (i.e., the ground state of the spin- $f$  AKLT model on  $X'$ ). With fine-tuned interactions,  $|\text{GS}_{f,X}\rangle$  can be exactly mapped to  $|\text{AKLT}_{f,X'}\rangle$ , provided that the lattice structures of  $X$  and  $X'$  satisfy a certain relation. This proves that  $|\text{GS}_{f,X}\rangle$  is the exact and unique ground state of the itinerant spin- $f$  model. The spin fluctuations of  $|\text{GS}_{f,X}\rangle$  are inherited from  $|\text{AKLT}_{f,X'}\rangle$ . Therefore, with respect to the spin rotation symmetry or the combination of spin rotation and translation symmetry, the  $d$ -dimensional symmetry-protected phase of  $|\text{GS}_{f,X}\rangle$  is identical to that of  $|\text{AKLT}_{f,X'}\rangle$ . Spins in  $|\text{AKLT}_{f,X'}\rangle$  are pinned to the lattice sites and cannot move. However,  $|\text{GS}_{f,X}\rangle$  is not a conventional Mott-insulating state (where a fixed number of bosons stay rigidly on each site), i.e., spin- $f$  bosons in

$|\text{GS}_{f,X}\rangle$  have nonvanishing charge fluctuations. It turns out that in terms of crystalline symmetries (i.e., point group or space group symmetries), both spin and charge fluctuations in  $|\text{GS}_{f,X}\rangle$  together determine its symmetry-protected phase. Hence, the crystalline-symmetry-protected phases of  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  may not be identical, because the charge fluctuations may play a nontrivial role in the former state. For example, as we will show later, interacting spin-3 bosons in the kagome lattice can be in an SPT phase protected by the point group  $D_2$  or  $D_3$ , and this SPT phase is purely a consequence of charge fluctuations at zero temperature.

This chapter is mainly based on my publication in Ref. [1].

## 4.1 Background: Ultracold spinful bosons in optical lattices

In reality, spinful (or spinor) bosons are atoms with integer hyperfine spin as an internal degree of freedom. Spinful bosons, when condensing in optical traps, interact with each other via spin-dependent scattering. When all particles are trapped in a single optical potential well, they form a continuous condensate (gas). *Spinful Bose-Hubbard models* physically refer to spinor bosons trapped in optical lattices (a set of discrete sites). Such systems can be viewed as the discrete versions of spinor boson gases.

The total spin  $S$  of an atom consists of two parts, the nuclear spin  $i$  and the total angular momentum  $j$  of partially filled electronic shell(s) <sup>2</sup>:

$$S = i + j. \quad (4.1)$$

For *alkali-metal atoms*, there is only a single electron in the outermost  $s$  orbital, so that  $j = 1/2$ . The two hyperfine spin levels  $f = |1/2 - i|$  and  $|1/2 + i|$  are not degenerate due to the hyperfine interaction  $V_{\text{hf}} = A i \cdot j$ . For most alkali-metal atoms, the level with smaller  $f$  has lower energy. This hyperfine energy splitting is much larger than the typical transition temperature of Bose–Einstein condensate (BEC)  $\sim 1\mu\text{K}$  [144]. Thus, the hyperfine spin  $f$  is a good quantum number. Table 4.1 shows how the hyperfine levels of some bosonic atoms are composed.

When atoms with  $f \neq 0$  are trapped in a magnetic potential, the degeneracy of each  $f$  is lost and the spin aligns along the magnetic field to lower the energy, which means that the internal degrees of freedom are frozen. The field operator  $\Psi(\mathbf{r})$  that annihilates an atom at position  $\mathbf{r}$  is therefore a scalar operator, and a scalar order parameter is used in the mean-field description. In contrast, when atoms are far-off resonance optically trapped, the internal degrees of freedom of atoms are liberated. In such cases one refers

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<sup>2</sup>According to Hund’s rules, a fully-filled electronic shell has  $s = l = 0$ , where  $s$  and  $l$  are the total spin and total orbital angular momentum of the shell, respectively. Hence  $j = s + l = 0$  for fully-filled shells.

to spinor atoms. Now the field operator  $\Psi(\mathbf{r})$  for hyperfine level  $f$  should have  $2f + 1$  components. Correspondingly, in the mean-field description, the order parameter should also be a vector over  $\mathbb{C}^{2f+1}$ .

atom	$s$	$l$	$j = s + l$	$i$	$f$
$^1\text{H}$	1/2	0	1/2	1/2	0, 1
$^7\text{Li}, ^{23}\text{Na}, ^{39}\text{K}, ^{41}\text{K}, ^{87}\text{Rb}$	1/2	0	1/2	3/2	1, 2
$^{85}\text{Rb}$	1/2	0	1/2	5/2	2, 3
$^{133}\text{Cs}$	1/2	0	1/2	7/2	3, 4

Table 4.1: List of some alkali-metal isotopes, where  $s$  and  $l$  are the total spin and the total orbital angular momentum quantum numbers of partially filled shell(s), respectively [126].

#### 4.1.1 Interaction between spinor bosons

In ultracold atom experiments, the atom density is usually very low, which makes it enough to consider only two-body interactions. The form of two-body interaction can be directly derived from two symmetry constraints. First, the interaction must be  $\text{SO}(3)$  rotationally invariant, i.e., the interaction can only depend on the total spin of two interacting atoms and not on the spatial orientation. Second, we assume that any two atoms interact via  $s$ -wave scattering, which means that the two-body spatial wave function is symmetric; then their total spin quantum number  $S$  can only take even values ( $S = 0, \dots, 2f - 2, 2f$ ) for two spin- $f$  bosonic atoms, while  $S$  must be odd for two spin- $f$  fermions. This guarantees that the quantum state of bosons and fermions are symmetric and antisymmetric, respectively. For the rest of this thesis we only focus on the interaction between identical spin- $f$  bosons, and therefore, from the above two symmetry constraints, the interaction of a many-body system must be of the form

$$H_{\text{int}} = \frac{1}{2} \sum_{i \neq j} \sum_{S=0,2,\dots,2f} v_S(\mathbf{r}_i - \mathbf{r}_j) P_{ij}^{(S)}, \quad (4.2)$$

where  $i$  and  $j$  are indices that label individual atoms,  $v_S$  is the interaction potential for the total spin  $S$  channel, and  $P_{ij}^{(S)}$  is the operator that projects the spin state of atoms  $i$  and  $j$  onto the subspace of the total spin  $S$ . The projection operator can be explicitly written as

$$P_{ij}^{(S)} = \sum_{M=-S}^S |S, M\rangle_{ij} \langle S, M| = \prod_{k=0,1,2,\dots,f \text{ \& } k \neq S/2} \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_{2k}}{\lambda_S - \lambda_{2k}}, \quad (4.3)$$

where  $|S, M\rangle_{ij}$  is the state with the total spin  $S$  and the Zeeman level  $M$ ,  $\mathbf{S}_i$  is the spin- $f$  operator for atom  $i$ , and  $\lambda_k = [k(k+1) - 2f(f+1)]/2$ ; see Appendix A for details. When ex-



pressed in terms of spin operators, it is clear that  $P_{ij}^{(S)}$  has  $\text{SO}(3)$  symmetry. Equation (4.3) follows from the identity [145]

$$(\mathbf{S}_i \cdot \mathbf{S}_j)^n = \sum_{S=0,2,\dots,2f} \lambda_S^n P_{ij}^{(S)}, \quad (4.4)$$

where  $n = 0, 1, 2, \dots, f$ . See also Appendix A in Ref. [146]. It is worth noting that taking  $n = 0$  in Eq. (4.4) yields the completeness relation. Defining

$$P^{(S)}(\mathbf{r}, \mathbf{r}') := \sum_{(i,j) \in \{(i,j) | \mathbf{r}_i = \mathbf{r}, \mathbf{r}_j = \mathbf{r}', i \neq j\}} P_{ij}^{(S)}, \quad (4.5)$$

we can therefore rewrite the interaction in Eq. (4.2) as <sup>3</sup>

$$H_{\text{int}} = \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \sum_{\mathcal{F}=0,2,\dots,2f} v_S(\mathbf{r} - \mathbf{r}') P^{(S)}(\mathbf{r}, \mathbf{r}'). \quad (4.6)$$

For alkali-metal atoms, the interaction potential  $v_S$  is usually approximated as

$$v_S(\mathbf{r}_i - \mathbf{r}_j) = g_S \delta(\mathbf{r}_i - \mathbf{r}_j), \quad (4.7)$$

where  $g_S = \frac{4\pi\hbar^2}{M} a_S$  is the interaction strength of total spin  $S$  channel and  $a_S$  is the  $s$ -wave scattering length [126, 144]. The interaction Hamiltonian then becomes

$$H_{\text{int}} = \frac{1}{2} \int d\mathbf{r} \sum_{S=0,2,\dots,2f} g_S P^{(S)}(\mathbf{r}, \mathbf{r}). \quad (4.8)$$

For  $f = 1$  bosons, by taking  $n = 0$  and 1 in Eq. (4.4), we get the solution

$$\begin{aligned} P^{(0)}(\mathbf{r}, \mathbf{r}) &= \sum_{i \neq j} P_{ij}^{(0)} = -\frac{1}{3} \sum_{i \neq j} [\mathbf{S}_i(\mathbf{r}) \cdot \mathbf{S}_j(\mathbf{r}) - 1] = \frac{1}{3} [-\mathbf{S}^2(\mathbf{r}) + n^2(\mathbf{r}) + n(\mathbf{r})], \\ P^{(2)}(\mathbf{r}, \mathbf{r}) &= \sum_{i \neq j} P_{ij}^{(2)} = \frac{1}{3} \sum_{i \neq j} [\mathbf{S}_i(\mathbf{r}) \cdot \mathbf{S}_j(\mathbf{r}) + 2] = \frac{1}{3} [\mathbf{S}^2(\mathbf{r}) + 2n^2(\mathbf{r}) - 4n(\mathbf{r})], \end{aligned} \quad (4.9)$$

where  $n(\mathbf{r})$  is the boson number at position  $\mathbf{r}$  and  $\mathbf{S}(\mathbf{r}) = \sum_{i=1}^{n(\mathbf{r})} \mathbf{S}_i(\mathbf{r})$  is the total spin operator at  $\mathbf{r}$ . Similarly, for  $f = 2$  bosons, from the identities given by  $n = 0$  and 1 in Eq. (4.4), we get

$$\begin{aligned} P^{(2)}(\mathbf{r}, \mathbf{r}) &= \frac{1}{7} [-\mathbf{S}^2(\mathbf{r}) - 10P^{(0)}(\mathbf{r}, \mathbf{r}) + 4n^2(\mathbf{r}) + 2n(\mathbf{r})], \\ P^{(4)}(\mathbf{r}, \mathbf{r}) &= \frac{1}{7} [\mathbf{S}^2(\mathbf{r}) + 3P^{(0)}(\mathbf{r}, \mathbf{r}) + 3n^2(\mathbf{r}) - 9n(\mathbf{r})]. \end{aligned} \quad (4.10)$$

Let us introduce the field operator  $\Psi(\mathbf{r}) = (\psi_{-f}(\mathbf{r}), \dots, \psi_f(\mathbf{r}))$  whose components satisfy the following canonical commutation relations:

$$\begin{aligned} [\psi_m(\mathbf{r}), \psi_n^\dagger(\mathbf{r}')] &= \delta_{mn} \delta(\mathbf{r} - \mathbf{r}'), \\ [\psi_m(\mathbf{r}), \psi_n(\mathbf{r}')] &= [\psi_m^\dagger(\mathbf{r}), \psi_n^\dagger(\mathbf{r}')] = 0, \end{aligned} \quad (4.11)$$

<sup>3</sup>Note that within this subsection,  $i$  and  $j$  label individual atoms instead of their space coordinates. Suppose that there are  $n$  bosons in the same position  $\mathbf{r}_1 = \mathbf{r}_2 = \dots = \mathbf{r}_n = \boldsymbol{\eta}$ ; then  $\boldsymbol{\eta}$  is summed over  $n$  times in Eq. (4.2), while  $\mathbf{r} = \boldsymbol{\eta}$  is summed over only once in Eq. (4.6).



where  $\psi_m(\mathbf{r})$  annihilates a boson with the Zeeman level  $m = -f, \dots, f$  at position  $\mathbf{r}$ . The second-quantized form of the spin operator  $\mathbf{S}(\mathbf{r}) = (S^x(\mathbf{r}), S^y(\mathbf{r}), S^z(\mathbf{r}))$  and the number operator  $n(\mathbf{r})$  are then given by

$$\begin{aligned} S^\alpha(\mathbf{r}) &= \sum_{m,n} S_{mn}^\alpha \psi_m^\dagger(\mathbf{r}) \psi_n(\mathbf{r}), \\ n(\mathbf{r}) &= \sum_m \psi_m^\dagger(\mathbf{r}) \psi_m(\mathbf{r}), \end{aligned} \quad (4.12)$$

where  $S_{mn}^\alpha$  is the spin matrix for spin- $f$  and  $\alpha = x, y, z$ . In general, the projection operator in the second-quantized form is given by

$$P^{(S)}(\mathbf{r}, \mathbf{r}') = \sum_{M=-S}^S A_{S,M}^\dagger(\mathbf{r}, \mathbf{r}') A_{S,M}(\mathbf{r}, \mathbf{r}'), \quad (4.13)$$

where

$$A_{S,M}(\mathbf{r}, \mathbf{r}') := \sum_{m_1, m_2=-f}^f \langle S, M | f, m_1; f, m_2 \rangle \psi_{m_1}(\mathbf{r}) \psi_{m_2}(\mathbf{r}') \quad (4.14)$$

with  $\langle S, M | f, m_1; f, m_2 \rangle$  being the Clebsch–Gordan coefficient. In other words,  $A_{S,M}(\mathbf{r}, \mathbf{r}')$  is the operator that annihilates a pair of bosons at position  $\mathbf{r}$  and  $\mathbf{r}'$  with total spin  $S$ . For example, the singlet annihilation operator is

$$A_{0,0}(\mathbf{r}, \mathbf{r}') = \frac{1}{\sqrt{2f+1}} \sum_{m=-f}^f (-1)^{f-m} \psi_m(\mathbf{r}) \psi_{-m}(\mathbf{r}'). \quad (4.15)$$

The completeness relation reads

$$\sum_{S=0,2,\dots,2f} P^{(S)}(\mathbf{r}, \mathbf{r}') =: n(\mathbf{r}) n(\mathbf{r}') :, \quad (4.16)$$

where the symbol  $: :$  denotes normal ordering of creation and annihilation operators.

The kinetic energy and one-body potential are respectively expressed as [144]

$$\begin{aligned} H_{\text{KE}} &= \int d\mathbf{r} \sum_m \psi_m^\dagger(\mathbf{r}) \left( -\frac{\hbar^2 \nabla^2}{2M} \right) \psi_m(\mathbf{r}), \\ H_{\text{PE}} &= \int d\mathbf{r} \sum_m V(\mathbf{r}) \psi_m^\dagger(\mathbf{r}) \psi_m(\mathbf{r}). \end{aligned} \quad (4.17)$$

Finally, we sum over Eq. (4.8) and Eq. (4.17):

$$H = H_{\text{KE}} + H_{\text{PE}} + H_{\text{int}}. \quad (4.18)$$

The Hamiltonians of spinor bosons always conserve the total particle number. In the absence of a magnetic field, the Hamiltonians do not depend on the spatial orientation, which means that the total spin is conserved too. The full symmetry group of the Hamiltonians of spinor bosons without a magnetic field is thus [147]

$$G = \text{U}(1) \times \text{SO}(3). \quad (4.19)$$

An element of  $G$  can be expressed with the combination of the Euler rotation  $e^{-i\alpha S_{\text{tot}}^z} e^{-i\beta S_{\text{tot}}^y} e^{-i\gamma S_{\text{tot}}^z}$  and the gauge transformation  $e^{i\phi}$ , where  $\alpha, \beta, \gamma$  are the Euler angles and  $\phi$  is the global phase.

### 4.1.2 Spin- $f$ Bose-Hubbard models

When spin- $f$  bosons are trapped in lattice systems, say, optical lattices, the Hamiltonian Eq. (4.18) effectively reduces to the *spin- $f$  Bose-Hubbard model*. Given a set of lattice sites, we define a set of bosonic operators that satisfy

$$\begin{aligned} [a_{i,\alpha}, a_{j,\beta}^\dagger] &= \delta_{ij} \delta_{\alpha\beta} \\ [a_{i,\alpha}, a_{j,\beta}] &= [a_{i,\alpha}^\dagger, a_{j,\beta}^\dagger] = 0, \end{aligned} \quad (4.20)$$

where  $a_{i,\alpha}^\dagger$  creates a spin- $f$  boson at the Zeeman level  $\alpha = -f, \dots, f$  with the spatial wave function localized at site  $i$ . We assume that the spatial wave function is independent of  $\alpha$ . Similarly to Eq. (4.13), the second-quantized projection operators at site  $i$  are given by <sup>4</sup>

$$P_i^{(S)} = \sum_{M=-S}^S A_{S,M}^\dagger(i) A_{S,M}(i), \quad (4.22)$$

where

$$A_{S,M}(i) := \frac{1}{\sqrt{2}} \sum_{\alpha, \beta=-f}^f \langle S, M | f, \alpha; f, \beta \rangle a_{i,\alpha} a_{i,\beta} \quad (4.23)$$

with  $\langle S, M | f, \alpha; f, \beta \rangle$  being the Clebsch–Gordan coefficient. For example, the singlet annihilation operator is

$$A_{0,0}(i) = \frac{1}{\sqrt{2(2f+1)}} \sum_{\alpha=-f}^f (-1)^{f-\alpha} a_{i,\alpha} a_{i,-\alpha}. \quad (4.24)$$

Other operators can also be expressed in terms of  $a^\dagger$  and  $a$ . For example, at site  $i$ , the number operator  $n_i$  and the spin  $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$  are given by

$$\begin{aligned} n_i &= \sum_{\alpha} a_{i,\alpha}^\dagger a_{i,\alpha}, \\ S_i^m &= \sum_{\alpha, \beta} S_{\alpha, \beta}^m a_{i,\alpha}^\dagger a_{i,\beta}, \end{aligned} \quad (4.25)$$

where  $S_{\alpha, \beta}^m$  is the spin matrix for spin- $f$  and  $m = x, y, z$ . The completeness relation in Eq. (4.16) now reads

$$\sum_{S=0,2,\dots,2f} P_i^{(S)} = \frac{1}{2} n_i (n_i - 1). \quad (4.26)$$

It follows from Eq. (4.9) that for spin-1 bosons,

$$\begin{aligned} P_i^{(0)} &= \frac{1}{6} (-\mathbf{S}_i^2 + n_i^2 + n_i), \\ P_i^{(2)} &= \frac{1}{6} (\mathbf{S}_i^2 + 2n_i^2 - 4n_i). \end{aligned} \quad (4.27)$$

---

<sup>4</sup>Let  $\mathbf{r}$  be the position of site  $i$ , then

$$\begin{aligned} P_i^{(S)} &= \frac{1}{2} P^{(S)}(\mathbf{r}, \mathbf{r}), \\ A_{S,M}(i) &= \frac{1}{\sqrt{2}} A_{S,M}(\mathbf{r}, \mathbf{r}). \end{aligned} \quad (4.21)$$

See Eq. (4.13) and Eq. (4.14).

Similarly, it follows from Eq. (4.10) that for spin-2 bosons, we have

$$\begin{aligned} P_i^{(2)} &= \frac{1}{14} \left( -S_i^2 - 20P_i^{(0)} + 4n_i^2 + 2n_i \right), \\ P_i^{(4)} &= \frac{1}{14} \left( S_i^2 + 6P_i^{(0)} + 3n_i^2 - 9n_i \right). \end{aligned} \quad (4.28)$$

In this formalism, it is natural that the two-body total spin quantum number  $S$  cannot be odd, because particles on the same site are assumed to have the same spatial wave function, but  $S = \text{odd}$  spin states are antisymmetric. Thus,  $S$  can only be even to guarantee the two-body bosonic state being symmetric. For example, if one tries to make an  $S = 1$  (triplet) state using two spin-1 bosons at site  $i$ , one will get nothing but zero:

$$\begin{aligned} A_{1,1}(i) &= a_{i,1}a_{i,0} - a_{i,0}a_{i,1} \equiv 0, \\ A_{1,0}(i) &= a_{i,1}a_{i,-1} - a_{i,-1}a_{i,1} \equiv 0, \\ A_{1,-1}(i) &= a_{i,-1}a_{i,0} - a_{i,0}a_{i,-1} \equiv 0. \end{aligned} \quad (4.29)$$

On the other hand,  $S = 0, 2$  states of two spin-1 bosons are always symmetric (ignore site index  $i$  in the following):

$$\begin{aligned} A_{0,0} &= \frac{1}{\sqrt{6}}(a_0a_0 - 2a_1a_{-1}), \\ A_{2,2} &= \frac{1}{\sqrt{2}}a_1a_1, \\ A_{2,1} &= a_0a_1, \\ A_{2,0} &= \frac{1}{\sqrt{3}}(a_0a_0 + a_1a_{-1}), \\ A_{2,-1} &= a_0a_{-1}, \\ A_{2,-2} &= \frac{1}{\sqrt{2}}a_{-1}a_{-1}. \end{aligned} \quad (4.30)$$

In the absence of a magnetic field, the Hamiltonian of the spin- $f$  Bose-Hubbard model is

$$H = - \sum_{i,j} t_{i,j} a_{i,\alpha}^\dagger a_{j,\alpha} + \sum_i V_i n_i + \sum_i \sum_{S=0,2,\dots,2f} g_S P_i^{(S)}, \quad (4.31)$$

where  $t_{i,j}$  is the hopping constant and  $V_i$  is the on-site potential. In general, the symmetry group  $G$  of such spinor Bose-Hubbard models follows from Eq. (4.19), which is  $U(1) \times SO(3)$ . Defining the total spin operator  $S_{\text{tot}} := \sum_i S_i$ , we can express an element of  $G$  as  $e^{i\phi} e^{-i\alpha S_{\text{tot}}^z} e^{-i\beta S_{\text{tot}}^y} e^{-i\gamma S_{\text{tot}}^z}$ , where  $\phi$  is the global phase and  $\alpha, \beta, \gamma$  are the Euler angles.

### 4.1.3 Effective spin models

For small but nonzero nearest-neighbor hopping  $t/g_S \ll 1$ , we can treat the hopping term as a perturbation and derive the effective Hamiltonian. The effective Hamiltonian should

preserve the symmetry of the original spinor (spinful) Bose-Hubbard model. For simplicity, we assume all the coefficients (including hopping and on-site potential) are site-independent in the following.

For spin-1 bosons, assuming  $g_2 - g_0 > 0$  and an unperturbed ground state given by  $n = 2k + 1$  bosons on each site, the total spin on each site is thus one [148]. Up to two-body interactions (second-order perturbation), the most general spin Hamiltonian that preserves the  $\text{SO}(3)$  symmetry is [149, 150]

$$H_{\text{eff1}} = \sum_{S=0,1,2} \epsilon_S \sum_{\langle i,j \rangle} P_{i,j}^{(S)}, \quad (4.32)$$

where  $P_{i,j}^{(S)}$  projects the state of two neighboring sites onto the state with total spin  $S$ . [Note that  $P_{i,j}^{(S)}$  is *different* from  $P_{ij}^{(S)}$  in Eq. (4.3).] On the other hand, in terms of spin operators, the most general  $\text{SO}(3)$ -invariant Hamiltonian should be of the form

$$H_{\text{BLBQ}} = \sqrt{a^2 + b^2} \sum_{\langle i,j \rangle} \left[ \cos \theta (\mathbf{S}_i \cdot \mathbf{S}_j) + \sin \theta (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \right] + c, \quad (4.33)$$

$$\theta = \arctan \frac{b}{a}.$$

There is no need to add higher order terms, such as  $(\mathbf{S}_i \cdot \mathbf{S}_j)^3$ , to  $H_{\text{BLBQ}}$ , because the product of any three spin operators for a spin-1 particle can always be expressed via the second order, first order, and constant terms [149]. The Hamiltonian  $H_{\text{BLBQ}}$  is more often referred to as the bilinear-biquadratic (BLBQ) model. From the identity (see Appendix A)

$$P_{i,j}^{(S)} = \prod_{k=0, \neq S}^{2f} \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_k}{\lambda_S - \lambda_k}, \quad (4.34)$$

$$\lambda_S = \frac{1}{2} [S(S+1) - 2f(f+1)],$$

where the coefficients in  $H_{\text{eff1}} \equiv H_{\text{BLBQ}}$  are related to each other by

$$\begin{aligned} \sqrt{a^2 + b^2} \sin \theta &= \frac{1}{3} \epsilon_0 - \frac{1}{2} \epsilon_1 + \frac{1}{6} \epsilon_2, \\ \sqrt{a^2 + b^2} \cos \theta &= -\frac{1}{2} \epsilon_1 + \frac{1}{2} \epsilon_2, \\ c &= -\frac{1}{3} \epsilon_0 - \epsilon_1 + \frac{1}{3} \epsilon_2. \end{aligned} \quad (4.35)$$

The parameters  $\epsilon_{0,1,2}$  can be obtained by perturbation theory<sup>5</sup>.

<sup>5</sup>A calculation gives [149, 150]

$$\epsilon_0 = -\frac{4t^2(k+1)(2k+3)}{3(c_0 - 2c_2)} - \frac{16t^2k(5+2k)}{15(c_0 + 4c_2)}, \epsilon_1 = -\frac{4t^2k(5+2k)}{5(c_0 + 4c_2)}, \epsilon_2 = -\frac{28t^2k(5+2k)}{75(c_0 + 4c_2)} - \frac{4t^2(15+20k+8k^2)}{15(c_0 + c_2)},$$

where  $c_0 = (g_0 + 2g_2)/3$  and  $c_2 = (g_2 - g_0)/3$ . Note that when there is only one boson per site,  $k = 0$  yields  $\epsilon_1 = 0$ . Physically, this means that any intermediate virtual state in which two spin-1 bosons form a triplet state on the same site is forbidden, as demonstrated in Eq. (4.29).

The phase diagram of the 1D spin-1 BLBQ model is shown in Fig. 4.1. The region  $-\pi/4 < \theta < \pi/4$  corresponds to the Haldane phase. At a special point  $\tan \theta = 1/3$ , the ground state is exactly solvable and the Hamiltonian is referred to as the AKLT model [45, 46]. On the other hand, the Hamiltonians with  $\theta = \pi/4$  and  $\theta = -\pi/4$  are referred to as the *Uimin-Lai-Sutherland model* [151–153] and the *Takhtajan-Babujian model* [154–156], respectively. In both cases the models are integrable by the Bethe ansatz and found to be gapless. The low-energy physics of the Takhtajan-Babujian model is described by the conformal field theory (CFT) with central charge  $c = 3/2$  [154–156].

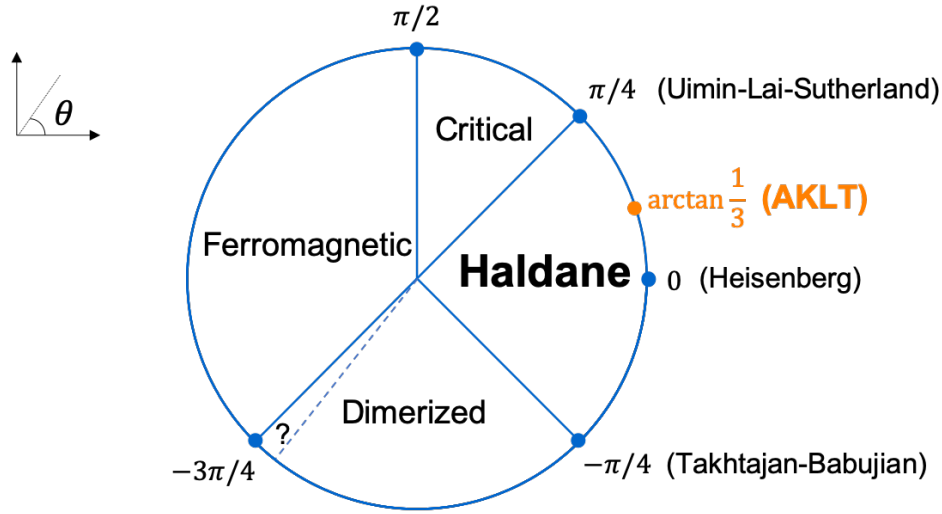


Figure 4.1: Phase diagram of the 1D spin-1 BLBQ model [157]. The question mark "?" stands for a nematic phase whose existence is still under debate.

For the spin-2 Bose-Hubbard model, we only consider one boson per site in the unperturbed ground state for simplicity. Up to two-body interactions (second-order perturbation), the most general spin Hamiltonian that preserves the  $SO(3)$  symmetry is [150, 158, 159]

$$H_{\text{eff}2} = \sum_{S=0,1,2,3,4} \epsilon_S \sum_{\langle i,j \rangle} P_{i,j}^{(S)}, \quad (4.36)$$

where the operator  $P_{i,j}^{(S)}$  projects two spin-2 bosons on neighboring sites  $i, j$  onto the subspace of the total spin  $S$ . Note that in the case of one boson per site,  $\epsilon_1 = \epsilon_3 = 0$ , because any intermediate virtual state in which two spin-2 bosons form an  $S = \text{odd}$  state on the same site is forbidden. The parameters  $\epsilon_{0,2,4}$  can be obtained by perturbation theory.<sup>6</sup> Again,  $P_{i,j}^{(S)}$  can be explicitly expressed by spin-2 operators according to Eq. (4.34).

<sup>6</sup>A direct calculation yields

$$\epsilon_0 = -\frac{4t^2}{c_0 + c_2 - 6c_1}, \epsilon_2 = -\frac{4t^2}{c_0 - 3c_1}, \epsilon_4 = -\frac{4t^2}{c_0 + 4c_1},$$

where  $c_0 = (4g_2 + 3g_4)/7$ ,  $c_1 = (g_4 - g_2)/7$ ,  $c_2 = (7g_0 - 10g_2 + 3g_4)/7$ .

## 4.2 A (1+1)D example: Spin-1 bosons on a sawtooth chain

Let us start from a simple but nontrivial model: the *spin-1 Bose-Hubbard model on the sawtooth chain (BHMSC)*.

### 4.2.1 Hamiltonian and exact ground states

Spin-1 atoms in optical lattices are effectively described by the spin-1 Bose-Hubbard model [160, 161], whose explicit form is obtained by taking  $f = 1$  in Eq. (4.31):

$$\begin{aligned} H &= H_{\text{hop}} + H_{\text{int}}, \\ H_{\text{hop}} &= - \sum_{\langle r, r' \rangle} \sum_{\alpha=-1}^1 t_{r, r'} a_{r, \alpha}^\dagger a_{r', \alpha} + \sum_r V_r n_r, \\ H_{\text{int}} &= \sum_r \left( g_{0, r} P_r^{(0)} + g_{2, r} P_r^{(2)} \right). \end{aligned} \quad (4.37)$$

The explicit form of the projection operator  $P_r^S$  is presented in Eqs. (4.22) and (4.27). We have assumed here that the interaction strength  $g_{S, r}$  can depend on the position  $r$ . As we will see later that in order to have an exact GS,  $g_{S, r}$  needs to be position-dependent. However, in order to realize an SPT phase,  $g_{S, r}$  does not have to depend on  $r$ , as suggested by the numerical calculation and the perturbation theory; see Sec. 4.2.3. We also assume the interaction strength  $g_{S, r} \geq 0$  as is the case of long-lived alkali-metal spin-1 condensates [126, 127];  $H_{\text{int}}$  is thus positive semidefinite.

On a sawtooth chain (see Fig. 4.2) with  $N$  unit cells ( $2N$  sites), the single-body Hamiltonian can be written in a compact form as [162–164]

$$H_{\text{hop}} = H_{\text{saw}} = \sum_{i=1}^N \sum_{\alpha=-1}^1 L_{i, \alpha}^\dagger L_{i, \alpha}, \quad (4.38)$$

where  $L_{i, \alpha}^\dagger := a_{2i-1, \alpha}^\dagger + \lambda a_{2i, \alpha}^\dagger + a_{2i+1, \alpha}^\dagger$  determines the values of  $t_{r, r'}$  and  $V_r$  in Eq. (4.37), and we assume  $\lambda \in \mathbb{R} \setminus \{0\}$ . The periodic boundary condition (PBC) has been imposed.  $H_{\text{saw}}$  is positive semi-definite, and it has two energy bands: a dispersive band with energy  $\lambda^2 + 2 + 2 \cos k > 0$  and a flat band with exactly zero energy. Every eigenstate of the flat band can be chosen to be localized on three sites (see Fig. 4.2):

$$B_{j, \alpha}^\dagger := \frac{1}{\sqrt{\lambda^2 + 2}} (a_{2j, \alpha}^\dagger - \lambda a_{2j+1, \alpha}^\dagger + a_{2j+2, \alpha}^\dagger), \quad (4.39)$$

where  $B_{j, \alpha}^\dagger$  creates a particle in a zero-energy eigenstate. In other words,  $B_{j, \alpha}^\dagger$  is a CLS creation operator. An experimental scheme for realizing an optical sawtooth chain has been proposed [165].

