

A study on antiferromagnetic spin-1 chains coupled
to environments: the ground-state properties and the
computational power of mixed states

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August 16, 2024

Abstract

This thesis explores antiferromagnetic spin-1 chains in one-dimensional space that interact with their environments. In Part I, the scenario where the spin-1 chain is coupled to a conduction electron system is considered. The spin-1 Kondo-Heisenberg model, which is analogous to the Kondo lattice model, is examined as the specific Hamiltonian of the entire system, and the magnetic and electric conductivity properties of the ground state are investigated. In Part II, without specifying a particular physical system for the environment, the stability of the symmetry-protected topological order in the AKLT chain within an open quantum system is investigated from a quantum information perspective, with a focus on its computational capability as a resource for measurement-based quantum computation.

Acknowledgement

I would like to express my sincere gratitude to all those who have contributed to the completion of this doctoral thesis.

First, I am deeply thankful to my supervisor, Prof. Keisuke Totsuka, for his invaluable guidance, encouragement, and support throughout my doctoral journey. His expertise and dedication have been instrumental in shaping my research and academic growth.

I am also grateful to the all members of Yukawa Institute for Theoretical Physics condensed matter group for their insightful feedback, constructive criticism, and encouragement during my doctoral studies. It is my pleasure to thank Prof. Yoshifumi Nakata for fruitful discussions and valuable advice. I would like to extend my thanks to Dr. Alex Turzillo for productive discussions in person and via emails. I also appreciate Prof. Keisuke Fujii for effective suggestions. I would like to express my gratitude to the administrative staff in the academic affairs office who supported my research activities, as well as to the administrative staff in the research institute.

I acknowledge the financial support provided by JST, the establishment of university fellowships towards the creation of science technology innovation, which enabled me to conduct my research.

Finally and foremost, I am deeply grateful to my mother, brother, and grandmother for their patient support throughout my research life, as well as to my father, who passed away suddenly last year while I was writing my doctoral thesis. I would like to express my strongest gratitude to them.

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Overview

When studying the properties of matter using quantum mechanics, understanding the nature of the ground state has been crucial for comprehending different phases of matter. Namely, many low temperature phases of matter are characterized by the ground states, which undergo phase transitions and exhibit different properties for each phase. Quantum mechanics allows us to predict and understand how matter behaves by closely examining these ground state properties at low temperatures. In closed systems, where isolation prevents external influences, states are unitarily developed and the law of energy conservation holds in the system. This makes theoretical studies and numerical simulations clear and enables to establish the fundamental characteristics of matter.

Real-world systems, however, are not completely isolated and inevitably interact with their external environments. In open quantum systems, interactions between the system and its environment can lead to the exchange of energy and information. As a result, considering open quantum systems allow for the exploration of new phases of matter that do not exist in closed systems [1]. Moreover, in the current era of quantum computing development known as the NISQ (Noisy Intermediate-Scale Quantum) era, understanding phenomena such as decoherence is critical. This is because we do not have logical quantum bits (qubits) robust enough for large-scale quantum computation. Decoherence poses challenges in maintaining coherence among qubits, significantly impacting the reliability and efficiency of quantum information processing. Research into open many-body systems aims to deepen our understanding of these phenomena and to contribute to improving quantum computations with a long-term goal of achieving the fault-tolerant quantum computing, and this needs to consider the robustness of properties of some quantum state against a quantum noise.

One of the important applications of quantum computers is, for instance, simulating quantum systems. When simulating the behavior of quantum systems with spin Hamiltonians introduced to study the magnetism of materials, it also becomes crucial

to investigate the effects of their interaction with the environment. Understanding how these quantum systems behave requires consideration of their interaction with the environment. In the case of spin systems, interactions with the external environment can alter the magnetic order of spins and other physical properties, essential for understanding the stability of them. Research on open quantum systems explores the effects of such interactions on material properties, aiming to generate new insights through both theoretical exploration and experimental validation.

In this thesis, antiferromagnetic spin-1 chains coupled with environment are discussed. The one-dimensional antiferromagnetic Heisenberg model is one of the most famous spin chain models. The ground state of this model has an interesting characteristic. That is, the ground state property depends on the spin degree of freedom: the ground state is gapless if the spin on each site is half-odd, and it is gapped if the spin is integer (Haldane conjecture [2, 3]). Along with this fact, magnetic orders of a half-odd spin chain and integer one are different. The former has quasi-long-range antiferromagnetic order,

$$\langle S_i^z S_{i+r}^z \rangle \sim (-1)^r \frac{(\log r)^{1/2}}{r}, \quad (1)$$

for the case of $S = 1/2$ and on the other hand, the latter has short-range antiferromagnetic order (disorder):

$$\langle S_i^z S_{i+r}^z \rangle \sim (-1)^r e^{-\xi r} \quad (\xi > 0). \quad (2)$$

Then, doesn't the integer spin chain have any order? In fact, it has a hidden non-local order called as string order¹ [5, 6], and the string order parameter, which has a form like

$$\mathcal{O}_{\text{str}}^z = \lim_{|i-j| \rightarrow \infty} \left\langle S_i^z \exp \left(i\pi \sum_{k=i}^{j-1} S_k^z \right) S_j^z \right\rangle, \quad (4)$$

actually detects this long-range hidden antiferromagnetic order. The value of the SOP is finite for the ground state of the spin-1 antiferromagnetic Heisenberg model and zero

¹The Affleck-Kennedy-Lieb-Tasaki (AKLT) model [4] is a representative spin-1 antiferromagnetic chain, which will be introduced later, and its ground state (AKLT state) has the almost same property as that of the spin-1 antiferromagnetic Heisenberg chain. The hidden antiferromagnetic order can be clearly seen in the AKLT state. If we expand this state in the basis of the eigenstates of S_i^z operator, each term has the form like

$$|\cdots - 110 - 1001 - 101 \cdots\rangle, \quad (3)$$

where $|S^z = 1\rangle$ and $|S^z = -1\rangle$ are alternatively arranged with $|S^z = 0\rangle$ in between. Namely, $|S^z = 0\rangle$ on each site hides the antiferromagnetic Néel order of $|S^z = 1\rangle$ and $|S^z = -1\rangle$ and makes the ground state disorder.

for that of spin-1/2. This string order is known to be related to the symmetry-protected topological (SPT) order [7] protected by $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. This will be reviewed in Part II in detail.

As mentioned earlier, considering the influence from the environment is crucial, and we have briefly outlined interesting properties of the antiferromagnetic spin-1 chain when considered as a closed system. Thus, this thesis will then discuss the stability of these properties of the antiferromagnetic spin-1 chain when coupled to environments. In Part I, we investigate the ground state of the whole system when the spin-1 Heisenberg chain is specifically coupled to the conduction electron system, whose Hamiltonian is described by the spin-1 Kondo-Heisenberg model. It contains the effect of the coupling on the magnetism of the ground state of the antiferromagnetic spin-1 Heisenberg chain.

On the other hand, in Part II we deal with the open quantum system rather than the ground state of the entire system, and we focus on the SPT order, which some group of the ground state of spin-1 antiferromagnetic chains possess, under general quantum noises that are not limited to the coupling with the conduction electron system and examine the stability of the SPT order from the quantum informationally motivated viewpoint.

Part I

Ground state of a spin-1 system coupled to itinerant fermions

Chapter 1

Introduction to Part I

In this Part I, we specifically consider the situation where the spin-1 antiferromagnetic chain is coupled with a conduction electron system (Fig. 1.1). The Hamiltonian of this system is described by the Kondo-Heisenberg model [8, 9, 10]; and we deal with this model in the Part I. The Hamiltonian of the Kondo-Heisenberg model can be written as the following:

$$\begin{aligned}\hat{H}_{\text{KH}} &= -t \sum_{i,\alpha} \left(c_{i,\alpha}^\dagger c_{i+1,\alpha} + \text{H.C.} \right) + J_K \sum_i \mathbf{s}_i \cdot \mathbf{S}_i + J_H \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ &=: \hat{H}_e + \hat{H}_K + \hat{H}_H .\end{aligned}\tag{1.1}$$

In Eq. (1.1), $c_{i,\alpha}$ ($c_{i,\alpha}^\dagger$) denotes the annihilation (creation) operator of the conduction electron with spin $\alpha = \uparrow, \downarrow$ at site i , so the first term $\hat{H}_e$ is the kinetic energy (the hoping term) of the conduction electron. On the other hand, the third one is the antiferromagnetic interaction between the nearest neighboring local spins. The second

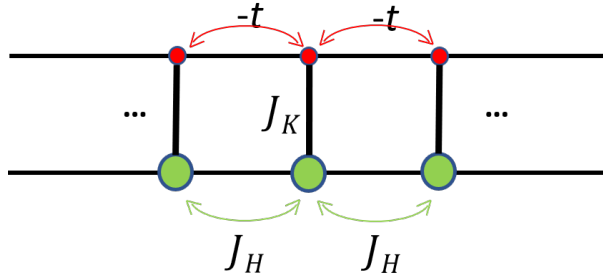


Figure 1.1: The schematic diagram of the Kondo Heisenberg model

interaction is called as Kondo coupling, which is the exchange interaction between the spin $\mathbf{s}_i = c_{i,\alpha}^\dagger [\boldsymbol{\sigma}]_{\alpha\beta} c_{i,\beta} / 2$ of the conduction electron (the symbols $\boldsymbol{\sigma}$ denote the Pauli matrices and the summation over repeated indices is implied) and the localized spin $\mathbf{S}_i$ (spin- S) at the same site, which is known as the Kondo coupling. From another perspective, this model can be seen as the model, in which the direct the spin-exchange interaction is taken into the *Kondo lattice model*. We approach to the Kondo-Heisenberg model from this perspective.

Firstly, we briefly review the Kondo lattice model (see, e.g., Refs. [11, 12], for detail reviews) underlying the Kondo-Heisenberg model. Heavy fermion systems are typical examples of the strongly correlated electron systems [13, 14], where the interaction among electrons plays crucial roles. In heavy fermion systems, the interaction among electrons results in quasi-particles with large effective mass, and realizes a variety of ground states depending on materials. The Kondo lattice model is one of the standard minimal theoretical models of heavy fermion system, in which tight-binding electrons interact with localized spins through the exchange interaction. Historically, the Kondo lattice model is derived from the Kondo model, where a single magnetic impurity exists in conduction electron system. In the ground state of the Kondo model, the conduction electron strongly couples to the impurity thereby screening its magnetic moment by forming the spin-singlet state (the Kondo singlet) [15]. On the other hand, when there are many magnetic impurities, the competition between the long-range spin-spin interaction mediated by the conduction electrons (the RKKY interaction [16, 17, 18]) and the Kondo screening is expected. The resulting global phase structure is summarized in the celebrated Doniach phase diagram [19]. The minimal lattice model that allows us to study the competition between the Kondo screening and the formation of magnetic order is the Kondo lattice model whose Hamiltonian is given by [19]:

$$\begin{aligned} \hat{H}_{\text{KL}} &= -t \sum_{i,\alpha} \left(c_{i,\alpha}^\dagger c_{i+1,\alpha} + \text{H.C.} \right) + J_{\text{K}} \sum_i \mathbf{s}_i \cdot \mathbf{S}_i \\ &= \hat{H}_{\text{e}} + \hat{H}_{\text{K}} . \end{aligned} \tag{1.2}$$

The Hamiltonian of this Kondo lattice model (1.2) clearly commutes with the z component of the total spin, $\sum_i (s_i^z + S_i^z)$ ($=: T^z$), and the total number of electrons, $\sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i,\alpha}$ ($=: \hat{N}_{\text{tot}}$). Regarding the number of conduction electrons, the occupancy rate $n = \langle \hat{N}_{\text{tot}} \rangle / L$, which is the eigenvalue of $\hat{N}_{\text{tot}}$ divided by the system size L , is often used as a label for the system. Furthermore, noting that the Kondo lattice model with N conduction electrons can be mapped to a Kondo lattice model with $2L - N$