Note that lattices with a bottom flat band (and CLSs) widely exist; they can actually be constructed systematically, see Sec. 4.3.2.

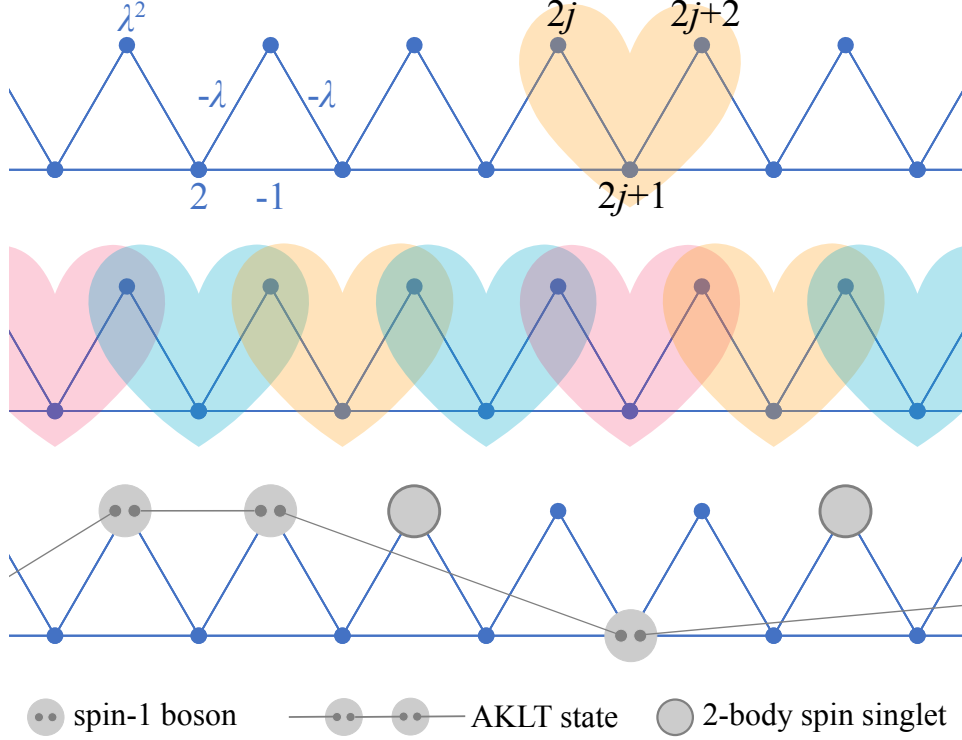


Figure 4.2: (Upper panel) The sawtooth lattice and one of its zero-energy state. The state is localized on three consecutive sites covered by the heart shape. The blue characters indicate the values of  $t_{r,r'}$  and  $V_r$ . (Middle panel) The state  $|\beta\rangle$  in Eq. (4.46) with a typical choice of  $\beta$ . Three different colors denote three different magnetic sublevels. Linearly independent CLSs cover the whole lattice, and two neighboring CLSs overlap on a top site. (Lower panel) The "hidden AKLT order" illustrated by a typical component of  $|\text{GS}\rangle$  in Eq. (4.55).

From now on, the total particle number on the sawtooth chain is assumed to be the same as the number of unit cells  $N$ . For simplicity, we also assume translation symmetry:

$$g_{S,r} = \begin{cases} g_S^t & \text{for top sites (r=even),} \\ g_S^b & \text{for bottom sites (r=odd).} \end{cases} \quad (4.40)$$

The phase diagram of the spin-1 BHMSC with respect to  $(g_0^t, g_2^t, 1/\lambda)$  is shown in Fig. 4.3(a).

For later purposes, let us recall the 1D spin-1 BLBQ model with PBC, whose Hamiltonian is given by [130]

$$\begin{aligned} H_{\text{BLBQ}} &= \sum_{j=1}^N \left( \tilde{g}_0 P_{j,j+1}^{(0)} + \tilde{g}_1 P_{j,j+1}^{(1)} + \tilde{g}_2 P_{j,j+1}^{(2)} \right), \\ &= J \sum_{j=1}^N \left[ \cos \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 \right] + c, \end{aligned} \quad (4.41)$$

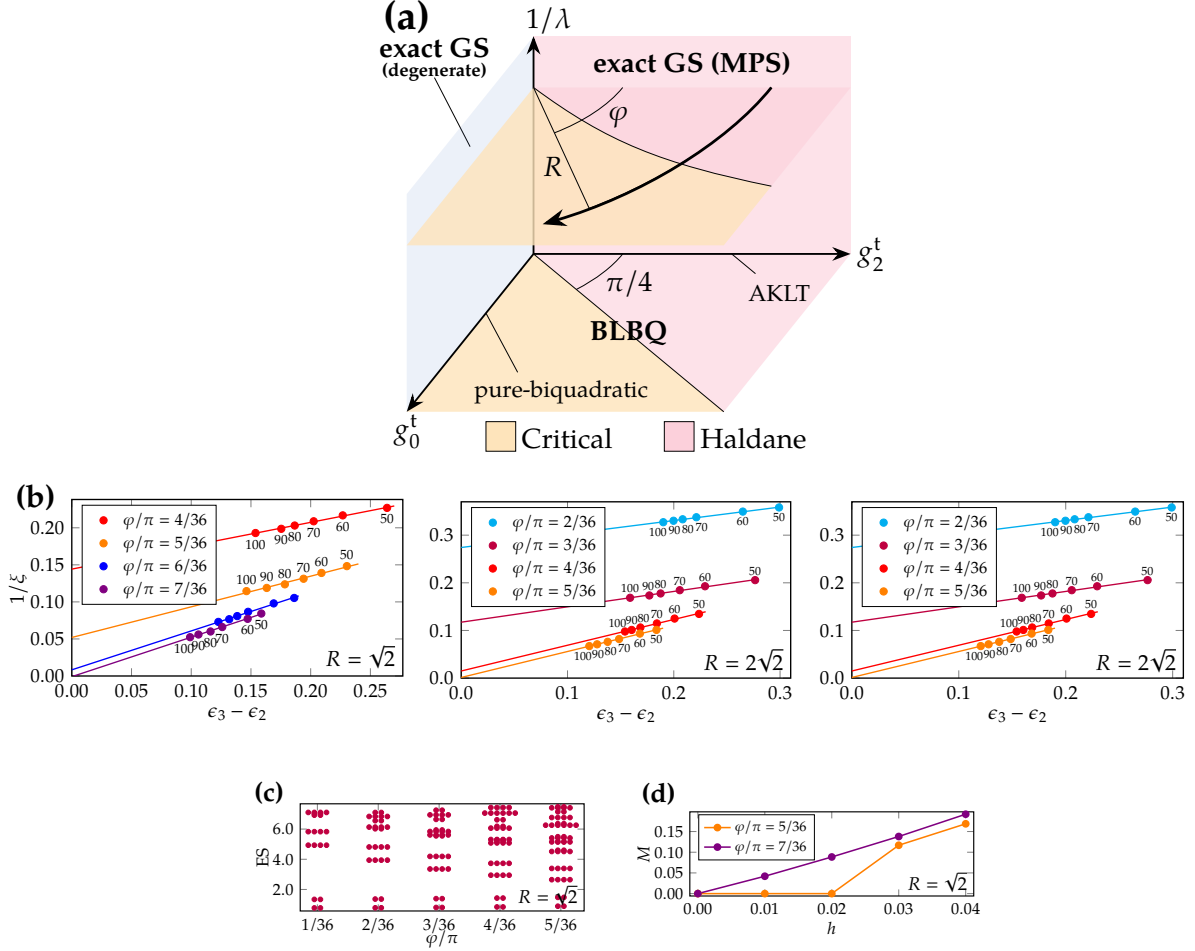


Figure 4.3: (a) Schematic phase diagram of spin-1 bosons on a sawtooth chain (in the thermodynamic limit  $N \rightarrow \infty$ ) in the parameter space  $(g_0^t, g_2^t, 1/\lambda)$ . In the phase diagram we have assumed  $g_0^t, g_2^t, \lambda \geq 0$  and  $g_0^b = g_2^b = 1/\lambda^2$ . In the  $g_0^t = 0$  plane,  $H$  has an exact and unique ground state (GS) given in Eq. (4.55). In the  $g_2^t = 0$  plane, the GS is massively degenerate, and the ferromagnetic states in Eq. (4.58) are exact ground states. Phase diagram in the  $1/\lambda \rightarrow 0$  plane, derived by perturbation theory, coincides with the phase diagram of the BLBQ model. Phase diagram in the  $1/\lambda = 1$  plane is determined by the numerical calculation based on the VUMPS algorithm. In particular, numerical results along the curved arrow parameterized by  $(\sqrt{2} \sin \varphi, \sqrt{2} \cos \varphi, 1)$  are shown in (b)–(d). (b) As we change the bond dimension, we calculate the scaling of the inverse correlation length  $1/\xi := \epsilon_2$  with respect to  $\epsilon_3 - \epsilon_2$  along the path parameterized by  $(R \sin \varphi, R \cos \varphi, 1)$ . We can see that when  $R = \sqrt{2}$ , a quantum phase transition occurs between  $\varphi = 6\pi/36$  and  $7\pi/36$ . As  $R$  grows, the phase transition occurs at smaller  $\varphi$ , which indicates that the phase boundary is curved instead of straight. Numbers near the data points denote the corresponding bond dimensions of each block, see Appendix E of Ref. [1] for details of the numerical calculation. (c) The whole entanglement spectrum (ES) in the Haldane phase region shows the even-fold degeneracy. For clarity, here we present only the lowest part of the ES. (d) Magnetization  $M$  with respect to the applied magnetic field  $h$  in the  $z$ -direction. In (c) and (d), the bond dimension of each block is 50 [1].



where  $P_{j,j+1}^{(S)}$  projects the state of two neighboring sites onto the state with total spin  $S = 0, 1, 2$ . Spin operators  $\{S_j\}$  act on the spin-chain Hilbert space spanned by the  $S^z$ -basis

$$|\psi_\alpha\rangle := |\alpha_1, \alpha_2, \dots, \alpha_N\rangle. \quad (4.42)$$

Parameters  $(J \cos \theta, J \sin \theta, c)$  with  $J > 0$  linearly depend on  $(\tilde{g}_0, \tilde{g}_1, \tilde{g}_2)$ . This model is in the Haldane phase when  $-\pi/4 < \theta < \pi/4$ , while it is in the critical phase when  $\pi/4 \leq \theta \leq \pi/2$ . At  $\theta = \arctan(1/3)$  and  $\pi/2$ , the model is particularly known as the AKLT model and the *pure-biquadratic model* [166, 167], respectively.

We notice the analogy between the  $s$ -wave collision Hamiltonian  $H_{\text{int}}$  and the BLBQ Hamiltonian  $H_{\text{BLBQ}}$ . This will help us find the exact ground state and the SPT phase in the spinful, itinerant, and short-range interacting bosonic systems.

Since both  $H_{\text{saw}}$  and  $H_{\text{int}}$  are positive semi-definite, a zero-energy ground state of  $H$ , if exists, must satisfy

$$(i) \quad H_{\text{saw}}|\text{GS}\rangle = 0,$$

$$(ii) \quad H_{\text{int}}|\text{GS}\rangle = 0.$$

In accordance with (i), there must be

$$|\text{GS}\rangle = \sum_{\sum_{j,\mu} n_{j,\mu} = N} x_{\mathbf{n}} \left( \prod_{j=1}^N \prod_{\mu=-1}^1 (B_{j,\mu}^\dagger)^{n_{j,\mu}} \right) |\text{vac}\rangle, \quad (4.43)$$

where  $x_{\mathbf{n}} \in \mathbb{C}$ ,  $\mathbf{n} = (\dots, n_{i,1}, n_{i,0}, n_{i,-1}, n_{i+1,1}, \dots)$ , and  $|\text{vac}\rangle$  is the vacuum state. Assuming  $g_0^b, g_2^b > 0$ , according to Eq. (4.26) and the positive semidefiniteness of  $P_r^{(S)}$ , one can conclude that

$$\begin{aligned} H_{\text{int}}|\text{GS}\rangle &= 0 \\ \iff (g_0^b P_{2j+1}^{(0)} + g_2^b P_{2j+1}^{(2)})|\text{GS}\rangle &= 0, \quad \forall j \\ \iff n_{2j+1} (n_{2j+1} - 1) |\text{GS}\rangle &= 0, \quad \forall j \\ \iff a_{2j+1,\alpha} a_{2j+1,\beta} |\text{GS}\rangle &= 0, \quad \forall j, \alpha, \beta \\ \implies x_{\mathbf{n}} = 0, \forall \mathbf{n} \text{ s.t. } n_{j,+1} + n_{j,0} + n_{j,-1} &> 1. \end{aligned} \quad (4.44)$$

Equation (4.43) thus reduces to

$$|\text{GS}\rangle = \sum_{\beta} y_{\beta} |\beta\rangle, \quad (4.45)$$

where  $y_{\beta} \in \mathbb{C}$ ,  $\beta = (\beta_1, \dots, \beta_N)$ , and

$$|\beta\rangle := \left( \prod_{j=1}^N B_{j,\beta_j}^\dagger \right) |\text{vac}\rangle. \quad (4.46)$$

A typical  $|\beta\rangle$  is illustrated in Fig. 4.2. Note that  $\{|\beta\rangle\}$  are linearly independent but not orthonormal because  $K_{jj'} := [B_{j,\mu}, B_{j',\mu}^\dagger] \neq \delta_{jj'}$ . We define the "dual operator" of  $B_{j,\mu}$  as [168]

$$C_{j,\mu} := \sum_{j'} (K^{-1})_{jj'} B_{j',\mu} \quad (4.47)$$

such that  $[C_{j,\mu}, B_{j',\mu'}^\dagger] = \delta_{jj'} \delta_{\mu\mu'}$ . Further defining

$$\langle \tilde{\alpha} | := \langle \text{vac} | \left( \prod_{j=1}^N C_{j,\alpha_j} \right) \quad (4.48)$$

such that  $\langle \tilde{\alpha} | \beta \rangle = \delta_{\alpha\beta}$ , eigenequation  $H|\text{GS}\rangle = 0$  then implies the matrix equation

$$\sum_{\beta} \langle \tilde{\alpha} | H | \beta \rangle y_{\beta} = 0. \quad (4.49)$$

Impressively, explicit calculation shows that

$$\langle \tilde{\alpha} | H | \beta \rangle = \langle \tilde{\alpha} | H_{\text{int}} | \beta \rangle = \langle \psi_{\alpha} | H_{\text{BLBQ}} | \psi_{\beta} \rangle, \quad (4.50)$$

provided that we take  $\tilde{g}_1 = 0$  and  $\tilde{g}_S = 2g_S^t d / (\lambda^2 + 2)$  in Eq. (4.41), where  $d > 0$  is a coefficient depending on the inverse matrix  $K^{-1}$  (matrix  $K$  is always invertible) [146]. The spin-chain basis states  $\{|\psi_{\beta}\rangle\}$  are defined in Eq. (4.42). Equation (4.50) indicates that there is a one-to-one correspondence between the zero-energy states of  $H$  and  $H_{\text{BLBQ}}$ . Note that such correspondence does not hold for eigenstates with nonzero energy, because  $P_{r=\text{odd}}^{(S)} |\beta\rangle = 0$  implies that nonzero-energy eigenstates cannot be purely spanned by  $\{|\beta\rangle\}$ . It is known that in the following two cases,  $H_{\text{BLBQ}}$  possesses zero-energy ground states:

- (1) AKLT point ( $\tilde{g}_0 = \tilde{g}_1 = 0$ ,  $\tilde{g}_2 > 0$ ),
- (2) pure-biquadratic point ( $\tilde{g}_1 = \tilde{g}_2 = 0$ ,  $\tilde{g}_0 > 0$ ).

Case (1) maps to  $g_0^t = 0$  and  $g_2^t > 0$  for  $H$ . In this case, the ground state of  $H$  is unique, which follows from the uniqueness of the ground state of the AKLT model [45, 46]. Despite the fact that the  $|\text{GS}\rangle$  in Eq. (4.45) is not represented in an orthonormal basis, the coefficient  $y_{\beta}$  is identical to that of the 1D AKLT state in Eq. (2.5):

$$y_{\beta} = \text{Tr}(M^{\beta_1} M^{\beta_2} \dots M^{\beta_N}). \quad (4.51)$$

Further expanding  $B_{j,\beta_j}^\dagger$  in terms of  $\{a^\dagger\}$ , we can see that  $|\text{GS}\rangle$  is a superposition of states of the form

$$(-\lambda)^b \sum_{\beta} \text{Tr}(M^{\beta_1} M^{\beta_2} \dots M^{\beta_N}) a_{r_1,\beta_1}^\dagger a_{r_2,\beta_2}^\dagger \dots a_{r_N,\beta_N}^\dagger, \quad (4.52)$$

where the integer  $b$  depends on  $\{r_1, \dots, r_N\}$ . In Eq. (4.52), we note that as long as two particles occupy the same top site  $\ell$ , there is the identity

$$\sum_{\beta_j, \beta_{j+1}} M^{\beta_j} M^{\beta_{j+1}} a_{\ell,\beta_j}^\dagger a_{\ell,\beta_{j+1}}^\dagger = \sqrt{6} b_\ell^\dagger I_2, \quad \ell = 2j, 2j+2 \quad (4.53)$$

where

$$b_r^\dagger := \frac{1}{\sqrt{6}}(a_{r,0}^\dagger a_{r,0}^\dagger - 2a_{r,1}^\dagger a_{r,-1}^\dagger) \quad (4.54)$$

creates a spin singlet. and  $I_2$  is a 2-by-2 identity matrix. Equation (4.53) implies that Eq. (4.52) has "hidden AKLT order", i.e., if we ignore all the vacant sites and sites occupied by a spin singlet, the remaining bosons form a perfect AKLT state, see Fig. 4.2. This enables us to express  $|\text{GS}\rangle$  in an orthonormal Fock basis as

$$|\text{GS}\rangle = \sum_{\tau_1, \dots, \tau_{2N} = -1}^3 \text{Tr} \left( \prod_{j=1}^N (F^{\tau_{2j-1}} E^{\tau_{2j}}) \right) \left( \prod_{r=1}^{2N} d_{r, \tau_r}^\dagger \right) |\text{vac}\rangle, \quad (4.55)$$

where

$$d_{r, \tau}^\dagger := \begin{cases} a_{r, \tau}^\dagger, & \tau = -1, 0, 1, \\ b_r^\dagger = (a_{r,0}^\dagger a_{r,0}^\dagger - 2a_{r,1}^\dagger a_{r,-1}^\dagger)/\sqrt{6}, & \tau = 2, \\ 1, & \tau = 3, \end{cases} \quad (4.56)$$

and

$$\begin{aligned} \sum_{\tau=-1}^3 F^\tau d_{r, \tau}^\dagger &= \frac{1}{\sqrt{\lambda^2 + 2}} \begin{pmatrix} I_2 & -\lambda \sum_\alpha M^\alpha a_{r, \alpha}^\dagger \\ 0 & I_2 \end{pmatrix}, \\ \sum_{\tau=-1}^3 E^\tau d_{r, \tau}^\dagger &= \begin{pmatrix} \sum_\alpha M^\alpha a_{r, \alpha}^\dagger & \sqrt{6} b_r^\dagger I_2 \\ I_2 & \sum_\alpha M^\alpha a_{r, \alpha}^\dagger \end{pmatrix}. \end{aligned} \quad (4.57)$$

Matrices  $F^\tau$  and  $E^\tau$  are determined from Eq. (4.57). Let  $\epsilon_i = -\ln |\lambda_i|$ , where  $\lambda_i$  is the  $i$ th largest absolute eigenvalue of the transfer matrix  $\sum_{\tau, \tau'} F^\tau E^{\tau'} \otimes F^\tau E^{\tau'}$ , and  $|\lambda_1|$  is normalized to 1. The matrix product state (MPS) in Eq. (4.55) is injective, because the largest absolute eigenvalue  $\lambda_1$  is non-degenerate. Using Eq. (4.57), one can easily see that the ground state in Eq. (4.55) is indeed a superposition of 1D AKLT states decorated with two-body singlets and/or vacant sites.

Case (2) maps to  $g_2^\dagger = 0$  and  $g_0^\dagger > 0$  for  $H$ . It is obvious that the ferromagnetic states

$$\left( \sum_{r=1}^{2N} S_r^- \right)^k \left( \prod_{j=1}^N B_{j,1}^\dagger \right) |\text{vac}\rangle, \quad k = 0, 1, \dots, 2N \quad (4.58)$$

with total spin  $S_{\text{tot}} = N$  are exact ground states of  $H$ . The spin-1 pure-biquadratic chain  $H_{\text{PB}} = \sum_{j=1}^N \tilde{g}_0 P_{j,j+1}^{(0)}$  (with  $\tilde{g}_0 > 0$ ) is integrable, and there are numerous ground states with  $S_{\text{tot}}$  ranging from 0 to  $N - 1$  that are degenerate with  $(\sum_j S_j^-)^k |\psi_{(1,1,\dots,1)}\rangle$  [166, 167, 169, 170]. The absence of a ferromagnetic phase in Fig. 4.3(a) can thus be understood from such degeneracy: after adding interaction  $\sum_{r=\text{even}} g_2^\dagger P_r^{(2)}$  (with  $g_2^\dagger > 0$ ) that disfavors the ferromagnetic states, states with smaller  $S_{\text{tot}}$  are picked up as the ground states.

### 4.2.2 The Haldane phase

In this section we investigate the properties of the MPS  $|\text{GS}\rangle$ . Let  $G$  be the symmetry group of  $H$  and  $U(q)$  be a symmetry operation (on the Hilbert space) corresponding to the group element  $q \in G$ , i.e.,  $[H, U(q)] = 0$ . Subjected to  $q$ , the unique ground state transforms as  $|\text{GS}\rangle \rightarrow U(q)|\text{GS}\rangle$ , while according to Theorem 2.8, the matrices in Eq. (4.55) transform as <sup>7</sup>

$$F^{\tau_{2j-1}} E^{\tau_{2j}} \rightarrow e^{i\phi_q} u_q^\dagger F^{\tau_{2j-1}} E^{\tau_{2j}} u_q, \quad (4.59)$$

where  $\{u_q\}_{q \in G}$  are unitary matrices which are used to classify the 1D SPT phases; see Sec. 2.1.2 for details.

The group  $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, U(x), U(y), U(z)\}$  is a symmetry group of  $H$ , where

$$U(\delta) := \exp\left(-i\pi \sum_r S_r^\delta\right) \quad (4.60)$$

is the spin rotation about the  $\delta = x, y, z$ -axis. The Hamiltonian is also invariant under time-reversal

$$U(\text{TR}) := U(y)K \quad (4.61)$$

(where  $K$  is a complex conjugation operator), space inversion

$$U(\mathcal{I}), \quad (4.62)$$

spin rotation together with inversion

$$U(z\mathcal{I}) := U(z)U(\mathcal{I}), \quad (4.63)$$

and pseudo-spin rotation together inversion

$$U(n\mathcal{I}) := \exp\left[-i\pi \sum_r (n_r - 1)\right] U(\mathcal{I}). \quad (4.64)$$

For  $U(\delta)$  and  $U(\text{TR})$ , we can define their respective topological indices using the corresponding unitary matrices in Eq. (4.59) as

$$\mathcal{Q}_{\mathbb{Z}_2 \times \mathbb{Z}_2} := \text{Tr}(u_x u_z u_x^\dagger u_z^\dagger) / \chi \quad (4.65)$$

and

$$\mathcal{Q}_{\text{TR}} := \text{Tr}(u_{\text{TR}} u_{\text{TR}}^*) / \chi, \quad (4.66)$$

where  $\chi$  is the bond dimension of the MPS [61]. It is known that  $\mathcal{Q}_{\mathbb{Z}_2 \times \mathbb{Z}_2}$  equals  $-1$  for the Haldane phase protected by  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry while  $+1$  for the trivial phase, similarly

<sup>7</sup>Theorem 2.8 is usually proved in the canonical form; see Ref. [60] or Theorem 7 in Ref. [43]. However, the equation holds regardless of the form of an injective MPS; see Ref. [4] or Sec. 7.3 in Ref. [44].

for  $\mathcal{Q}_{\text{TR}}$  [48]. When  $0 < |\lambda| < \infty$ , the system has inversion symmetry with respect to every lattice site. However, as explained in Sec. 3.3, the site-centered inversion symmetry cannot protect SPT phases. The groups  $\{1, U(\mathcal{I})\}$ ,  $\{1, U(z\mathcal{I})\}$ , and  $\{1, U(n\mathcal{I})\}$  can protect SPT phases only when  $U(\mathcal{I})$  is a bond-centered inversion; see Sec. 3.3 for details. When the bond-centered inversion symmetry is present, we can similarly define

$$\mathcal{Q}_{\mathcal{I}} := \text{Tr}(u_{\mathcal{I}} u_{\mathcal{I}}^*) / \chi, \quad \mathcal{Q}_{z\mathcal{I}} := \text{Tr}(u_{z\mathcal{I}} u_{z\mathcal{I}}^*) / \chi, \quad \mathcal{Q}_{n\mathcal{I}} := \text{Tr}(u_{n\mathcal{I}} u_{n\mathcal{I}}^*) / \chi, \quad (4.67)$$

which are quantized to +1 and -1 for trivial and Haldane phases, respectively [48, 49, 61]. The state  $|\text{GS}\rangle$  at  $\lambda = 0$  and  $|\lambda| \rightarrow \infty$  has bond-centered inversion symmetry. At  $|\lambda| \rightarrow \infty$ ,  $|\text{GS}\rangle$  reduces to Eq. (2.5). At  $\lambda = 0$ , although  $|\text{GS}_{\lambda=0}\rangle$  is not the unique ground state of  $H|_{\lambda=0}$ , one can (in principle) always find a parent Hamiltonian that has  $|\text{GS}_{\lambda=0}\rangle$  as the unique ground state (see Theorem 2.5), and hence the state itself is still worth studying. Actually, it turns out that  $|\text{GS}_{\lambda=0}\rangle$  can be viewed as a spinful generalization of the Haldane insulator state in spinless bosons; see Appendix A of Ref. [1]. Table 4.2 summarizes the unitary matrices  $\{u_q\}$  with respect to different symmetry operations on  $|\text{GS}\rangle$ . It is then clear that the Haldane phase of  $|\text{GS}_{0<|\lambda|<\infty}\rangle$  is protected by  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry or time-reversal symmetry. Interestingly, when the inversion symmetry is involved,  $|\text{GS}_{\lambda=0}\rangle$  and  $|\text{GS}_{|\lambda|\rightarrow\infty}\rangle$  can be in different phases. This difference originates from the charge fluctuations in  $|\text{GS}_{\lambda=0}\rangle$ . We claim that in general, charge fluctuations can play a nontrivial role in the SPT orders protected by crystalline symmetries, see Sec. 4.3.3 for details.

Using the exact MPS in Eq. (4.55) and Eq. (4.57), various quantities that characterize the Haldane phase can be calculated analytically. For example, the spin-spin correlation length is exactly given by

$$\xi = \left( \ln \frac{\lambda_1}{\lambda_2} \right)^{-1} = \left( \ln \frac{3\lambda^2 + \sqrt{9\lambda^4 + 36\lambda^2 + 24} + 6}{\lambda^2 + \sqrt{\lambda^4 + 4\lambda^2 + 24} + 2} \right)^{-1}, \quad (4.68)$$

where  $\lambda_1$  and  $\lambda_2$  are the eigenvalues of the transfer matrix  $\sum_{\tau, \tau'} F^\tau E^{\tau'} \otimes F^\tau E^{\tau'}$  with the largest and the second largest absolute values, respectively. The symmetry flux of  $\mathbb{Z}_2 \times \mathbb{Z}_2$  can be chosen to be

$$\mathcal{F}_r^\delta = \prod_{k=-\infty}^{r-2} \exp(i\pi S_k^\delta) (S_{r-1}^\delta + S_r^\delta), \quad \delta = x, y, z. \quad (4.69)$$

The string order parameter is found to be exactly equals

$$\begin{aligned} \mathcal{O}_{\text{str}}^\delta &= - \lim_{L \rightarrow \infty} \frac{1}{\langle \text{GS} | \text{GS} \rangle} \langle \text{GS} | \mathcal{F}_r^{\delta\dagger} \mathcal{F}_{r+2L}^\delta | \text{GS} \rangle \\ &= \frac{16[9\lambda^6 + (5Q + 48)\lambda^2 + 3(Q + 11)\lambda^4 + 24]^2}{Q^2(3\lambda^2 + Q + 6)^2(Q + 3\lambda^2)^2}, \end{aligned} \quad (4.70)$$

Table 4.2: Unitary matrices in Eq. (4.59) with respect to various symmetry operations on  $|\text{GS}\rangle$ . In accordance with the values of  $\mathcal{Q}_{\mathbb{Z}_2 \times \mathbb{Z}_2}$ ,  $\mathcal{Q}_{\text{TR}}$ ,  $\mathcal{Q}_{\mathcal{I}}$ ,  $\mathcal{Q}_{z\mathcal{I}}$ , and  $\mathcal{Q}_{n\mathcal{I}}$ , the two shadowed matrices denote trivial phases, while the other matrices denote the SPT phase. N/A means the symmetry group cannot give an SPT/trivial classification.

	$\lambda = 0$	$0 <  \lambda  < \infty$	$ \lambda  \rightarrow \infty$
$U(\delta) \ (\delta = x, y, z)$	$u_\delta = \begin{pmatrix} \sigma^\delta & 0 \\ 0 & \sigma^\delta \end{pmatrix}$	$u_\delta = \begin{pmatrix} \sigma^\delta & 0 \\ 0 & \sigma^\delta \end{pmatrix}$	$u_\delta = \sigma^\delta$
$U(\text{TR})$	$u_{\text{TR}} = \begin{pmatrix} \sigma^y & 0 \\ 0 & \sigma^y \end{pmatrix}$	$u_{\text{TR}} = \begin{pmatrix} \sigma^y & 0 \\ 0 & \sigma^y \end{pmatrix}$	$u_{\text{TR}} = \sigma^y$
$U(\mathcal{I})$	$u_{\mathcal{I}} = \begin{pmatrix} 0 & -\sigma^y \\ \sigma^y & 0 \end{pmatrix}$	N/A	$u_{\mathcal{I}} = \sigma^y$
$U(z\mathcal{I})$	$u_{z\mathcal{I}} = \begin{pmatrix} 0 & -\sigma^x \\ \sigma^x & 0 \end{pmatrix}$	N/A	$u_{z\mathcal{I}} = \sigma^x$
$U(n\mathcal{I})$	$u_{n\mathcal{I}} = \begin{pmatrix} 0 & \sigma^y \\ \sigma^y & 0 \end{pmatrix}$	N/A	$u_{n\mathcal{I}} = \sigma^y$

where  $Q := \sqrt{9\lambda^4 + 36\lambda^2 + 24}$ . It can be shown that  $4/(\sqrt{6} + 3)^2 < \mathcal{O}_{\text{str}}^\delta < 4/9$ . In fact, in the large  $\lambda$  limit,

$$\begin{aligned} \lim_{\lambda \rightarrow \pm\infty} \xi &= \frac{1}{\ln 3}, \\ \lim_{\lambda \rightarrow \pm\infty} \mathcal{O}_{\text{str}}^\delta &= \frac{4}{9}, \quad \delta = x, y, z, \end{aligned} \tag{4.71}$$

which exactly agree with those of the AKLT model.