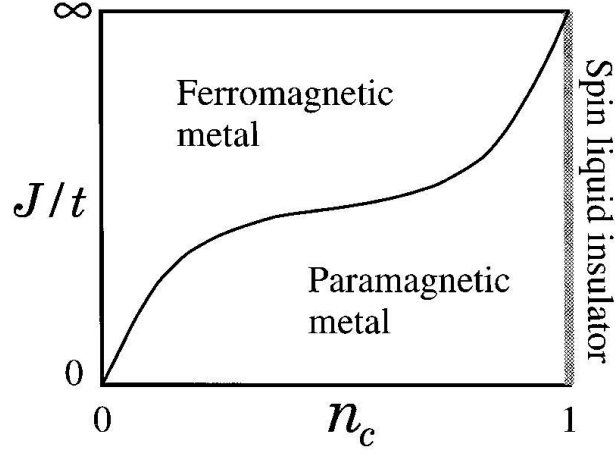


Figure 1.2: The rough sketch of the phase diagram of the Kondo lattice model (Ref. [11]). The J on the vertical axis in the diagram corresponds to J_K in this thesis, and the n_c horizontal axis represents the conduction electron density n .

conduction electrons via particle-hole transformation, it is sufficient to consider only the case $0 \leq n \leq 1$. Additionally, regarding spin, if we define $\mathbf{T} := \sum_i (\mathbf{S}_i + \mathbf{s}_i)$, $\hat{H}_{KL}$ also commutes with $(\mathbf{T})^2$ (and since T^z also commutes with $(\mathbf{T})^2$), the eigenstates of $\hat{H}_{KL}$ can be labeled by the eigenvalues of the two operators $(\mathbf{T})^2$ and T^z . Therefore, similar to the Heisenberg model, there is $SU(2)$ symmetry regarding spin, and all eigenstates of T^z belonging to the same eigenvalue of $\mathbf{T}^2$ have the same energy eigenvalue. Thus, when investigating the ground state of $\hat{H}_{KL}$, it is sufficient to examine the subspace of the Hilbert space where $T_{tot}^z = 0$. In general, utilizing such symmetries of the Hamiltonian is important not only in theory but also in numerical calculations such as exact diagonalization and DMRG, as it can reduce the size of the matrices being handled [20, 21]. Since the localized spins $\mathbf{S}_i$ in the Kondo lattice model (1.2) originate from the spin degree of freedom of d or f -electrons, the case $S = 1/2$ has been mainly studied [11]. The properties of the ground state of the conduction electron Kondo lattice model vary depending on the occupancy rate n of the conduction electrons and the coupling constant ratio (J_K/t) . The Fig. 1.2 shows a schematic phase diagram of the Kondo lattice model with local one-half spins that was considered in the 1990s.

Based on Fig. 1.2, the properties of the ground state of the one-dimensional Kondo lattice model can be briefly described. At half-filling, where the number of conduction electrons equals the number of sites, it has been shown through numerical diagonalization of small systems [22, 23], numerical calculations using the density matrix renormal-

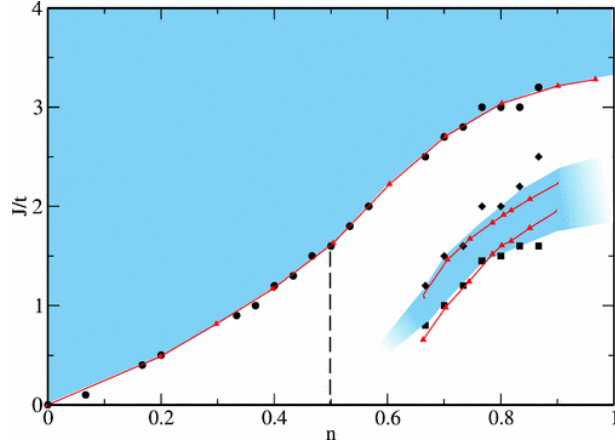


Figure 1.3: The phase diagram of the Kondo lattice model as of 2012. [32]

ization group (DMRG) [24], and analytical methods using bosonization [25] that the system is in a spin-liquid phase with both spin and charge gaps. On the other hand, in the case $0 < n < 1$ of the KL model (1.2), the ground state is the ferromagnetic metal when J_K is sufficiently large [26, 27]. Specifically, in the low electron density limit, it has been analytically proven that the system becomes ferromagnetic for any finite J_K/t [26], and numerical calculations using the quantum Monte Carlo method [28] have suggested that the system becomes ferromagnetic in the strong coupling region of large J_K/t even at finite electron densities. We can derive this ferromagnetism by considering the second order perturbation of the hopping term $\hat{H}_e$ to Kondo coupling term $\hat{H}_K$ in the strong-coupling region. Furthermore, numerical calculations using the DMRG for the Kondo lattice model with certain occupancy rates and parameter ratios J_K/t have shown that the ground state becomes a paramagnetic metallic phase for small J_K/t in systems with tens of sites [29]. The paramagnetic metal phase is described as a Tomonaga-Luttinger liquid [30] with both the charge gap and spin gap closed. One of the non-Fermi liquid characteristics of a Tomonaga-Luttinger liquid is that the momentum distribution function is continuous at the Fermi surface (in one-dimensional systems, it consists of two discrete Fermi points), but its derivative $dn(k)/dk$ is discontinuous [31]. Subsequently, studies using methods such as the DMRG for a wider range of parameter sets ($n, J_K/t$) resulted in the phase diagram shown in Figure 1.3 [32]. Compared to Figure 1.2, it has been newly revealed that there is another ferromagnetic phase within the region previously considered to be a paramagnetic metal phase. Even after this phase diagram was obtained, detailed studies [33, 34] of the paramagnetic phase have continued. For example, it has also been found that at quarter-filling, where the occupancy rate of

conduction electrons is half the number of sites in the system, there exists a region of parameters J_K/t where both the spin gap and charge gap open [33], and there is also a region of J_K/t where the localized spins form a dimerized state [35, 36]. On the other hand, it has been also experimentally proposed that the model (1.2) itself can be quantum-simulated in a well-controlled manner using alkaline-earth-like fermionic cold atoms (e.g., ^{171}Yb) loaded on optical lattices [37, 38]. However, the phase diagram of the ground state of the Kondo lattice model has not yet been completely clarified.

Recently, the possibility that the $S = 1$ Kondo lattice model with a uniaxial anisotropy under a transverse magnetic field can describe the coexistence of ferromagnetism and superconductivity in materials like URhGe has been pointed out [39, 40]. This motivates us to study the Kondo lattice model with spin S larger than $1/2$ and broaden the range of materials to which the Kondo lattice model can apply¹. Another interesting aspect of considering the higher-spin (S) generalization is that, in one dimension, the magnetically-ordered region of the Doniach phase diagram may exhibit intrinsically different properties depending on, e.g., the parity of $2S$.

On top of considering higher-spin cases, we shall incorporate below the *direct* interaction between the adjacent localized spins. Here, by “direct” we mean that the spin-spin interaction is not mediated by the conduction electrons. In order to incorporate these two generalizations to the Kondo lattice model, we consider the aforementioned spin- S Kondo-Heisenberg (KH) Hamiltonian. In the context of the Kondo lattice model, the Heisenberg term $\hat{H}_h$ in Eq. (1.1) corresponds to the superexchange interaction among f electrons which would arise when small hopping of the f -electrons is taken into account.

For the case of $S = 1/2$, we shortly present the effect of the Heisenberg term $\hat{H}_h$ on the Kondo lattice model. As already noted, in the case $0 < n < 1$ of the KL model (1.2), the electron motion favors ferromagnetism when J_K is sufficiently large. One of the important effects of the J_H term is to suppress this ferromagnetic ground state and stabilize the paramagnetic one [41]. Another interesting effect is that moderate J_H term can open the spin gap even away from half-filling $0 < n < 1$ [42]. The KH model (1.1) with the localized spin- $1/2$ has been studied in the context of, e.g., the uranium-based heavy-fermion superconductors [43], the pair density wave in superconducting state of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ [42], and the topological Kondo insulators [44, 45, 46]. The model $\hat{H}_{\text{KH}}$ with $S = 1/2$ is also used as a simplest model that may describe the interplay between

¹If $S = 1$ or higher, the ground state multiplet of the corresponding f-ion must be four-degenerate by spin-orbit coupling. This degeneracy will be lifted under the crystalline field, so the realization of the magnitude $S = 1$ has the delicate problem.

two different orders in a certain class of organic compounds [e.g., $(\text{Per})_2\text{Pt}(\text{mnt})_2$] in which the systems consist of partially-filled metallic part and half-filled insulating one [47, 48, 49].

As the first step toward the understanding of the physics of the generalized KH model (1.1), we study in this Part I its phase structure in the region of strong Kondo coupling where we can determine the ground-state properties accurately (sometimes rigorously).

The organization of the rest of the part I of this thesis is as follows. In Chap. 2, we derive the low-energy effective Hamiltonian in the strong-coupling region (i.e., $J_K \gg t, J_H$) both at half-filling and away from half-filling, which gives an important insight into the structure of the phase diagram. In particular, we will show that, in the strong-coupling region, the ferromagnetic phase is generically stabilized (except at half-filling) through a mechanism similar to the double-exchange interaction and that this tendency competes with antiferromagnetism stabilized by the direct antiferromagnetic interaction J_H .

In Chap. 3, in order to investigate this competition between the ferromagnetism and the J_H -induced antiferromagnetism, we carry out numerical density-matrix-renormalization-group (DMRG) simulations [50, 20, 21] combined with the sine-square-deformation (SSD) technique [51, 52, 53] for the special case of $S = 1$ to find that the competition indeed stabilizes a new dimerized (i.e., bond-centered) phase with power-law spin correlation and a finite charge gap. We summarize the main results in Chap. 4, and some technical details including the proof of ferromagnetism are presented in the appendices.

Chapter 2

Strong-coupling effective Hamiltonian

In this chapter, we carry out the perturbation theory from the strong-coupling limit ($J_K \rightarrow \infty$) to derive the low-energy effective Hamiltonian that enables us to map out the strong-coupling phases. As already noted in the last chapter, since $\hat{H}_{\text{KH}}$ can commute with the total electron number $N_e = \sum_{i,\alpha} c_{i,\alpha}^\dagger c_{i,\alpha} = \sum_i n_i$, the electron density $n = N_e/L$ (with L being the system size) of the conduction electrons is a conserved quantum number to be fixed. Moreover, since the particle-hole transformation $c_{i,\alpha} \leftrightarrow c_{i,\alpha}^\dagger$ maps the KH model at filling n onto the same model at filling $2 - n$ as in the KL model [11], we can safely restrict ourselves to $n \leq 1$ without the loss of generality. Another important conserved quantum number is: $T_{\text{tot}}^z = \sum_i T_i^z = \sum_i (s_i^z + S_i^z)$. Throughout this part, we reserve the notation $\mathbf{T}_i$ to denote the composite spin on each site:

$$\mathbf{T}_i := \mathbf{s}_i + \mathbf{S}_i . \quad (2.1)$$

To be specific, unless otherwise stated, we set $S = 1$ in what follows, although the generalization to arbitrary S is straightforward. Some of the generalizations are discussed in appendices.

2.1 Half-filling ($n = 1$)

2.1.1 Strong-coupling limit

At half-filling $n = 1$, the number of conduction electrons N_e equals to the number of the sites L . In the strong-coupling limit $J_K \rightarrow \infty$, where we can ignore the other

two terms $\hat{H}_e$ and $\hat{H}_H$, we can find the ground state of $\hat{H}_K$ by minimizing the Kondo coupling $J_K \mathbf{s}_i \cdot \mathbf{S}_i$ site by site; the ground state has no doubly-occupied or vacant sites, and at each site the spin-1/2 from a conduction electron and the localized spin-1 form a doublet:

$$\begin{aligned} |\uparrow\uparrow\rangle_i &:= \sqrt{\frac{2}{3}} \left| \begin{array}{c} \downarrow \\ 1 \end{array} \right\rangle_i - \sqrt{\frac{1}{3}} \left| \begin{array}{c} \uparrow \\ 0 \end{array} \right\rangle_i, \\ |\downarrow\downarrow\rangle_i &:= \sqrt{\frac{2}{3}} \left| \begin{array}{c} \uparrow \\ -1 \end{array} \right\rangle_i - \sqrt{\frac{1}{3}} \left| \begin{array}{c} \downarrow \\ 0 \end{array} \right\rangle_i. \end{aligned} \tag{2.2}$$

On the right-hand sides of (2.2), we have introduced the symbols $\left| \begin{array}{c} \alpha \\ S^z \end{array} \right\rangle_i$ to denote the tensor-product state $|\alpha\rangle_{i,\text{c-electron}} \otimes |S^z\rangle_{i,\text{local spin}}$ with $|\alpha\rangle$ being one of the four electronic states $|\text{emp}\rangle = |0\rangle$, $|\uparrow\rangle = c_{i,\uparrow}^\dagger|0\rangle$, $|\downarrow\rangle = c_{i,\downarrow}^\dagger|0\rangle$, and $|\uparrow\downarrow\rangle = c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger|0\rangle$, and $S^z = \pm 1, 0$. From now on, we call this effective spin-1/2 state as the *Kondo doublet*. In addition, as the Kondo doublets at the individual sites do not interact with each other in this limit, the ground state of the entire system is 2^L -fold degenerate; all the possible tensor-products of these local Kondo doublet states $\otimes_i |A\rangle_i$ ($A = \uparrow\uparrow, \downarrow\downarrow$) span the basis of the huge ground-state eigenspace $\mathcal{H}_{\text{hf}}$ in the strong-coupling limit.

2.1.2 Perturbation theory from strong-coupling limit

Now, we consider the parameter region where the Kondo coupling is finite but still much larger than the other two terms, i.e. where the hopping term and the Heisenberg term can be viewed as the small perturbation.

(i) Second-order perturbation in the hopping t .

At half-filling, the first-order perturbation of the hopping term is prohibited because the application of the hopping to the unperturbed ground state always gives rise to the states with exactly one pair of a doubly-occupied and a vacant (“emp”) sites which is

out of the ground-state subspace:

$$\left\{ \begin{array}{l} c_{i+1,\uparrow}^\dagger c_{i,\uparrow} |\uparrow\uparrow\rangle_i \otimes |\uparrow\uparrow\rangle_{i+1} = -\frac{\sqrt{2}}{3} \left| \begin{array}{c} \text{emp} \\ 0 \end{array} \right\rangle_i \otimes \left| \begin{array}{c} \uparrow\downarrow \\ 1 \end{array} \right\rangle_{i+1}, \\ c_{i+1,\uparrow}^\dagger c_{i,\uparrow} |\uparrow\uparrow\rangle_i \otimes |\downarrow\downarrow\rangle_{i+1} = \frac{1}{3} \left| \begin{array}{c} \text{emp} \\ 0 \end{array} \right\rangle_i \otimes \left| \begin{array}{c} \uparrow\downarrow \\ 0 \end{array} \right\rangle_{i+1}, \\ c_{i+1,\uparrow}^\dagger c_{i,\uparrow} |\downarrow\downarrow\rangle_i \otimes |\uparrow\uparrow\rangle_{i+1} = \frac{2}{3} \left| \begin{array}{c} \text{emp} \\ -1 \end{array} \right\rangle_i \otimes \left| \begin{array}{c} \uparrow\downarrow \\ 1 \end{array} \right\rangle_{i+1}, \\ c_{i+1,\uparrow}^\dagger c_{i,\uparrow} |\downarrow\downarrow\rangle_i \otimes |\downarrow\downarrow\rangle_{i+1} = -\frac{\sqrt{2}}{3} \left| \begin{array}{c} \text{emp} \\ -1 \end{array} \right\rangle_i \otimes \left| \begin{array}{c} \uparrow\downarrow \\ 0 \end{array} \right\rangle_{i+1}. \end{array} \right. \quad (2.3)$$

Here, the sign of the right-hand side comes from the definition of the doubly-occupied state $|\uparrow\downarrow\rangle_i = c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger |\text{emp}\rangle_i$. Therefore, we need to go to the second-order perturbation in the hopping t to find the effective interaction among the Kondo doublets.

As is illustrated in Fig. 2.1, the second-order process consists of (i) hopping from i to $i+1$ (from $i+1$ to i) that excites $\hat{H}_K$ to the intermediate state with exactly one pair of a doubly-occupied and a vacant sites, and (ii) hopping from $i+1$ to i (from i to $i+1$). Therefore, the second-order processes induce the following transitions among the four states ($|\uparrow\uparrow\rangle |\uparrow\downarrow\rangle |\downarrow\uparrow\rangle |\downarrow\downarrow\rangle$) of the neighboring Kondo doublets ($i, i+1$):

$$\begin{aligned} & P_{\text{G.S.}} \left(\sum_{\alpha=\uparrow,\downarrow} c_{i,\alpha}^\dagger c_{i+1,\alpha} + \text{H.C.} \right) \frac{1}{E_{\text{G.S.}} - \hat{H}_K} \left(\sum_{\alpha} c_{i+1,\alpha}^\dagger c_{i,\alpha} + \text{H.C.} \right) P_{\text{G.S.}} \\ &= -\frac{t^2}{9J_K} \begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 5 & -1 & 0 \\ 0 & -1 & 5 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix}, \end{aligned} \quad (2.4)$$

where $E_{\text{G.S.}} = -J_K L$ is the ground-state energy of $\hat{H}_K$ and $P_{\text{G.S.}}$ is the projector onto the ground-state subspace. In deriving the above, we have used the fact that we can substitute the denominator $E_{\text{G.S.}} - \hat{H}_K$ on the left-hand side with the constant $-2J_K$ because any allowed intermediate states have exactly one pair of a doubly-occupied and a vacant sites each of which contributes the energy cost J_K . Similar effective interactions arise from any neighboring doublet pairs ($i, i+1$), and we finally obtain the following effective antiferromagnetic spin exchange among the Kondo doublets:

$$\sum_i \left(\frac{2t^2}{9J_K} \mathbf{D}_i \cdot \mathbf{D}_{i+1} - \frac{t^2}{2J_K} \right). \quad (2.5)$$

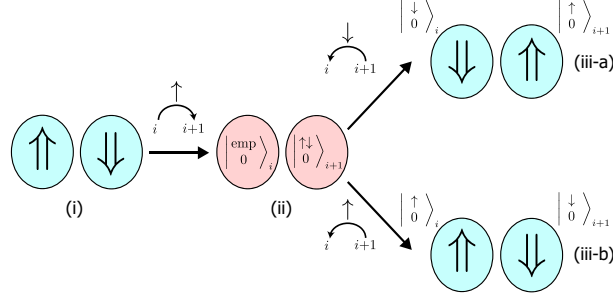


Figure 2.1: A process of second-order perturbation of hopping term. (i) One of neighboring sites in the non-perturbed ground state. Thick arrow in an oval describes a Kondo doublet in the strong-coupling limit. (ii) shows a possible first-order process. This picture describes the state after an electron with up-spin hops from the left site to the right one. This state is not included in vastly degenerated ground states. (iii) Second-order process. We can take two possible ways to back to the eigenspace which is spanned by non-perturbed ground states. (Reproduced from Ref. [54])

Here, $\mathbf{D}_i$ denotes the spin-1/2 operator for the Kondo doublet at site i .

(ii) First-order perturbation in the Heisenberg interaction J_H .

On top of the second-order kinetic exchange, there is the contribution from the Heisenberg term $\hat{H}_H$. As the Heisenberg interaction J_H does not change the electronic state, it can generate first-order processes within the half-filled ground-state subspace $\mathcal{H}_{\text{hf}}$. In the basis (2.2) spanning $\mathcal{H}_{\text{hf}}$, the matrix elements of the localized spin-1 operators $\mathbf{S}_i$ are:

$$\begin{aligned} \langle \uparrow \uparrow |_i S_i^z | \uparrow \uparrow \rangle_i &= 2/3 = 4/3 \langle \uparrow \uparrow |_i D_i^z | \uparrow \uparrow \rangle_i \\ \langle \uparrow \uparrow |_i S_i^z | \uparrow \downarrow \rangle_i &= \langle \uparrow \downarrow |_i S_i^z | \uparrow \uparrow \rangle_i = 0 \end{aligned} \quad (2.6)$$

$$\begin{aligned} \langle \uparrow \downarrow |_i S_i^z | \uparrow \downarrow \rangle_i &= -2/3 = 4/3 \langle \uparrow \downarrow |_i D_i^z | \uparrow \downarrow \rangle_i, \\ \langle \uparrow \uparrow |_i S_i^+ | \uparrow \uparrow \rangle_i &= \langle \uparrow \downarrow |_i S_i^+ | \uparrow \downarrow \rangle_i = 0 \\ \langle \uparrow \uparrow |_i S_i^+ | \uparrow \downarrow \rangle_i &= -4/3 \\ \langle \uparrow \downarrow |_i S_i^+ | \uparrow \uparrow \rangle_i &= 0, \end{aligned} \quad (2.7)$$

which means that the localized spin $\mathbf{S}_i$ projected onto $\mathcal{H}_{\text{hf}}$ is given by $\mathbf{S}_i \xrightarrow{\mathcal{H}_{\text{hf}}} (4/3)\mathbf{D}_i$ [see Eq. (A.8) for the expression for general S]. Therefore, the first-order degenerate perturbation of the Heisenberg term $\hat{H}_H$ gives the following effective antiferromagnetic

spin exchange among the neighboring Kondo doublets:

$$J_H \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \xrightarrow{\mathcal{H}_{\text{hf}}} \frac{16}{9} J_H \sum_i \mathbf{D}_i \cdot \mathbf{D}_{i+1} . \quad (2.8)$$

Combining Eqs. (2.5) and (2.8), we obtain the following spin-1/2 antiferromagnetic Heisenberg model for the Kondo doublets as the strong-coupling effective Hamiltonian at half-filling $n = 1$:

$$H_{\text{eff}}^{(n=1)} = \left(\frac{2t^2}{9J_K} + \frac{16}{9} J_H \right) \sum_{i=1}^L \mathbf{D}_i \cdot \mathbf{D}_{i+1} + E_0 . \quad (2.9)$$

[with the constant E_0 given by $-(t^2/2J_K + J_K)L$]. Therefore, the ground state of the half-filled KH model in the strong-coupling region exhibits the quasi-long-range antiferromagnetic order with gapless spinon excitations (a spin Luttinger liquid) [31]. Moreover, as adding an electron or changing the electron configuration in the ground state costs a finite energy ($\sim J_K$), the ground state is expected to be insulating. Hence, we conclude that the ground state of strongly-coupled spin-1 KH chain at half-filling is an insulator with power-law antiferromagnetic spin-spin correlation regardless of the value of $J_H (\ll J_K)$ [31]. This is in stark contrast to the spin-gapped insulating ground state (the Kondo insulator) found in the $S = 1/2$ KL model [22, 55].

In general, the spin sector of spin- S half-filled KH chain is described effectively by the antiferromagnetic spin- $(S - 1/2)$ Heisenberg model for the partially-screened moments (see Appendix A.1 for the details):

$$H_{\text{eff}}^{(n=1)} = \left\{ \frac{4t^2}{(2S+1)^2(S+1)J_K} + \left(\frac{2(S+1)}{2S+1} \right)^2 J_H \right\} \sum_i \mathfrak{S}_i \cdot \mathfrak{S}_{i+1} \quad (2.10)$$

where $\mathfrak{S}_i$ is the effective spin- $(S-1/2)$ operator which replaces the doublet $\mathbf{D}_i$ in the case of $S = 1$. The ground state of the above effective Hamiltonian depends on the value of S [2, 3]; when $2S$ is even, the insulating ground state has gapless spin excitations, while the ground state is fully gapped (i.e., both the charge and spin gaps are finite) when $2S$ is odd. This conclusion is consistent with that of a field-theory argument [56, 57]. In Sec. 3.1, we will numerically check this prediction for $S = 1$ by increasing J_H up to $\sim J_K$ while keeping $J_K \gg t$.

2.2 Other filling ($n < 1$)

Now let us consider the filling less than half-filling, i.e., $N_e < L$. In this case, the strong-coupling ground state is ${}_L C_{N_e} \times 2^{N_e} \times 3^{L-N_e}$ -fold degenerate. This degree of

degeneracy includes the value 2^L at half-filling as a special case $N_e = L$. Unlike at half-filling, there exist some sites without conduction electrons (since $n < 1$, doubly-occupied sites are not allowed in the strong-coupling ground state), and electrons can move even in the limit $J_K \rightarrow \infty$. As we will see, this difference dramatically changes the magnetism.