### 4.2.3 Perturbation theory and numerical analysis

Beyond the cases in which the ground state is exactly solvable, the phase of  $H$  can still be determined analytically when  $|\lambda|$  is large enough. See Fig. 4.3(a). In the limit  $|\lambda| \rightarrow \infty$ , if we assume  $g_0^b$  and  $g_2^b$  are around the magnitude of  $\lambda^2$ , the unperturbed ground state will have each bottom site occupied by exactly one particle. In this case, perturbation theory tells us that the low-energy effective Hamiltonian of  $H$  is given by  $H_{\text{BLBQ}}$  in Eq. (4.41) with  $J \propto \lambda^{-2}$  and [146]

$$\theta = \arctan \left( \frac{1}{3} \cdot \frac{3g_0^t + 4g_0^t \lambda^2 / g_2^t + 2\lambda^2}{g_0^t + 2\lambda^2} \right) \geq \arctan \frac{1}{3}, \tag{4.72}$$

where  $J$  and  $\theta$  are independent of  $g_S^b$ . From Eq. (4.72), we know that the effective model is in the Haldane phase when  $0 \leq g_0^t < g_2^t$  while in the critical phase when  $0 < g_2^t \leq g_0^t$ . In particular,  $g_0^t = 0$  and  $g_2^t = 0$  corresponds to the AKLT and pure-quadratic point, respectively.

Beyond the three special planes in Fig. 4.3(a) where either exact ground states can be found or perturbation theory works, the phase diagram of the spin-1 BHMSC can in general be determined by numerical calculations. In the thermodynamic limit  $N \rightarrow \infty$ , we find the phase diagram in the  $\lambda = 1$  plane in Fig. 4.3(a) with the variational uniform matrix product state (VUMPS) algorithm [171, 172]. (In the phase diagram we have assumed  $g_0^t, g_2^t, \lambda \geq 0$  and  $g_0^b = g_2^b = 1/\lambda^2$ .) Due to the fact that the total number of particles and unit cells are the same, matrices in the MPS ansatz used in the algorithm are assumed to be block-banded [173]. Also, the maximum particle number on each site is truncated to three. See Appendix E of Ref. [1] for details of the MPS ansatz. Let  $\epsilon_i := -\ln|\lambda_i|$ , where  $\lambda_i$  is the  $i$ th largest absolute eigenvalue of the transfer matrix, and  $|\lambda_1|$  is normalized to 1. When the bond dimension  $\chi$  is extrapolated to infinity, the correlation length  $\xi := 1/\epsilon_2$  diverges for gapless phases while it converges to a finite value for gapped phases. This fact is known to be well reflected in the scaling relation of the inverse correlation length  $1/\xi(\chi)$  with respect to  $\epsilon_3(\chi) - \epsilon_2(\chi)$  [174, 175]. As shown in Fig. 4.3(b), with different choices of the bond dimension, we calculate the scaling relation along the path parameterized by  $(g_0^t, g_2^t, 1/\lambda) = (R \sin \varphi, R \cos \varphi, 1)$ . We can see that when  $R = \sqrt{2}$ , a quantum phase transition occurs between  $\varphi = 6\pi/36$  and  $7\pi/36$ . As  $R$  grows, the phase transition occurs at smaller  $\varphi$ , which indicates that the phase boundary is curved instead of straight. In the region of the gapped phase in Fig. 4.3(a), we find that  $\mathcal{Q}_{\mathbb{Z}_2 \times \mathbb{Z}_2} = \mathcal{Q}_{\text{TR}} = -1$ , which suggests that the gapped phase is the Haldane phase. The Haldane phase is characterized by an even-fold degenerate entanglement spectrum (ES) [48], see Fig. 4.3(c). The ground state magnetization  $M := \lim_{N \rightarrow \infty} \langle \sum_{r=1}^{2N} S_r^z \rangle / N$  is calculated after adding  $-h \sum_r S_r^z$  to  $H$ , where  $h$  is the magnetic field; see Fig. 4.3(d). In the gapless region,  $M$  grows almost linearly with  $h$ , which suggests that the gapless phase is the critical phase [176]. In the Haldane phase region, however,  $M$  is expected to exhibit a zero plateau for small  $h$  [176], which is indeed the case as in Fig. 4.3(d).

### 4.3 General construction

The sawtooth chain is not special in the sense that there are many other lattices possessing a bottom flat band. It is thus natural to expect that the SPT phases can be realized with spinful bosons loaded on these lattices. Our approach in the previous section can be generalized. In this section, we present a general theory for the SPT phases of spin- $f$  bosons with a bottom flat band. We first show in Sec. 4.3.1 that the AKLT model and AKLT state can be generalized to higher spins and higher dimensional lattices. Let  $|\text{AKLT}_{f,X'}\rangle$  be the exact and unique ground state of the spin- $f$  AKLT model defined on a lattice  $X'$ . On the other hand, bottom-flat-band lattices can be constructed systematically. Let  $|\text{GS}_{f,X}\rangle$  be the ground state of  $N$  spin- $f$  bosons on a bottom-flat-band lattice  $X$  with  $N$  unit cells.

In Sec. 4.3.2, we show that with fine-tuned parameters,  $|\text{GS}_{f,X}\rangle$  can be exactly mapped to  $|\text{AKLT}_{f,X'}\rangle$ , provided that  $f$ ,  $X$ , and  $X'$  satisfy a certain relation. This means that  $|\text{GS}_{f,X}\rangle$  is the exact and unique ground state of the itinerant spin- $f$  model. In Sec. 4.3.3, with various  $f$  and  $X$ , we classify the quantum phases of  $|\text{GS}_{f,X}\rangle$ 's from the viewpoint of SPT orders. In particular, we find that in terms of crystalline symmetries, not only spin fluctuations but also charge fluctuations in  $|\text{GS}_{f,X}\rangle$  determine its symmetry-protected phase.

### 4.3.1 Generalized AKLT models

It is known that AKLT states can be constructed on any lattice in any dimensions [46, 73, 74]. In this chapter, we consider only bosonic spin- $f$  AKLT states ( $f = \text{integer}$ ). Let  $X' = (\Lambda_{X'}, \mathcal{B}_{X'})$  be a lattice (graph) where  $\Lambda_{X'}$  is the set of sites (vertices) and  $\mathcal{B}_{X'}$  is the set of bonds (edges). A bond is defined by two sites  $\{j, j'\}$  with  $j, j' \in \Lambda_{X'}$ . We assume that every site in  $X'$  is directly connected to  $2f$  other sites, i.e.,

$$|\{j' \in \Lambda_{X'} | \{j, j'\} \in \mathcal{B}_{X'}\}| = 2f, \forall j. \quad (4.73)$$

(In other words,  $X'$  is a regular graph of degree  $2f$ .) When there is a spin- $f$  degree of freedom (DOF) residing in every site of  $X'$ , an AKLT-type quantum spin model can be defined on  $X'$  as

$$H_{\text{AKLT}}^{f,X'} := \tilde{g}_{2f} \sum_{\{j,j'\} \in \mathcal{B}_{X'}} P_{j,j'}^{(2f)} \quad (\tilde{g}_{2f} > 0), \quad (4.74)$$

where the operator  $P_{j,j'}^{(2f)}$  projects the state of two spin- $f$ 's on two sites  $j, j'$  onto the state with total spin  $2f$ . The operator  $P_{j,j'}^{(2f)}$  can be explicitly expressed in terms of spin operators; see Eq. (4.34).

It has been proved that when  $|\Lambda_{X'}| = N < \infty$ ,  $H_{\text{AKLT}}^{f,X'}$  has an exact and unique ground state [4, 177]<sup>8</sup>:

$$|\text{AKLT}_{f,X'}\rangle = \sum_{\alpha_1, \dots, \alpha_N = -f}^f S_{\alpha_1, \dots, \alpha_N} |\psi_{\alpha_1, \dots, \alpha_N}\rangle, \quad (4.75)$$

where  $\{|\psi_{\alpha_1, \alpha_2, \dots, \alpha_N}\rangle\}$  is the spin  $S^z$ -basis and the coefficient  $S_{\alpha_1, \dots, \alpha_N}$  encodes short-range entanglement between the spins. When  $X'$  is the simple 1D linear chain with  $f = 1$ ,  $H_{\text{AKLT}}^{f,X'}$  reduces to Eq. (2.4), and its ground state is the 1D spin-1 AKLT state in Eq. (2.5), and  $S_{\alpha_1, \dots, \alpha_N} = y_{\alpha}$  in Eq. (4.51). For  $H_{\text{AKLT}}^{f,X'}$  on a general  $X'$ , the ground state  $|\text{AKLT}_{f,X'}\rangle$  can be interpreted as follows: each spin- $f$  is regarded as a composite state of  $2f$  spin-1/2's, and a singlet is formed between two spin-1/2's in every bond  $\{j, j'\} \in \mathcal{B}_{X'}$  [46, 73]. Some other graph representations of AKLT states in 2D and 3D are given in Fig. 2.1.

<sup>8</sup>So far, for a general AKLT model, the existence of gap generally has no rigorous mathematical proof yet.



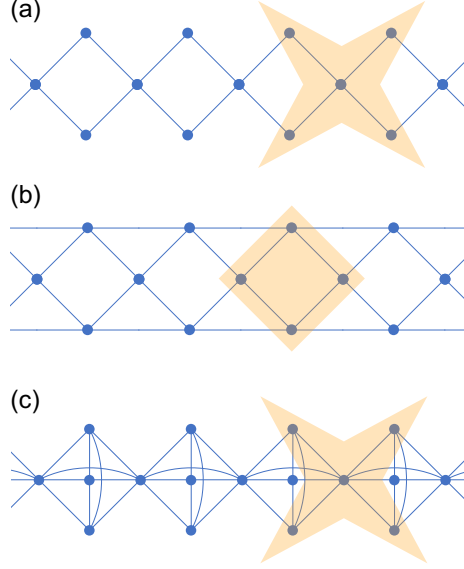


Figure 4.4: Other examples of 1D lattices that can be used to construct nontrivial ground states with spin-1 bosons. Allowed hopping process between two sites is illustrated by a bond. (a) Diamond chain. A  $\pi$  flux threads each plaquette [186]. A CLS covers five sites, as denoted by the four-pointed star. (b) Kagome ladder, an example of the line graph construction [74, 179]. A CLS is denoted by the square. (c) Pyramid chain, an example of the cell construction [4]. A CLS is denoted by the four-pointed star.

### 4.3.2 Ground states of spin- $f$ bosons with a bottom flat band

We have seen that the single-particle CLSs play a crucial role in constructing the many-body ground state. The CLSs exist not only in the sawtooth chain but also in all the finite-range hopping lattices possessing a flat band [142, 143]. In fact, there are various systematic approaches to construct flat-band lattices [4, 142, 162, 163, 178–185], among which Tasaki’s cell construction [162, 163] and Mielke’s line graph construction [178–180] always yield a bottom flat band<sup>9</sup>. These systematic constructions generate infinitely many kinds of lattices in  $d \geq 1$  dimensions, such as those shown in Fig. 4.4 for  $d = 1$  and Fig. 4.5 for  $d = 2, 3$ .

Let  $X = (\Lambda_X, \mathcal{B}_X)$  be a bottom-flat-band lattice, where  $\Lambda_X$  is the set of sites and  $\mathcal{B}_X$  is the set of bonds. A bond is defined by two sites  $\{r, r'\}$  with  $r, r' \in \Lambda_X$ . Let  $H_{\text{hop}}^{f,X}$  be a single-body Hamiltonian for spin- $f$  bosons on  $X$ :

$$H_{\text{hop}}^{f,X} = - \sum_{\{r,r'\} \in \mathcal{B}_X} \sum_{\alpha=-f}^f t_{r,r'} a_{r,\alpha}^\dagger a_{r',\alpha} + \sum_{r \in \Lambda_X} V_r n_r, \quad (4.76)$$

where  $a_{r,\alpha}^\dagger$  creates a boson with magnetic sublevel  $\alpha$  at site  $r$ . Let  $N$  be the total number of unit cells in  $X$ . The assumption that  $X$  has a bottom flat band means that the

<sup>9</sup>In fact, the sawtooth chain can be produced by either the cell construction or the line graph construction.

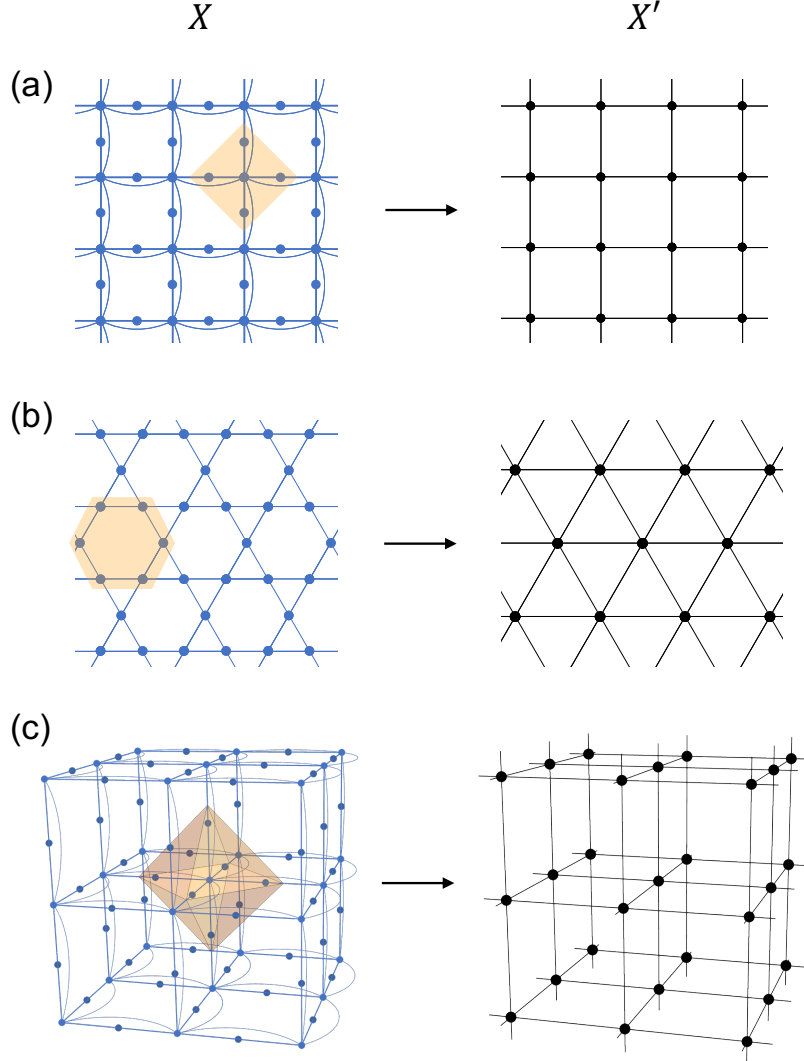


Figure 4.5: Examples of higher dimensional lattices  $X$  with a bottom flat band (left column) and their corresponding lattices  $X'$  where the AKLT models are defined (right column). In  $X$ , allowed hopping processes are illustrated by bonds. In  $X'$ , a bond represents interaction between two spins. (a) 2D Tasaki lattice (left), an example of the cell construction [162, 163]. A CLS is localized on five sites, as pictured by the square. All the CLSs are related to each other by lattice translation vectors. Every CLS overlaps with four other CLSs, thus  $f$  should be  $4/2 = 2$ . The corresponding AKLT model lives on a square lattice (right). We symbolize the 2D Tasaki lattice as  $\boxplus$  and the square lattice as  $\square$ . (b) Kagome lattice (left), an example of the line graph construction [179]. A CLS is localized on a hexagon. Every CLS overlaps with  $2f = 6$  other CLSs, and the corresponding AKLT model lives on a triangular lattice (right). We symbolize the kagome lattice as  $\star$  and the triangular lattice as  $\triangle$ . An optical kagome lattice has been realized experimentally [187]. (c) 3D Tasaki lattice (left), another example of the cell construction [162, 163]. A CLS is localized on seven sites, as covered by the octahedron. Every CLS overlaps with  $2f = 6$  other CLSs, the corresponding AKLT model thus lives on a cubic lattice (right). We symbolize the cubic lattice as  $\boxtimes$ .

single-particle ground state degeneracy of  $H_{\text{hop}}^{f,X}$  is  $N(2f+1)$ . The corresponding CLSs are localized on  $N$  different positions and are related to each other by lattice translation vectors<sup>10</sup>. The shapes of some CLSs are shown in Fig. 4.4 and 4.5. Let  $(B_{j,\alpha}^{f,X})^\dagger$  be the creation operator of a CLS, where  $j = 1, 2, \dots, N$  labels different positions. A *fully packed state (FPS)* on  $X$  is defined as a product of  $N$  CLSs:

$$(B_{1,\alpha_1}^{f,X})^\dagger (B_{2,\alpha_2}^{f,X})^\dagger \dots (B_{N,\alpha_N}^{f,X})^\dagger |\text{vac}\rangle. \quad (4.77)$$

In an FPS, the lattice is "fully packed" by  $N$  particles. For example,  $|\beta\rangle$  in Eq. (4.46) is an FPS in the sawtooth chain.

We now consider another lattice  $X' = (\Lambda_{X'}, \mathcal{B}_{X'})$  with  $|\Lambda_{X'}| = N$ , and each site  $j \in \Lambda_{X'}$  represents a CLS in the FPS of  $X$ . Two sites in  $X'$  are directly connected iff the two corresponding CLSs in the FPS (partially) overlap. For example, as shown in Fig. 4.5, if  $X$  is the 2D (3D) Tasaki lattice,  $X'$  will be the square (cubic) lattice, while if  $X$  is the kagome lattice,  $X'$  will then be the triangular lattice. Define  $\Lambda_X^{[k]} \subset \Lambda_X$  as a set of sites where  $k$  CLSs in the FPS overlap. For example, in the sawtooth chain  $\Lambda_X = \Lambda_X^{[1]} \cup \Lambda_X^{[2]}$ , where  $\Lambda_X^{[1]}$  is the set of all the bottom sites and  $\Lambda_X^{[2]}$  is all the top sites. In the following, we require that

1. every site  $r \in \Lambda_X$  is shared by no more than two CLSs in the FPS, i.e.,  $\Lambda_X^{[k]} = \emptyset$  for  $k > 2$ ;
2.  $f$  and  $X$  are chosen such that  $X'$  satisfies the condition  $|\{j' \in \Lambda_{X'} | \{j, j'\} \in \mathcal{B}_{X'}\}| = 2f, \forall j \in \Lambda_{X'}$ .

We then define the spin model  $H_{\text{AKLT}}^{f,X'}$  on  $X'$ , as introduced in Sec. 4.3.1.

For interaction between alkali-metal atoms, it is sufficient to consider the short-range  $s$ -wave scattering [126, 127]. As introduced in Sec. 4.1.2, spin- $f$  bosons in optical lattices are described by the spin- $f$  Bose-Hubbard model. On the lattice  $X$ , the model is given by

$$\begin{aligned} H^{f,X} &:= H_{\text{hop}}^{f,X} + H_{\text{int}}^{f,X}, \\ H_{\text{int}}^{f,X} &:= \sum_{r \in \Lambda_X} \sum_{S=0,2,\dots,2f} g_{S,r} P_r^{(S)}. \end{aligned} \quad (4.78)$$

The  $s$ -wave scattering Hamiltonian is reminiscent of the AKLT Hamiltonians. If

- $N$  spin- $f$  bosons are loaded on  $X$ ,
- $g_{2f,r} > 0$  and  $g_{S<2f,r} = 0$  for all  $r \in \Lambda_X^{[2]}$ ,

<sup>10</sup>Ignore spin for the moment, i.e., take  $f = 0$ . In  $d = 1$ ,  $N$  different CLSs can always be chosen to be linearly independent. However, in  $d > 1$  with PBC, these  $N$  CLSs can be linearly dependent in some cases, such as in kagome lattice [142]. Nevertheless, they can still be linearly independent in  $d > 1$  with OBC.

then following Sec. 4.2.1, the zero-energy ground states of  $H^{f,X}$  in Eq. (4.78) and  $H_{\text{AKLT}}^{f,X'}$  in Eq. (4.74) can be exactly mapped to each other, just as Eq. (4.50).

Let us see some concrete examples. In  $d = 1$  dimension, besides the sawtooth chain, spin-1 bosons can be loaded on the lattices in Fig. 4.4 as well. In  $d = 2$ , the 2D Tasaki lattice matches spin-2 bosons, and the corresponding spin-2 AKLT model lives on a square lattice with the AKLT ground state in Fig. 2.1(b). The kagome lattice is suitable for spin-3 bosons, while the corresponding AKLT model has the spin-3 AKLT ground state on a triangular lattice as shown in Fig. 2.1(c). On the other hand, spin-3 bosons are also compatible with the 3D Tasaki lattice, which corresponds to a 3D spin-3 AKLT state in Fig. 2.1(d). In fact, the Tasaki lattice can be constructed in any dimensions, and the sawtooth chain can actually be regarded as the 1D Tasaki lattice [162, 163]. In general, the  $d$ -dimensional Tasaki lattice matches spin- $d$  bosons, and the corresponding AKLT model lives on a  $d$ -dimensional hypercubic lattice.

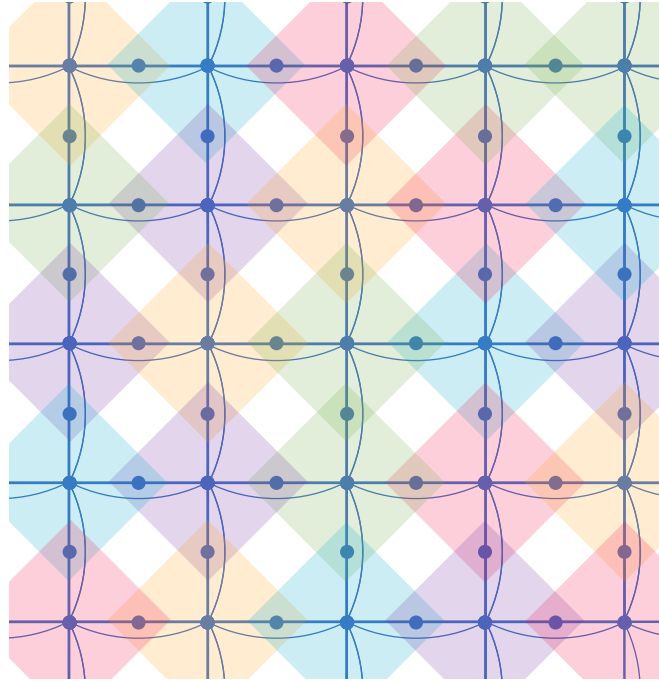


Figure 4.6: An FPS spin-2 bosons on the 2D Tasaki lattice with a typical choice of  $\alpha_1, \dots, \alpha_N$ . The five possible values of  $\alpha_j$  are represented by five different colors.

Let  $|\text{GS}_{f,X}\rangle$  be the exact and unique ground state of  $H^{f,X}$ . It can be expressed as

$$\begin{aligned} |\text{GS}_{f,X}\rangle &= \sum_{\alpha_1, \dots, \alpha_N = -f}^f S_{\alpha_1, \dots, \alpha_N} \sum_{\mathbf{r}_1, \dots, \mathbf{r}_N} C_{\mathbf{r}_1, \dots, \mathbf{r}_N} a_{\mathbf{r}_1, \alpha_1}^\dagger \dots a_{\mathbf{r}_N, \alpha_N}^\dagger |\text{vac}\rangle \\ &= \sum_{\alpha_1, \dots, \alpha_N = -f}^f S_{\alpha_1, \dots, \alpha_N} (B_{1, \alpha_1}^{f,X})^\dagger (B_{2, \alpha_2}^{f,X})^\dagger \dots (B_{N, \alpha_N}^{f,X})^\dagger |\text{vac}\rangle, \end{aligned} \quad (4.79)$$

where  $S_{\alpha_1, \dots, \alpha_N}$  and  $C_{r_1, \dots, r_N}$  are coefficients that correspond to different spin and charge configurations, respectively. We can see that  $|\text{GS}_{f,X}\rangle$  is a linear combination of FPSs with different spin configurations, and the coefficients  $S_{\alpha_1, \dots, \alpha_N}$  in Eq. (4.79) and Eq. (4.75) are identical. Figure 4.6 gives an example of an FPS of spin-2 bosons on the 2D Tasaki lattice.

Mathematically, the uniqueness of the ground state of  $H^{f,X}$  can be proved with additional assumptions:

- $\Lambda_X^{[1]} \neq \emptyset$  and  $g_{S,r} > 0$  for  $\forall S$  and  $\forall r \in \Lambda_X^{[1]}$ .

With the "completeness relation"  $\sum_S P_r^{(S)} = n_r(n_r - 1)/2$  in mind and following the deduction in Eq. (4.44), one can show that the ground state can only be a linear combination of FPSs. The uniqueness of the ground state of  $H^{f,X}$  then follows from the uniqueness of  $|\text{AKLT}_{f,X'}\rangle$ . The assumption  $\Lambda_X^{[1]} \neq \emptyset$  is always satisfied in lattices generated by the cell construction, see, for example, Fig. 4.4(b) and Fig. 4.5(a). However, for the kagome lattice shown in Fig. 4.5(b),  $\Lambda_X^{[1]} = \emptyset$ . Nevertheless, we propose the following conjecture:

**Conjecture 4.1** *In the flat-band lattice  $X$  with  $\Lambda_X^{[1]} = \emptyset$  and  $\Lambda_X^{[k]} = \emptyset$  for  $k > 2$ , the exact ground state of  $H^{f,X}$  is unique when  $X'$  is not a bipartite lattice.*

The conjecture clearly makes sense in physics yet seems difficult to prove mathematically. Nevertheless, let us take a look at some examples. For the kagome lattice,  $X'$  is a triangular lattice which is not bipartite. Note that if  $X'$  is bipartite and  $\Lambda_X^{[1]} = \emptyset$ , the ground state of  $H^{f,X}$  will be degenerate. For example, for the Creutz ladder in Fig. 4.7(a), let  $(B_{j,\beta_j}^{1,\boxtimes})^\dagger$  create a CLS of spin-1 boson, it is easy to see that the following two states both have zero energy:

$$\text{Tr} \prod_{j=1}^N \left[ \sum_{\beta_j} M^{\beta_j} (B_{j,\beta_j}^{1,\boxtimes})^\dagger \right] |\text{vac}\rangle, \quad (4.80a)$$

$$\prod_{\ell=1}^{N/2} \left[ (B_{2\ell,0}^{1,\boxtimes})^\dagger (B_{2\ell,0}^{1,\boxtimes})^\dagger - 2 (B_{2\ell,1}^{1,\boxtimes})^\dagger (B_{2\ell,-1}^{1,\boxtimes})^\dagger \right] |\text{vac}\rangle. \quad (4.80b)$$

These two states are depicted in Fig. 4.7(a). The first "nontrivial" state is a linear combination of FPSs, while the second state is a product state. A similar thing happens in spin-2 bosons loaded on the checkerboard lattice, see Fig. 4.7(b).

In the followings, we will only focus on lattices with a unique ground state.

Let us note that although an exact ground state  $|\text{GS}_{f,X}\rangle$  is a result of fine-tuned interactions, one can readily believe that the quantum phase represented by  $|\text{GS}_{f,X}\rangle$  (to be discussed in Sec. 4.3.3) exists in rather broad parameter regions, as supported by the evidences shown in Sec. 4.2.3 for the sawtooth chain.

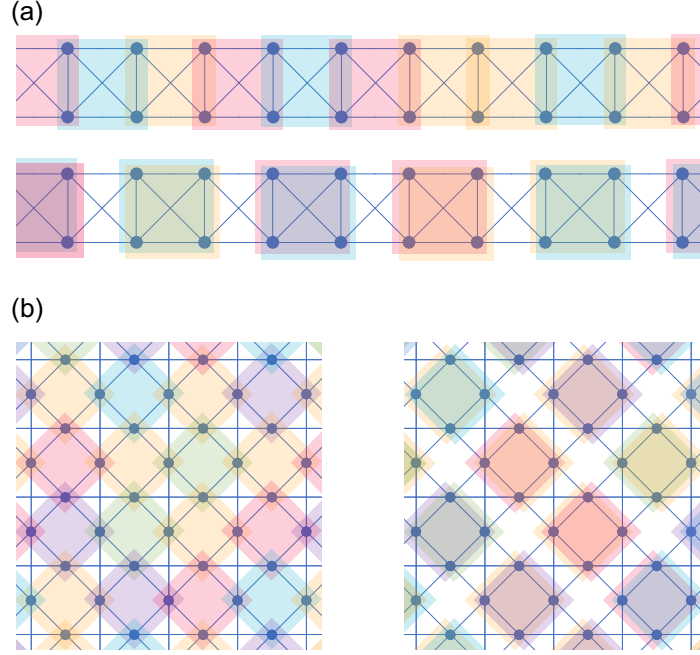


Figure 4.7: A "nontrivial" ground state is degenerated with product states, if  $\Lambda_X^{[1]} = \emptyset$  and the corresponding quantum spin model lives on a bipartite lattice. (a) Spin-1 bosons on a Creutz ladder. Each colored square denotes a CLS with spin degree of freedom. Note that the ground states are superpositions of all allowed spin configurations. (b) Spin-2 bosons on a checkerboard lattice.  $X'$  in this case is a square lattice.

### 4.3.3 Classification of the ground states

As the unique ground state,  $|\text{GS}_{f,X}\rangle$  preserves all the symmetries of the system. One can always think of  $|\text{GS}_{f,X}\rangle$  as a representative state of a certain disordered, gapped, short-range entangled, and symmetry-protected quantum phase. In order to classify the phases represented by  $|\text{GS}_{f,X}\rangle$  with various  $f$  and  $X$ , there are two main questions that we need to answer. First, what is the phase of the corresponding state  $|\text{AKLT}_{f,X'}\rangle$ ? Second, are the two states  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  in exactly the same phase?

Recall that for  $f = 1$  and  $X$  being the sawtooth chain, the answers to the two questions have been completely listed in Table 4.2. The two states Eq. (4.55) and Eq. (2.5) are in the same phase except when the inversion symmetry is involved. In  $d > 1$  dimensions, however, regarding the first question, given an arbitrary  $f$  and  $X'$ , there is so far no complete answer about the phase of  $|\text{AKLT}_{f,X'}\rangle$  in terms of all of its symmetry groups. Nevertheless, as discussed in Sec. 3.1, with on-site symmetry alone,  $|\text{AKLT}_{f,X'}\rangle$  always represents a trivial phase in  $d > 1$  dimensions, while the combination of certain on-site and spatial symmetry can give an SPT/trivial classification. In addition, as shown in Sec. 3.3, crystalline symmetries alone can also give an SPT/trivial classification for  $|\text{AKLT}_{f,X'}\rangle$ . Regarding the second question, we claim that  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  are always in the same phase

protected by on-site symmetry alone or the combination of on-site and translation symmetry, see Sec. 4.3.3.1. However, their phases should be investigated on a case-by-case basis when crystalline symmetries come into play, see Sec. 4.3.3.2 and Sec. 4.3.3.3. In particular, we find that the charge fluctuations in  $|\text{GS}_{f,X}\rangle$  can play a nontrivial role in the SPT orders protected by crystalline symmetries. In the following, for simplicity, we focus only on several concrete examples. The analysis, however, applies to general cases.

#### 4.3.3.1 Smooth path argument

In terms of the combination of  $\text{SO}(3)$  spin rotation and translation symmetry [denote the symmetry group as  $\text{SO}(3) \times \text{trn}$ ], the spin-2 AKLT state on a square lattice  $|\text{AKLT}_{2,\square}\rangle$  is in an SPT phase, while the spin-3 AKLT state on a triangular lattice  $|\text{AKLT}_{3,\triangle}\rangle$  represents a trivial phase. A key observation is that

**Proposition 4.2**  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  can always be smoothly connected to each other without breaking the  $\text{SO}(3) \times \text{trn}$  symmetry. Therefore, the two states are in the same phase protected by  $\text{SO}(3) \times \text{trn}$  according to Definition 1.7.