In deriving the effective Hamiltonian, we first note that the Kondo doublets carry the spin degrees of freedom in contrast to the case of spin-1/2 KL model [11], where the spin degrees of freedom are quenched at the sites occupied by the conduction electrons by forming the Kondo singlets. For these reasons, at $n < 1$, the electron motion contributes to the magnetism already at the first-order in t . The first-order effective Hamiltonian reads:

$$H_{\text{eff}}^{(n<1)} = -t \sum_i \left\{ \hat{d}_{i+1}^\dagger \hat{d}_i f_{i \rightarrow i+1}^{(S=1)}(\mathbf{D}_i \cdot \mathbf{S}_{i+1}) \hat{n}_{d,i} (1 - \hat{n}_{d,i+1}) + \hat{d}_i^\dagger \hat{d}_{i+1} f_{i+1 \rightarrow i}^{(S=1)}(\mathbf{S}_i \cdot \mathbf{D}_{i+1}) (1 - \hat{n}_{d,i}) \hat{n}_{d,i+1} \right\}, \quad (2.11)$$

where $\hat{n}_{d,i}$ ($= 0, 1$) denotes the number of the Kondo doublets at site i , which are created (annihilated) by the fermionic operator $\hat{d}_i^\dagger$ ($\hat{d}_i$), and the effective spin-dependent hopping amplitudes of the doublets are given by:

$$\begin{aligned} f_{i \rightarrow i+1}^{(S=1)}(\mathbf{D}_i \cdot \mathbf{S}_{i+1}) &= (2/3) \mathbf{D}_i \cdot \mathbf{S}_{i+1} + 1/3 \\ f_{i+1 \rightarrow i}^{(S=1)}(\mathbf{S}_i \cdot \mathbf{D}_{i+1}) &= (2/3) \mathbf{S}_i \cdot \mathbf{D}_{i+1} + 1/3 \end{aligned} \quad (2.12)$$

[see Eq. (A.16) for the expression for general S]. The derivation of the above equation (2.11) and the generalization to the arbitrary spin- S (≥ 1) are given in Appendix A.2.

The amplitude of the doublet hopping $\hat{d}_{i\pm 1}^\dagger \hat{d}_i$ in the Hamiltonian (2.11) takes its maximal value ($-2t/3$) when a doublet ($D = 1/2$) and the localized spin ($S = 1$) on the adjacent site are coupled ferromagnetically, which suggests a ferromagnetic ground state similar to that of the double-exchange model [58, 59, 60, 61]. In fact, as is discussed in Appendix A.3, exploiting the non-positivity and the indecomposability of the effective Hamiltonian (2.11), we can rigorously show that the ground state of the effective Hamiltonian (2.11) is unique (up to trivial degeneracy associated with the rotational symmetry) and ferromagnetic with the maximal total spin $S_{\text{tot}} = L - N_e/2$ for $1 \leq N_e \leq L - 1$. Hence, the ground state of the spin-1 KL model in the strong-coupling region is ferromagnetic for generic filling $0 < n < 1$ (and for $1 < n < 2$ by the particle-hole symmetry) [in fact, the statement can be generalized to arbitrary $S \geq 1$

in which the maximal total spin is $S_{\text{tot}} = LS - N_e/2$; see Appendix A.3]. This is consistent with the recent numerical observation for the spin-1 KL model [39, 40]. The ferromagnetic phase in the large- J_K region is reminiscent of the situation in the spin-1/2 KL model [26, 27, 62, 32], but the way how the hopping of conduction electrons causes ferromagnetism is different from each other; the mechanism of ferromagnetic ground state of spin-1 KL model (1.2) rather resembles the double-exchange interaction first-order in t , while, in the latter case, the ferromagnetism occurs through the second-order ($\propto t^2$) effective interactions [27]. The ferromagnetic-metal phase found in the strong-coupling region persists down to $J_K \rightarrow 0$ at least in the low-density ($n \rightarrow 0$) limit as in the $S = 1/2$ case [63]. In fact, it is straightforward to generalize the proof in Ref. [26] to $S \geq 1$ to show that the ground state of the *single-electron* spin- S KL model is ferromagnetic.

Now let us consider the effects of the Heisenberg term $\hat{H}_H$. By the same argument as that leading to (2.8), we see that the projection $\tilde{\mathbf{S}}_i$ of the localized spin $\mathbf{S}_i$ onto the ground-state subspace is given by:

$$\tilde{\mathbf{S}}_i = \begin{cases} \mathbf{S}_i & \text{when site-}i \text{ is unoccuied} \\ (4/3)\mathbf{D}_i & \text{when site-}i \text{ is occuied} . \end{cases} \quad (2.13)$$

Then, the first-order perturbation in J_H results in the following antiferromagnetic spin-spin exchange on the adjacent spins (either $S = 1$ or $S = 1/2$ depending on how the individual sites are occupied by the conduction electrons):

$$J_H \sum_i \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} . \quad (2.14)$$

Therefore, in the strong-coupling region of the KH model ($J_H > 0$), the ferromagnetic order found above for the KL model may be destabilized by the antiferromagnetic interaction generated by the Heisenberg term J_H . A rough estimate of the critical value of J_H may be obtained by comparing the spin-dependent hopping amplitude (2.12) and the projected Heisenberg interaction (2.14): $J_H^c/t \sim 1/2$. A more precise calculation for the two-site system shows that the ferromagnetic ground state ends at $J_H/t = 1/6$.

Note that the effects of the Heisenberg term $\hat{H}_H$ is very different for $n = 1$ (half-filling) and $n < 1$; in the former, $\hat{H}_H$ stabilizes the antiferromagnetic correlation in the insulating phase, while it competes with the hopping-assisted (double-exchange) ferromagnetism in the latter. We will closely investigate this competition in the next chapter.

Chapter 3

Numerical results for Kondo-Heisenberg model

In this chapter, we report the numerical results for a particular case of the spin-1 localized moments. To obtain the ground state of the $S = 1$ KH model (1.1), we carried out density-matrix renormalization group (DMRG) simulations using an open source library ITensor [64] for the DMRG algorithm. In addition, in some DMRG simulations, we adopted the sine-square-deformed Hamiltonian [51, 52] in order to reduce the effects of the open boundary condition, in which the DMRG algorithm works better [50, 20]. Specifically, we simulated the following Hamiltonian instead of the original one (1.1):

$$\begin{aligned} H_{\text{KH,SSD}} &= -t \sum_{i=1, \alpha}^{i=L-1} f_1(i) \left(c_{i, \alpha}^\dagger c_{i, \alpha} + \text{H.C.} \right) - \mu \sum_{i=1, \alpha}^{i=L} f_0(i) c_{i, \alpha}^\dagger c_{i, \alpha} \\ &\quad + J_K \sum_{i=1}^{i=L} f_0(i) \mathbf{s}_i \cdot \mathbf{S}_i + J_H \sum_{i=1}^{i=L-1} f_1(i) \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \end{aligned} \quad (3.1a)$$

where the deformation functions are given by:

$$f_l(i) = \sin^2 \left[\frac{\pi}{L} \left(i + \frac{l-1}{2} \right) \right] \quad (l = 0, 1) \quad (3.1b)$$

and $l = 0$ ($l = 1$) is used for the on-site (on-bond) operators. With the Sine-Square Deformation (SSD) [65], the vicinity of the center of a finite system well approximates the bulk of the infinite system. In our simulations, we considered finite systems of the sizes $L \leq 100$ under open boundary condition, and set the block sizes $m \leq 720$. In all

the cases, we found that the truncation errors were less than $\sim 10^{-7}$. Throughout this chapter, we set $t = 1$ as the unit of energy.

3.1 half-filling

In Sec. 2.1, we have studied the ground state in the strong-coupling limit ($J_K \gg t, J_H$), where the perturbation theory in t and J_H predicts that the ground state is insulating; the low-energy physics is described, when $S = 1$, by the spin-1/2 Heisenberg model (2.9), which indicates the power-law antiferromagnetic spin-spin correlation. To check this for increasing J_H ($0 \leq J_H \lesssim J_K$), we numerically investigate in this section the ground-state spin-spin correlation at half-filling. Specifically, we fixed $J_K/t = 10$, and increased J_H/t from the Kondo-lattice limit ($J_H = 0$) up to $J_H \sim J_K$ to calculate the spin correlation between distant sites for each J_H/t . In doing so, we used the uniform (i.e., undeformed) Hamiltonian (1.1). The results for the correlation functions of (a) the composite spins $\langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle$ [$\mathbf{T}_i$ is defined in (2.1)] and (b) the localized spins $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$, as well as those for the spin-1 and 1/2 Heisenberg models, are plotted in Fig. 3.1.

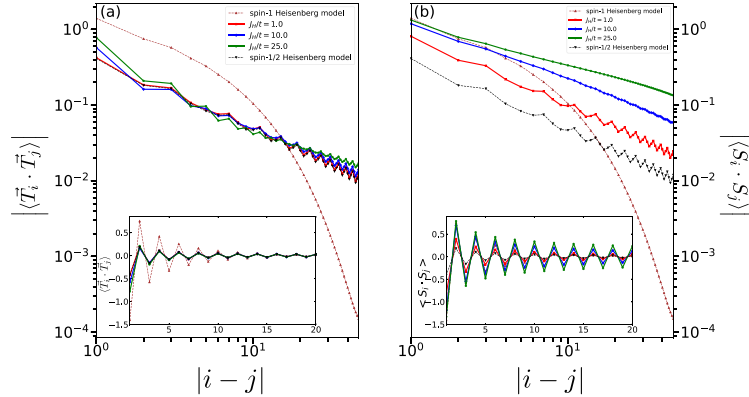


Figure 3.1: Correlation functions (log-log plots) of (a) the total spin $\langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle := \langle (\mathbf{s}_i + \mathbf{S}_i) \cdot (\mathbf{s}_j + \mathbf{S}_j) \rangle$ and (b) the $S = 1$ localized spins $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ in the ground state of the *uniform* (i.e., without SSD) spin-1 KH model (1.1) at half-filling. Both are calculated at the fixed $J_K/t = 10.0$ for varying J_H/t . For comparison, the spin-spin correlation functions of the $S = 1/2, 1$ Heisenberg models are also plotted (dashed curves). The zoom-up of the short-range part is shown in the insets which clearly indicates the antiferromagnetic nature of the correlation. (Reproduced from Ref. [54])

From the numerical results, we can first read off that the composite-spin correlation function $\langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle$ essentially coincides with the ordinary spin-spin correlation of the spin-1/2 Heisenberg chain (shown by the dashed line), up to fairly large J_H/t [see Fig. 3.1(a)]. As the system is insulating and in the strong-coupling region, this quasi-long-range antiferromagnetic correlation is not attributed to the RKKY interaction which requires metallicity and is valid in the weak-coupling regime. Rather, this implies that the strong-coupling picture discussed in Sec. 2.1 remains valid even for large $J_H (\sim J_K)$, suggesting that the Kondo doublets, which are well-defined when $J_K \gg t, J_H$, are rather robust against the interaction (J_H) among the localized spins.

We can also confirm this persistence of the Kondo doublets by the results shown in Fig. 3.1(b). According to the strong-coupling argument in Sec. 2.1, the correlation function of the localized $S = 1$ spins in the KH model (1.1) should behave like that of the spin-1/2 Heisenberg chain (2.9):

$$\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\text{KH}} \xrightarrow{\mathcal{H}_{\text{hf}}} (4/3)^2 \langle \mathbf{D}_i \cdot \mathbf{D}_j \rangle_{\text{Heisenberg}} . \quad (3.2)$$

In fact, the plots in Fig. 3.1(b) clearly show that the localized-spin correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\text{KH}}$ and the spin-spin correlation function of the spin-1/2 Heisenberg chain (dashed line) behave similarly¹ even when J_H is fairly large; the correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle_{\text{KH}}$ exhibits behavior essentially different from the short-range (i.e., exponentially-decaying) correlation in the spin-1 Heisenberg chain which describes the physics of the localized spins when $J_K = 0$. All these suggest that the exchange interaction J_H does not really interfere with the antiferromagnetism stabilized by the motion of the conduction electrons, and that the Kondo-doublet physics dominates a wide range of the parameter space (i.e., $0 \leq J_H \lesssim J_K$) at half-filling.

3.2 Away from half-filling

In the last section, we have seen that the inclusion of antiferromagnetic J_H does not essentially affect the insulating ground state with gapless antiferromagnetic spinon excitations at half-filling found in the strong-coupling limit. Away from half-filling (i.e., $0 < n < 1$), on the other hand, the situation is very different. In fact, the strong-coupling argument tells us that the electron hopping tends to stabilize the ferromagnetic ground state which may be eventually destabilized by the antiferromagnetic interaction

¹Almost parallel shifts of the four curves in Fig. 3.1(b) suggest that $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ and $\langle \mathbf{D}_i \cdot \mathbf{D}_j \rangle$ differ only by numerical factors.

(2.14). In this section, we consider various ground-state phases resulting from the competition between the kinetic-energy-driven ferromagnetism and the J_H -induced antiferromagnetism. Specifically, we fix J_K large, i.e., $J_K/t = 5.0$ and numerically investigate the stability of the ferromagnetic order found in the KL-model limit $J_H = 0$ against the antiferromagnetic interaction J_H . As long as we know from the preliminary calculations, the quarter-filling case $n = 1/2$ seems most interesting, and we mainly focus on the case with $n = 1/2$ in this section unless otherwise stated.

3.2.1 Magnetic properties

To investigate how the magnetic properties change as the direct antiferromagnetic interaction J_H is increased, we calculated the correlation function of the total spin $\mathbf{T}_i (= \mathbf{s}_i + \mathbf{S}_i)$ at each site as the probe. First, we show in Fig. 3.2(a) and (b) the nearest-neighbor spin-spin correlation functions $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ [(a)] and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ [(b)] between neighboring sites for various J_H/t at a fixed Kondo coupling $J_K/t = 5.0$.

It can be seen from Fig. 3.2(a) that for sufficiently weak J_H , i.e., $0 \leq J_H/t \lesssim 0.053$, the value of the neighboring spin correlation $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ is site(i)-independent and takes a positive constant value (i.e. ferromagnetic) regardless of the value of J_H , while for $J_H/t \gtrsim 0.054$, it is alternating between two values. A similar behavior was observed for the localized spins as well [see Fig. 3.2(b)]. The period-two behavior in the bond-centered operators $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ suggests that the localized spins are dimerized for $J_H/t \gtrsim 0.054$.

If we further increase J_H , the clear period-2 behavior disappears at around $J_H/t \sim 0.45$ and both $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ become negatively constant, which means that, when $J_H/t \gtrsim 0.45$, the dimerized phase is taken over by a new phase in which short-range antiferromagnetic correlation develops [see Figs. 3.8(a)-(d)]. This is consistent with that the system asymptotically approach the spin-1 Heisenberg model, which exhibits short-range antiferromagnetic correlation, if we increase J_H to a large value with J_K/t fixed. In contrast to the naive expectation based on the energetic argument in Sec. 2.2, the ferromagnetic phase yields first to the dimerized one at much smaller value of J_H before the antiferromagnetic tendency due to J_H finally wins.

Despite the usual lore that the spin dimerization is accompanied by a finite spin gap, the intermediate “dimerized” phase found above in fact has quasi-long-range antiferromagnetic correlation, i.e., the correlation function $\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle$ exhibits power-law

decay [see Fig. 3.3 (a)], indicating a vanishing spin gap². To check whether the spin gap vanishes, we calculated the magnetization $\langle M \rangle = \sum_i T_i^z / L$ with increasing external magnetic field h (in the z -direction). To this end, we used the SSD Hamiltonian (3.1a) with the (deformed) Zeeman term $-h \sum_i f_0(i)(S_i^z + s_i^z)$ added. The results are shown in Fig. 3.3(b). The linear increase of the magnetization $\langle M \rangle \propto h$ ($h \ll 1$) strongly suggests that the spin gap indeed vanishes in the dimerized phase.

All these properties of the dimerized phase may be best understood in the strong-coupling limit in which the system is described only in terms of spin-1/2 (the Kondo doublets $\mathbf{D}_i$) and the unscreened localized spin-1 ($\mathbf{S}_i$) [see Eq. (2.11)]. Let us consider the situation where J_H is much larger than t and we can neglect the order- t perturbation (2.11). Depending on the configurations, $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ is given by

$$\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle = \begin{cases} \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1, 1) \\ \langle \mathbf{S}_i \cdot \mathbf{D}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1, 1/2) \\ \langle \mathbf{D}_i \cdot \mathbf{S}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1/2, 1) \\ \langle \mathbf{D}_i \cdot \mathbf{D}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1/2, 1/2) . \end{cases} \quad (3.3)$$

Similarly, for the (projected) localized spins [see Eq. (2.13)], we have:

$$\begin{aligned} & \langle \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} \rangle \\ &= \begin{cases} \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1, 1) \\ (4/3) \langle \mathbf{S}_i \cdot \mathbf{D}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1, 1/2) \\ (4/3) \langle \mathbf{D}_i \cdot \mathbf{S}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1/2, 1) \\ (16/9) \langle \mathbf{D}_i \cdot \mathbf{D}_{i+1} \rangle & \text{when } (T_i, T_{i+1}) = (1/2, 1/2) . \end{cases} \end{aligned} \quad (3.4)$$

The value $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle = 1/2$ means that neighboring $S = 1/2$ and $S = 1$ form spin-3/2 pairs for, e.g., $J_H = 0.054$ [see Fig. 3.5(b)]. The expected value $\langle \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} \rangle = 2/3$ is consistent with the numerical results in Fig. 3.2(b). On the other hand, the value $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle = -1$ allows the two possibilities $(T_i, T_{i+1}) = (1, 1)$ and $(1/2, 1)$ [or $(1, 1/2)$]. However, looking at the value $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \approx -4/3$ [see Fig. 3.2(b)], we may conclude that the second realizes for, e.g., $J_H/t \gtrsim 0.1$ and that the spin pairs $(1/2, 1)$ form doublets [Fig. 3.5(c)].

²Although in critical isotropic spin systems, the spin-spin correlation function is generically expected to behave like $(\ln|i-j|)^{1/2}/|i-j|$ [31] except at the fine-tuned points, we did not find such logarithmic corrections in our simulations. We do not know whether this absence of the logarithmic correction is explained by some effective long-range spin-spin interactions generated by the electron motion or not.

From these observations, the following picture emerges. First we note that this dimerized state is in fact insulating as will be shown in the next subsection, which allows us to treat the spin-1/2 and 1 (there are equal numbers of them at quarter-filling) as immobile. The numerical results indicate that these spin-1/2 and 1 alternate in the insulating dimerized phase. For small values of J_H/t ($\gtrsim 0.054$), local ferromagnetic correlation still remains and magnetism is described by the *preformed* quartets on the A-B bonds [see the red ovals in Fig. 3.5(b)]. The weak fluctuations among these quartets may be captured by the spin-3/2 Heisenberg chain which eventually leads to a gapless collective singlet ground state. For larger values of J_H/t ($\gtrsim 0.1$), on top of the ferromagnetic correlation on the A-B bonds, short-range antiferromagnetic correlation develops on the B-A bonds, and doublets are formed on these bonds [see the blue ovals Fig. 3.5(c)]. Note that, in contrast to the usual spin-singlet dimerization, these two different kinds of correlation do *not* interfere with each other, and the state shown in Fig. 3.5(b) smoothly crosses over to Fig. 3.5(c). Again, the fluctuations among these doublets may be taken into account by the spin-1/2 Heisenberg chain, which exhibits power-law antiferromagnetic correlation. A remark is in order here about the nature of “antiferromagnetic” correlation. As the effective “spin”-1/2s are formed on dimers, the π -oscillating correlation in the effective model translates to the period-4 oscillation in the original model. In fact, we numerically observed such power-law decaying period-4 behavior in the spin-spin correlation $\langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle$ at $J_H/t = 0.1$.

A similar “gapless dimerized phase” has also been found recently in the quarter-filled Kondo lattice model ($S = 1/2$, $J_H = 0$) at *small* Kondo coupling $J_K/t = 0.6$ [36]. However, we would like to stress here that the above dimerized phase found in the strong-coupling region does not exist in the $S = 1/2$ KH model at quarter-filling. In fact, as is seen in Fig. 3.4(a) and (b), a similar intermediate spin-dimerized state is absent in the $S = 1/2$ case, and instead there seems to be a jump at $J_H/t \sim 0.1$ in both $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ from a positive value to a negative one. This sudden suppression of ferromagnetism by J_H in the $S = 1/2$ case is consistent with the analytic argument in Ref. [41]. Therefore, the existence of this intermediate gapless dimerized phase is one of the unique properties of the $S = 1$ KH model at quarter-filling. In Fig. 3.5, we illustrate how the ferromagnetic order is lost via the dimerized phase as we increase the interaction J_H among the localized spins.

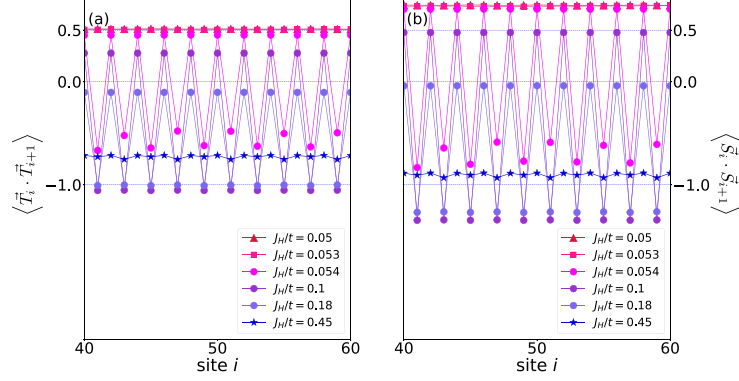


Figure 3.2: The nearest-neighbor spin-spin correlation (a) $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and (b) $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ in the ground state of strongly coupled spin-1 KH model at quarter-filling. $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ are calculated for fixed $J_K/t = 5.0$ and $L = 100$. (Reproduced from Ref. [54])

3.2.2 Electrical properties

In the previous subsection, we have investigated the spin correlation $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ and concluded that the competition between the hopping-induced ferromagnetism and the direct antiferromagnetic interaction J_H leads to two quantum phase transitions; one at $J_H/t \approx 0.054$ from the ferromagnetic phase to the new *gapless* dimerized phase, and another at $J_H/t \approx 0.45$ from the dimerized phase to a non-dimerized one with short-range antiferromagnetic correlation. In this subsection, we investigate the phase structure and the quantum phase transition(s) from the viewpoint of the electrical transport.

To this end, we calculated the charge gap Δ_c for various J_H/t with the Kondo coupling J_K/t fixed. In doing so, we first fixed the chemical potential μ and calculated the bulk electron density $\langle n(\mu) \rangle$ by averaging the *local* density $\langle n_i \rangle$ around the center of the system. In Fig. 3.6, we plot the electron density $\langle n(\mu) \rangle$ obtained at $(J_K/t, J_H/t) = (5.0, 0.1)$ for several system sizes L . There is a clear jump in μ *only* at $\langle n \rangle = 0.5$, which suggests that a finite charge gap opens at quarter-filling and that the system is metallic for other densities around $n = 1/2$. This seems consistent with the field-theoretical prediction in Ref. [57] which concludes that a metallic phase with collinear spin fluctuations (*collinear metal*) occupies the region around $n = 1/2$ (when $J_H = 0$).

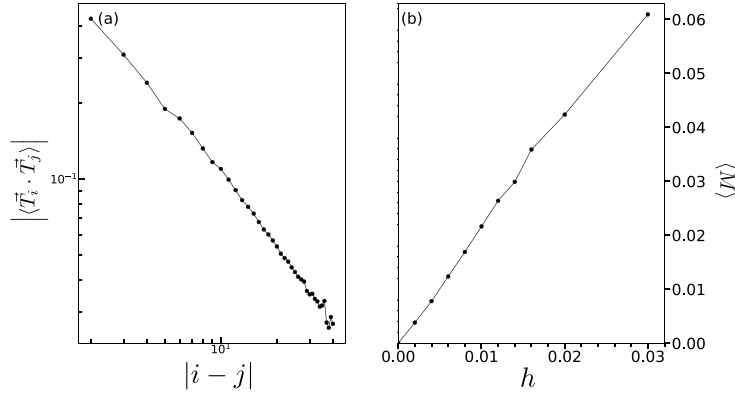


Figure 3.3: (a) Spin-spin correlation $\langle \mathbf{T}_i \cdot \mathbf{T}_j | \mathbf{T}_i \cdot \mathbf{T}_j \rangle$ and (b) the ground-state magnetization process of the quarter-filled spin-1 KH model in the dimerized phase: $(J_K/t, J_H/t) = (5.0, 0.1)$. The correlation function seems to decay as $|\langle \mathbf{T}_i \cdot \mathbf{T}_j | \mathbf{T}_i \cdot \mathbf{T}_j \rangle| \sim |i - j|^{-1}$. In obtaining (b), the SSD Hamiltonian (3.1a) was used. (Reproduced from Ref. [54])

Also the size-dependence seems to be relatively small. The charge gap Δ_c is obtained by appropriately extrapolating the width of the jump to $L \rightarrow \infty$ [52].