For example, let  $B_{1,\alpha}^{3,\star}$  be one of the CLS operators on the kagome lattice, whose exact form is given by

$$B_{1,\alpha}^{3,\star} = \frac{1}{\sqrt{6}} \sum_{x=1}^6 (-1)^x a_{x,\alpha}, \quad (4.81)$$

where the six sites labeled by  $x$  form vertices of a hexagon, as shown in Fig. 4.8. We then define a  $\lambda$ -deformed CLS operator as

$$B_{1,\alpha}^{3,\star}(\lambda) = \frac{1}{\sqrt{\lambda^2 + 5}} \left( \sum_{x=1}^5 (-1)^x a_{x,\alpha} + \lambda a_{6,\alpha} \right), \quad (4.82)$$

which satisfies  $B_{1,\alpha}^{3,\star}(1) = B_{1,\alpha}^{3,\star}$  and  $\lim_{\lambda \rightarrow \infty} B_{1,\alpha}^{3,\star}(\lambda) = a_{6,\alpha}$ . By applying lattice translation vectors, we can get all the other  $B_{j,\alpha}^{3,\star}(\lambda)$  with  $j = 2, \dots, N$ . Now consider the state defined on the kagome lattice

$$|\text{GS}_{3,\star}(\lambda)\rangle = \sum_{\alpha_1, \dots, \alpha_N = -3}^3 S_{\alpha_1, \dots, \alpha_N} \prod_{j=1}^N \left( B_{j,\alpha_j}^{3,\star}(\lambda) \right)^\dagger |\text{vac}\rangle, \quad (4.83)$$

where  $\{S_{\alpha_1, \dots, \alpha_N}\}$  are chosen such that  $|\text{GS}_{3,\star}(1)\rangle = |\text{GS}_{3,\star}\rangle$  is the original ground state of  $H^{3,\star}$ . One can then easily see that  $\lim_{\lambda \rightarrow \infty} |\text{GS}_{3,\star}(\lambda)\rangle = |\text{AKLT}_{3,\triangle}\rangle$  and the state  $|\text{GS}_{3,\star}(\lambda)\rangle$  remains  $(\text{SO}(3) \times \text{trn})$ -symmetric and short-range entangled for  $1 < \lambda < \infty$ . Therefore,  $|\text{GS}_{3,\star}\rangle$  and  $|\text{AKLT}_{3,\triangle}\rangle$  are smoothly connected and are in the same trivial phase protected by  $\text{SO}(3) \times \text{trn}$ . For an arbitrary  $f$  and  $X$ , a smooth path between  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  can always be explicitly constructed by smoothly deforming every CLS in  $X$  to one single site while preserving the  $\text{SO}(3)$  or  $\text{SO}(3) \times \text{trn}$  symmetry, and thus the two states always represent the same phase protected by the symmetry. Let  $|\text{GS}_{2,\square}\rangle$  be the exact ground

	SO(3)	SO(3) $\times$ trn
$ \text{AKLT}_{2,\square}\rangle$	trivial	<b>SPT</b>
$ \text{GS}_{2,\mathbb{D}}\rangle$		
$ \text{AKLT}_{3,\triangle}\rangle$	trivial	trivial
$ \text{GS}_{3,\star}\rangle$		

Table 4.3: In terms of on-site symmetry or on-site $\times$ trn symmetry,  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  are always in the same phase.

state of spin-2 bosons in the 2D Tasaki lattice; for the above reason,  $|\text{GS}_{2,\mathbb{D}}\rangle$  and  $|\text{AKLT}_{2,\square}\rangle$  are in the same SPT phase protected by  $\text{SO}(3) \times \text{trn}$ . (Recall that the phases of  $|\text{AKLT}_{2,\square}\rangle$  and  $|\text{AKLT}_{3,\triangle}\rangle$  have been discussed in Sec. 3.1.)

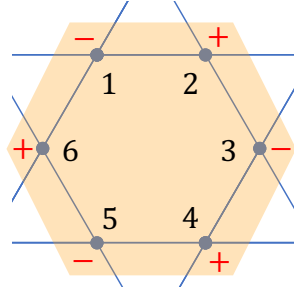


Figure 4.8: A CLS in the kagome lattice. Sign of the amplitude alternates from site 1 to 6. The CLS carries nontrivial charges of point groups  $D_2$ ,  $D_3$ , and  $D_6$ .

Table 4.3 summarizes current results. The purpose of this section (Sec. 4.3.3.1) is to demonstrate the smooth path argument. More on the on-site  $\times$  trn symmetries will be discussed in Sec. 4.3.3.3.

#### 4.3.3.2 SPT/trivial phases protected by crystalline symmetries alone

For general crystalline symmetries, however, the smooth path argument does not always apply. For simplicity, we consider only point group symmetries in  $d = 2$  spatial dimension in this chapter. Let  $G$  be a point group of a Hamiltonian with a unique gapped ground state  $|\Psi\rangle$ . Let  $U(q)$  be the symmetry operation (on the Hilbert space) corresponding to the group element  $q \in G$ . Subjected to  $q$ , the unique ground state transforms as,

$$|\Psi\rangle \rightarrow U(q)|\Psi\rangle = e^{i\theta_q}|\Psi\rangle. \quad (4.84)$$

As introduced in Sec. 3.3, the phase factors  $\{e^{i\theta_q}\}_{q \in G}$  form a 1D representation of  $G$ , and different 1D representations label different phases protected by the point group  $G$ . When  $\{e^{i\theta_q}\}_{q \in G}$  is a trivial representation, that is,  $e^{i\theta_q} = 1$  for all  $q \in G$ ,  $|\Psi\rangle$  is in a trivial phase. On



the other hand,  $|\Psi\rangle$  is in an SPT phase if  $\{e^{i\theta_q}\}_{q \in G}$  is a nontrivial representation [65, 97]. As also emphasized in Sec. 3.3, for point group symmetries alone in  $d < 3$  dimensions, the SPT/trivial classifications become meaningless when there are microscopic DOF lying precisely at symmetry centers. In other words, it is only legal to put the symmetry centers in vacuum.

We have already discussed how to classify the pgSPT/trivial phases of  $|\text{AKLT}_{2,\square}\rangle$  and  $|\text{AKLT}_{3,\triangle}\rangle$  in Sec. 3.3, and the results are summarized in Table 4.4. (Pay attention to the positions of symmetry centers we assumed in Table 4.4!)

In general, a smooth path between  $|\text{GS}_{f,X}\rangle$  and  $|\text{AKLT}_{f,X'}\rangle$  that preserve on-site  $\times$  trn symmetry may or may not break crystalline symmetries. For example, by smoothly deforming every CLS into the single site at its center,  $|\text{GS}_{2,\square}\rangle$  reduces to  $|\text{AKLT}_{2,\square}\rangle$  while preserving the plaquette-centered  $D_2$  symmetry, see Fig. 4.6(a). For  $|\text{GS}_{3,\star}\rangle$ , however, the smooth path described by Eq. (4.83) breaks the  $D_2$  symmetry. In general, when we are not able to find a path that is both crystalline-symmetry-preserving and smooth, such a path either is too complicated to be explicitly found or simply does not exist. Nevertheless, it is always possible to investigate the crystalline-symmetry-protected phase of  $|\text{GS}_{f,X}\rangle$  case-by-case. We again use  $|\text{GS}_{3,\star}\rangle$  as an example. As shown in Fig. 4.9(a), we put the symmetry center at the geometric center of a hexagonal plaquette. A CLS in the kagome lattice can actually be regarded as a 0D SPT phase protected by  $D_2$ , because, for example, according to Eq. (4.81) and Fig. 4.8,

$$U(\sigma_2) \left( B_{1,\alpha}^{3,\star} \right)^\dagger \bigotimes_{k=1}^6 |\text{vac}\rangle_k = - \left( B_{1,\alpha}^{3,\star} \right)^\dagger \bigotimes_{k=1}^6 |\text{vac}\rangle_k, \quad (4.85)$$

where  $\sigma_2$  is the mirror plane in vertical direction; see Fig. 4.9. The nontrivial charge  $-1$  in Eq. (4.85) cannot be eliminated.<sup>11</sup> The many-body ground state  $|\text{GS}_{3,\star}\rangle$  is a fully packing of CLSs with entangled spin DOF. The spin configuration of  $|\text{GS}_{3,\star}\rangle$ , which is inherited from  $|\text{AKLT}_{3,\triangle}\rangle$ , transforms trivially, as shown in Figs. 4.9(b) and 4.9(c). Nevertheless,  $|\text{GS}_{3,\star}\rangle$  yields a nontrivial representation of  $D_2$  thanks to how CLSs transform. We thus see that  $|\text{GS}_{3,\star}\rangle$  is in an SPT phase protected by  $D_2$ ; the SPT phase is purely a result of charge fluctuations at zero temperature, as the spin DOF contribute trivially. On the other hand, the phase of  $|\text{AKLT}_{3,\triangle}\rangle$  is not well-defined because the symmetry  $D_2$  in Fig. 4.9(b) is site-centered. Similarly, with the symmetry center in Fig. 4.9, one can also show that  $|\text{GS}_{3,\star}\rangle$  represents an SPT phase protected by point group  $D_3$  or  $D_6$ , while the phase of  $|\text{AKLT}_{3,\triangle}\rangle$  is not well-defined with respect to the site-centered  $D_3$  or  $D_6$ . Once again, the SPT phase of  $|\text{GS}_{3,\star}\rangle$  protected by  $D_3$  or  $D_6$  originates from the charge fluctuation of each CLS. Results of the current section are summarized in Table 4.4. Note that according to Proposition 3.4,  $|\text{GS}_{3,\star}\rangle$  has no anomalous edge states.

<sup>11</sup>It is natural to require that  $U(\sigma_2)a_1^\dagger U(\sigma_2) = a_2^\dagger$  and so on. Whether we define  $U(\sigma_2)|\text{vac}\rangle_1 = |\text{vac}\rangle_2$  or  $U(\sigma_2)|\text{vac}\rangle_1 = -|\text{vac}\rangle_2$ , Eq. (4.85) is invariant, because there are even number of sites in total.

	$ \text{AKLT}_{2,\square}\rangle$	$ \text{GS}_{2,\square}\rangle$	$ \text{AKLT}_{3,\triangle}\rangle$	$ \text{GS}_{3,\triangle}\rangle$
$D_1$	trivial	trivial	trivial	trivial
$D_2$	trivial	trivial	not well-defined	<b>SPT</b>
$D_3$	—	—	not well-defined	<b>SPT</b>
$D_4$	trivial	trivial	—	—
$D_6$	—	—	not well-defined	<b>SPT</b>

Table 4.4: Classifying the phases of 2D states in terms of point group symmetries. For  $|\text{AKLT}_{2,\square}\rangle$  and  $|\text{GS}_{2,\square}\rangle$ ,  $D_2$  and  $D_4$  are assumed to be plaquette-centered symmetries; see Fig. 3.6(b). For  $|\text{AKLT}_{3,\triangle}\rangle$  and  $|\text{GS}_{3,\triangle}\rangle$ , the symmetry centers of  $D_2$ ,  $D_3$ , and  $D_6$  are assumed to be those in Fig. 4.9. The phase is not well-defined if the symmetry is site-centered. Note that as demonstrated in Fig. 3.6, if we change the positions of symmetry centers, the results can change.

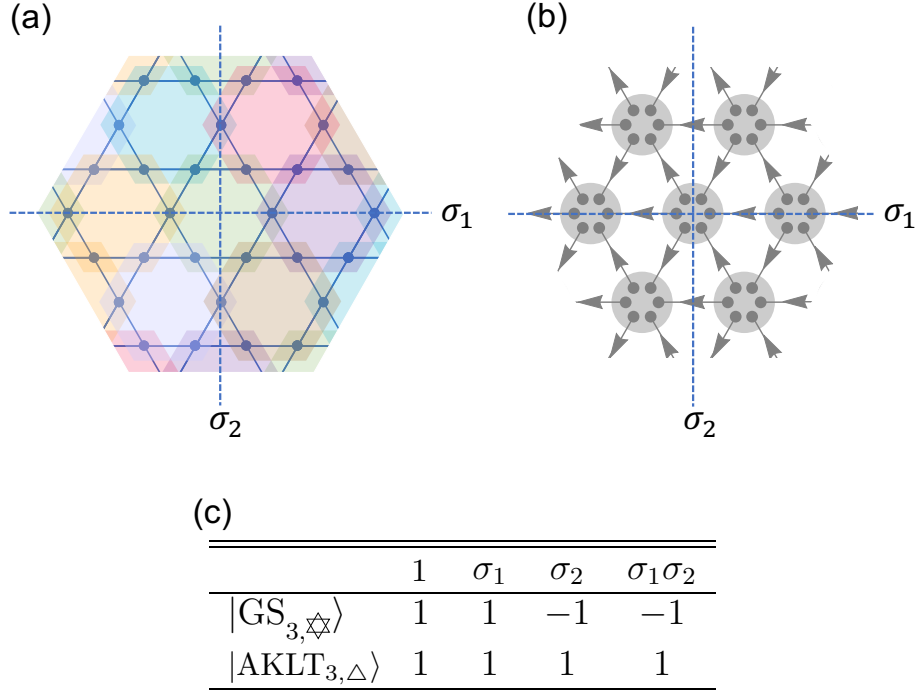


Figure 4.9: (a) An FPS on the kagome lattice. ( $|\text{GS}_{3,\triangle}\rangle$  is  $D_2$  symmetric, and it is a superposition of FPSs with different spin configurations.) We require that the symmetry center of  $D_2$  lies at the geometric center of a hexagon. (b) For  $|\text{AKLT}_{3,\triangle}\rangle$ , the symmetry center should lie at a site (spin) in order to be compatible with (a). See Fig. 3.5(a) for the meaning of the arrows. (c) 1D representations of  $D_2$  associated with  $|\text{GS}_{3,\triangle}\rangle$  and  $|\text{AKLT}_{3,\triangle}\rangle$ . The latter state transforms trivially, because there are always even number of bonds being reversed.

For a specific symmetry, to identify the phase of  $|\text{GS}_{f,X}\rangle$ , we can first try to find a both symmetry-preserving and smooth path that connects  $|\text{GS}_{f,X}\rangle$  to  $|\text{AKLT}_{f,X'}\rangle$ , provided that the phase of  $|\text{AKLT}_{f,X'}\rangle$  is already known. (For point group symmetries, we require that there are no microscopic DOF lying at the symmetry center all along the path.) When such a path cannot be explicitly found, it is either too complicated to be found or simply absent. Nevertheless, for point group symmetries, based on Eq. (4.84), one can always classify the phase of  $|\text{GS}_{f,X}\rangle$  without the help of the smooth path argument.

I would like to mention some related research. The "fragile Mott insulator" studied in Ref [188] can be understood as pgSPT phases. In contrast, the "featureless Mott insulator" of spinless bosons studied in Refs. [189, 190] should be classified into trivial phases protected by point group symmetries.

#### 4.3.3.3 SPT phases protected by on-site $\times$ crystalline symmetries: a result of the LSM theorems

	$ \text{AKLT}_{2,\square}\rangle$	$ \text{GS}_{2,\square}\rangle$	$ \text{AKLT}_{3,\boxplus}\rangle$	$ \text{GS}_{3,3\text{DTas}}\rangle$
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times (\mathbb{Z}^{\text{trn}})^{d-1}$	<b>SPT</b>	<b>SPT</b>	<b>SPT</b>	<b>SPT</b>
$\text{TR} \times (\mathbb{Z}^{\text{trn}})^{d-1}$	<b>SPT</b>	<b>SPT</b>	<b>SPT</b>	<b>SPT</b>
$\mathbb{Z}_2 \times \mathbb{Z}_2 \times D_1$	<b>SPT</b>	<b>SPT</b>	trivial	trivial
$\text{TR} \times D_1$	<b>SPT</b>	<b>SPT</b>	trivial	trivial

Table 4.5: Classifying the phases of 2D and 3D states in terms of some on-site  $\times$  crystalline symmetries.  $D_1$  in this table refers to mirror reflection symmetry *along an array of sites*. All the SPT phases on the table are a result of LSM theorems; see also Sec. 3.1. The spin-3 AKLT state on a cubic lattice  $|\text{AKLT}_{3,\boxplus}\rangle$  represents a trivial phase in terms of  $\mathbb{Z}_2 \times \mathbb{Z}_2 \times D_1$  or  $\text{TR} \times D_1$ , because its surface state can be trivially gapped out without breaking these two symmetries.  $|\text{GS}_{3,3\text{DTas}}\rangle$  refers to the exact ground state of spin-3 bosons on the 3D Tasaki lattice, and it is smoothly connected to  $|\text{AKLT}_{3,\boxplus}\rangle$  while preserving the four symmetries on the table.

As introduced in Sec. 3.1, some AKLT states in  $d > 1$  dimensions are in (weak) SPT phases, which are closely related to the LSM theorems. As explained in Sec. 4.3.3.1,  $|\text{GS}_{f,X}\rangle$  is always smoothly connected to  $|\text{AKLT}_{f,X'}\rangle$  while preserving on-site  $\times (\mathbb{Z}^{\text{trn}})^{d-1}$  symmetries, where  $(d-1)$  is the spatial dimension of the boundary. However, for on-site  $\times$  point group or on-site  $\times$  space group symmetries, a symmetry-preserving smooth path may not exist.<sup>12</sup> In the case where a symmetry-preserving smooth path cannot be found, the phase of  $|\text{GS}_{f,X}\rangle$  can always be judged by examining if one can trivially gap out the edge

<sup>12</sup>Luckily, for  $\mathbb{Z}_2 \times \mathbb{Z}_2 \times D_1$  and  $\text{TR} \times D_1$ ,  $|\text{GS}_{2,\square}\rangle$  and  $|\text{GS}_{3,3\text{DTas}}\rangle$  are smoothly connected to their corresponding AKLT states.

state without out breaking the symmetry:  $|\text{GS}_{f,X}\rangle$  is in an SPT phase if its edge state cannot be trivially gapped out.

## 4.4 Discussions

It is known that the Haldane phase can also be realized in a spin-1/2 two-leg ladder [118, 125]. In the Mott insulating limit shown in Fig. 4.10(a), there are two spin-1/2 fermions in each unit cell, such that the symmetry of each unit cell is  $\text{SO}(3)$  (assuming Heisenberg interaction). However, it is known that if one tunes away from the Mott limit, the distinction between the SPT and trivial phases breaks down [118, 125, 191, 192]. This is because with nonvanishing charge fluctuations, one unit cell may contain odd number of spin-1/2 fermions; see Fig. 4.10(b). In such a case, the symmetry of the system becomes  $\text{SU}(2)$ , and the Haldane phase is unstable under  $\text{SU}(2)$  because  $H^2[\text{SU}(2), \text{U}(1)] = \{1\}$  [31, 64, 118, 125, 191]. In fact, there is the following *short exact sequence* [64, 94]:

$$1 \rightarrow \mathbb{Z}_2 \rightarrow \text{SU}(2) \rightarrow \text{SO}(3) \rightarrow 1, \quad (4.86)$$

where  $\text{SU}(2)$  is said to be the *extension* of  $\text{SO}(3)$ . In this sense, we say that the Haldane phase can be trivialized by the symmetry extension. On the contrary, for spinful bosons (interacting through  $s$ -wave scattering), the on-site symmetry is always  $\text{SO}(3)$  even if one introduces charge fluctuations, and hence the Haldane phase and the weak SPT phases are always stable under charge fluctuations.

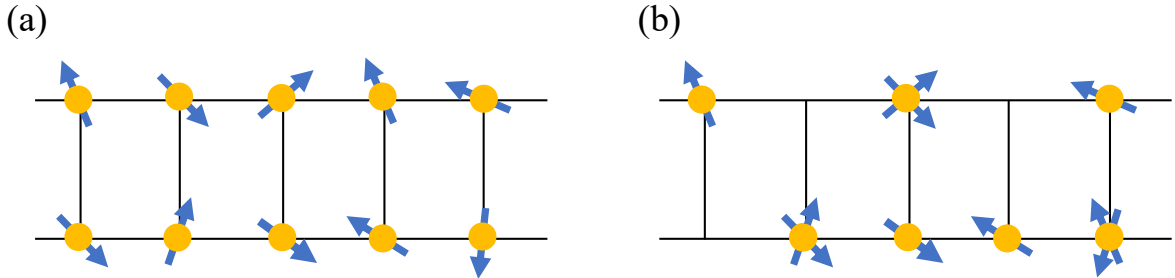


Figure 4.10: (a) A spin-1/2 two-leg ladder in the Mott limit, where each unit cell contains two spin-1/2 fermions. (b) With charge fluctuations, a unit cell may contain odd number of fermions, leading to the  $\text{SU}(2)$  symmetry.

We have been ignoring the long-range *dipole-dipole interaction (DDI)*, and this can be justified in many alkali-metal atom experiments. However, several kinds of *transition-metal atoms* can also be regarded as spinful bosons, such as  $^{52}\text{Cr}$  (spin-3),  $^{164}\text{Dy}$  (spin-8), and  $^{168}\text{Er}$  (spin-6) [126, 127]. Interestingly, these transition-metal atoms have very strong magnetic DDI [193–195]. It is also known that even for bosonic alkali-metal atoms, the

magnetic DDI can have a significant effect in certain cases [126, 127]. When taking the DDI into account (in addition to the short-range  $s$ -wave collision), it is probably impossible to exactly write down the many-body ground states. Nevertheless, we expect that the DDI induces new phases, such as charge density wave and supersolid, due to its long-range nature. Hunting new phases, including the SPT phases, in itinerant spinful bosonic systems with DDI will be an interesting future direction. Note that systems with magnetic DDI no longer have spin rotation symmetry. Instead, the magnetic DDI is invariant under simultaneous rotation in both spin and real spaces  $V^\delta(\theta) := \exp[-i\theta \sum_r (S_r^\delta + L_r^\delta)]$ , where  $L_r^\delta$  is the orbital angular momentum operator in the  $\delta(=x, y, z)$ -direction for particles at position  $r$  [126, 127, 196]. In other words, such systems conserve total angular momentum in free space. When constrained on a lattice, the systems can still preserve some discrete rotation symmetries, though such rotation symmetries are not on-site. In the future studies, it is worth investigating how such symmetries classify the SPT phases.

Finally, we would like to make some remarks about the flat band. The flat band has been gaining much attention these years because it was found to give rise to various collective phenomena, such as ferromagnetism [163, 168] and superconductivity [185, 197], in quantum many-body systems. In this chapter, we discover that the flat band can also be an origin of interacting SPT phases. We believe that this work stimulates future research on the relation between flat bands and topological quantum physics.

Interestingly, there exists many kinds of lattices where the flat band appears in the middle or top of the band structure [142, 181–183]. One can certainly follow the scheme in this chapter to construct the many-body eigenstates in these lattices with the help of the CLSs of the flat bands. The resulting many-body eigenstates, due to their short-range entangled nature, are actually *quantum many-body scars* [198–202], which lead to weak ergodicity breaking of the systems. Exploring quantum many-body scars in spinful atoms with a flat band will be another intriguing future direction.



造化賦形，支體必雙，神理為用，  
事不孤立。夫心生文辭，運裁百慮，  
高下相須，自然成對。

南北朝·劉勰『文心雕龍·麗辭』

## DUALITY, CRITICALITY, ANOMALY, AND TOPOLOGY IN QUANTUM SPIN-1 CHAINS

The concept of duality plays an important role in physics, in particular in the study of quantum phases of matter. Since a duality usually relates different phases of matter, when the duality becomes a symmetry (i.e., the system is *self-dual*), the self-duality must force the system to stay on the phase boundary between the two duality-related phases, often leading to criticality or multicriticality [203–207]. A prominent example is the transverse field Ising chain  $H_{\text{Ising}} = -\sum_j (\sigma_j^z \sigma_{j+1}^z + h \sigma_j^x)$ , in which the Kramers-Wannier duality [7, 8] exchanges the symmetric phase and the  $\mathbb{Z}_2$  SSB phase. At the self-dual point  $h = 1$ ,  $H_{\text{Ising}}$  is at a critical point described by the Ising conformal field theory (CFT).

In quantum spin-1 chains the Kennedy-Tasaki (KT) transformation  $U_{\text{KT}}$  defines a duality between the Haldane phase and the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry-breaking phase; see Sec. 2.1.1. In this chapter, we focus on the KT duality and study a Hamiltonian of the form  $H(\lambda) = (1 - \lambda)H_{\text{Hal}} + (1 + \lambda)U_{\text{KT}}H_{\text{Hal}}U_{\text{KT}}$ , where  $H_{\text{Hal}}$  is an SO(3) symmetric and short-range interacting spin-1 chain in the Haldane phase (for example, the AFM Heisenberg model). In other words,  $H(\lambda)$  with  $-1 \leq \lambda \leq 1$  interpolates between the Haldane phase and its KT dual phase ( $\mathbb{Z}_2 \times \mathbb{Z}_2$  SSB phase). Note that  $U_{\text{KT}}H(\lambda)U_{\text{KT}} = H(-\lambda)$ . Surprisingly, we find that the self-dual model  $H(0)$  is *exactly equivalent* to a  $(1+1)\text{D}$  spin-1/2 XXZ model doped by immobile holes, and the holes are completely absent from the low-energy theory. This means that the self-dual point is indeed a critical point described by a Gaussian CFT (with central charge  $c = 1$ ). Furthermore, we find that the effective model for  $H(|\lambda| \ll 1)$  is given by the famous  $(1+1)\text{D}$  spin-1/2 XYZ model, which implies that there is an *emergent quantum anomaly* around the self-dual point  $\lambda = 0$ . To our knowledge, the idea of

emergent anomaly can be found in Refs. [30, 64, 94, 208, 209].

In fact,  $H(\lambda)$  hosts more phases other than the Haldane and the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  SSB phases: there are two  $\mathbb{Z}_2$  SSB phases in the region  $-\lambda_c < \lambda < 0$  and  $0 < \lambda < \lambda_c$  (with  $\lambda_c < 1$ ), where  $\pm\lambda_c$  are two Ising critical points; the former one is a  $\mathbb{Z}_2 \times \mathbb{Z}_2$  trivial Ising criticality while the latter is a  $\mathbb{Z}_2 \times \mathbb{Z}_2$  SPT Ising criticality. (The concept of SPT Ising criticality has been discussed in Sec. 2.2 of this thesis.) This means that the KT transformation also defines a duality between the SPT and trivial Ising criticality. If we introduce an additional parameter  $\theta$  to the model, then the two critical lines  $\pm\lambda_c(\theta)$  meet at  $(\lambda, \theta) = (0, \arctan \frac{1}{2})$ , on which the model  $H(\lambda, \theta)$  is exactly equivalent to a spin-1/2 ferromagnetic (FM) Heisenberg chain doped by immobile holes. This means that the two KT duality-related Ising criticalities meet at a self-dual point which is indeed multicritical. See Fig. 5.1(a) for the phase diagram of  $H(\lambda, \theta)$ .

This chapter is mainly based on my publication in Ref. [2].

Let us review some basic facts about the KT transformation. For a quantum spin-1 chain with open boundary condition (OBC), let  $S_j = (S_j^x, S_j^y, S_j^z)$  be the spin-1 operator on the lattice site  $j \in \{1, 2, \dots, L\}$ . The KT transformation is defined as [50–53]

$$U_{\text{KT}} = \prod_{1 \leq u < v \leq L} \exp(i\pi S_u^z S_v^x), \quad (5.1)$$

which satisfies  $U_{\text{KT}} = U_{\text{KT}}^\dagger$  and  $U_{\text{KT}}^2 = 1$ . An AFM Heisenberg interaction  $S_j \cdot S_{j+1}$  is KT-dual to an FM interaction in both  $x$  and  $z$  directions; more precisely, according to Eqs. (2.20) and (2.21),

$$S_j \cdot S_{j+1} \xleftrightarrow{U_{\text{KT}}} U_{\text{KT}} S_j \cdot S_{j+1} U_{\text{KT}} = -S_j^x S_{j+1}^x + S_j^y e^{i\pi(S_j^z + S_{j+1}^z)} S_{j+1}^y - S_j^z S_{j+1}^z. \quad (5.2)$$

Let  $Y_\theta = \prod_j \exp(-i\theta S_j^y)$ ,  $Z_\theta = \prod_j \exp(-i\theta S_j^z)$ ,  $X_\pi = Y_\pi Z_\pi = \prod_j \exp(-i\pi S_j^x)$ ,  $\mathbb{Z}_2^z = \{1, Z_\pi\}$ , and

$$\mathbb{Z}_2^y = \{1, Y_\pi\} \subset \mathbb{Z}_4^y = \{1, Y_{\pi/2}, Y_\pi, Y_{3\pi/2}\}. \quad (5.3)$$

The left-hand side of Eq. (5.2) respects the on-site  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  symmetry<sup>1</sup>, where

$$\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z = \{1, X_\pi, Y_\pi, Z_\pi, Y_{\pi/2}, Y_{3\pi/2}, Z_\pi Y_{\pi/2}, Y_{\pi/2} Z_\pi\}. \quad (5.4)$$

The semidirect product group  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  is isomorphic to  $D_4$  (the dihedral group of order 8), while

$$\mathbb{Z}_2^y \times \mathbb{Z}_2^z = \{1, X_\pi, Y_\pi, Z_\pi\} \quad (5.5)$$

<sup>1</sup>The Hamiltonian  $\sum_\ell S_j \cdot S_{j+1}$  has an on-site  $\text{SO}(3)$  symmetry whose group element  $g$  looks like  $g = \prod_j \exp(-i\theta_x S_j^x - i\theta_y S_j^y - i\theta_z S_j^z)$ . The dual Hamiltonian  $U_{\text{KT}} (\sum_j S_j \cdot S_{j+1}) U_{\text{KT}}$  also has an  $\text{SO}(3)$  symmetry, but elements in this  $\text{SO}(3)$  group take the form  $\tilde{g} = U_{\text{KT}} g U_{\text{KT}}$  which is *not* on-site in general. We are only interested in on-site symmetries in this chapter. Theorem 2.7 guarantees the on-site  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry of  $U_{\text{KT}} (\sum_j S_j \cdot S_{j+1}) U_{\text{KT}}$ . However, the on-site  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  symmetry is rather a coincidence in spin-1 chains. For an integer spin  $S > 1$ ,  $U_{\text{KT}} (\sum_j S_j \cdot S_{j+1}) U_{\text{KT}}$  in general has no on-site  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  symmetry.



is isomorphic to the dihedral group  $D_2$ . For the Haldane phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ , the symmetry flux associated to  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  is defined as

$$F_j^\alpha = \exp\left(-i\pi \sum_{k < j} S_k^\alpha\right) S_j^\alpha \quad (5.6)$$

where  $\alpha = x, y, z$  [23]. The correlation of two symmetry fluxes gives the nonlocal string order parameter  $\mathcal{O}_{\text{str}}^\alpha = -\lim_{r \rightarrow \infty} \langle F_j^{\alpha\dagger} F_{j+r}^\alpha \rangle$  [47]. It is known that  $\mathcal{O}_{\text{str}}^\alpha > 0$  serves as an order parameter for the Haldane phase [50–52, 60, 61]. For the spins in  $\alpha = x, z$  direction, the following duality holds:

$$-(F_j^\alpha)^\dagger F_{j+r}^\alpha = -S_j^\alpha \exp\left(i\pi \sum_{k=j+1}^{j+r-1} S_k^\alpha\right) S_{j+r}^\alpha \xleftrightarrow[\alpha=x,z]{U_{\text{KT}}} S_j^\alpha S_{j+r}^\alpha. \quad (5.7)$$

As for the  $y$  direction, see Eq. (5.36).

## 5.1 Model

For a spin-1 chain with only nearest-neighbor interaction and  $\text{SO}(3)$  spin rotation symmetry, the most general Hamiltonian is the bilinear-biquadratic (BLBQ) model [157, 210]

$$H_{\text{BLBQ}}(\theta) = \sum_{j=1}^{L-1} \left[ \cos \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1}) + \sin \theta (\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2 \right]. \quad (5.8)$$

In particular,  $\theta = 0$  and  $\arctan(1/3)$  correspond to the Heisenberg model and the AKLT model [45, 46], respectively. In fact, the GS of  $H_{\text{BLBQ}}(\theta)$  is in the Haldane phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  as long as  $-\pi/4 < \theta < \pi/4$  [157], and in that case the dual Hamiltonian  $\tilde{H}_{\text{BLBQ}}(\theta) = U_{\text{KT}} H_{\text{BLBQ}}(\theta) U_{\text{KT}}$  is in the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SSB phase. [An explicit expression of  $\tilde{H}_{\text{BLBQ}}$  can be obtained by substituting Eq. (5.2) into Eq. (5.8).] In the following, we study a one-parameter interpolation between the two duality-related models as

$$H(\lambda, \theta) = (1 - \lambda) H_{\text{BLBQ}}(\theta) + (1 + \lambda) \tilde{H}_{\text{BLBQ}}(\theta) \quad (5.9)$$

where we have assumed the model is defined on a chain of length  $L$  with OBC and  $-1 \leq \lambda \leq 1$ . For a general  $(\lambda, \theta)$ , the largest on-site symmetry group of  $H(\lambda, \theta)$  is  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$ , where  $\mathbb{Z}_4^y = \{1, Y_{\pi/2}, Y_\pi, Y_{3\pi/2}\}$ . Obviously,  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z \subset \mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$ . In the thermodynamic limit  $L \rightarrow \infty$ , the model has translation symmetry (denote the group as  $\mathbb{Z}^{\text{trn}}$ ), thus the whole symmetry group  $G$  of  $H(\lambda, \theta)$  is

$$G = \mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z \times \mathbb{Z}^{\text{trn}}. \quad (5.10)$$

A phase diagram for  $H(\lambda, \theta)$  is presented in Fig. 5.1(a). Note that the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SSB phase is also a fully  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  breaking phase, because, according to Eq. (3.7),

$$H^1[\mathbb{Z}_2^y \times \mathbb{Z}_2^z, \text{U}(1)] = H^1[\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z, \text{U}(1)] = \mathbb{Z}_2 \times \mathbb{Z}_2, \quad (5.11)$$

which means that fully breaking of either symmetry gives four-fold (quasi-)degeneracy.

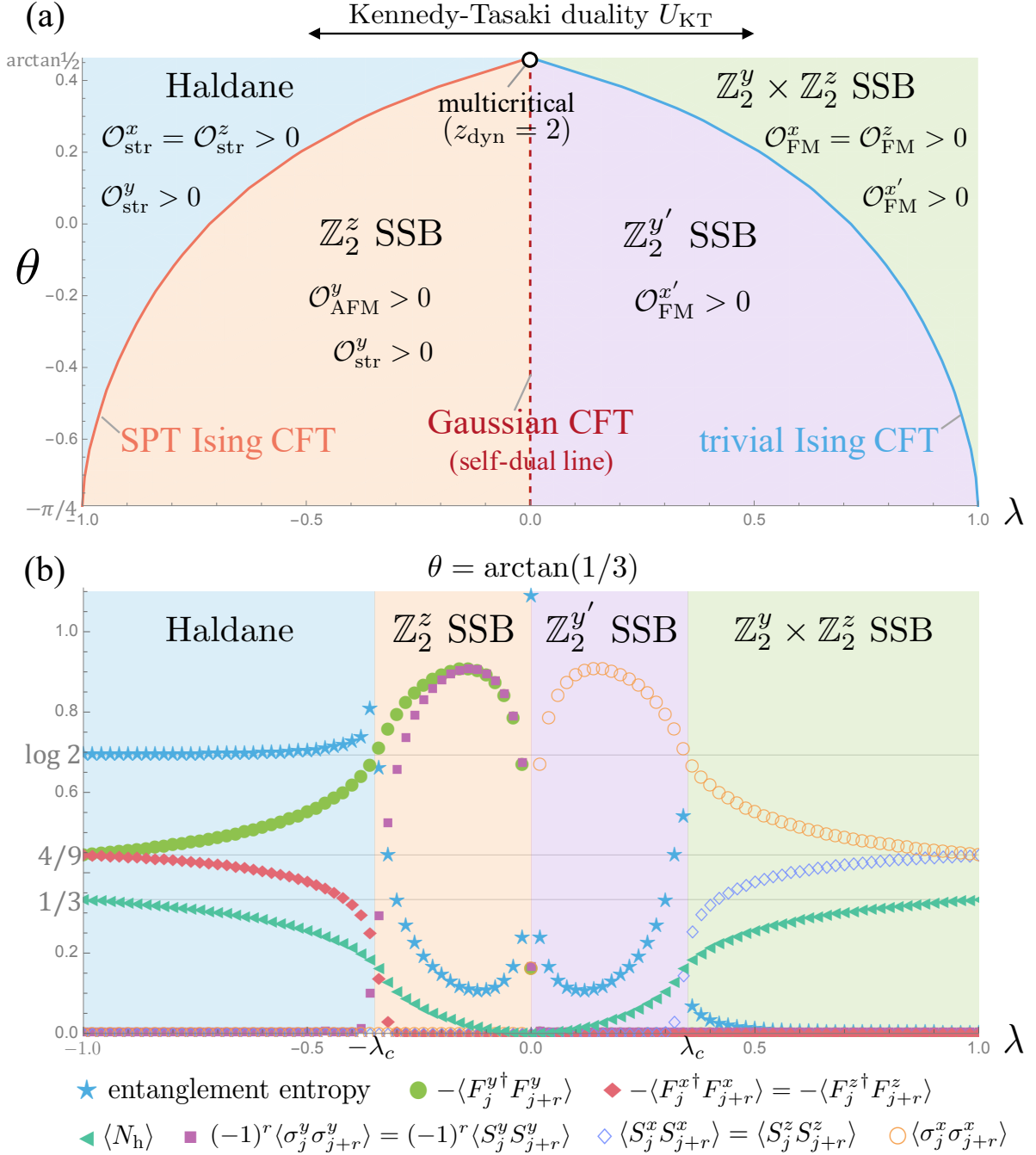


Figure 5.1: (a) Schematic phase diagram of  $H(\lambda, \theta)$  in the region  $(\lambda, \theta) \in [-1, 1] \times (-\pi/4, \arctan(1/2)]$ . There is an emergent LSM anomaly when  $|\lambda| \ll 1$ . Note that  $\mathbb{Z}_2^y$  is a normal subgroup of  $\mathbb{Z}_4^y$ , while  $\mathbb{Z}_2^{y'} = \mathbb{Z}_4^y / \mathbb{Z}_2^y$ . The  $\mathbb{Z}_2^{y'}$  SSB phase can also be viewed as another  $\mathbb{Z}_2^z$  SSB phase. Due to the global  $\mathbb{Z}_4^y$  symmetry,  $\mathcal{O}_{\text{str}}^x = \mathcal{O}_{\text{str}}^z$  and  $\mathcal{O}_{\text{FM}}^x = \mathcal{O}_{\text{FM}}^z$ . (b) DMRG results at  $\theta = \arctan(1/3)$ . The total hole number  $\langle N_h \rangle$  is obtained by infinite DMRG, while the correlation functions are calculated on an open chain with  $L = 64$  and  $r = 40$ . Due to Eq. (5.37),  $\mathcal{O}_{\text{str}}^y \approx \mathcal{O}_{\text{AFM}}^y$  when  $-\lambda_c \ll \lambda < 0$ . It is also clear that  $\mathcal{O}_{\text{str}}^y > 0$  at the SPT Ising critical point  $-\lambda_c$ . The half-chain entanglement entropy ( $L = 64$ ) shows a sudden change at the critical points.

## 5.2 Self-duality

Since  $U_{\text{KT}}H(\lambda, \theta)U_{\text{KT}} = H(-\lambda, \theta)$ , the model  $H_{\text{SD}}(\theta) = H(0, \theta)$  is self-dual at  $\lambda = 0$ . Let  $\{|+\rangle_j, |0\rangle_j, |-\rangle_j\}$  be a basis of local Hilbert space satisfying  $S_j^z |\pm\rangle_j = \pm |\pm\rangle_j$  and  $S_j^z |0\rangle_j = 0$ . We define a "p-wave basis"  $\{|\uparrow\rangle_j, |\downarrow\rangle_j, |\text{h}\rangle_j\}$  as [211, 212]

$$\begin{aligned} |\uparrow\rangle_j &= \frac{1}{\sqrt{2}}(|+\rangle_j - |-\rangle_j), \\ |\downarrow\rangle_j &= |0\rangle_j, \\ |\text{h}\rangle_j &= \frac{1}{\sqrt{2}}(|+\rangle_j + |-\rangle_j). \end{aligned} \quad (5.12)$$

We will often abbreviate  $|\cdot\rangle_j$  to  $|\cdot\rangle$  for simplicity. Let us treat  $|\uparrow\rangle/|\downarrow\rangle$  as the up/down spin of a spin-1/2 particle (qubit) and  $|\text{h}\rangle$  as a hole. Define the Pauli operators as

$$\begin{aligned} \sigma_j^x &= |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|, \\ \sigma_j^y &= S_j^y = -i|\uparrow\rangle\langle\downarrow| + i|\downarrow\rangle\langle\uparrow|, \\ \sigma_j^z &= |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|. \end{aligned} \quad (5.13)$$

Note that  $\sigma_j^y$  and  $S_j^y$  happen to be identical. Also define two number operators

$$\begin{aligned} n_j &= |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|, \\ h_j &= |\text{h}\rangle\langle\text{h}| \end{aligned} \quad (5.14)$$

satisfying  $n_j + h_j = 1$ . The self-dual Hamiltonian can then be *exactly* written as

$$H_{\text{SD}}(\theta) = H_{\text{XXZ}} + \sin \theta \sum_{j=1}^{L-1} (2h_j h_{j+1} + n_j n_{j+1} + 2), \quad (5.15)$$

where

$$H_{\text{XXZ}} = (\cos \theta - \sin \theta) \sum_{j=1}^{L-1} (-\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y) + \sin \theta \sum_{j=1}^{L-1} \sigma_j^z \sigma_{j+1}^z \quad (5.16)$$

is the *spin-1/2 XXZ model*. The minus sign in front of  $\sigma_j^x \sigma_{j+1}^x$  can be eliminated by a unitary transformation

$$V = \prod_{k=\text{odd}} \sigma_k^y. \quad (5.17)$$

The Hilbert space of a spin-1 chain is given by

$$\mathcal{H}_1 = \bigotimes_{j=1}^L \text{span}(|+\rangle_j, |0\rangle_j, |-\rangle_j), \quad (5.18)$$

while we define the Hilbert space of a spin-1/2 chain by

$$\mathcal{H}_{1/2} = \bigotimes_{j=1}^L \text{span}(|\uparrow\rangle_j, |\downarrow\rangle_j). \quad (5.19)$$

For  $H_{\text{SD}}$ , the holes are completely decoupled from the qubits, making  $\mathcal{H}_{1/2}$  an invariant subspace. We emphasize that a system is specified by a pair consisting of the Hamiltonian and its underlying Hilbert space. The pair  $(H_{\text{SD}}, \mathcal{H}_1)$  completely specifies the self-dual model. On the other hand,  $(H_{\text{SD}}, \mathcal{H}_{1/2})$  is equal to  $(H_{\text{XXZ}}, \mathcal{H}_{1/2})$  up to a constant, meaning that

$$PH_{\text{SD}}P = PH_{\text{XXZ}}P + 3(L-1)\sin\theta P, \quad (5.20)$$

where

$$P = \bigotimes_{j=1}^L n_j = \bigotimes_{j=1}^L (|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) \quad (5.21)$$

is the projection operator onto  $\mathcal{H}_{1/2}$ . Luckily,  $(H_{\text{XXZ}}, \mathcal{H}_{1/2})$  is exactly solvable by the Bethe ansatz [213, 214]: Let

$$\Delta(\theta) = \frac{\sin\theta}{|\cos\theta - \sin\theta|}. \quad (5.22)$$

The GS of  $(H_{\text{XXZ}}, \mathcal{H}_{1/2})$  is

- (i) a Gaussian CFT ( $c = 1$ ) when  $-1 \leq \Delta < 1$ ;
- (ii) gapped and degenerate when  $|\Delta| > 1$ ;
- (iii) gapless, degenerate, and has a dynamical critical exponent  $z_{\text{dyn}} = 2$  when  $\Delta = 1$ . (In this case, the model is unitarily equivalent to the FM Heisenberg chain.)

For the low-energy theory of  $(H_{\text{SD}}, \mathcal{H}_1)$  in the thermodynamic limit, we have the following

**Proposition 5.1** *When  $-\infty < \Delta < 1$ , holes do not appear in the low-energy eigenstates of  $(H_{\text{SD}}, \mathcal{H}_1)$ , meaning that states with holes are "gapped degrees of freedom (DOF)". On the other hand, when  $\Delta \geq 1$  or  $\Delta \rightarrow -\infty$ , let  $W_1$  and  $W_{1/2}$  be the GS eigenspace of  $(H_{\text{SD}}, \mathcal{H}_1)$  and  $(H_{\text{SD}}, \mathcal{H}_{1/2})$ , respectively. Then  $W_1 \not\supset W_{1/2}$ , implying that holes appear in  $W_1$ .*

An intuitive picture for the case  $-\infty < \Delta < 1$  is shown in Fig. 5.2. A "general proof" of the Proposition 5.1 is presented in Appendix C, but let us take a look at two special points as intuitive examples. At  $\theta = 0$ ,  $(VH_{\text{SD}}V, \mathcal{H}_1)$  simply becomes a spin-1/2 XX model doped by immobile holes. A spin-1/2 XX chain in  $\mathcal{H}_{1/2}$  can be exactly mapped to a free-fermion chain. When  $L \rightarrow \infty$ , the GS energy density of the fermion chain is given by  $e_\infty = -4/\pi$  [213, 214]. In this case, if we cut the fermion chain somewhere, two edges will be created, which will raise the GS energy by  $f = 2 - 4/\pi$  [215]. Replacing a qubit (in the XX chain) by an immobile hole is equivalent to cutting the fermion chain and in the mean time shorten the total length of the fermion chains by one. This in total changes the GS energy by  $f - e_\infty = 2 > 0$ . Therefore, holes are energetically unfavorable when  $\theta = 0$ . On the other hand, at  $\theta = \pi/4$ ,  $(H_{\text{SD}}, \mathcal{H}_1)$  is precisely the classical AFM 3-state Potts model (when representing in the  $p$ -wave basis), implying that  $\{|h\rangle_j\}$  are involved in the GS eigenspace.

A direct corollary of Proposition 5.1 is that following the same  $\Delta$ -dependence of the spin-1/2 XXZ model, the GS of  $(H_{\text{SD}}, \mathcal{H}_1)$  can only be in any of the three cases (i), (ii), and

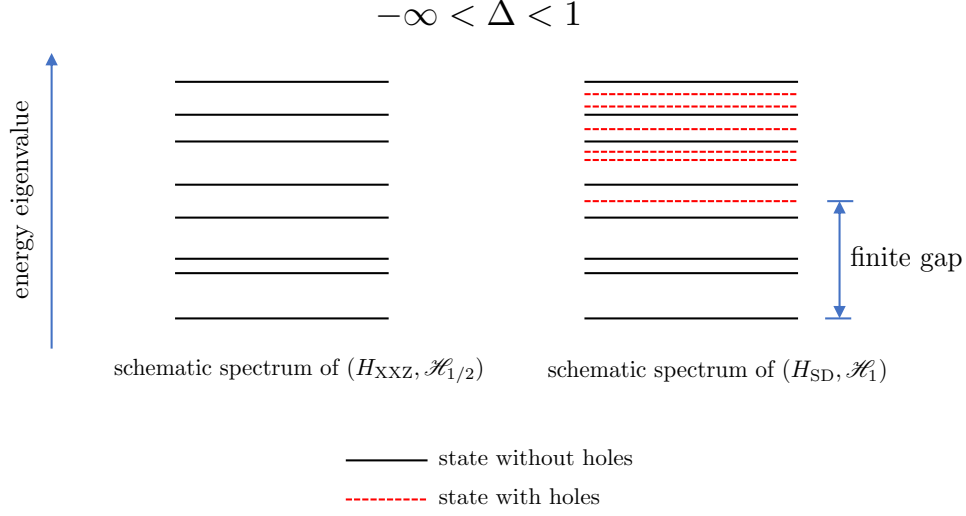


Figure 5.2: According to Eq. (5.20), the spectrum of  $(H_{XXZ}, \mathcal{H}_{1/2})$  is completely embedded in that of  $(H_{SD}, \mathcal{H}_1)$ . When  $-\infty < \Delta < 1$ , in the thermodynamic limit, eigenstates of  $(H_{SD}, \mathcal{H}_1)$  with holes are separated from the GS by a finite energy gap, making the low-energy physics of  $(H_{XXZ}, \mathcal{H}_{1/2})$  and  $(H_{SD}, \mathcal{H}_1)$  completely identical. In this figure, we have ignored the constant shift such that the GS energy of both models is the same.

(iii) as  $(H_{XXZ}, \mathcal{H}_{1/2})$ . Let us now focus on the region  $-\infty < \Delta(\theta) < 1$ ; in such a case the low-energy theory of  $(H_{SD}, \mathcal{H}_1)$  and  $(H_{XXZ}, \mathcal{H}_{1/2})$  are identical. Let

$$\begin{aligned} Y'_\pi &= Y_{\pi/2} = \prod_j \exp(-i\pi\sigma_j^y/2), \\ Z'_\pi &= \prod_j \exp(-i\pi\sigma_j^z/2). \end{aligned} \quad (5.23)$$

Since

$$\exp(-i\pi\sigma_j^y) = \exp(-i\pi\sigma_j^z) = -n_j + h_j, \quad (5.24)$$

we see that  $Y_\pi = (Y'_\pi)^2$  and  $(Z'_\pi)^2$  can only act nontrivially on the gapped DOF. We thus call  $\mathbb{Z}_2^y$  a "gapped symmetry". In the low-energy theory (which lies in  $\mathcal{H}_{1/2}$ ),  $\mathbb{Z}_4^y$  reduces to the quotient group

$$\mathbb{Z}_2^{y'} = \mathbb{Z}_4^y / \mathbb{Z}_2^y. \quad (5.25)$$

Similarly, one can also define

$$\mathbb{Z}_2^{z'} = \{1, Z'_\pi, (Z'_\pi)^2, (Z'_\pi)^3\} / \{1, (Z'_\pi)^2\}. \quad (5.26)$$

The fact that the GS of  $(H_{XXZ}, \mathcal{H}_{1/2})$  always belongs to the cases (i), (ii), and (iii) is nowadays understood as a *Lieb–Schultz–Mattis (LSM) anomaly*. The anomaly essentially states that a spin-1/2 system with certain symmetries can never have a unique gapped GS; see Theorem 3.1 and Corollary 3.2. The LSM anomaly of  $H_{XXZ}$  (and also  $H_{SD}$ ) is a

result of the  $\mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times \mathbb{Z}^{\text{trn}}$  symmetry in  $\mathcal{H}_{1/2}$  [79, 82, 84, 86]. Since a self-duality in various cases implies a quantum phase transition, one may wonder if the anomaly of  $H_{\text{SD}}$  can also be regarded as a result of the KT self-duality  $\mathbb{Z}_2^{\text{KT}} = \{1, U_{\text{KT}}\}$ . Let us consider a trivial model  $H_{\text{triv}} = \sum_j (S_j^z)^2$  satisfying  $[H_{\text{triv}}, U_{\text{KT}}] = 0$ . Clearly,  $(H_{\text{triv}}, \mathcal{H}_{1/2})$  has a unique gapped GS, because  $PH_{\text{triv}}P = \sum_j P(\sigma_j^z/2 + 1/2)P$ . This tells us that neither  $\mathbb{Z}_2^{\text{KT}}$  nor  $\mathbb{Z}_2^{\text{KT}} \times \mathbb{Z}^{\text{trn}}$  in  $\mathcal{H}_{1/2}$  has an anomaly. However, a direct calculation shows that  $PY'_\pi U_{\text{KT}} Y'_\pi U_{\text{KT}} P = (-i)^L P Z'_\pi P$  when  $L$  is even, which means that within  $\mathcal{H}_{1/2}$ , a system with both  $\mathbb{Z}_2^{\text{KT}}$  and  $\mathbb{Z}_2^{y'}$  symmetries must also have  $\mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'}$  symmetry. Therefore, we claim that the anomaly of  $H_{\text{SD}}$  is protected by  $\mathbb{Z}_2^{\text{KT}}$ ,  $\mathbb{Z}_2^{y'}$ , and  $\mathbb{Z}^{\text{trn}}$  symmetries together in  $\mathcal{H}_{1/2}$ . This is actually an emergent anomaly; details will be discussed in Sec. 5.5.

In the remainder of this chapter, we will assume that  $\theta$  takes the value such that  $H(-1, \theta)$  is in the Haldane phase while  $H_{\text{SD}}(\theta)$  is critical, namely

$$\theta \in \mathcal{R} := \left(-\frac{\pi}{4}, \arctan \frac{1}{2}\right), \quad (5.27)$$

which is included in the region  $-\infty < \Delta(\theta) < 1$ .

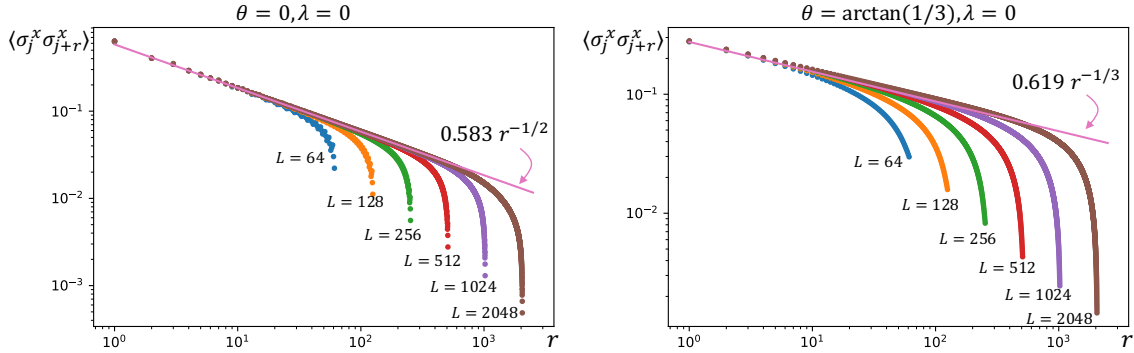


Figure 5.3: The correlation function  $\langle \sigma_j^x \sigma_{j+r}^x \rangle$  on an open chain with length  $L$  is calculated with various  $L$  at  $\theta = 0$  (Left) and  $\arctan(1/3)$  (Right). From the log-log plots, it is clear that the data are well-fitted by  $r^{-\eta(\theta)}$  when  $1 \ll r \ll L$ .

The fact that the self-dual point in the region  $\theta \in \mathcal{R}$  stands for a Gaussian criticality ( $c = 1$  CFT) is also supported by our density matrix renormalization group (DMRG) calculations of the critical exponent  $\eta$ . According to  $(H_{\text{XXZ}}, \mathcal{H}_{1/2})$  in Eq. (5.16) [see also the effective Hamiltonian in Eq. (5.32) with  $\lambda = 0$ ] the spin correlation function behaves as

$$\langle \sigma_j^x \sigma_{j+r}^x \rangle \sim r^{-\eta(\theta)}, \quad (5.28)$$

where [216]

$$\eta(\theta) = \frac{1}{2} - \frac{1}{\pi} \arcsin[\Delta(\theta)]. \quad (5.29)$$

In particular,  $\eta(0) = 1/2$  and  $\eta(\arctan \frac{1}{3}) = 1/3$ , which are consistent with the numerical results presented in Fig. 5.3.

### 5.3 Perturbation theory

Our model can be written as

$$H(\lambda, \theta) = H_{\text{SD}}(\theta) + \lambda H_{\text{pert}}(\theta), \quad (5.30)$$

where in the  $p$ -wave basis,  $H_{\text{SD}}$  is given by Eq. (5.15), and the second term reads

$$\begin{aligned} H_{\text{pert}}(\theta) &= U_{\text{KT}} H_{\text{BLBQ}}(\theta) U_{\text{KT}} - H_{\text{BLBQ}}(\theta) \\ &= -\cos \theta \sum_j \left( \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right) \\ &\quad - 2 \cos \theta \sum_j \left( |\uparrow \mathbf{h}\rangle \langle \mathbf{h} \uparrow| + |\downarrow \mathbf{h}\rangle \langle \mathbf{h} \downarrow| + |\mathbf{h} \uparrow\rangle \langle \uparrow \mathbf{h}| + |\mathbf{h} \downarrow\rangle \langle \downarrow \mathbf{h}| \right) \\ &\quad - 2(\cos \theta - \sin \theta) \sum_j \left( |\uparrow \uparrow\rangle \langle \mathbf{h} \mathbf{h}| + |\downarrow \downarrow\rangle \langle \mathbf{h} \mathbf{h}| + |\mathbf{h} \mathbf{h}\rangle \langle \uparrow \uparrow| + |\mathbf{h} \mathbf{h}\rangle \langle \downarrow \downarrow| \right), \end{aligned} \quad (5.31)$$

where  $|\cdot\rangle$  stands for a two-site state  $|\cdot\rangle_{j,j+1}$ . Around the self-dual point, we can treat  $\lambda H_{\text{pert}}$  as a perturbation to  $H_{\text{SD}}$ . Thanks to the Proposition 5.1 and Eq. (5.31), we know that holes are absent from the low-energy states of  $(H(\lambda, \theta), \mathcal{H}_1)$  when  $|\lambda| \ll 1$  and  $\theta \in \mathcal{R}$ . Let  $N_{\text{h}} = \sum_j h_j$ , this means that  $\lim_{\lambda \rightarrow 0} \langle N_{\text{h}} \rangle_{\text{GS}} = 0$ , which is also verified by our numerical calculations; see Fig. 5.1(b). Up to first order in  $\lambda$ , Eq. (5.31) tells us that the effective theory for  $(H(\lambda, \theta), \mathcal{H}_1)$  is given by  $(H_{\text{XYZ}}, \mathcal{H}_{1/2})$ , where

$$H_{\text{XYZ}}(\lambda, \theta) = -[(1+\lambda) \cos \theta - \sin \theta] \sum_{j=1}^{L-1} \sigma_j^x \sigma_{j+1}^x + [(1-\lambda) \cos \theta - \sin \theta] \sum_{j=1}^{L-1} \sigma_j^y \sigma_{j+1}^y + \sin \theta \sum_{j=1}^{L-1} (\sigma_j^z \sigma_{j+1}^z + 3). \quad (5.32)$$

The *spin-1/2 XYZ model*  $H_{\text{XYZ}}$  obviously has  $\mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times \mathbb{Z}^{\text{trn}}$  symmetry in  $\mathcal{H}_{1/2}$ . Let us note that

$$P Z_{\pi} P = i^L P Z'_{\pi} P, \quad (5.33)$$

which means that we can identify  $Z_{\pi}$  with  $Z'_{\pi}$  in the low-energy theory. The exact solutions by Bethe ansatz [217–220] tells us that when  $\lambda < 0$ ,  $(H_{\text{XYZ}}, \mathcal{H}_{1/2})$  is in a phase with

$$\mathcal{O}_{\text{AFM}}^y = \lim_{r \rightarrow \infty} (-1)^r \langle \sigma_j^y \sigma_{j+r}^y \rangle = \lim_{r \rightarrow \infty} (-1)^r \langle S_j^y S_{j+r}^y \rangle > 0, \quad (5.34)$$

implying the breaking of  $\mathbb{Z}_2^{z'}$  in  $\mathcal{H}_{1/2}$  (or equivalently,  $\mathbb{Z}_2^z$  SSB in  $\mathcal{H}_1$ ). On the other hand, when  $\lambda > 0$ , the XYZ model is in the  $\mathbb{Z}_2^{y'}$  SSB phase with

$$\mathcal{O}_{\text{FM}}^{x'} = \lim_{r \rightarrow \infty} \langle \sigma_j^x \sigma_{j+r}^x \rangle > 0. \quad (5.35)$$

In fact, from the following duality

$$-F_j^{y\dagger} F_{j+r}^y \xleftrightarrow{U_{\text{KT}}} \sigma_j^x \sigma_{j+r}^x, \quad (5.36)$$

it is clear that the two  $\mathbb{Z}_2$  SSB phases are dual to each other, because

$$-PF_j^{y\dagger}F_{j+r}^yP = (-1)^rP\sigma_j^y\sigma_{j+r}^yP. \quad (5.37)$$

The whole phase diagram for  $(\lambda, \theta) \in [-1, 1] \times \mathcal{R}$  is determined by DMRG calculations, and the results are presented in Fig. 5.1. The DMRG results suggest that a direct transition between the  $\mathbb{Z}_2^y$  SSB phase and the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SSB phase happens at  $\lambda_c(\theta) > 0$ . Due to the KT duality, there is also a direct transition between the Haldane phase and the  $\mathbb{Z}_2^z$  SSB phase at  $-\lambda_c(\theta) < 0$ .

On the other hand, when  $\theta \in \mathcal{S} = [\arctan \frac{1}{2}, \pi/2]$ , although the GS eigenspace of  $H_{\text{SD}}$  contains holes, Eq. (C.16) tells us that two holes are never adjacent. Therefore, the effective Hamiltonian around the self-dual point is given by  $(H_{tJ}, \mathcal{H}_1)$ , where

$$\begin{aligned} H_{tJ}(\lambda, \theta \in \mathcal{S}) = & -[(1+\lambda)\cos\theta - \sin\theta] \sum_j \sigma_j^x \sigma_{j+1}^x + [(1-\lambda)\cos\theta - \sin\theta] \sum_j \sigma_j^y \sigma_{j+1}^y \\ & + \sin\theta \sum_j (\sigma_j^z \sigma_{j+1}^z + n_j n_{j+1} + 2) \\ & + 2\lambda \cos\theta \sum_j \left( |\uparrow \mathbf{h}\rangle \langle \mathbf{h} \uparrow| + |\downarrow \mathbf{h}\rangle \langle \mathbf{h} \downarrow| + |\mathbf{h} \uparrow\rangle \langle \uparrow \mathbf{h}| + |\mathbf{h} \downarrow\rangle \langle \downarrow \mathbf{h}| \right). \end{aligned} \quad (5.38)$$

We can see that  $H_{tJ}$  is like a  $t$ - $J$  model without double occupancy. A detailed study of  $H_{tJ}$  will be a future direction. In the following, we will keep focusing on the region  $\mathcal{R} = (-\pi/4, \arctan \frac{1}{2})$ .

## 5.4 KT duality in low-energy theory

As shown in the previous sections, when

$$|\lambda| \ll 1, \quad \theta \in \mathcal{R} = \left(-\frac{\pi}{4}, \arctan \frac{1}{2}\right), \quad (5.39)$$

the low-energy eigenspace of the model  $(H(\lambda, \theta), \mathcal{H}_1)$  completely lies in  $\mathcal{H}_{1/2}$ . The projection onto  $\mathcal{H}_{1/2}$  gives

$$P U_{\text{KT}} P = \prod_{1 \leq u < v \leq L} P \exp \left[ \frac{i\pi}{4} (1 + \sigma_u^z)(1 - \sigma_v^z) \right] P. \quad (5.40)$$

From Eq. (5.40), it can be shown that within  $\mathcal{H}_{1/2}$ , the following duality holds:

$$\begin{aligned} -\sigma_j^y \sigma_{j+1}^y & \xleftrightarrow[1 \leq j < L-1]{U_{\text{KT}}} \sigma_j^x \sigma_{j+1}^x, \\ (-1)^{L-1} \sigma_L^y \sigma_1^y & \xleftrightarrow{U_{\text{KT}}} \sigma_L^x \sigma_1^x. \end{aligned} \quad (5.41)$$

Interestingly, although we have been dealing with the case of OBC, Eq. (5.41) shows that even if we impose PBC on Eq. (5.32), the effective theory around the self-dual point still respects the KT duality as long as  $L$  is even.



Within  $\mathcal{R}$ , it follows from  $(H_{\text{XXZ}}, \mathcal{H}_{1/2})$  that the low-energy theory of  $(\mathcal{H}_{\text{SD}} = V H_{\text{SD}} V, \mathcal{H}_1)$  can be exactly mapped to a U(1) symmetric spinless fermion chain by the Jordan-Wigner transformation

$$c_j^\dagger = \sigma_j^+ \prod_{k < j} (-\sigma_k^z), \quad (5.42)$$

where  $V$  is defined in Eq. (5.17) and  $c_j^\dagger$  is a fermion creation operator. Let  $\mathcal{U}_{\text{KT}} = V U_{\text{KT}} V$  satisfying  $[\mathcal{H}_{\text{SD}}, \mathcal{U}_{\text{KT}}] = 0$ . It then follows from Eq. (5.40) that within  $\mathcal{H}_{1/2}$ , the following duality holds for fermions:

$$c_j^\dagger \xrightarrow{\mathcal{U}_{\text{KT}}} (-1)^{L(L-1)/2} c_j^\dagger (-1)^F, \quad (5.43)$$

where  $F = \sum_j c_j^\dagger c_j$ . Note that  $(-1)^F$  cannot be simply regarded as a phase, because it anti-commutes with  $c_j^\dagger$ .

## 5.5 Emergent anomaly

The symmetry

$$G = \mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z \times \mathbb{Z}^{\text{trn}} \quad (5.44)$$

of the complete theory reduces to

$$G' = \mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times \mathbb{Z}^{\text{trn}} \quad (5.45)$$

in the low-energy theory. In other words, in the low-energy theory,  $G = \mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z \times \mathbb{Z}^{\text{trn}}$  leads to an LSM anomaly, which accounts for the absence of a unique gapped GS for  $(H_{\text{XYZ}}, \mathcal{H}_{1/2})$  [79, 82, 84, 86]. However,  $G$  in  $\mathcal{H}_1$  has no anomaly, which can be seen from the toy model  $H_{\text{toy}} = \sum_j (S_j^y)^2$  whose GS is trivially gapped. In other words,  $H(|\lambda| \ll \lambda_c, \theta \in \mathcal{R})$  has an *emergent* anomaly. In order to recover the complete anomaly-free theory in  $\mathcal{H}_1$ , the emergent anomaly has to be cancelled by some mechanism. Note that for the gapped symmetry  $\mathbb{Z}_2^y$ ,  $\exp(-i\pi S_j^y)$  is identical to  $-1$  in the low-energy theory. This indicates that the GS is "stacked" on a gapped (weak) SPT phase protected by  $\mathbb{Z}_2^y \times \mathbb{Z}^{\text{trn}}$ . It is this SPT phase that cancels the emergent anomaly, because  $Y_\pi' Z_\pi' = Y_\pi Z_\pi Y_\pi'$ . Below I will explain how this works in detail <sup>2</sup>.