The value of the charge gap Δ_c at $n = 1/2$ (quarter-filling) obtained in this way is shown as a function of J_H/t ($J_K/t = 5.0$ is fixed) in Fig. 3.7. It clearly shows that for $0 \leq J_H \lesssim 0.053$ the ground state is metallic with a vanishing charge gap, while for $J_H \gtrsim 0.054$ the ground state is an insulator. Moreover, Fig. 3.7 shows that, after attaining a maximum at around $J_H \sim 0.07$, the charge gap Δ_c decreases monotonically until it vanishes at around $J_H/t = 0.45$. Combining all these with the results of the last subsection, we conclude that the region where the system has a finite charge gap matches that of the dimerized phase. To put it another way, the two magnetic quantum phase transitions into and out of the dimerized phase (at $J_H/t \approx 0.054$ and $J_H/t \approx 0.45$), and the metal-insulator transitions found here occur simultaneously. The final phase diagram at quarter-filling along J_H/t axis is shown in Fig. 3.8. Note that the third phase (“AFM”) is determined only by the order parameter $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and the charge gap Δ_c , and the precise characterization, e.g., in the light of the heavy Luttinger liquid [66] is yet to be done.

The mechanism of this dimerization-induced metal-insulator transitions at quarter-filling is an intriguing question. One may naively expect that magnetic dimerization

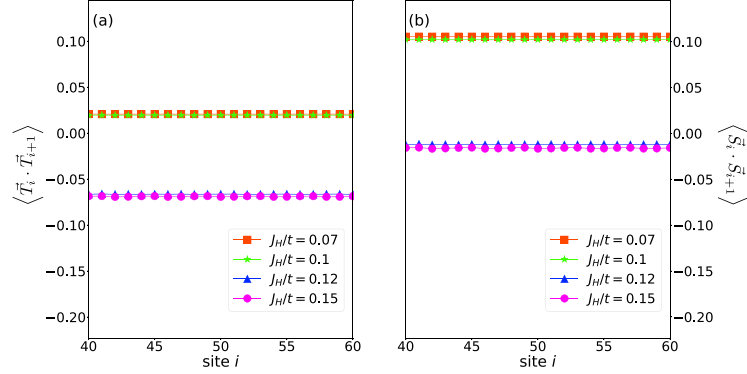


Figure 3.4: The same correlation functions as in Fig. 3.2 for $S = 1/2$. Again $J_K/t = 5.0$ was used. Note that no alternating (period-2) behavior is observed for $S = 1/2$. (Reproduced from Ref. [54])

somehow induces the modulation of the hopping amplitude thereby halving the Brillouin zone and leading to a Mott-insulating state in the *half-filled* bonding band [67]. To clarify this point, we measured the hopping amplitude $\langle \sum_{\alpha} c_{i\alpha}^{\dagger} c_{i+1,\alpha} + \text{h.c.} \rangle$ in the dimerized phase to find no sign of alternation. Therefore, this appealing scenario does not seem to work in our situation.

However, once we assume the spin-dimerization in the local moments, a combination of bosonization and a mean-field-like argument seems to reasonably explain the opening of the charge gap at quarter-filling. When the spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ exhibits alternation, second-order perturbation in J_K induces the following effective interaction among the conduction electrons [68]:

$$(-1)^i g_d (\mathbf{s}_i \cdot \mathbf{s}_{i+1}) \quad (3.5)$$

where the coupling constant g_d is proportional to the amplitude of the spin-dimerization. Then, it is straightforward to treat the above interaction in the framework of bosonization [31], and we see that, at $n = 1/2$, the charge sector of the conduction electron acquires the interaction $\cos(\sqrt{8}\phi_{\rho})$ whose scaling dimension is $2/K_{\rho}$ (with ϕ_{ρ} and K_{ρ} respectively being the charge boson field and the corresponding Luttinger-liquid parameter)³, which, when $K_{\rho} > 1$, opens the charge gap. Note that the period-2 component of the hopping amplitude $\sin(\sqrt{8}\phi_{\rho})$ has a zero expectation value consistent

³We follow the convention of Ref. [31]. Precisely, we have one more interaction of the form

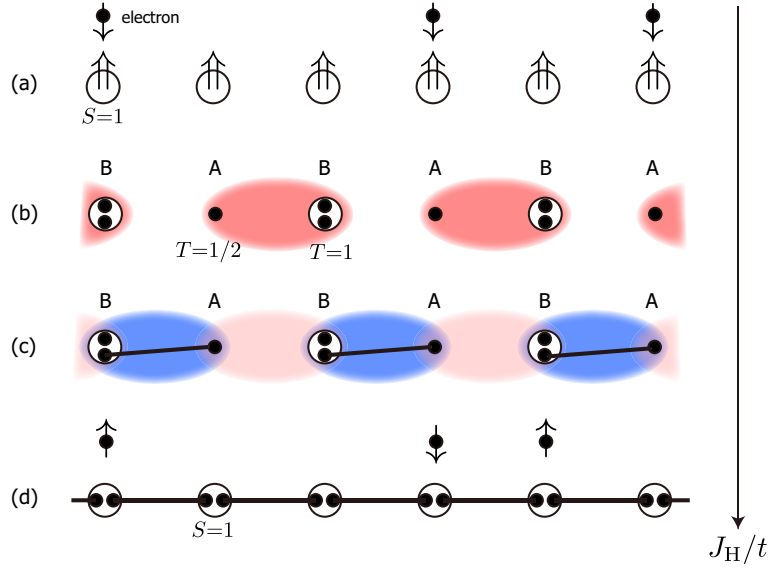


Figure 3.5: Schematic pictures illustrating how magnetic property changes as J_H/t increases. (a) ferromagnetic phase, (b) dimerized phase for small J_H in which spin-3/2s (i.e., local ferromagnetic correlation between $T = 1/2$ and $T = 1$) are formed on A-B bonds (red ovals), (c) dimerized phase for larger J_H where doublets develop on B-A bonds (blue ovals), and (d) metallic phase with short-range antiferromagnetic correlation. Note that there is no transition between (b) and (c). (Reproduced from Ref. [54])

with the above numerical observation. Although this argument seems reasonable, the spin-dimerization and the opening of the charge gap actually occur hand in hand, and a clear explanation of the mechanism of the magnetic dimerization still remains to be an important open question.

$\cos(\sqrt{8}\phi_\rho)\cos(\sqrt{8}\phi_\sigma)$ with the scaling dimension $2 + 2/K_\rho > 2$. This is irrelevant and we can safely drop it.

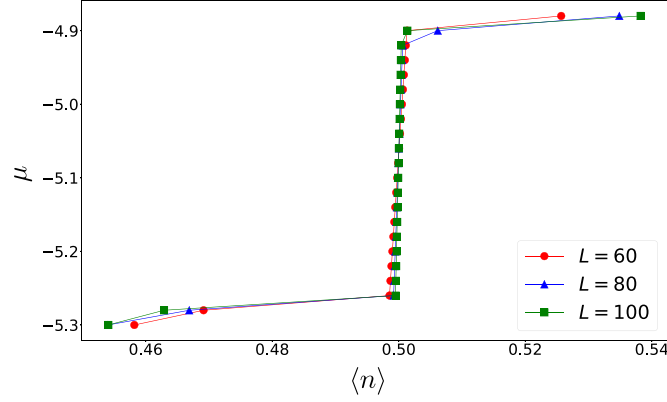


Figure 3.6: A typical behavior of μ as a function of the electron density $\langle n \rangle$ around $n = 1/2$ for various system sizes $L = 60, 80, 100$. The clear jump at $n = 1/2$ indicates a finite charge gap at quarter-filling and the absence of the charge gap for other fillings (around $n = 1/2$). $(J_K/t, J_H/t) = (5.0, 0.1)$ is used. (Reproduced from Ref. [54])

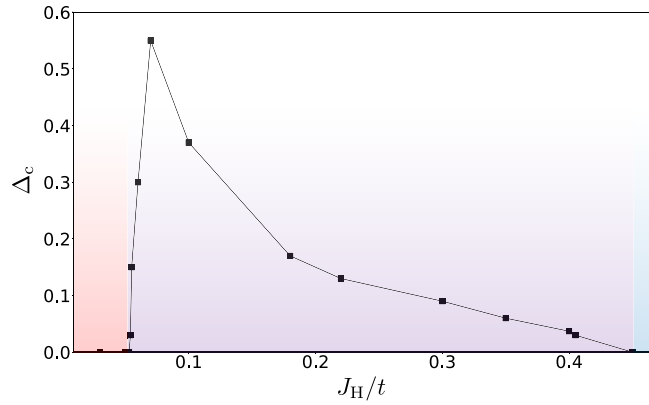


Figure 3.7: Relation between J_H/t and the charge gap Δ_c for fixed $J_K/t = 5.0$. The charge gap is obtained by extrapolating the finite-size values (which are given by the jump in the n - μ plot; see Fig. 3.6). Note that the charge gap Δ_c is finite only in the dimerized phase ($0.054 < J_H/t \lesssim 0.45$). (Reproduced from Ref. [54])

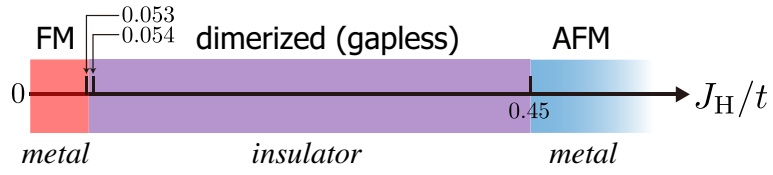


Figure 3.8: Phase diagram at quarter-filling ($n = 1/2$) along the J_H/t axis with fixed $J_K/t = 5.0$. The magnetic and electrical properties of the phases are determined by $\langle T_i \cdot T_{i+1} \rangle$ ($\langle S_i \cdot S_{i+1} \rangle$) and the charge gap Δ_c . In the dimerized phase, the spin-spin correlation is power-law decaying with period-4 oscillation. (Reproduced from Ref. [54])

Chapter 4

Summary of Part I

In this part, we investigated the ground-state phases of the spin- S Kondo-Heisenberg model in one dimension by means of analytical calculations in the limit of strong Kondo coupling (J_K) and the numerical DMRG simulations for $S = 1$. The main results are summarized schematically in Fig. 4.1. First, we derived the strong-coupling effective Hamiltonian both for and away from half-filling to obtain the insight into the global phase structure. At half-filling, the charge gap of the order of J_K opens and the magnetic sector is described solely by the partially screened local moments [with spin- $(S-1/2)$], whose dynamics is governed by the antiferromagnetic Heisenberg model. The resulting physics of the magnetic sector depends on the parity of $2S$; when $2S$ is odd, the half-filled ground state is a spin-gapped insulator while when $2S$ is even the system is an insulator with power-law antiferromagnetic correlation (i.e., a spin Luttinger liquid). As far as the direct interaction J_H is much smaller than J_K , the two do not compete with each other and the only effect of J_H is to renormalize the effective antiferromagnetic interaction among the partially screened local moments. Away from half-filling, on the other hand, we can prove that the system (at $J_H = 0$) in strong coupling is generically in the ferromagnetic metallic phase (see Fig. 4.1) in which the unscreened moments (spin- S) and the (partially) screened ones [spin- $(S-1/2)$] form a collective ferromagnetic state. Now this ferromagnetic state is challenged by the direct antiferromagnetic interaction J_H among the local moments.

To substantiate these expectations quantitatively for large but finite J_K , we carried out the DMRG simulations combined with the SSD method for the case of $S = 1$. At half-filling ($n = 1$), the spin-spin correlation indeed exhibits a power-law antiferromagnetic behavior, which agrees very well with that of the spin-1/2 ($S-1/2 = 1/2$ here)

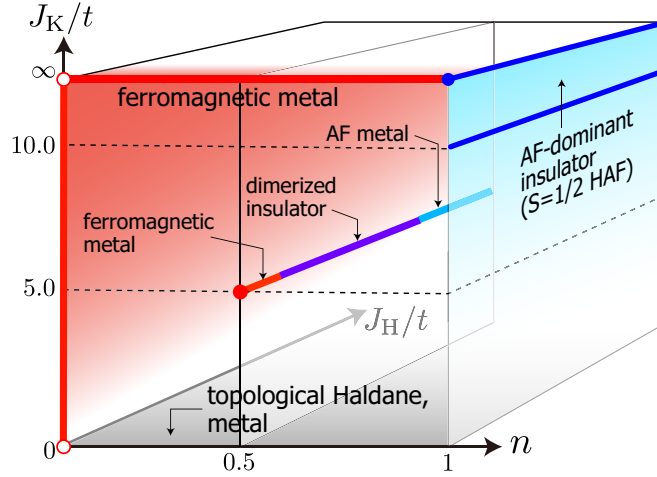


Figure 4.1: Schematic phase diagram of the spin-1 Kondo-Heisenberg model obtained from strong-coupling expansions and numerical simulations. The parameter regions studied in this thesis are shown by the thick lines. On the line $J_K = \infty$, $0 < n < 1$, the system is rigorously shown to be ferromagnetic metal. On the plane $n = 1$ (half-filling), an insulating phase with power-law antiferromagnetic spin correlation is stable. At quarter-filling ($n = 1/2$), we found at least three different phases at $J_K/t = 5.0$: (i) ferromagnetic metal, (ii) dimerized insulator with power-law period-4 spin correlation, and (iii) metallic phase with antiferromagnetic correlation. (Reproduced from Ref. [54])

Heisenberg chain up to fairly large values of J_H ($\gtrsim J_K$). This implies that the picture of the insulating phase with correlated Kondo-doublets, which is established in the perturbative regime (i.e., $J_H \ll J_K$), in fact extends over a wide range of the parameter space (see “AF-dominant insulator” in Fig. 4.1). Combining this with the results of the weak-coupling approach [56, 57], we expect that the AF-dominant insulator persists all the way down to small J_K .