The model  $H(|\lambda| \ll 1, \theta \in \mathcal{R})$  is effectively described by  $(H_{\text{XYZ}}, \mathcal{H}_{1/2})$  and hence has an emergent LSM anomaly protected by  $G' = \mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times \mathbb{Z}^{\text{trn}}$  in the low-energy eigenspace. Let  $M_d$  be a  $d$ D manifold in the real space and  $S^1$  be a circle standing for the imaginary time  $\tau$  with PBC. Now let us put the model on a circle  $M_1 = S^1$  [i.e., a chain with PBC. Recall that in the low-energy theory, the KT duality also holds for PBC; see Eq. (5.41).], and consider the anomaly as the boundary of an SPT phase defined on  $M_2 \times S^1$  with  $\partial M_2 = M_1 = S^1$ . Due

<sup>2</sup>Contents of this section are mainly done by my collaborator Linhao Li, but I include them in this thesis for completeness.

to the bulk-boundary correspondence (Theorem. 3.3), the SPT phase is also protected by  $G' = \mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times \mathbb{Z}^{\text{trn}}$ . The partition function on  $M_2 \times S^1$  coupled to the  $G'$ -gauge field should be [101, 221]<sup>3</sup>:

$$Z[A^{y'}, A^{z'}, A^{\text{trn}}] = Z[0, 0, 0] \exp \left( i\pi \int_{M_2 \times S^1} A^{y'} \wedge A^{z'} \wedge A^{\text{trn}} \right), \quad (5.46)$$

where  $A^{y'}$ ,  $A^{z'}$ , and  $A^{\text{trn}}$  are gauge fields associated with  $\mathbb{Z}_2^{y'}$ ,  $\mathbb{Z}_2^{z'}$ , and  $\mathbb{Z}^{\text{trn}}$ , respectively<sup>4</sup>. In general, a  $\mathbb{Z}_2$ -gauge field should satisfy the restriction,

$$\begin{aligned} \int A_s^{y'} ds \mod 2 &= 0, 1 \quad (\text{for all components of } A^{y'}), \\ dA^{y'} &= 0 \quad (\text{almost everywhere}), \\ dA^{y'} &\neq 0 \quad (\text{at monodromy defects}), \\ \int_{M_d \times S^1} dA^{y'} \mod 2 &= 0. \end{aligned} \quad (5.47)$$

On the other hand, the  $\mathbb{Z}$ -gauge field  $A^{\text{trn}}$  satisfies the restriction

$$\begin{aligned} \int A_s^{\text{trn}} ds &= 0, 1, 2, 3, \dots \quad (\text{for all components of } A^{\text{trn}}), \\ dA^{\text{trn}} &= 0. \end{aligned} \quad (5.48)$$

Similar to the example in Eq. (2.71), Eq. (5.46) is not gauge invariant due to the (emergent) anomaly on  $\partial M_2$ . Be aware that introducing the  $G'$ -gauge field is sort of “illegal” because  $G'$  is not really the symmetry of the complete theory which is anomaly-free. The true symmetry of the complete theory is  $G = \mathbb{Z}_4^y \times \mathbb{Z}_2^z \times \mathbb{Z}^{\text{trn}}$  in  $\mathcal{H}_1$ . Nevertheless,  $G$  reduces to  $G'$  in the low-energy theory. Therefore, for consistency, the partition function coupled to the  $G$ -gauge field should take the form

$$Z[A^{\bar{y}}, A^z, A^{\text{trn}}] = Z[A^{y'}, A^{z'}, A^{\text{trn}}] Z_{\text{others}}, \quad (5.49)$$

where  $A^{\bar{y}}$  is a  $\mathbb{Z}_4^y$ -gauge field, and  $Z_{\text{others}}$  is some other phase factor that should be able to cancel the emergent anomaly on  $\partial M_2 \times S^1$  and thus guarantees the gauge invariance of  $Z[A^{\bar{y}}, A^z, A^{\text{trn}}]$ .

Recall that  $\mathbb{Z}_2^y$  is a symmetry associated with gapped DOF. An important observation is that  $\exp(-i\pi S_j^y)$  is identical to  $-1$  in the low-energy theory, which means that each lattice site is in a (0+1)D “gapped” SPT phase protected by  $\mathbb{Z}_2^y$ . Together with the translation symmetry, the GS of our model can be regarded as “stacking” on a (1+1)D gapped SPT phase protected by the  $\mathbb{Z}_2^y \times \mathbb{Z}^{\text{trn}}$  symmetry [11, 31]. [This is a weak SPT phase, because

<sup>3</sup>In general, the partition function of an SPT phase on  $M_d \times S^1$  and the partition function of its corresponding anomalous theory on  $\partial M_d \times S^1$  differ by a gauge invariant term, which is not important.

<sup>4</sup>Strictly speaking, the gauge field of a discrete group is a cochain rather than a differential form. Therefore, a more precise expression of Eq. (5.46) is to use the cup product  $\smile$  instead of the wedge product  $\wedge$ . See Appendix B of Ref. [68], Appendix J.4.e of Ref. [31], and Refs. [67, 69] for details.

it is essentially equivalent to a translational copy of (0+1)D SPT phases.] Under the  $G$ -gauge field, this (1+1)D weak SPT phase manifests itself via the following contribution to  $Z_{\text{others}}$ :

$$\exp\left(i\pi \int_{\partial M_2 \times S^1} A^y \wedge A^{\text{trn}}\right), \quad (5.50)$$

where  $A^y$  is a  $\mathbb{Z}_2^y$ -gauge field. We now show that Eq. (5.50) cancels the emergent anomaly in Eq. (5.46). Note that there is an identity

$$Y'_\pi Z'_\pi = Y_\pi Z'_\pi Y'_\pi, \quad (5.51)$$

which implies that [222]

$$\left(\int_{N_2} dA^y - \int_{N_2} A^{y'} \wedge A^{z'}\right) \bmod 2 = 0, \quad (5.52)$$

where  $N_2$  is any 2D submanifold of  $M_2 \times S^1$ . Using Eq. (5.52) and the Stokes theorem, Eq. (5.46) becomes

$$Z[A^{y'}, A^{z'}, A^{\text{trn}}] = Z[0, 0, 0] \exp\left(i\pi \int_{\partial M_2 \times S^1} A^y \wedge A^{\text{trn}}\right). \quad (5.53)$$

Since the two phases in Eq. (5.50) and Eq. (5.53) combine into

$$\exp\left(2\pi i \int_{\partial M_2 \times S^1} A^y \wedge A^{\text{trn}}\right) = \exp\left(2\pi i \int_{S^1} A_\mu^y d\mu \int_{S^1} A_\tau^{\text{trn}} d\tau - 2\pi i \int_{S^1} A_\tau^y d\tau \int_{S^1} A_\mu^{\text{trn}} d\mu\right) = 1, \quad (5.54)$$

it is now clear that Eq. (5.49) is indeed gauge invariant and anomaly-free.

In fact, Eq. (5.51) can also be written as  $Y'_\pi Z_\pi = Y_\pi Z_\pi Y'_\pi$ , which implies the following *short exact sequence*:

$$1 \rightarrow \mathbb{Z}_2^y \rightarrow \mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z \rightarrow \mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \rightarrow 1. \quad (5.55)$$

We say that  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$  is the *extension* of  $\mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'}$ . We also notice that the idea of the anomaly cancellation by symmetry extension can be found in in Refs. [30, 64, 94, 208, 209].

Finally, we note that *higher dimensional emergent anomaly* may be realized by simply defining our model  $H(\lambda, \theta)$  on higher dimensional lattices, where  $\tilde{H}_{\text{BLBQ}}(\theta)$  is defined by the right hand side of Eq. (5.2). If one can show that holes are absent from the low-energy theory (though might not be a easy task), then the effective spin-1/2 Hamiltonian  $H_{\text{XYZ}}$  in Eq. (5.32) holds regardless of dimensions. In that case, we have emergent LSM anomaly protected by  $\mathbb{Z}_2^{y'} \times \mathbb{Z}_2^{z'} \times (\text{crystalline symmetry})$  in higher dimensions.

## 5.6 Duality of SPT/trivial Ising criticality

From Eq. (5.35), one can easily see that the  $\mathbb{Z}_2^{y'}$  SSB phase also breaks the  $\mathbb{Z}_2^z$  symmetry, so that the  $\mathbb{Z}_2^y$  symmetry is broken or restored every time we cross the critical line  $\lambda_c(\theta) > 0$ , indicating the Ising universality class. Similarly,  $-\lambda_c(\theta) < 0$  is also an Ising critical line.

The transition at  $\lambda_c > 0$  is a *trivial Ising criticality* (protected by  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ ) in the sense that the phases on both sides have SSB. At  $\lambda_c$ ,  $\mathbb{Z}_2^y$  is the "critical symmetry", thus [9]

$$\langle S_j^x S_{j+r}^x \rangle = \langle S_j^z S_{j+r}^z \rangle \sim r^{-1/4}. \quad (5.56)$$

Due to the duality in Eq. (5.36), we know that  $\mathcal{O}_{\text{FM}}^{x'} > 0$  for the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SSB phase. Since  $\mathcal{O}_{\text{FM}}^{x'}$  is also nonzero for the  $\mathbb{Z}_2^{y'}$  SSB phase, it is easy to believe that at the Ising critical point between the two SSB phases ( $\lambda_c > 0$ ),

$$\mathcal{O}_{\text{FM}}^{x'} = \lim_{r \rightarrow \infty} \langle \sigma_j^x \sigma_{j+r}^x \rangle > 0. \quad (5.57)$$

It then directly follows from Eq. (5.7) and Eq. (5.36) that at  $-\lambda_c < 0$ ,

$$\langle F_j^x F_{j+r}^x \rangle = \langle F_j^z F_{j+r}^z \rangle \sim r^{-1/4}, \quad (5.58a)$$

$$\mathcal{O}_{\text{str}}^y = - \lim_{r \rightarrow \infty} \langle F_j^{y\dagger} F_{j+r}^y \rangle > 0. \quad (5.58b)$$

Since the nonlocal symmetry fluxes  $F_j^x$  and  $F_j^z$  carry nontrivial charges under  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  (for example,  $Z_\pi F_j^x Z_\pi = -F_j^x$ )<sup>5</sup>, we claim that the transition at  $-\lambda_c$  represents a  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  *SPT Ising criticality* [23]. Since  $\mathbb{Z}_2^z$  is broken as long as  $0 < \lambda \leq 1$ , it is obvious that the GS has two-fold degeneracy at  $\lambda_c$ ; so is that at  $-\lambda_c$  due to the KT duality (remember that we always assume OBC). The two-fold degeneracy at  $-\lambda_c$  is actually associated with topological edge states [23]; this can be seen by noting that  $0 \neq \langle F_1^{y\dagger} F_L^y \rangle = \langle S_1^y e^{i\pi S_1^y} Y_\pi e^{i\pi S_L^y} S_L^y \rangle = \pm \langle S_1^y e^{i\pi S_1^y} e^{i\pi S_L^y} S_L^y \rangle$  implies edge magnetization  $\langle S_1^y e^{i\pi S_1^y} \rangle = -\langle S_1^y \rangle \neq 0$  and  $\langle S_L^y \rangle \neq 0$ , where we have used the clustering property  $\langle S_1^y e^{i\pi S_1^y} e^{i\pi S_L^y} S_L^y \rangle \approx \langle S_1^y e^{i\pi S_1^y} \rangle \langle e^{i\pi S_L^y} S_L^y \rangle$  [30]. Moreover,  $\mathcal{O}_{\text{str}}^y > 0$  at  $-\lambda_c$  indicates that the topological criticality is partially protected by the gapped symmetry  $\mathbb{Z}_2^y$ , which further implies that the two-fold (quasi-)degenerate GS has an energy splitting proportional to  $e^{-L/\xi}$  [23]. From the above discussions, we can see that the KT duality also provides a *hidden  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry breaking* picture for the SPT criticality: The algebraic decay or the long-range order of  $\langle F_j^{\alpha\dagger} F_{j+r}^\alpha \rangle$  at  $-\lambda_c$  can be easily understood from the classical Landau transition at  $\lambda_c$ .

Our DMRG results in Fig. 5.4 show that  $\langle S_j^z S_{j+r}^z \rangle = \langle S_j^x S_{j+r}^x \rangle \sim r^{-1/4}$  at the critical point  $\lambda_c > 0$ , which indeed suggests the Ising universality class [9]. The fact that  $\mathcal{O}_{\text{FM}}^{x'} > 0$  at  $-\lambda_c$  and  $\mathcal{O}_{\text{str}}^y > 0$  at  $\lambda_c$  is also supported by DMRG calculations; see Fig. 5.1(b).

<sup>5</sup> Instead of  $\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z$ , it is sufficient to consider its subgroup  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$ , because their second cohomology groups are the same:  $H^2[\mathbb{Z}_4^y \rtimes \mathbb{Z}_2^z, U(1)] = H^2[\mathbb{Z}_2^y \times \mathbb{Z}_2^z, U(1)] = \mathbb{Z}_2$  [31].

We expect that the finite-size energy splitting of the four low-lying states should behave like those depicted Fig. 5.5. At  $\pm\lambda_c$ , the energy splitting of the two lowest states is exponentially small due to the existence of gapped DOF; see also Sec. 2.2.

In Fig. 5.1(a), one can see that the trivial and topological Ising criticalities related by the KT duality meet at the self-dual point  $(\lambda, \theta) = (0, \arctan \frac{1}{2})$ , forcing the model  $H_{\text{SD}}(\arctan \frac{1}{2})$  to be at a multicritical point. Indeed,  $\theta = \arctan \frac{1}{2}$  corresponds to  $\Delta = 1$ , thus  $(H_{\text{SD}}, \mathcal{H}_1)$  is equivalent to a spin-1/2 FM Heisenberg model doped by immobile holes, which has  $z_{\text{dyn}} = 2$ . To numerically show that there is indeed a direct transition between the Haldane phase and the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  phase at  $(\lambda, \theta) = (0, \arctan \frac{1}{2})$ , we estimate  $\mathcal{O}_{\text{str}}^{x,z}$  and  $\mathcal{O}_{\text{FM}}^{x,z}$  around that point; see Fig. 5.6. The DMRG results clearly suggest that the two  $\mathbb{Z}_2$  SSB phases vanish at  $\theta = \arctan(1/2)$ .

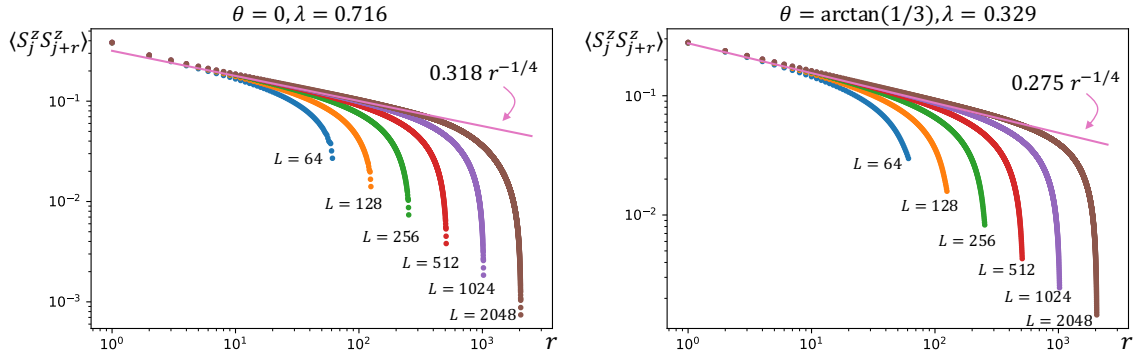


Figure 5.4: The correlation function  $\langle S_j^z S_{j+r}^z \rangle$  on an open chain with length  $L$  is calculated with various  $L$  at  $\theta = 0$  and  $\arctan(1/3)$ . From the log-log plots, it is clear that the data are well-fitted by  $r^{-1/4}$  when  $1 \ll r \ll L$ .

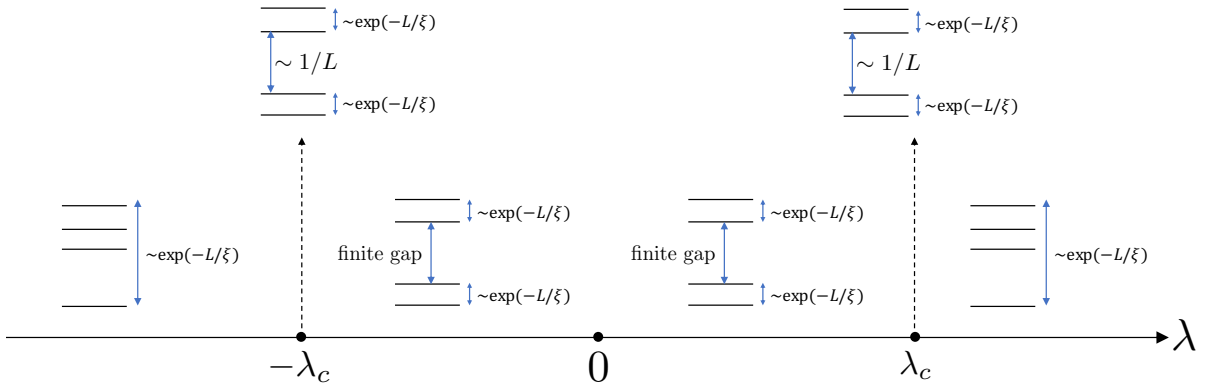


Figure 5.5: Finite-size energy splitting of four edge states.

On the other direction, the Ising critical lines terminate at  $H(\pm 1, -\pi/4)$ , whose low-energy physics is the CFT with  $c = 3/2$  [154–156].

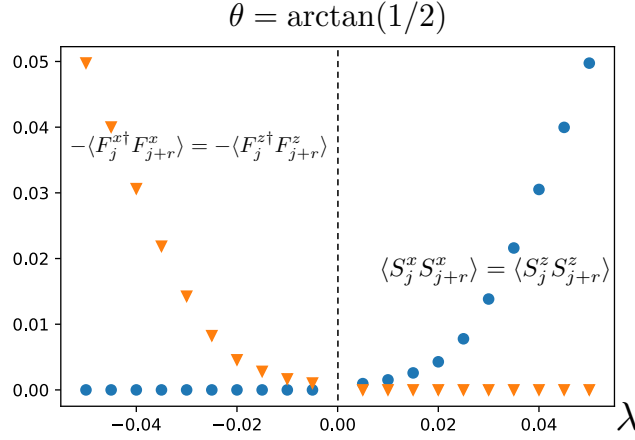


Figure 5.6: DMRG calculations at  $\theta = \arctan(1/2)$  and  $-0.05 \leq \lambda \leq 0.05$ . The order parameters  $\mathcal{O}_{\text{str}}^{x,z}$  and  $\mathcal{O}_{\text{FM}}^{x,z}$  are estimated by taking  $L = 1024$  and  $r = 512$ .

## 5.7 Conjecture and discussions

We have been focusing on the spin-1 chains, but in fact, the KT transformation directly applies to *any integer* spin quantum number  $S$ , as long as we take  $S_u^z$  and  $S_v^x$  in Eq. (5.1) to be the spin- $S$  operators [52]. Let  $H_S = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$  be the spin- $S$  AFM Heisenberg chain; it is believed that the GS of  $H_S$  is in the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SPT phase when  $S$  is odd, while the GS is trivial when  $S$  is even [see also Eq. (2.26)] [4, 52]. Note that  $H_{\text{triv}} = \sum_j (S_j^z)^2$  suggests that the KT dual of the trivial phase is still trivial. Therefore, we propose the following conj

**Conjecture 5.2** *Let  $H_{\text{SD}}^{(S)} = H_S + U_{\text{KT}} H_S U_{\text{KT}}$ ; the GS of  $H_{\text{SD}}^{(S)}$  is gapless when  $S$  is odd, while it is trivially gapped when  $S$  is even.*

Moreover, the KT transformation can be generalized to (1+1)D systems with a broad class of symmetries beyond  $\mathbb{Z}_2 \times \mathbb{Z}_2$ , such as  $\mathbb{Z}_n \times \mathbb{Z}_n$  and  $\text{SO}(2n-1)$  [55–58], thus providing the hidden symmetry breaking picture for the SPT phases in such systems. Exploring the relationship between the KT duality, criticality, anomaly, and topology in such systems will also be interesting.

孟子曰：「博學而詳說之，將以反說約也。」

『孟子·離婁下』

## SUMMARY

After giving an introduction to bosonic SPT phases in the first three chapters, I presented two main research projects of myself [1, 2], which are included in Chapter 4 and Chapter 5, respectively. Chapter 4 is about realizing the SPT phases in spinful boson systems [1], while Chapter 5 studied the relation between KT duality, SPT/trivial Ising criticality, and emergent LSM anomaly in quantum spin chains [2].

In Chapter 4, we show that the SPT phases can be realized with short-range interacting spinful bosons that are loaded on the lattices with a bottom flat band. Such systems are described by the spinful Bose-Hubbard models. The ground states of such systems have both spin and charge fluctuations. The single-body eigenstates of a flat band can usually be chosen to be strictly localized on a finite number of sites, known as compact localized states (CLSs). When  $N$  spin- $f$  bosons are loaded on a bottom-flat-band lattice  $X$  with  $N$  unit cells, at low temperatures, the particles' wave functions tend to avoid overlapping each other in order to minimize the system's energy. In particular, when the interaction strength between spin- $f$  bosons is fine-tuned, in the ground state  $|\text{GS}_{f,X}\rangle$ ,  $N$  bosons exactly occupy  $N$  CLSs on different patches. We make use of the analogy between the Hamiltonian that describes the  $s$ -wave collision among spin- $f$  bosons and the spin- $f$  AKLT Hamiltonian. This analogy enables us to exactly map  $|\text{GS}_{f,X}\rangle$  onto  $|\text{AKLT}_{f,X'}\rangle$ , where the latter state is the spin- $f$  AKLT state on the lattice  $X'$ . This implies that  $|\text{GS}_{f,X}\rangle$  is the exact and unique many-body ground state of the spin- $f$  Bose-Hubbard model. The choice of  $f$  and  $X'$  is determined by the geometry of  $X$ . Over the years, exact results have proved to be highly valuable in quantum and statistical physics. Our work features the exact many-body ground states  $|\text{GS}_{f,X}\rangle$  of spinful itinerant systems. The spin fluctuations of  $|\text{GS}_{f,X}\rangle$  is inherited from  $|\text{AKLT}_{f,X'}\rangle$ . Therefore, with respect to the spin rotation



symmetry or the spin rotation  $\times$  translation symmetry, the symmetry-protected phase of  $|\text{GS}_{f,X}\rangle$  is identical to that of  $|\text{AKLT}_{f,X'}\rangle$ . However, unlike  $|\text{AKLT}_{f,X'}\rangle$ , the state  $|\text{GS}_{f,X}\rangle$  also possesses nonvanishing charge fluctuations, and in terms of crystalline symmetries, both spin and charge fluctuations in  $|\text{GS}_{f,X}\rangle$  together determine its phase. Hence, one cannot simply conclude that the crystalline-symmetry-protected phase of  $|\text{GS}_{f,X}\rangle$  is also inherited from  $|\text{AKLT}_{f,X'}\rangle$ , because charge fluctuations may play a nontrivial role in the former state, which is indeed the case for spin-3 bosons in the kagome lattice. Although our analysis in  $d > 1$  dimensions is based on the exact ground states  $|\text{GS}_{f,X}\rangle$  (as a consequence of fine-tuned parameters), we expect that just like what has been shown in the spin-1 BHMSC, the SPT phases survive in wider parameter regions, and  $|\text{GS}_{f,X}\rangle$  just serves as a representative state of the phases.

In Chapter 5, we focus on the KT duality  $U_{\text{KT}}$ . In quantum spin-1 chains,  $U_{\text{KT}}$  defines a duality between the Haldane phase and the  $\mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry-breaking phase. We study a spin-1 chain of the form

$$H(\lambda, \theta) = (1 - \lambda)H_{\text{BLBQ}}(\theta) + (1 + \lambda)U_{\text{KT}}H_{\text{BLBQ}}(\theta)U_{\text{KT}}, \quad -1 \leq \lambda \leq 1,$$

which satisfies  $U_{\text{KT}}H(\lambda, \theta)U_{\text{KT}} = H(-\lambda, \theta)$ . When  $-\pi/4 < \theta < \arctan(1/2)$ , the model experiences four phases as we increase  $\lambda$ : the Haldane phase, the  $\mathbb{Z}_2^z$  SSB phase, the  $\mathbb{Z}_2^{y'}$  SSB phase, and the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  SSB phase. Around the self-dual point, holes are absent from the low-energy physics because they are gapped DOF, thus the model  $H(\lambda, \theta)$  effectively reduces to a spin-1/2 chain. Surprisingly, we find that the self-dual model  $H(0, \theta)$  is *exactly equivalent* to a (1+1)D spin-1/2 XXZ model doped by immobile holes, and the holes are completely absent from the low-energy theory when  $-\pi/4 < \theta < \arctan(1/2)$ . This means that the self-dual point is indeed a critical point described by a Gaussian CFT. Furthermore, we find that the effective model for  $H(|\lambda| \ll 1, -\pi/4 < \theta < \arctan \frac{1}{2})$  is given by the famous (1+1)D spin-1/2 XYZ model, which implies that there is an emergent LSM anomaly around the self-dual point  $\lambda = 0$ . We explained how the anomaly can be cancelled by symmetry extension. At the two critical values  $\lambda = \pm\lambda_c$ , the model is in the Ising critical phase. With the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  symmetry, the criticality at  $-\lambda_c < 0$  is SPT and the other is trivial. This thus provides a hidden symmetry breaking picture for the SPT Ising criticality. The SPT Ising criticality is the transition between the Haldane phase and the  $\mathbb{Z}_2^z$  SSB phase, while the trivial Ising criticality is the transition between the  $\mathbb{Z}_2^{y'}$  SSB phase and the  $\mathbb{Z}_2^y \times \mathbb{Z}_2^z$  phase. In the two-dimensional phase diagram with the coordinate  $(\lambda, \theta)$ , the two critical lines  $\pm\lambda_c(\theta)$  meet at  $(\lambda, \theta) = (0, \arctan \frac{1}{2})$ , on which the model  $H(\lambda, \theta)$  is exactly equivalent to a spin-1/2 ferromagnetic (FM) Heisenberg chain doped by immobile holes. This means that the two KT duality-related Ising criticalities meet at a self-dual point which is indeed multicritical. We expect that our discussions can be generalized to other symmetries beyond the spin-1 chains. Finally, we proposed a conjecture on the difference between even-spin and odd-spin self-dual models.





## SPIN PROJECTION OPERATORS

Let  $i$  and  $j$  represent two different spin- $f$  particles ( $i \neq j$ );  $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$  be the spin operator of particle  $i$ . In this Appendix we prove the identity related to the spin projection operator  $P_{ij}^{(S)}$  defined as

$$P_{ij}^{(S)} = \sum_{M=-S}^S |S, M\rangle_{ij} {}_{ij}\langle S, M|, \quad (\text{A.1})$$

where  $|S, M\rangle_{ij}$  is the eigenstate of  $(\mathbf{S}_i + \mathbf{S}_j)^2$  and  $(S_i^z + S_j^z)$  with eigenvalues  $S(S+1)$  and  $M$ , respectively. The following scheme is based on Ref. [145]. Let us first note that

$$\begin{aligned} \mathbf{S}_i \cdot \mathbf{S}_j |S, M\rangle &= \frac{1}{2} [(\mathbf{S}_i + \mathbf{S}_j)^2 - 2f(f+1)] |S, M\rangle \\ &= \frac{1}{2} [S(S+1) - 2f(f+1)] |S, M\rangle \\ &\equiv \lambda_S |S, M\rangle. \end{aligned} \quad (\text{A.2})$$

We thus have

$$(\mathbf{S}_i \cdot \mathbf{S}_j)^n |S, M\rangle = \lambda_S^n |S, M\rangle. \quad (\text{A.3})$$

If there is *no* restriction on the parity of  $S$ , we then have the completeness relation

$$\sum_{S=0}^{2f} \sum_{M=-S}^S |S, M\rangle_{ij} {}_{ij}\langle S, M| = \sum_{S=0}^{2f} P_{ij}^{(S)} = \mathbb{1}. \quad (\text{A.4})$$

Equation (A.3) yields  $2f+1$  independent equations

$$(\mathbf{S}_i \cdot \mathbf{S}_j)^n \mathbb{1} = \sum_{S=0}^{2f} \sum_{M=-S}^S \lambda_S^n |S, M\rangle_{ij} {}_{ij}\langle S, M| = \sum_{S=0}^{2f} \lambda_S^n P_{ij}^{(S)} \quad (\text{A.5})$$

with  $n = 0, 1, 2, \dots, 2f$ . Absence of the higher order terms, such as  $(\mathbf{S}_i \cdot \mathbf{S}_j)^{2f+1}$ , follows from the fact that the product of any  $2f+1$  spin operators for an spin- $f$  particle can be expressed via the lower-order terms [149]. Equation (A.5) in matrix form reads

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ \lambda_0 & \lambda_1 & \dots & \lambda_{2f} \\ \lambda_0^2 & \lambda_1^2 & \dots & \lambda_{2f}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_0^{2f} & \lambda_1^{2f} & \dots & \lambda_{2f}^{2f} \end{pmatrix} \begin{pmatrix} P_{ij}^{(0)} \\ P_{ij}^{(1)} \\ P_{ij}^{(2)} \\ \vdots \\ P_{ij}^{(2f)} \end{pmatrix} = \begin{pmatrix} 1 \\ \mathbf{S}_i \cdot \mathbf{S}_j \\ (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \\ \vdots \\ (\mathbf{S}_i \cdot \mathbf{S}_j)^{2f} \end{pmatrix}. \quad (\text{A.6})$$

The solution of  $P_{ij}^{(S)}$  is given by Cramer's rule as

$$P_{ij}^{(S)} = \frac{\begin{vmatrix} 1 & \dots & 1 & 1 & 1 & \dots & 1 \\ \lambda_0 & \dots & \lambda_{S-1} & \mathbf{S}_i \cdot \mathbf{S}_j & \lambda_{S+1} & \dots & \lambda_{2f} \\ \lambda_0^2 & \dots & \lambda_{S-1}^2 & (\mathbf{S}_i \cdot \mathbf{S}_j)^2 & \lambda_{S+1}^2 & \dots & \lambda_{2f}^2 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \lambda_0^{2f} & \dots & \lambda_{S-1}^{2f} & (\mathbf{S}_i \cdot \mathbf{S}_j)^{2f} & \lambda_{S+1}^{2f} & \dots & \lambda_{2f}^{2f} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ \lambda_0 & \lambda_1 & \dots & \lambda_{2f} \\ \lambda_0^2 & \lambda_1^2 & \dots & \lambda_{2f}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_0^{2f} & \lambda_1^{2f} & \dots & \lambda_{2f}^{2f} \end{vmatrix}}, \quad (\text{A.7})$$

where both the denominator and the numerator are of the form of Vandermonde determinant, which can be calculated as

$$\begin{aligned} \text{denominator} &= \prod_{k < l} (\lambda_k - \lambda_l), \\ \text{numerator} &= \prod_{k < l \text{ \& } k, l \neq S} (\lambda_k - \lambda_l) \prod_{m \neq S} (\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_m). \end{aligned} \quad (\text{A.8})$$

Equation (A.7) is then finally simplified to

$$P_{ij}^{(S)} = \frac{\prod_{k < l \text{ \& } k, l \neq S} (\lambda_k - \lambda_l) \prod_{k \neq S} (\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_k)}{\prod_{k < l \text{ \& } k, l \neq S} (\lambda_k - \lambda_l) \prod_{k \neq S} (\lambda_S - \lambda_k)} = \prod_{k=0, \neq S}^{2f} \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_k}{\lambda_S - \lambda_k}. \quad (\text{A.9})$$