At quarter-filling ($n = 1/2$) where ferromagnetism and antiferromagnetic J_H compete with each other, the phase diagram is much richer (Figs. 3.8 and 4.1). The ferromagnetic metal which is found for rather small J_H is destabilized by increasing J_H and

yields to a dimerized insulating phase with period-4 power-law spin-spin correlation (labeled as “dimerized insulator” in Fig. 4.1). The critical value of J_H is much smaller than we expect from the strong-coupling effective Hamiltonian. We also characterized the magnetic structure in the dimerized phase by a simple phenomenological argument. If J_H is further increased, we encountered another quantum phase transition at $J_H/t \approx 0.45$ where the system becomes metallic again. It remains open to understand how magnetic dimerization is stabilized by J_H and opens a charge gap. Perhaps direct simulations for the large- J_K effective Hamiltonian (2.11) might give an important hint. Also, as already noted in §3.2.2, the third phase with short-range antiferromagnetic correlation (“AF metal”) is determined only by the behavior of $\langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ and the absence of the charge gap, and the full characterization of it is an important open problem.

In this Part, we have focused on the strong-coupling phases of the spin-1 KH chain with small J_H . On the other hand, when the spin-1 moments are replaced with spin-1/2s, the model at weak coupling $J_K \ll J_H$ is known to possess co-existing CDW and superconducting orders [42], and, when inter-chain couplings are turned on, it even exhibits a topologically nontrivial ground state [69]. These facts hint at a possibility that, in the weak-coupling region, our spin-1 KH model might have a rich phase structure. Therefore, it is also an important future problem to study whether this is the case or not for $S > 1/2$.

We approached the investigation of the ground state of a composite system consisting of an antiferromagnetic spin-1 chain and a conduction electron system from the perspective of a model incorporating direct local spin interactions in the Kondo lattice model. Here, we summarize the influence of the conduction electron system on the antiferromagnetic spin-1 chain.

Firstly, at half-filling, as shown by the numerical results in section 3.1, the coupling with the conduction electron system shifted the correlation between localized spins from short-range to quasi-long-range with power-law decay.

On the other hand, at quarter-filling, we observed that the behavior of the correlation between adjacent localized spins changes depending on the ratio of J_H/t to J_K/t . More specifically, in the absence of coupling with the conduction electron system, the system exhibits antiferromagnetic-like correlations. However, when J_H/t is extremely weak, ferromagnetic-like correlations mediated by the conduction electrons dominate. In the intermediate regime of J_H/t values, there is competition between this ferromagnetic order mediated by the conduction electrons and the intrinsic antiferromagnetic order of the spin-1 chain, and interestingly, it was found that under certain conditions

of J_H/t , the system undergoes dimerization. On the contrary, regarding the influence of the localized spin system on the conduction electron system, in this intermediate parameter regime, the presence of localized spins leads to the opening of a charge gap, resulting in the insulating behavior of the conduction electron system.

In this way, from the perspective of the influence of coupling with the conduction electron system on the localized spin system, we here have primarily discussed the magnetic properties in the strong coupling regime. However, what will become of the important property of spin-1 antiferromagnetic chains, namely the Symmetry-Protected Topological (SPT) order [7]?

Regarding this matter, in Part II, we will discuss the coupling of the spin-1 chain with an environment that is not limited to the conduction electron system in general terms. However, let's briefly summarize the results of addressing this issue within the context established in Part I.

For this purpose, we numerically calculated one of the string order parameters (SOP) [5, 6]:

$$\mathcal{O}_{\text{str}}^z = \lim_{|i-j| \rightarrow \infty} \left\langle S_i^z \exp \left(i\pi \sum_{k=i}^{j-1} S_k^z \right) S_j^z \right\rangle, \quad (4.1)$$

an indicator of SPT order respecting $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, which we will introduce in the § 6.1.2, by extrapolating from calculations in finite systems. This is shown in Fig. 4.2

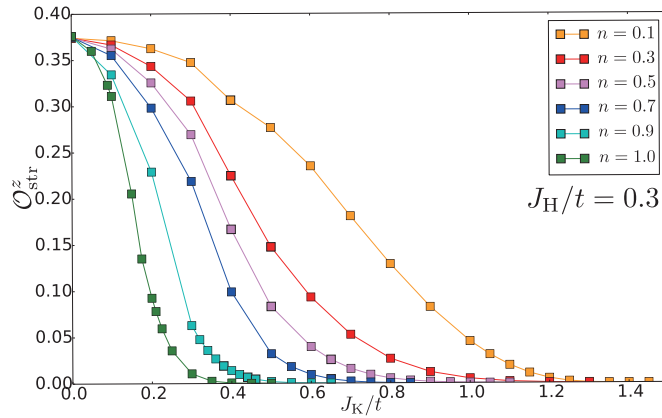


Figure 4.2: The decay of the string order parameter caused by the Kondo-coupling for each fixed density of the electrons.

Each graph corresponds to the results for each density of the conduction electrons $\langle n \rangle$, showing that as the coupling with the conduction electron system increases, the

SOP decreases, as indicated by these results. Furthermore, it was found that the SOP decays faster with higher numbers of conduction electrons, consistent with intuitive expectations. This decline indicates that the SPT order inherent in the spin-1 chain weakens and ultimately disappears. Part II will address questions such as why the SPT order disappears and whether there exist environments where the coupling does not diminish the SPT order.

Part II

Computational characterization of decohered symmetry-protected topological orders in a spin-1 system

Chapter 5

Introduction to Part II

Studying the character of many different quantum phases is mainly based on classification of gapped Hamiltonians, which is equivalent to the classification of gapped ground states. Some quantum phases exist without spontaneous breaking of global symmetries, and we cannot characterize them with local order parameters such as the magnetization. These relatively new phases (often said as “beyond Landau paradigm”) which we call “topological” include quantum spin liquids, the quantum Hall states, the fractonic states, and so on [70, 71]. One useful way to distinguish these phases from other trivial ones is to use quantum entanglement [72]. In this respect, “trivial phases” are those which can be deformed into product states by local unitary transformations (or finite-depth quantum circuits). In contrast, a state that cannot be transformed into a product state by such transformations without closing the gap is referred to as long-range entangled. In this sense, it is known [73, 74] that long-range entangled states with “genuine” topological order are forbidden in one-dimensional (bosonic) systems. However, if we consider only local unitary transformations respecting a certain symmetry, some sets of states become distinct from the set of product states. This is how the concept of the symmetry-protected topological (SPT) phases arises [7]. One of the best known examples of the SPT phases in one dimension would be the Haldane phase [2, 3], which is protected by one of (i) spatial inversion, (ii) time-reversal, and (iii) $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetries. For example, the ground state of the spin-1 antiferromagnetic Heisenberg model and the Affleck-Kennedy-Lieb-Tasaki (AKLT) state [4] belong to this phase. The Haldane phase has no local order parameter, and instead, is characterized by, e.g., the non-vanishing string order parameter [5, 6] which is associated with the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, the even-fold degeneracy of the entanglement spectrum [75], and

the emergent fractionalized edge spins [76, 77, 78] which are essentially different from those constituting the bulk.

In one dimension, gapped ground states are well approximated by the matrix product states (MPS) [79] which automatically satisfy the area law of the entanglement entropy [80], and the aforementioned non trivial properties of the Haldane phase can be altogether understood using the MPS representation [75, 74, 73, 81]. The most important message from this MPS-based approach would be that the symmetry group acts on the fractionalized edge state as a projective representation [6]. Therefore, when the group G of the on-site symmetry is given, the classification of one-dimensional G -symmetric SPT phases amounts to enumerating all the possible projective representations of G [73, 74, 82].

On the other hand, measurement-based quantum computation (MBQC) [83, 84] is a computational model known to be mathematically equivalent to the quantum circuit model. In this formulation, the quantum teleportation in which the state sent by one person is the same as that received by the other is applied. The sender teleports some qubit to the receiver by the specific two-qubit measurement based on the entangled state which the sender and receiver share. MBQC utilizes the fact that the unitarily transformed state can be sent by appropriate measurements or by sharing appropriate entangled state between the sender and the receiver [85, 86]. Therefore, in MBQC, the computation is literally implemented by the measurement on what is called the resource states. It is known [87, 88, 89, 90, 91, 92] that states in non-trivial SPT phases can be used as resource states of MBQC (the so-called computational phases of matter), and in simplest cases, the corresponding qubits are encoded in the physical edge states of the SPT phases [89, 90]. Furthermore, the computational power is retained throughout a given SPT phase and the feasibility of MBQC is thought of as associated not with a particular state but with the phase itself [88, 91].

Then, it would be natural from both topological and quantum-computational points of view to ask how robust SPT phases are against the coupling to the environment. While, in the case of pure states, SPT phases, have been fairly well understood as already stated, there have been relatively few discussions about how to characterize SPT phases in generic mixed states. Some attempts in this direction include characterizing the topological nature by the indices based on the Uhlmann phase [93, 94, 95, 96], generalizing the MPS-based markers (e.g., projective representations, entanglement spectrum, etc.) to density operators via the doubled-Hilbert-space formalism [97, 98, 99], and order-parameter-based approaches using the strange correlators [100], the string

order parameters [101], etc.

The main challenge here consists in how to capture the topological nature in the density operators, since most of the existing approaches (the entanglement spectrum, the projective representations, etc.) which have been successfully applied to the pure cases are based on the ground-state wave functions and are not directly generalized to mixed states. For instance, in Ref. [101], de Groot et al. discuss the robustness of SPT phases of one-dimensional spin systems by focusing on the non-local string order parameters [102, 81]. Specifically, they showed that if the quantum channel $\mathcal{E}$ describing the system-environment coupling and the protecting symmetry G satisfy a certain condition (the strong-symmetry condition defined below), the G -protected SPT phases in closed systems are robust against $\mathcal{E}$ in the sense that the corresponding string order parameter survives.

On the other hand, since the computational ability of MBQC is an inherent property of a given SPT phase as has been described above, it should be possible to capture its topological nature also by the performance of MBQC on it. In this part, we propose to use the computational power of a given SPT phase to characterize the topological property behind. Specifically, we use the gate fidelity [see Eq. (6.52)] that measures the performance of MBQC to judge whether the phase still retains its topological properties even under decoherence. The merit of this approach is that it is applicable regardless of whether the state is pure or mixed. It also uncovers a remarkable connection between the feasibility of MBQC and the non-local string order parameters which have been used in assessing the robustness of SPT phases under decoherence [101] thereby giving a physical interpretation to the recent observation made in Ref. [103] concerning the relation between the computational power (of a *pure* SPT state) and the string order parameter.

Chapter 6

Preliminaries

6.1 Haldane phase in the closed system

One of the most famous symmetry-protected topological (SPT) phases is the Haldane phase in one-dimensional spin-1 systems. For example, the ground state of spin-1 antiferromagnetic Heisenberg model and Affleck-Kennedy-Lieb-Tasaki (AKLT) state [4] belong to this phase. As already stated in the introduction (Chap. 5), the Haldane phase has no local order parameter, and instead, this phase is characterized by, for example, the finite string order parameter [5] and the even degeneracy of entanglement spectrum [75], and topologically protected edge states [77]. The Haldane phase is protected by (i) $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, (ii) spatial inversion symmetry, and (iii) time-reversal symmetry. The string order parameter is a non-local order parameter respecting the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

In this chapter, first we briefly review the matrix product state (MPS), and second we will see that we can extract the non-triviality from the MPS form of the pure ground state in SPT phases.