For  $f = 1$  particles,  $\lambda_0 = -2$ ,  $\lambda_1 = -1$  and  $\lambda_2 = 1$ , three projection operators are

$$\begin{aligned} P_{ij}^{(0)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_1}{\lambda_0 - \lambda_1} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_2}{\lambda_0 - \lambda_2} = \frac{1}{3}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 - 1], \\ P_{ij}^{(1)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_0}{\lambda_1 - \lambda_0} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_2}{\lambda_1 - \lambda_2} = -\frac{1}{2}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + (\mathbf{S}_i \cdot \mathbf{S}_j) - 2], \\ P_{ij}^{(2)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_0}{\lambda_2 - \lambda_0} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_1}{\lambda_2 - \lambda_1} = \frac{1}{6}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + 3(\mathbf{S}_i \cdot \mathbf{S}_j) + 2]. \end{aligned} \quad (\text{A.10})$$

However, as discussed at beginning of Sec. 4.1.1, for two spin- $f$  bosons interacting via  $s$ -wave scattering, their total spin  $S$  can only be even. The completeness relation thus becomes

$$\sum_{S=0,2,\dots,2f} \sum_{M=-S}^S |S, M\rangle_{ij} \langle S, M| = \sum_{S=0,2,\dots,2f} P_{ij}^{(S)} = \mathbb{1}. \quad (\text{A.11})$$

Similarly, this results in  $f + 1$  independent equations

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ \lambda_0 & \lambda_2 & \dots & \lambda_{2f} \\ \lambda_0^2 & \lambda_2^2 & \dots & \lambda_{2f}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_0^S & \lambda_2^S & \dots & \lambda_{2f}^S \end{pmatrix} \begin{pmatrix} P_{ij}^{(0)} \\ P_{ij}^{(2)} \\ P_{ij}^{(4)} \\ \vdots \\ P_{ij}^{(2f)} \end{pmatrix} = \begin{pmatrix} 1 \\ \mathbf{S}_i \cdot \mathbf{S}_j \\ (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \\ \vdots \\ (\mathbf{S}_i \cdot \mathbf{S}_j)^S \end{pmatrix} \quad (\text{A.12})$$

with solutions

$$P_{ij}^{(S)} = \prod_{k=0, \neq S/2}^f \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_{2k}}{\lambda_S - \lambda_{2k}}. \quad (\text{A.13})$$

For  $f = 1$  particles,  $\lambda_0 = -2$  and  $\lambda_2 = 1$ , two projection operators are

$$\begin{aligned} P_{ij}^{(0)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_2}{\lambda_0 - \lambda_2} = -\frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_j - 1), \\ P_{ij}^{(2)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_0}{\lambda_2 - \lambda_0} = \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_j + 2). \end{aligned} \quad (\text{A.14})$$

For  $f = 2$  particles,  $\lambda_0 = -6$ ,  $\lambda_2 = -3$ , and  $\lambda_4 = 4$ , three projection operators are

$$\begin{aligned} P_{ij}^{(0)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_2}{\lambda_0 - \lambda_2} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_4}{\lambda_0 - \lambda_4} = \frac{1}{30}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 - \mathbf{S}_i \cdot \mathbf{S}_j - 12], \\ P_{ij}^{(2)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_0}{\lambda_2 - \lambda_0} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_4}{\lambda_2 - \lambda_4} = -\frac{1}{21}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + 2\mathbf{S}_i \cdot \mathbf{S}_j - 24] = -\frac{1}{7}[\mathbf{S}_i \cdot \mathbf{S}_j + 10P_{ij}^{(0)} - 4], \\ P_{ij}^{(4)} &= \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_0}{\lambda_4 - \lambda_0} \cdot \frac{\mathbf{S}_i \cdot \mathbf{S}_j - \lambda_2}{\lambda_4 - \lambda_2} = \frac{1}{70}[(\mathbf{S}_i \cdot \mathbf{S}_j)^2 + 9\mathbf{S}_i \cdot \mathbf{S}_j + 18] = \frac{1}{7}[\mathbf{S}_i \cdot \mathbf{S}_j + 3P_{ij}^{(0)} + 3]. \end{aligned} \quad (\text{A.15})$$



## GROUP COHOMOLOGY

**M**athematical details of group cohomology will be presented in this appendix.

**Definition B.1 (group homomorphism and group isomorphism)** *Let  $G$  and  $G'$  be two groups. A map  $\psi : G \rightarrow G'$  is a group homomorphism if*

$$\psi(ab) = \psi(a)\psi(b), \quad \forall a, b \in G. \quad (\text{B.1})$$

*If the homomorphism  $\psi$  is a bijection, then  $\psi$  is called a group isomorphism. We use  $G \cong G'$  to denote that  $G$  and  $G'$  are isomorphic.*

**Definition B.2 ( $n$ -cochain)** *Let  $G$  be an arbitrary group and  $M$  an abelian group. An  $n$ -cochain is a map  $f : G^n = G \times \cdots \times G \rightarrow M$ . The set of all  $n$ -cochains of  $G$  in  $M$  is denoted as  $C^n(G, M)$ , where the multiplication, identity and the inverse are defined by:*

1.  $fg : (x_1, \dots, x_n) \mapsto f(x_1, \dots, x_n)g(x_1, \dots, x_n)$ , for all  $x_i \in G$  and  $f, g \in C^n(G, M)$ ;
2.  $e : (x_1, \dots, x_n) \mapsto e_M$ ;
3.  $f^{-1} : (x_1, \dots, x_n) \mapsto f(x_1, \dots, x_n)^{-1}$ ;

*The identity in  $M$  is denoted as  $e_M$  above. In particular,  $C^0(G, M) \cong M$  since  $G^0$  only contains a trivial element.*

The group  $C^n(G, M)$  is abelian because  $M$  is abelian.

**Definition B.3 ( $G$ -module)** *Let  $G$  be a group. A  $G$ -module is an abelian group  $M$  on which  $G$  acts compatibly with the abelian group structure on  $M$ . A left  $G$ -module consists*

of an abelian group  $M$  together with a left group action

$$\begin{aligned} G \times M &\rightarrow M \\ (x, a) &\mapsto x.a \end{aligned} \tag{B.2}$$

such that

$$x.(ab) = (x.a)(x.b), \quad \forall x \in G, a, b \in M. \tag{B.3}$$

In particular,  $M$  is a trivial  $G$ -module if  $x.a = a$  for all  $x \in G, a \in M$ .

**Example B.4** In the main text of this thesis, we always choose  $M = \text{U}(1)$ . We also define the action of  $G$  on  $\text{U}(1)$  as

$$x.a = \begin{cases} a^{-1} = a^*, & \text{if } x \text{ contains complex conjugation} \\ a, & \text{elsewise} \end{cases}, \quad \forall x \in G, a \in \text{U}(1). \tag{B.4}$$

In other words, if  $G$  is a unitary symmetry group, then  $\text{U}(1)$  is a trivial  $G$ -module, but if  $G$  contains anti-unitary symmetry operation, then  $M = \text{U}_T(1)$  is a nontrivial  $G$ -module, where  $\text{U}_T(1)$  is just the group  $\text{U}(1)$  and we use the subscript T to emphasize the nontrivial action of  $G$ .

**Definition B.5 (coboundary homomorphism)**  $\delta^n : C^n(G, M) \rightarrow C^{n+1}(G, M), f \mapsto \delta^n f$

$$\delta^n f(x_1, \dots, x_{n+1}) := f(x_1, \dots, x_n)^{(-1)^{n+1}} \left( \prod_{i=1}^n f(x_1, \dots, x_{i-1}, x_i x_{i+1}, x_{i+2}, \dots, x_{n+1})^{(-1)^i} \right) (x_1 \cdot f(x_2, \dots, x_{n+1})). \tag{B.5}$$

**Example B.6**  $\delta^0 : C^0(G, M) \rightarrow C^1(G, M)$  is naturally defined by  $\delta^0 a(x) = a^{-1}(x.a)$  with  $a \in M$  because  $C^0(G, M) \cong M$ . If  $M$  is a trivial  $G$ -module, then  $\text{im } \delta^0 = \{e_{C^1}\}$ .

**Proposition B.7** For all  $f, g \in C^n(G, M)$ , the following two identities hold:

1.  $\delta^n(fg) = (\delta^n f)(\delta^n g),$
2.  $\delta^n(\delta^{n-1} f) = e_{C^{n+1}},$

where  $e_{C^{n+1}}$  is the identity element in  $C^{n+1}(G, M)$ .

The first identity, which directly follows from Eq. (B.5), is nothing more than the assertion that  $\delta^n$  is a group homomorphism. The second identity implies that

$$\text{im } \delta^{n-1} \subseteq \ker \delta^n \subseteq C^n(G, M); \tag{B.6}$$

see Fig. B.1.

**Definition B.8 ( $n$ -cocycle and  $n$ -coboundary)** Let  $Z^n(G, M) = \ker \delta^n$  and  $B^n(G, M) = \text{im } \delta^{n-1}$ . An  $n$ -cochain  $f$  is called an  $n$ -cocycle if  $f \in Z^n(G, M)$ . An  $n$ -cocycle  $f$  is called an  $n$ -coboundary if  $f \in B^n(G, M)$ . We also define  $B^0(G, M) = \{e_{C^0}\} \cong \{e_M\}$ .

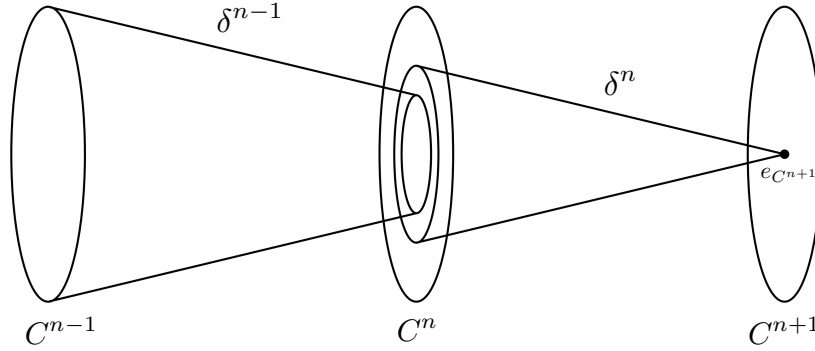


Figure B.1:  $\delta^n$  is a function from  $C^n$  to  $C^{n+1}$ . The image of  $\delta^{n-1}$  is in the kernel of  $\delta^n$ .

Let us note that  $\delta^n$  is a group homomorphism. Its kernel is thus defined as

$$Z^n(G, M) = \ker \delta^n = \{f \in C^n(G, M) \mid \delta^n f = e_{C^{n+1}}\}. \quad (\text{B.7})$$

The condition  $\delta^n f = e_{C^{n+1}(G, M)}$  simply means that  $\delta^n f(x_1, \dots, x_{n+1}) = e_M$  for all  $x_1, \dots, x_{n+1} \in G$ .

Since  $B^n(G, M)$  is a subgroup of  $Z^n(G, M)$ , we can define an equivalence relation between  $\zeta_1, \zeta_2 \in Z^n(G, M)$  as

$$\zeta_1 \sim \zeta_2 \iff \exists \beta \in B^n(G, M) \text{ s.t. } \zeta_1 = \beta \zeta_2. \quad (\text{B.8})$$

**Definition B.9 (*n*th-cohomology group)** The *n*th-cohomology group is defined to be the quotient group

$$H^n(G, M) = \frac{Z^n(G, M)}{B^n(G, M)}. \quad (\text{B.9})$$

**Example B.10 (zeroth-cohomology group)** Since  $B^0(G, M)$  is trivial,  $H^0(G, M) \cong Z^0(G, M) = \ker \delta^0 = \{a \in M \mid x.a = a, \forall x \in G\}$ ; see also Example B.6. In particular, if  $M$  is a trivial  $G$ -module, then  $H^0(G, M) = M$ . On the other hand, if  $M = \text{U}(1)$  and  $G$  contains complex conjugation, then  $H^0(G, M) = \{1, -1\}$ ; see Example B.4.

**Example B.11 (first-cohomology group)** In the case of  $n = 1$ , we have

$$\delta^1 f(x_1, x_2) = f(x_1)f(x_1x_2)^{-1}[x_1.f(x_2)], \quad (\text{B.10})$$

so a 1-cocycle  $\zeta \in Z^1(G, M)$  must satisfy

$$\zeta(x_1)\zeta(x_1x_2)^{-1}[x_1.\zeta(x_2)] = e_M, \quad \forall x_1, x_2 \in G. \quad (\text{B.11})$$

On the other hand,

$$B^1(G, M) = \{\zeta \in C^1(G, M) \mid \zeta(x) = a^{-1}(x.a), \forall x \in G, a \in M\}. \quad (\text{B.12})$$

In particular, if  $M = \text{U}(1)$  and  $G$  is a unitary symmetry group, then  $B^1(G, M) = \{e_{C^1}\}$  is trivial, so  $H^1(G, M) \cong Z^1(G, M)$ . The first-cohomology group is the set of all 1D representations of  $G$ , and the set has an Abelian group structure.

However, if  $G$  contains an anti-unitary symmetry operation, then Eq. (B.11) becomes

$$\zeta(x_1 x_2) = \zeta(x_1) \zeta(x_2)^{-1} = \begin{cases} \zeta(x_1) \zeta(x_2)^*, & \text{if } x_1 \text{ contains complex conjugation} \\ \zeta(x_1) \zeta(x_2), & \text{elsewise.} \end{cases} \quad (\text{B.13})$$

Equation (B.13) is nothing but the representation of  $G$ ; see Ref. [63] and Appendix B of Ref. [31]. Besides,

$$B^1[G, \text{U}_T(1)] = \{\zeta \in C^1 \mid \zeta(x) = \begin{cases} a^{-2}, & \text{if } x \text{ contains complex conjugation} \\ 1, & \text{elsewise} \end{cases}, \forall x \in G, a \in \text{U}(1)\} \quad (\text{B.14})$$

defines the equivalence of two 1D representations [63]. To sum up,  $H^1[G, \text{U}_T(1)]$  is the set of all the inequivalent 1D representations of  $G$ .

**Example B.12 (second-cohomology group)** In the case of  $n = 2$ , we have

$$\delta^2 f(x_1, x_2, x_3) = f(x_1, x_2)^{-1} f(x_1 x_2, x_3)^{-1} f(x_1, x_2 x_3) [x_1 \cdot f(x_2, x_3)], \quad (\text{B.15})$$

so a 2-cocycle  $\zeta \in Z^2(G, M)$  must satisfy

$$\zeta(x_1, x_2)^{-1} \zeta(x_1 x_2, x_3)^{-1} \zeta(x_1, x_2 x_3) [x_1 \cdot \zeta(x_2, x_3)] = e_M, \quad \forall x_1, x_2 \in G. \quad (\text{B.16})$$

A 2-coboundary  $\beta \in B^2(G, M)$  is an image of  $\delta^1$ , which means that for any  $f \in C^1(G, M)$ , we have

$$\beta(x_1, x_2) = f(x_1) f(x_1 x_2)^{-1} [x_1 \cdot f(x_2)], \quad \forall x_1, x_2 \in G. \quad (\text{B.17})$$

Therefore,  $\zeta_1 \sim \zeta_2 \iff \exists f \in C^1(G, M)$  s.t.  $\zeta_1(x_1, x_2) = \zeta_2(x_1, x_2) f(x_1) f(x_1 x_2)^{-1} [x_1 \cdot f(x_2)]$ ,  $\forall x_1, x_2 \in G$ .

In particular, when  $G$  is a unitary symmetry group and  $M = \text{U}(1)$ , Eq. (B.16) and Eq. (B.17) simply reduce to Eq. (2.44) and Eq. (2.43), respectively. For a general  $G$  that contains anti-unitary operations and  $M = \text{U}_T(1)$ , Eq. (B.16) and Eq. (B.17) become Eq. (2.66) and Eq. (2.64), respectively.

In general, the cohomology group can be calculated with some advanced tools, see the appendices in Refs. [31, 223]. Here we present an elementary calculation of  $H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)]$ , which was presented in Problem 8.3.4a in Sec. 8.3.4 of Ref. [4].

**Example B.13 (projective representation of  $\mathbb{Z}_2 \times \mathbb{Z}_2$ )** Let  $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{e, a, b, c\}$ . Let  $\rho(\cdot)$  be a projective representation of  $\mathbb{Z}_2 \times \mathbb{Z}_2$  such that  $\rho(g)\rho(h) = e^{i\phi(g,h)}\rho(gh)$  for all  $g, h \in \mathbb{Z}_2 \times \mathbb{Z}_2$ . One can always choose a gauge such that

$$\rho(e) = 1, \quad e^{i\phi(g,g)} = 1, \quad \forall g \in \mathbb{Z}_2 \times \mathbb{Z}_2. \quad (\text{B.18})$$



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This further implies that  $e^{i\phi(e,g)} = e^{i\phi(g,e)} = 1$  for all  $g$ . By setting  $(g_1, g_2, g_3) = (a, b, c)$  and  $(b, c, a)$ , Eq. (2.44) implies that

$$e^{i\phi(a,b)} = e^{i\phi(b,c)} = e^{i\phi(c,a)} := \xi. \quad (\text{B.19})$$

Similarly, we also have

$$e^{i\phi(a,c)} = e^{i\phi(c,b)} = e^{i\phi(b,a)} := \xi'. \quad (\text{B.20})$$

By setting  $(g_1, g_2, g_3) = (a, b, b)$ , we obtain

$$\xi\xi' = e^{i\phi(a,b)}e^{i\phi(c,b)} = 1. \quad (\text{B.21})$$

By setting  $(g_1, g_2, g_3) = (a, b, a)$ , we obtain

$$\xi^2 = e^{i\phi(a,b)}e^{i\phi(c,a)} = \xi'^2 = e^{i\phi(b,a)}e^{i\phi(a,c)}, \quad (\text{B.22})$$

The above two equations imply that  $\xi^4 = 1$  and thus  $\xi = \pm 1, \pm i$ . By redefining  $\{\rho(a), \rho(b), \rho(c)\} \rightarrow \{-\rho(a), -\rho(b), -\rho(c)\}$ , we see that  $\xi \rightarrow -\xi$ . Hence, we only need to consider  $\xi = 1, i$ . When  $\xi = 1$ ,  $\rho(\cdot)$  is a trivial projective representation. When  $\xi = i$ , we have  $\rho(a)\rho(b) = i\rho(c)$  and  $\rho(b)\rho(a) = -i\rho(c)$ , so  $\rho(a)\rho(b) = -\rho(b)\rho(a)$ . To sum up,

$$H^2[\mathbb{Z}_2 \times \mathbb{Z}_2, \text{U}(1)] = \mathbb{Z}_2. \quad (\text{B.23})$$

Many contents in this appendix also have interesting geometric interpretations; details can be found in Ref. [224] and Appendix D.3 of Ref. [31].



## EXISTENCE OR ABSENCE OF HOLES

A proof of the Proposition 5.1 is presented here. Although our proof might not be entirely rigorous in the mathematical point of view, it nevertheless makes sense for physicists. Let us begin by first noting that by properly rotating the spins. Then  $H_{\text{SD}}$  in Eq. (5.15) is always unitarily equivalent to

$$H'_{\text{SD}}(\theta) = 2\sqrt{2} \left| \sin\left(\frac{\pi}{4} - \theta\right) \right| \times H_{\text{XXZ}}(\theta) + \sin \theta \sum_{j=1}^{L-1} (2h_j h_{j+1} + n_j n_{j+1} + 2), \quad (\text{C.1})$$

where

$$H_{\text{XXZ}}(\theta) = \frac{1}{2} \sum_{j=1}^{L-1} \left[ \sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y - \Delta(\theta) \sigma_j^z \sigma_{j+1}^z \right]. \quad (\text{C.2})$$

Note that in the definition of  $H_{\text{XXZ}}$  here is different from the main text. Within this appendix we will adapt the definition in Eq. (C.2). The parameter

$$\Delta(\theta) = \frac{\sin \theta}{|\cos \theta - \sin \theta|} \quad (\text{C.3})$$

determines the phase of  $H_{\text{XXZ}}(\theta)$  and hence  $H_{\text{SD}}(\theta)$ . The results are summarized in Fig. C.1.

### C.0.1 Absence of holes

Let

$$\mathcal{A} = \left[-\frac{\pi}{2}, \arctan \frac{1}{2}\right) \cup \left(\frac{\pi}{2}, \arctan \frac{1}{2} + \pi\right], \quad (\text{C.4})$$

$$\mathcal{B} = \left(\arctan \frac{1}{2} - \pi, -\frac{\pi}{2}\right) \setminus \left\{-\frac{3\pi}{4}\right\}. \quad (\text{C.5})$$

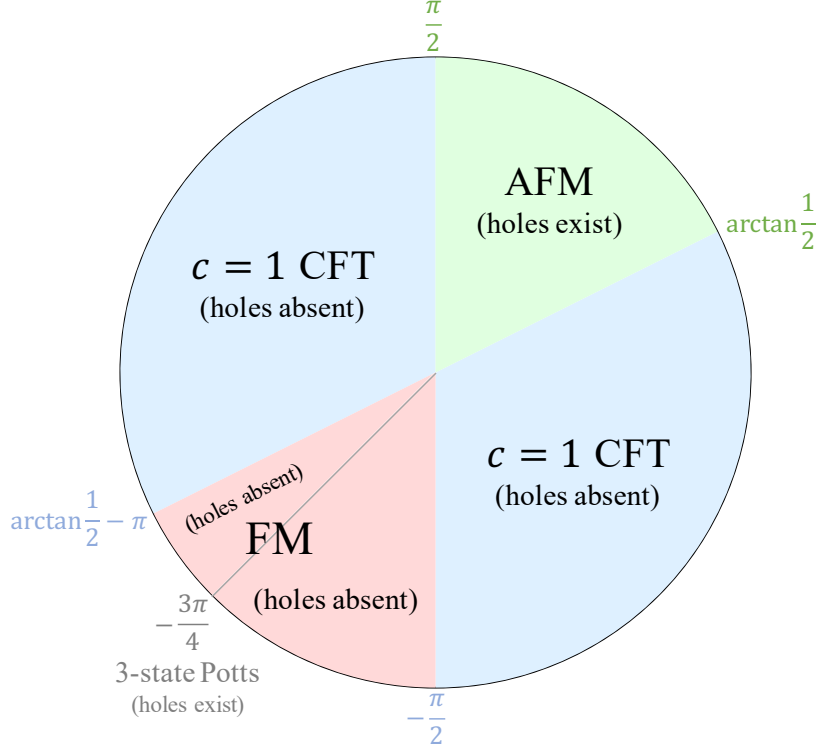


Figure C.1: Phase diagram for the ground state of  $H_{\text{SD}}(\theta)$  in Eq. (5.15). Holes are absent from the low-energy eigenstates when  $\theta \in (\pi/2, 2\pi + \arctan \frac{1}{2}) \setminus \{5\pi/4\}$ , which means that the low-energy physics of  $H_{\text{SD}}$  in this region is exactly the same as the spin-1/2 XXZ model. Note that  $H_{\text{SD}}$  and  $H'_{\text{SD}}$  are related to each other by  $V = \prod_{k=\text{odd}} \sigma_k^y$ , so that an FM (AFM) ground state of  $H_{\text{SD}}$  corresponds to an AFM (FM) ground state of  $H'_{\text{SD}}$ .

When  $\theta \in \mathcal{A}$ ,  $-1 \leq \Delta(\theta) < 1$ , and thus  $H_{\text{XXZ}}$  is gapless and the low-energy physics is described by a  $c = 1$  CFT. When  $\theta \in \mathcal{B}$ ,  $\Delta(\theta) < -1$  and  $H_{\text{XXZ}}$  has two degenerate and antiferromagnetic (AFM) ground states in the thermodynamic limit  $L \rightarrow \infty$ . Let  $\gamma = \arccos[-\Delta(\theta)]$  when  $\theta \in \mathcal{A}$  and  $\xi = \text{arccosh}[-\Delta(\theta)]$  when  $\theta \in \mathcal{B}$ . The ground-state (GS) energy density of  $H_{\text{XXZ}}$  in the thermodynamic limit, denoted as  $e_\infty$ , was exactly obtained by Yang and Yang back in 1966 [213, 214]:

$$e_\infty(\theta) = \begin{cases} \frac{1}{2} \cos \gamma - (\sin \gamma)^2 \int_{-\infty}^{\infty} \frac{dx}{\cosh(\pi x) [\cosh(2\gamma x) - \cos \gamma]}, & -1 \leq -\cos \gamma = \Delta(\theta) < 1, \\ \frac{1}{2} \cosh \xi - \left[ 1 + 4 \sum_{n=1}^{\infty} \frac{1}{1 + e^{2\xi n}} \right] \sinh \xi, & -\cosh \xi = \Delta(\theta) < -1. \end{cases} \quad (\text{C.6})$$

When  $1 \ll L < \infty$ , we need to consider finite-size corrections. For OBC, the finite-size GS energy density  $e_L^{\text{OBC}}$  takes the form [215, 225]:

$$e_L^{\text{OBC}} = e_\infty + \frac{f}{L} + O\left(\frac{1}{L}\right), \quad (\text{C.7})$$

where  $f$  is called the "surface energy" and is given by

$$f(\theta) = \begin{cases} \frac{\pi \sin \gamma}{2\gamma} - \frac{\cos \gamma}{2} - \frac{\sin \gamma}{4} \int_{-\infty}^{\infty} dx \left[ 1 - \tanh\left(\frac{\pi x}{4}\right) \tanh\left(\frac{\gamma x}{2}\right) \right], & -1 \leq -\cos \gamma = \Delta(\theta) < 1 \\ -\frac{1}{2} \cosh \xi + 4 \left[ \frac{1}{4} + \sum_{n=1}^{\infty} \frac{e^{2n\xi} - 1}{1 + e^{4n\xi}} + \sum_{n=1}^{\infty} \frac{(-1)^n}{1 + e^{2n\xi}} \right] \sinh \xi, & -\cosh \xi = \Delta(\theta) < -1 \end{cases}. \quad (\text{C.8})$$

Note that Eq. (C.1) is defined on a chain with OBC. For a sufficiently long chain, in  $\mathcal{H}_{1/2}$  (the subspace without holes), the GS energy of  $H_{\text{SD}}$  (up to the order of  $L^0$ ) is given by

$$E_0 = 2\sqrt{2} \left| \sin\left(\frac{\pi}{4} - \theta\right) \right| (Le_{\infty} + f) + 3(L-1) \sin \theta. \quad (\text{C.9})$$

Now consider the subspace of  $m$  holes. When the  $m$  holes are disjoint, sufficiently far away from each other, and sufficiently far away from the boundary, the GS energy of  $H_{\text{SD}}$  in this subspace is (up to the order of  $L^0$ )

$$E_m = 2\sqrt{2} \left| \sin\left(\frac{\pi}{4} - \theta\right) \right| [(L-m)e_{\infty} + (m+1)f] + (L-1-2m) \sin \theta + 2(L-1) \sin \theta. \quad (\text{C.10})$$

The energy difference is given by

$$\Delta E_m = E_m - E_0 = m \left[ 2\sqrt{2} \left| \sin\left(\frac{\pi}{4} - \theta\right) \right| (f - e_{\infty}) - 2 \sin \theta \right] = m \Delta E_1. \quad (\text{C.11})$$

As long as  $\Delta E_1 = 2\sqrt{2} \left| \sin(\pi/4 - \theta) \right| (f - e_{\infty}) - 2 \sin \theta > 0$ , eigenstates with disjoint holes are gapped from the ground state. The value of  $\Delta E_1$  can be easily obtained numerically, see Fig. C.2(a). We can see that  $\Delta E_1$  is indeed positive when  $\theta \in \mathcal{A} \cup \mathcal{B}$ .

We have not yet ruled out the possibility of "phase separation", meaning that holes form a domain, like  $|\dots \uparrow\uparrow \text{hhh}\dots \text{hh} \downarrow\uparrow \dots\rangle$ . In fact, the energy density of the hole domain is given by  $4 \sin \theta$ , while the energy density of the spin-1/2 domain is  $2\sqrt{2} \left| \sin(\pi/4 - \theta) \right| e_{\infty} + 3 \sin \theta$  (up to the order of  $L^0$ ). We can numerically show that the former energy density is always higher than the latter when  $\theta \in \mathcal{A} \cup \mathcal{B}$ , see Fig. C.2(b), which means that the phase separation does not occur.

To sum up, holes  $\{|\text{h}\rangle_j\}$  are gapped from the ground state of  $H_{\text{SD}}(\theta)$  when  $\theta$  is in the region described by Eq. (C.4) and Eq. (C.5), which is in accordance with our DMRG results.

## C.0.2 Existence of holes

At two special points  $\theta = \pi/4$  and  $-3\pi/4$ ,  $H_{\text{SD}}$  (but not  $H'_{\text{SD}}$ ) reduces to the classical *three-state Potts model*. This can be seen by noting that

$$\sigma_j^z \sigma_{j+1}^z + 2h_j h_{j+1} + n_j n_{j+1} = 2 \left( |\uparrow\uparrow\rangle \langle \uparrow\uparrow| + |\downarrow\downarrow\rangle \langle \downarrow\downarrow| + |\text{hh}\rangle \langle \text{hh}| \right), \quad (\text{C.12})$$

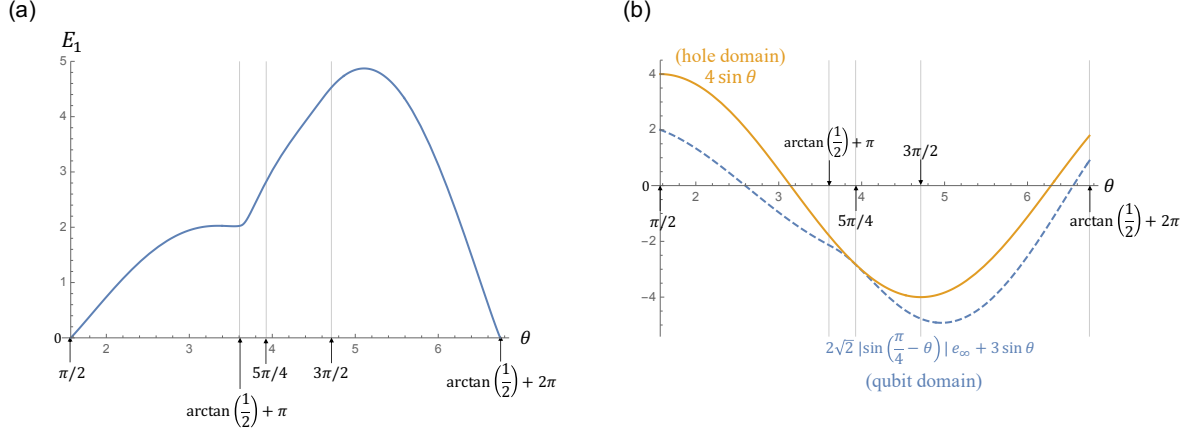


Figure C.2: (a)  $E_1 > 0$  for all  $\theta \in (\pi/2, \arctan \frac{1}{2} + 2\pi)$ . (b) Energy density of the hole domain is higher than that of the qubit domain when  $\theta \in A \cup B = (\pi/2, \arctan \frac{1}{2} + 2\pi) \setminus \{5\pi/4\}$ , implying the absence of the phase separation.

where  $\theta = \pi/4$  is AFM and  $\theta = -3\pi/4$  is FM. The ground states at these two points are thus degenerate, and holes  $\{|\mathbf{h}\rangle_j\}$  appear in the GS eigenspace.

In the region

$$\theta \in \left[ \arctan \frac{1}{2}, \frac{\pi}{2} \right], \quad (\text{C.13})$$

$\Delta(\theta) \geq 1$ , and the ground state of  $H_{\text{XXZ}}$  is FM. The GS energy of  $H_{\text{XXZ}}$  exactly equals  $-(L-1)\Delta(\theta)/2$ . In the subspace without holes, the GS energy of  $H_{\text{SD}}$  is then given by

$$E_0 = 2\sqrt{2} \left| \sin \left( \frac{\pi}{4} - \theta \right) \right| \times [-(L-1)\Delta(\theta)/2] + 3(L-1) \sin \theta = 2(L-1) \sin \theta. \quad (\text{C.14})$$

In the subspace of  $m$  holes, when the holes are all disjoint, the GS energy becomes

$$E_m = 2\sqrt{2} \left| \sin \left( \frac{\pi}{4} - \theta \right) \right| \times [-(L-1-2m)\Delta(\theta)/2] + (L-1-2m) \sin \theta + 2(L-1) \sin \theta = 2(L-1) \sin \theta = E_0, \quad (\text{C.15})$$

which means that adding disjoint holes to the ground state does not cost energy. On the other hand, if the  $m$  holes form a domain,

$$\begin{aligned} E_m &= 2\sqrt{2} \left| \sin \left( \frac{\pi}{4} - \theta \right) \right| \times [-(L-m-2)\Delta(\theta)/2] + 2(m-1) \sin \theta + (L-m-2) \sin \theta + 2(L-1) \sin \theta \\ &= 2(L+m-2) \sin \theta. \end{aligned} \quad (\text{C.16})$$

We see that  $E_m > E_0$  as long as  $m \geq 2$ . In other words, phase separation does not occur in the ground state.

## BIBLIOGRAPHY

- [1] H. Yang, H. Nakano, and H. Katsura, [Phys. Rev. Research \*\*3\*\*, 023210 \(2021\)](#).
- [2] H. Yang, L. Li, K. Okunishi, and H. Katsura, [arXiv:2203.15791 \(2022\)](#).
- [3] [“Phase diagram of water \(simplified\),”](#) Wikimedia Commons (2022).
- [4] H. Tasaki, *Physics and Mathematics of Quantum Many-Body Systems* (Springer, 2020).
- [5] B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen, *Quantum Information Meets Quantum Matter* (Springer, New York, 2019).
- [6] J. Goldstone, A. Salam, and S. Weinberg, [Phys. Rev. \*\*127\*\*, 965 \(1962\)](#).
- [7] H. A. Kramers and G. H. Wannier, [Phys. Rev. \*\*60\*\*, 252 \(1941\)](#).
- [8] D. Aasen, R. S. K. Mong, and P. Fendley, [J. Phys. A: Math. Theor. \*\*49\*\*, 354001 \(2016\)](#).
- [9] P. Di Francesco, P. Mathieu, and D. Sénéchal, *Conformal Field Theory* (Springer Science & Business Media, New York, 2012).
- [10] X. Chen, Z.-C. Gu, and X.-G. Wen, [Phys. Rev. B \*\*82\*\*, 155138 \(2010\)](#).
- [11] X. Chen, Z.-C. Gu, and X.-G. Wen, [Phys. Rev. B \*\*83\*\*, 035107 \(2011\)](#).
- [12] X. Chen, Z.-C. Gu, and X.-G. Wen, [Phys. Rev. B \*\*84\*\*, 235128 \(2011\)](#).
- [13] N. Schuch, D. Pérez-García, and I. Cirac, [Phys. Rev. B \*\*84\*\*, 165139 \(2011\)](#).
- [14] Y. Ogata, [Commun. Math. Phys. \*\*348\*\*, 847 \(2016\)](#).
- [15] Y. Ogata, [Commun. Math. Phys. \*\*348\*\*, 897 \(2016\)](#).
- [16] Y. Ogata, [Commun. Math. Phys. \*\*352\*\*, 1205 \(2017\)](#).
- [17] A. Y. Kitaev, [Phys.-Uspekhi \*\*44\*\*, 131 \(2001\)](#).
- [18] R. Verresen, R. Moessner, and F. Pollmann, [Phys. Rev. B \*\*96\*\*, 165124 \(2017\)](#).

- [19] X.-G. Wen, [“Definition of short range entanglement,”](#) Physics Stack Exchange (2014).
- [20] X.-G. Wen, [Rev. Mod. Phys. \*\*89\*\*, 041004 \(2017\).](#)
- [21] S.-Q. Ning, Y. Qi, Z.-C. Gu, and C. Wang, [arXiv:2109.15307 \(2021\).](#)
- [22] W. Son, L. Amico, R. Fazio, A. Hamma, S. Pascazio, and V. Vedral, [EPL \*\*95\*\*, 50001 \(2011\).](#)
- [23] R. Verresen, R. Thorngren, N. G. Jones, and F. Pollmann, [Phys. Rev. X \*\*11\*\*, 041059 \(2021\).](#)
- [24] T. Scaffidi, D. E. Parker, and R. Vasseur, [Phys. Rev. X \*\*7\*\*, 041048 \(2017\).](#)
- [25] L. Li, M. Oshikawa, and Y. Zheng, [arXiv:2204.03131 \(2022\).](#)
- [26] D. E. Parker, T. Scaffidi, and R. Vasseur, [Phys. Rev. B \*\*97\*\*, 165114 \(2018\).](#)
- [27] R. Verresen, N. G. Jones, and F. Pollmann, [Phys. Rev. Lett. \*\*120\*\*, 057001 \(2018\).](#)
- [28] N. G. Jones and R. Verresen, [J. Stat. Phys. \*\*175\*\*, 1164 \(2019\).](#)
- [29] C. M. Duque, H.-Y. Hu, Y.-Z. You, V. Khemani, R. Verresen, and R. Vasseur, [Phys. Rev. B \*\*103\*\*, L100207 \(2021\).](#)
- [30] R. Thorngren, A. Vishwanath, and R. Verresen, [Phys. Rev. B \*\*104\*\*, 075132 \(2021\).](#)
- [31] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, [Phys. Rev. B \*\*87\*\*, 155114 \(2013\).](#)
- [32] M. B. Hastings, [Phys. Rev. B \*\*69\*\*, 104431 \(2004\).](#)
- [33] M. B. Hastings and T. Koma, [Commun. Math. Phys. \*\*265\*\*, 781 \(2006\).](#)
- [34] M. B. Hastings, [J. Stat. Phys. \*\*2007\*\*, P08024 \(2007\).](#)
- [35] I. Arad, A. Kitaev, Z. Landau, and U. Vazirani, [arXiv:1301.1162 \(2013\).](#)
- [36] A. Kitaev and J. Preskill, [Phys. Rev. Lett. \*\*96\*\*, 110404 \(2006\).](#)
- [37] F. G. Brandão and M. Horodecki, [Commun. Math. Phys. \*\*333\*\*, 761 \(2015\).](#)
- [38] F. G. Brandão and M. Horodecki, [Nat. Phys. \*\*9\*\*, 721 \(2013\).](#)
- [39] F. Verstraete and J. I. Cirac, [Phys. Rev. B \*\*73\*\*, 094423 \(2006\).](#)
- [40] G. Vidal, [Phys. Rev. Lett. \*\*91\*\*, 147902 \(2003\).](#)



- [41] D. Perez-Garcia, F. Verstraete, J. I. Cirac, and M. M. Wolf, [Quantum Inf. Comput.](#) **8**, 0650 (2008).
- [42] R. Orús and G. Vidal, [Phys. Rev. B](#) **78**, 155117 (2008).
- [43] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, [Quantum Inf. Comput.](#) **7**, 401 (2007).
- [44] M. Fannes, B. Nachtergaele, and R. F. Werner, [Commun. Math. Phys.](#) **144**, 443 (1992).
- [45] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, [Phys. Rev. Lett.](#) **59**, 799 (1987).
- [46] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, [Commun. Math. Phys.](#) **115**, 477 (1988).
- [47] M. den Nijs and K. Rommelse, [Phys. Rev. B](#) **40**, 4709 (1989).
- [48] F. Pollmann, A. M. Turner, E. Berg, and M. Oshikawa, [Phys. Rev. B](#) **81**, 064439 (2010).
- [49] F. Pollmann, E. Berg, A. M. Turner, and M. Oshikawa, [Phys. Rev. B](#) **85**, 075125 (2012).
- [50] T. Kennedy and H. Tasaki, [Phys. Rev. B](#) **45**, 304 (1992).
- [51] T. Kennedy and H. Tasaki, [Comm. Math. Phys.](#) **147**, 431 (1992).
- [52] M. Oshikawa, [J. Phys. Condens. Matter](#) **4**, 7469 (1992).
- [53] K. Okunishi, [Phys. Rev. B](#) **83**, 104411 (2011).
- [54] D. Maekawa and H. Tasaki, [arXiv:2205.00653](#) (2022).
- [55] D. V. Else, S. D. Bartlett, and A. C. Doherty, [Phys. Rev. B](#) **88**, 085114 (2013).
- [56] H.-H. Tu, G.-M. Zhang, and T. Xiang, [Phys. Rev. B](#) **78**, 094404 (2008).
- [57] K. Duivenvoorden and T. Quella, [Phys. Rev. B](#) **88**, 125115 (2013).
- [58] W.-J. Rao, G.-M. Zhang, and K. Yang, [Phys. Rev. B](#) **89**, 125112 (2014).
- [59] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, [Science](#) **338**, 1604 (2012).
- [60] D. Pérez-García, M. M. Wolf, M. Sanz, F. Verstraete, and J. I. Cirac, [Phys. Rev. Lett.](#) **100**, 167202 (2008).
- [61] F. Pollmann and A. M. Turner, [Phys. Rev. B](#) **86**, 125441 (2012).

- [62] A. M. Turner, F. Pollmann, and E. Berg, [Phys. Rev. B \*\*83\*\*, 075102 \(2011\)](#).
- [63] [“Corepresentations of unitary and antiunitary groups,” Wikipedia](#).
- [64] A. Prakash, J. Wang, and T.-C. Wei, [Phys. Rev. B \*\*98\*\*, 125108 \(2018\)](#).
- [65] S.-J. Huang, H. Song, Y.-P. Huang, and M. Hermele, [Phys. Rev. B \*\*96\*\*, 205106 \(2017\)](#).
- [66] J. C. Wang, Z.-C. Gu, and X.-G. Wen, [arXiv:1405.7689 \(2014\)](#).
- [67] X.-G. Wen, [Phys. Rev. B \*\*95\*\*, 205142 \(2017\)](#).
- [68] A. Kapustin and N. Seiberg, [J. High Energy Phys. \*\*2014\*\*, 1 \(2014\)](#).
- [69] N. E. Steenrod, [Ann. Math. , 290 \(1947\)](#).
- [70] J. L. Cardy, [Nucl. Phys. B \*\*275\*\*, 200 \(1986\)](#).
- [71] J. L. Cardy, [Nucl. Phys. B \*\*324\*\*, 581 \(1989\)](#).
- [72] W. Chen, K. Hida, and B. C. Sanctuary, [Phys. Rev. B \*\*67\*\*, 104401 \(2003\)](#).
- [73] A. N. Kirillov and V. E. Korepin, [Leningrad Math. J. \*\*1\*\*, 343 \(1990\)](#), [arXiv:0909.2211](#).
- [74] H. Katsura, I. Maruyama, A. Tanaka, and H. Tasaki, [EPL \(Europhysics Letters\) \*\*91\*\*, 57007 \(2010\)](#).
- [75] E. Lieb, T. Schultz, and D. Mattis, [Ann. Phys. \*\*16\*\*, 407 \(1961\)](#).
- [76] I. Affleck and E. H. Lieb, [Lett. Math. Phys. \*\*12\*\*, 57 \(1986\)](#).
- [77] M. Oshikawa, [Phys. Rev. Lett. \*\*84\*\*, 1535 \(2000\)](#).
- [78] Y. Yao and M. Oshikawa, [Phys. Rev. X \*\*10\*\*, 031008 \(2020\)](#).
- [79] Y. Fuji, [Phys. Rev. B \*\*93\*\*, 104425 \(2016\)](#).
- [80] S. A. Parameswaran, A. M. Turner, D. P. Arovas, and A. Vishwanath, [Nat. Phys. \*\*9\*\*, 299 \(2013\)](#).
- [81] H. Watanabe, H. C. Po, A. Vishwanath, and M. Zaletel, [Proc. Natl. Acad. Sci. USA \*\*112\*\*, 14551 \(2015\)](#).
- [82] Y. Ogata and H. Tasaki, [Commun. Math. Phys. \*\*372\*\*, 951 \(2019\)](#).
- [83] H. Tasaki, [arXiv:2202.06243 \(2022\)](#).
- [84] Y. Yao and M. Oshikawa, [Phys. Rev. Lett. \*\*126\*\*, 217201 \(2021\)](#).

- [85] T. Hirano, H. Katsura, and Y. Hatsugai, [Phys. Rev. B \*\*78\*\*, 054431 \(2008\)](#).
- [86] Y. Ogata, Y. Tachikawa, and H. Tasaki, [Commun. Math. Phys. \*\*385\*\*, 79 \(2021\)](#).
- [87] H. C. Po, H. Watanabe, C.-M. Jian, and M. P. Zaletel, [Phys. Rev. Lett. \*\*119\*\*, 127202 \(2017\)](#).
- [88] D. V. Else and R. Thorngren, [Phys. Rev. B \*\*101\*\*, 224437 \(2020\)](#).
- [89] X. Chen, Z.-X. Liu, and X.-G. Wen, [Phys. Rev. B \*\*84\*\*, 235141 \(2011\)](#).
- [90] S. Takayoshi, P. Pujol, and A. Tanaka, [Phys. Rev. B \*\*94\*\*, 235159 \(2016\)](#).
- [91] M. Cheng, M. Zaletel, M. Barkeshli, A. Vishwanath, and P. Bonderson, [Phys. Rev. X \*\*6\*\*, 041068 \(2016\)](#).
- [92] Y. Yao, C.-T. Hsieh, and M. Oshikawa, [Phys. Rev. Lett. \*\*123\*\*, 180201 \(2019\)](#).
- [93] R. Dijkgraaf and E. Witten, [Comm. Math. Phys. \*\*129\*\*, 393 \(1990\)](#).
- [94] J. Wang, X.-G. Wen, and E. Witten, [Phys. Rev. X \*\*8\*\*, 031048 \(2018\)](#).
- [95] M. Levin and Z.-C. Gu, [Phys. Rev. B \*\*86\*\*, 115109 \(2012\)](#).
- [96] A. Kapustin, [arXiv:1403.1467 \(2014\)](#).
- [97] H. Song, S.-J. Huang, L. Fu, and M. Hermele, [Phys. Rev. X \*\*7\*\*, 011020 \(2017\)](#).
- [98] D. V. Else and C. Nayak, [Phys. Rev. B \*\*90\*\*, 235137 \(2014\)](#).
- [99] Z.-C. Gu and X.-G. Wen, [Phys. Rev. B \*\*80\*\*, 155131 \(2009\)](#).
- [100] Y. Fuji, F. Pollmann, and M. Oshikawa, [Phys. Rev. Lett. \*\*114\*\*, 177204 \(2015\)](#).
- [101] R. Thorngren and D. V. Else, [Phys. Rev. X \*\*8\*\*, 011040 \(2018\)](#).
- [102] T. A. Hilker, G. Salomon, F. Grusdt, A. Omran, M. Boll, E. Demler, I. Bloch, and C. Gross, [Science \*\*357\*\*, 484 \(2017\)](#).
- [103] S. de Léséleuc, V. Lienhard, P. Scholl, D. Barredo, S. Weber, N. Lang, H. P. Büchler, T. Lahaye, and A. Browaeys, [Science \*\*365\*\*, 775 \(2019\)](#).
- [104] E. G. Dalla Torre, E. Berg, and E. Altman, [Phys. Rev. Lett. \*\*97\*\*, 260401 \(2006\)](#).
- [105] E. Berg, E. G. Dalla Torre, T. Giamarchi, and E. Altman, [Phys. Rev. B \*\*77\*\*, 245119 \(2008\)](#).
- [106] D. Rossini and R. Fazio, [New J. Phys. \*\*14\*\*, 065012 \(2012\)](#).

- [107] J. Xu, Q. Gu, and E. J. Mueller, [Phys. Rev. Lett. \*\*120\*\*, 085301 \(2018\)](#).
- [108] G. G. Batrouni, R. T. Scalettar, V. G. Rousseau, and B. Grémaud, [Phys. Rev. Lett. \*\*110\*\*, 265303 \(2013\)](#).
- [109] S. Ejima, F. Lange, and H. Fehske, [Phys. Rev. Lett. \*\*113\*\*, 020401 \(2014\)](#).
- [110] F. Lange, S. Ejima, and H. Fehske, [Phys. Rev. Lett. \*\*118\*\*, 120401 \(2017\)](#).
- [111] M. Dalmonte, M. Di Dio, L. Barbiero, and F. Ortolani, [Phys. Rev. B \*\*83\*\*, 155110 \(2011\)](#).
- [112] K. Sugimoto, S. Ejima, F. Lange, and H. Fehske, [Phys. Rev. A \*\*99\*\*, 012122 \(2019\)](#).
- [113] J. Zhao, S. Hu, and P. Zhang, [Phys. Rev. Lett. \*\*115\*\*, 195302 \(2015\)](#).
- [114] B. Grémaud and G. G. Batrouni, [Phys. Rev. B \*\*95\*\*, 165131 \(2017\)](#).
- [115] J. J. García-Ripoll, M. A. Martin-Delgado, and J. I. Cirac, [Phys. Rev. Lett. \*\*93\*\*, 250405 \(2004\)](#).
- [116] H. Nonne, P. Lecheminant, S. Capponi, G. Roux, and E. Boulat, [Phys. Rev. B \*\*81\*\*, 020408\(R\) \(2010\)](#).
- [117] V. Bois, S. Capponi, P. Lecheminant, M. Moliner, and K. Totsuka, [Phys. Rev. B \*\*91\*\*, 075121 \(2015\)](#).
- [118] S. Moudgalya and F. Pollmann, [Phys. Rev. B \*\*91\*\*, 155128 \(2015\)](#).
- [119] F. Lange, S. Ejima, and H. Fehske, [Phys. Rev. B \*\*92\*\*, 041120\(R\) \(2015\)](#).
- [120] M. Nakagawa and N. Kawakami, [Phys. Rev. B \*\*96\*\*, 155133 \(2017\)](#).
- [121] H. Ueda, T. Morimoto, and T. Momoi, [Phys. Rev. B \*\*98\*\*, 045128 \(2018\)](#).
- [122] P. Fromholz, S. Capponi, P. Lecheminant, D. J. Papoular, and K. Totsuka, [Phys. Rev. B \*\*99\*\*, 054414 \(2019\)](#).
- [123] S. Fazzini, L. Barbiero, and A. Montorsi, [Phys. Rev. Lett. \*\*122\*\*, 106402 \(2019\)](#).
- [124] A. Montorsi, S. Fazzini, and L. Barbiero, [Phys. Rev. A \*\*101\*\*, 043618 \(2020\)](#).
- [125] P. Sompet, S. Hirth, D. Bourgund, T. Chalopin, J. Bibo, J. Koepsell, P. Bojović, R. Verresen, F. Pollmann, G. Salomon, *et al.*, [Nature](#) , 1 (2022).
- [126] Y. Kawaguchi and M. Ueda, [Phys. Rep. \*\*520\*\*, 253 \(2012\)](#).
- [127] D. M. Stamper-Kurn and M. Ueda, [Rev. Mod. Phys. \*\*85\*\*, 1191 \(2013\)](#).

- [128] H. Katsura and H. Tasaki, [Phys. Rev. Lett. \*\*110\*\*, 130405 \(2013\)](#).
- [129] H. Yang and H. Katsura, [Phys. Rev. Lett. \*\*122\*\*, 053401 \(2019\)](#).
- [130] A. Läuchli, G. Schmid, and S. Trebst, [Phys. Rev. B \*\*74\*\*, 144426 \(2006\)](#).
- [131] A. Eckardt, C. Weiss, and M. Holthaus, [Phys. Rev. Lett. \*\*95\*\*, 260404 \(2005\)](#).
- [132] A. Eckardt, P. Hauke, P. Soltan-Panahi, C. Becker, K. Sengstock, and M. Lewenstein, [Europhys. Lett. \*\*89\*\*, 10010 \(2010\)](#).
- [133] D. H. Dunlap and V. M. Kenkre, [Phys. Rev. B \*\*34\*\*, 3625 \(1986\)](#).
- [134] F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, [Phys. Rev. Lett. \*\*67\*\*, 516 \(1991\)](#).
- [135] F. Großmann and P. Hänggi, [Europhys. Lett. \*\*18\*\*, 571 \(1992\)](#).
- [136] K. Drese and M. Holthaus, [Phys. Rev. Lett. \*\*78\*\*, 2932 \(1997\)](#).
- [137] H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo, [Phys. Rev. Lett. \*\*99\*\*, 220403 \(2007\)](#).
- [138] A. Eckardt, M. Holthaus, H. Lignier, A. Zenesini, D. Ciampini, O. Morsch, and E. Arimondo, [Phys. Rev. A \*\*79\*\*, 013611 \(2009\)](#).
- [139] E. Kierig, U. Schnorrberger, A. Schietinger, J. Tomkovic, and M. K. Oberthaler, [Phys. Rev. Lett. \*\*100\*\*, 190405 \(2008\)](#).
- [140] A. Zenesini, H. Lignier, D. Ciampini, O. Morsch, and E. Arimondo, [Phys. Rev. Lett. \*\*102\*\*, 100403 \(2009\)](#).
- [141] J. Struck, C. Ölschläger, R. Le Targat, P. Soltan-Panahi, A. Eckardt, M. Lewenstein, P. Windpassinger, and K. Sengstock, [Science \*\*333\*\*, 996 \(2011\)](#).
- [142] J.-W. Rhim and B.-J. Yang, [Phys. Rev. B \*\*99\*\*, 045107 \(2019\)](#).
- [143] N. Read, [Phys. Rev. B \*\*95\*\*, 115309 \(2017\)](#).
- [144] M. Ueda, *Fundamentals and New Frontiers of Bose-Einstein Condensation* (World Scientific, Singapore, 2010).
- [145] G.-M. Zhang and X. Wang, [J. Phys. A: Math. Gen. \*\*39\*\*, 8515 \(2006\)](#).
- [146] H. Yang, *Rigorous Results for the Ground States of Spinor Bose-Hubbard Models*, Master's thesis, The University of Tokyo, Tokyo (2019).
- [147] M. Kobayashi, Y. Kawaguchi, M. Nitta, and M. Ueda, [J. Low Temp. Phys. \*\*162\*\*, 299 \(2011\)](#).

- [148] H. Katsura and H. Tasaki, [Phys. Rev. Lett. \*\*110\*\*, 130405 \(2013\)](#).
- [149] A. Imambekov, M. Lukin, and E. Demler, [Phys. Rev. A \*\*68\*\*, 063602 \(2003\)](#).
- [150] M. Lewenstein, A. Sanpera, and V. Ahufinger, *Ultracold Atoms in Optical Lattices: Simulating Quantum Many-body Systems* (Oxford University, New York, 2012).
- [151] G. Uimin, *ZhETF Pisma Redaktsiiu* **12**, 332 (1970).
- [152] C. K. Lai, [J. Math. Phys. \*\*15\*\*, 1675 \(1974\)](#).
- [153] B. Sutherland, [Phys. Rev. B \*\*12\*\*, 3795 \(1975\)](#).
- [154] L. Takhtajan, [Phys. Lett. A \*\*87\*\*, 479 \(1982\)](#).
- [155] H. Babujian, [Phys. Lett. A \*\*90\*\*, 479 \(1982\)](#).
- [156] A. Kitazawa and K. Nomura, [Phys. Rev. B \*\*59\*\*, 11358 \(1999\)](#).
- [157] A. Läuchli, G. Schmid, and S. Trebst, [Phys. Rev. B \*\*74\*\*, 144426 \(2006\)](#).
- [158] R. Barnett, A. Turner, and E. Demler, [Phys. Rev. Lett. \*\*97\*\*, 180412 \(2006\)](#).
- [159] K. Eckert, Ł. Zawitkowski, M. J. Leskinen, A. Sanpera, and M. Lewenstein, [New J. Phys. \*\*9\*\*, 133 \(2007\)](#).
- [160] A. Imambekov, M. Lukin, and E. Demler, [Phys. Rev. A \*\*68\*\*, 063602 \(2003\)](#).
- [161] S. Tsuchiya, S. Kurihara, and T. Kimura, [Phys. Rev. A \*\*70\*\*, 043628 \(2004\)](#).
- [162] H. Tasaki, [Phys. Rev. Lett. \*\*69\*\*, 1608 \(1992\)](#).
- [163] H. Tasaki, [Prog. Theor. Phys. \*\*99\*\*, 489 \(1998\)](#).
- [164] K. Tamura and H. Katsura, [Phys. Rev. B \*\*100\*\*, 214423 \(2019\)](#).
- [165] T. Zhang and G.-B. Jo, [Sci. Rep. \*\*5\*\*, 16044 \(2015\)](#).
- [166] J. B. Parkinson, [J. Phys. C \*\*20\*\*, L1029 \(1987\)](#).
- [167] J. B. Parkinson, [J. Phys. C \*\*21\*\*, 3793 \(1988\)](#).
- [168] A. Mielke and H. Tasaki, [Comm. Math. Phys. \*\*158\*\*, 341 \(1993\)](#).
- [169] Y.-T. Oh, H. Katsura, H.-Y. Lee, and J. H. Han, [Phys. Rev. B \*\*96\*\*, 165126 \(2017\)](#).
- [170] M. Andres, I. Schneider, and S. Eggert, [Phys. Rev. B \*\*77\*\*, 014429 \(2008\)](#).
- [171] V. Zauner-Stauber, L. Vanderstraeten, M. T. Fishman, F. Verstraete, and J. Haegeman, [Phys. Rev. B \*\*97\*\*, 045145 \(2018\)](#).

- [172] L. Vanderstraeten, J. Haegeman, and F. Verstraete, [SciPost Phys. Lect. Notes](#) , **7** (2019).
- [173] V. Zauner-Stauber, L. Vanderstraeten, J. Haegeman, I. P. McCulloch, and F. Verstraete, [Phys. Rev. B](#) **97**, 235155 (2018).
- [174] M. M. Rams, P. Czarnik, and L. Cincio, [Phys. Rev. X](#) **8**, 041033 (2018).
- [175] L. Tagliacozzo, T. R. de Oliveira, S. Iblisdir, and J. I. Latorre, [Phys. Rev. B](#) **78**, 024410 (2008).
- [176] S. R. Manmana, A. M. Läuchli, F. H. L. Essler, and F. Mila, [Phys. Rev. B](#) **83**, 184433 (2011).
- [177] T. Kennedy, E. H. Lieb, and H. Tasaki, [J. Stat. Phys.](#) **53**, 383 (1988).
- [178] A. Mielke, [Phys. Lett. A](#) **174**, 443 (1993).
- [179] A. Mielke, [J. Phys. A](#) **25**, 4335 (1992).
- [180] A. Mielke, [J. Phys. A](#) **24**, 3311 (1991).
- [181] L. Morales-Inostroza and R. A. Vicencio, [Phys. Rev. A](#) **94**, 043831 (2016).
- [182] W. Maimaiti, A. Andreanov, H. C. Park, O. Gendelman, and S. Flach, [Phys. Rev. B](#) **95**, 115135 (2017).
- [183] R. Dias and J. Gouveia, [Sci. Rep.](#) **5**, 16852 (2015).
- [184] A. Tanaka, [J. Stat. Phys.](#) **181**, 897 (2020).
- [185] Z. Liu, F. Liu, and Y.-S. Wu, [Chin. Phys. B](#) **23**, 077308 (2014).
- [186] Z. Gulácsi, A. Kampf, and D. Vollhardt, [Phys. Rev. Lett.](#) **99**, 026404 (2007).
- [187] G.-B. Jo, J. Guzman, C. K. Thomas, P. Hosur, A. Vishwanath, and D. M. Stamper-Kurn, [Phys. Rev. Lett.](#) **108**, 045305 (2012).
- [188] H. Yao and S. A. Kivelson, [Phys. Rev. Lett.](#) **105**, 166402 (2010).
- [189] S. A. Parameswaran, I. Kimchi, A. M. Turner, D. M. Stamper-Kurn, and A. Vishwanath, [Phys. Rev. Lett.](#) **110**, 125301 (2013).
- [190] I. Kimchi, S. Parameswaran, A. M. Turner, F. Wang, and A. Vishwanath, [Proc. Natl. Acad. Sci. USA](#) **110**, 16378 (2013).
- [191] R. Verresen, J. Bibo, and F. Pollmann, [arXiv:2102.08967](#) (2021).

- [192] F. Anfuso and A. Rosch, [Phys. Rev. B \*\*76\*\*, 085124 \(2007\)](#).
- [193] A. Griesmaier, J. Werner, S. Hensler, J. Stuhler, and T. Pfau, [Phys. Rev. Lett. \*\*94\*\*, 160401 \(2005\)](#).
- [194] M. Lu, N. Q. Burdick, S. H. Youn, and B. L. Lev, [Phys. Rev. Lett. \*\*107\*\*, 190401 \(2011\)](#).
- [195] K. Aikawa, A. Frisch, M. Mark, S. Baier, A. Rietzler, R. Grimm, and F. Ferlaino, [Phys. Rev. Lett. \*\*108\*\*, 210401 \(2012\)](#).
- [196] Y. Kawaguchi, H. Saito, and M. Ueda, [Phys. Rev. Lett. \*\*96\*\*, 080405 \(2006\)](#).
- [197] Y. Cao, V. Fatemi, S. Fang, K. Watanabe, T. Taniguchi, E. Kaxiras, and P. Jarillo-Herrero, [Nature \*\*556\*\*, 43 \(2018\)](#).
- [198] C. J. Turner, A. A. Michailidis, D. A. Abanin, M. Serbyn, and Z. Papić, [Nat. Phys. \*\*14\*\*, 745 \(2018\)](#).
- [199] W. W. Ho, S. Choi, H. Pichler, and M. D. Lukin, [Phys. Rev. Lett. \*\*122\*\*, 040603 \(2019\)](#).
- [200] Y. Kuno, T. Mizoguchi, and Y. Hatsugai, [Phys. Rev. B \*\*102\*\*, 241115\(R\) \(2020\)](#).
- [201] O. Hart, G. De Tomasi, and C. Castelnovo, [Phys. Rev. Research \*\*2\*\*, 043267 \(2020\)](#).
- [202] N. Shibata, N. Yoshioka, and H. Katsura, [Phys. Rev. Lett. \*\*124\*\*, 180604 \(2020\)](#).
- [203] D.-C. Lu, C. Xu, and Y.-Z. You, [Phys. Rev. B \*\*104\*\*, 205142 \(2021\)](#).
- [204] E. O'Brien and P. Fendley, [SciPost Phys. \*\*9\*\*, 88 \(2020\)](#).
- [205] N. Tantivasadakarn, R. Thorngren, A. Vishwanath, and R. Verresen, [arXiv:2110.07599 \(2021\)](#).
- [206] D. Aasen, P. Fendley, and R. S. Mong, [arXiv:2008.08598 \(2020\)](#).
- [207] J. C. Bridgeman and D. J. Williamson, [Phys. Rev. B \*\*96\*\*, 125104 \(2017\)](#).
- [208] G. Y. Cho, C.-T. Hsieh, and S. Ryu, [Phys. Rev. B \*\*96\*\*, 195105 \(2017\)](#).
- [209] M. A. Metlitski and R. Thorngren, [Phys. Rev. B \*\*98\*\*, 085140 \(2018\)](#).
- [210] A. Imambekov, M. Lukin, and E. Demler, [Phys. Rev. A \*\*68\*\*, 063602 \(2003\)](#).
- [211] T. Kennedy, [J. Phys. Condens. Matter \*\*6\*\*, 8015 \(1994\)](#).
- [212] K. Okunishi and K. Harada, [Phys. Rev. B \*\*89\*\*, 134422 \(2014\)](#).
- [213] C. N. Yang and C. P. Yang, [Phys. Rev. \*\*150\*\*, 321 \(1966\)](#).



- [214] C. N. Yang and C. P. Yang, *Phys. Rev.* **150**, 327 (1966).
- [215] C. Hamer, G. Quispel, and M. Batchelor, *J. Phys. A: Math. Gen.* **20**, 5677 (1987).
- [216] A. Luther and I. Peschel, *Phys. Rev. B* **12**, 3908 (1975).
- [217] S. Lukyanov and V. Terras, *Nucl. Phys. B* **654**, 323 (2003).
- [218] R. J. Baxter and S. B. Kelland, *J. Phys. C: Solid State Phys.* **7**, L403 (1974).
- [219] R. J. Baxter, *Phys. Rev. Lett.* **26**, 832 (1971).
- [220] R. J. Baxter, *Phys. Rev. Lett.* **26**, 834 (1971).
- [221] L. Zou, Y.-C. He, and C. Wang, *Phys. Rev. X* **11**, 031043 (2021).
- [222] Y. Tachikawa, *SciPost Phys.* **8**, 15 (2020).
- [223] T. Morimoto, H. Ueda, T. Momoi, and A. Furusaki, *Phys. Rev. B* **90**, 235111 (2014).
- [224] T. Tao, “Cayley graphs and the algebra of groups,”  
<https://terrytao.wordpress.com/2012/05/11/cayley-graphs-and-the-algebra-of-groups/> (2012).
- [225] A. Kapustin and S. Skorik, *J. Phys. A: Math. Gen.* **29**, 1629 (1996).



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