6.1.1 AKLT state and its matrix product state form

In this subsection, we will briefly review the AKLT state as a representative of the Haldane phase and its matrix product state (MPS) form. Through this process, we will see the non-triviality of Haldane phase as a SPT phase. The AKLT Hamiltonian is

$$H = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] \quad (6.1)$$

The ground state of this Hamiltonian can be constructed as the following:

- (i) Prepare the tensor product state of spin-1/2 singlet pairs.
- (ii) Project neighboring spin-1/2, which are not paired as singlets, onto spin-1.

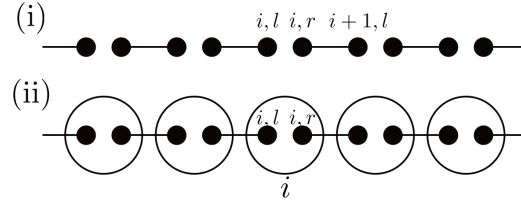


Figure 6.1: A schematic diagram of the construction of the AKLT state.

Let me formulate this process mathematically and actually construct the AKLT state in the MPS form.

$$\begin{aligned}
 \bullet^{i,r} \text{---} \bullet^{i+1,l} &= \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{i,r} |\downarrow\rangle_{i+1,l} - |\downarrow\rangle_{i,r} |\uparrow\rangle_{i+1,l} \right) \\
 &= A_{\sigma_{i,r} \sigma_{i+1,l}} |\sigma_{i,r}\rangle |\sigma_{i+1,l}\rangle
 \end{aligned} \tag{6.2}$$

Here,

$$A := \begin{pmatrix} 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix} \tag{6.3}$$

On the other hand, we can acquire the spin-1 degree of freedom on each site from two spin-1/2's by

$$\begin{aligned}
 |1\rangle_i &= |\uparrow\rangle_{i,l} |\uparrow\rangle_{i,r} \\
 |0\rangle_i &= \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{i,l} |\downarrow\rangle_{i,r} + |\downarrow\rangle_{i,l} |\uparrow\rangle_{i,r} \right) \\
 |-1\rangle_i &= |\downarrow\rangle_{i,l} |\downarrow\rangle_{i,r}
 \end{aligned} \tag{6.4}$$

We can unify these equation into one equation

$$|m_i\rangle = \sum_{\sigma_{i,l}, \sigma_{i,r}} P_{\sigma_{i,l} \sigma_{i,r}}^{(m_i)} |\sigma_{i,l}\rangle |\sigma_{i,r}\rangle \quad m_i \in \{1, 0, -1\} \tag{6.5}$$

Here, we define the $P^{(m_i)}$ for each m_i as

$$P^{(1)} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P^{(0)} := \begin{pmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix}, \quad P^{(-1)} := \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad (6.6)$$

And, the identity operator on the spin-1 degree of freedom is

$$\begin{aligned} I_i &= \sum_{m_i=0,\pm 1} |m_i\rangle \langle m_i| \\ &= \sum_{m_i=0,\pm 1} |m_i\rangle \sum_{\sigma_{i,l}, \sigma_{i,r}} \left(P_{\sigma_{i,l} \sigma_{i,r}}^{(m_i)} \right)^* \langle \sigma_{i,l} | \langle \sigma_{i,r} | \\ &= \sum_{m_i} |m_i\rangle \sum_{\sigma_{i,l}, \sigma_{i,r}} P_{\sigma_{i,l} \sigma_{i,r}}^{(m_i)} \langle \sigma_{i,l} | \langle \sigma_{i,r} | \end{aligned} \quad (6.7)$$

Finally, we get the MPS form of the AKLT state in the periodic N -site system:

$$\begin{aligned} |\text{AKLT}\rangle &= I^{\otimes L} \sum_{\{\sigma_{i,x}\}} A_{\sigma_{1,r} \sigma_{2,l}} \dots A_{\sigma_{L,r} \sigma_{1,l}} |\sigma_{1,l}\rangle |\sigma_{1,r}\rangle \dots |\sigma_{L,l}\rangle |\sigma_{L,r}\rangle \\ &= \sum_{\{m_i\}} |m_1\rangle \dots |m_L\rangle \sum_{\{\sigma'_{i,x}\}} P_{\sigma'_{1,l} \sigma'_{1,r}}^{(m_1)} \dots P_{\sigma'_{L,l} \sigma'_{L,r}}^{(m_L)} \langle \sigma'_{1,l} | \langle \sigma'_{1,r} | \dots \langle \sigma'_{L,l} | \langle \sigma'_{L,r} | \\ &\quad \sum_{\{\sigma_{i,x}\}} A_{\sigma_{1,r} \sigma_{2,l}} \dots A_{\sigma_{L,r} \sigma_{1,l}} |\sigma_{1,l}\rangle |\sigma_{1,r}\rangle \dots |\sigma_{L,l}\rangle |\sigma_{L,r}\rangle \\ &= \sum_{\{m_i\}} |m_1\rangle \dots |m_L\rangle \sum_{\{\sigma_{i,x}\}} P_{\sigma_{1,l} \sigma_{1,r}}^{(m_1)} A_{\sigma_{1,r} \sigma_{2,l}} P_{\sigma_{2,l} \sigma_{2,r}}^{(m_2)} A_{\sigma_{2,r} \sigma_{3,l}} \dots P_{\sigma_{L,l} \sigma_{L,r}}^{(m_L)} A_{\sigma_{L,r} \sigma_{1,l}} \\ &= \sum_{\{m_i\}} \text{Tr} \left[\underline{P^{(m_1)} A} \underline{P^{(m_2)} A} \dots \underline{P^{(m_L)} A} \right] |m_1\rangle \dots |m_L\rangle \\ &=: \sum_{\{m_i\}} \text{Tr} \left[A^{(m_1)} A^{(m_2)} \dots A^{(m_L)} \right] |m_1\rangle \dots |m_L\rangle \end{aligned} \quad (6.8)$$

This So, this is an MPS representation of the unique ground state of the AKLT Hamiltonian. The $\text{Tr} [A^{(m_1)} A^{(m_2)} \dots A^{(m_L)}]$ in the last line of this equation can be drawn as a diagram (Fig.6.2)

Apparently, the MPS representation of a pure state is not unique. If there exists a unitary matrix V satisfying $A = V^\dagger B V$, this pure state can also be described as an MPS with MPS tensor B . In other words, the MPS description of a pure state has the gauge degree of freedom, and one pure state $|\psi\rangle$ corresponds to an equivalence

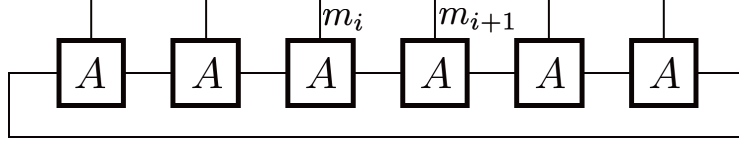


Figure 6.2: Schematic diagram of MPS representation of AKLT state. Each square corresponds to the MPS tensor of (6.8). Horizontal lines connecting the adjacent squares means entanglement bond, and the connection does the matrix product in (6.8). Vertical lines denotes physical degrees of freedom on each site, which are labeled as m_i . The MPS tensor A associated to each site is the same, so this MPS has translationally invariance.

class of MPS in which every MPS form of $|\psi\rangle$ can transform to another MPS form by gauge transformation. The canonical form of the MPS is the representative of each equivalence class useful to calculate expectation values or correlation functions and to know the entanglement structure. Now let us consider a pure state schematically described as Fig. 6.3, where Γ is a χ by χ real diagonal matrix. The canonical MPS is defined by the following conditions:

$$\sum_{m_i} \Gamma^{(m_i)\dagger} \Lambda^2 \Gamma^{(m_i)} = \sum_{m_i} \Gamma^{(m_i)} \Lambda^2 \Gamma^{(m_i)\dagger} = \mathbb{I}_\chi. \quad (6.9)$$

These equations can be translated diagrammatically,

$$\begin{array}{c} \Lambda \\ \bullet \\ \Gamma^* \\ | \\ \Lambda \\ \bullet \\ \Gamma \end{array} = \left[\begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \right] \quad (6.10)$$

$$\begin{array}{c} \\ \\ \Gamma^* \\ | \\ \Gamma \\ \end{array} \begin{array}{c} \Lambda \\ \bullet \\ \\ \\ \Lambda \\ \bullet \\ \end{array} = \left[\begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \right] \quad (6.11)$$

Here, right-hand sides of these equations are identity matrices $\mathbb{I}_\chi$.

Similarly, the MPS form of the AKLT state in L -site system (i.e. in the open boundary condition) is described as

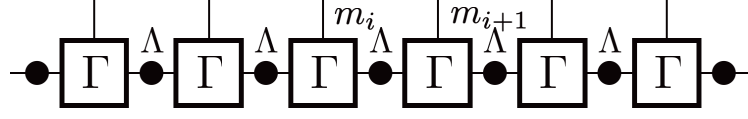


Figure 6.3: Schematic diagram of MPS in canonical form. Each square corresponds to the MPS tensor of (6.8). Horizontal lines connecting the adjacent squares means entanglement bond, and the connection does the matrix product in (6.8). Vertical lines denotes physical degrees of freedom on each site, which are labeled as m_i . In this case, the Γ is a translationally invariant MPS tensor and the Λ is a diagonal matrix, whose component is related to the Schmidt value. These two kinds of matrix satisfy the canonical condition in Eq. 6.9

$$\begin{aligned}
|\text{AKLT}\rangle &= I^{\otimes L} \sum_{\{\sigma_{i,x}\}} A_{\sigma_{1,r}\sigma_{2,l}} \dots A_{\sigma_{L-1,r}\sigma_{L,l}} |\sigma_{1,l}\rangle |\sigma_{1,r}\rangle \dots |\sigma_{L,l}\rangle |\sigma_{L,r}\rangle \\
&= \sum_{\{m_i\}} |m_1\rangle \dots |m_L\rangle \sum_{\{\sigma'_{i,x}\}} P_{\sigma'_{1,l}\sigma'_{1,r}}^{(m_1)} \dots P_{\sigma'_{L,l}\sigma'_{L,r}}^{(m_L)} \langle \sigma'_{1,l} | \langle \sigma'_{1,r} | \dots \langle \sigma'_{L,l} | \langle \sigma'_{L,r} | \\
&\quad \sum_{\sigma_{1,r}} \sum_{\{\sigma_{2,x}\}} \dots \sum_{\{\sigma_{L-1,x}\}} \sum_{\sigma_{L,l}} A_{\sigma_{1,r}\sigma_{2,l}} \dots A_{\sigma_{L-1,r}\sigma_{L,l}} |\sigma_{1,l}\rangle |\sigma_{1,r}\rangle \dots |\sigma_{L,l}\rangle |\sigma_{L,r}\rangle \\
&= \sum_{\{m_i\}} |m_1\rangle \dots |m_L\rangle \sum_{\sigma_{1,r}} \sum_{\{\sigma_{i,x}\}_{i=2}^{L-1}} \sum_{\sigma_{L,l}} P_{\sigma_{1,l}\sigma_{1,r}}^{(m_1)} A_{\sigma_{1,r}\sigma_{2,l}} P_{\sigma_{2,l}\sigma_{2,r}}^{(m_2)} \dots A_{\sigma_{L-1,r}\sigma_{L,l}} P_{\sigma_{L,l}\sigma_{L,r}}^{(m_L)} \\
&= \sum_{\{m_i\}} [P^{(m_1)} A P^{(m_2)} A \dots A P^{(m_L)}]_{\sigma_{1,l}\sigma_{L,r}} |m_1\rangle \dots |m_L\rangle \\
&= \sum_{\{m_i\}} [A^{(m_1)} A^{(m_2)} \dots A^{(m_{L-1})} P^{(m_L)}]_{\sigma_{1,l}\sigma_{L,r}} |m_1\rangle \dots |m_L\rangle \tag{6.12}
\end{aligned}$$

The subscript of the square bracket in the rightmost-hand-side indicates that the ground state of the AKLT Hamiltonian has a four-fold degeneracy under open boundary conditions. Let me briefly confirm that this is indeed the ground state of the previously provided AKLT Hamiltonian (6.1). Since the total spin operator between site i and site $i+1$ is $\mathbf{S}_{i,i+1}^{\text{tot}} = \mathbf{S}_i + \mathbf{S}_{i+1}$ and generally, the $(\mathbf{S}_i)^2$ takes the value $S_i(S_i+1)$ for each irreducible representation space of spin operator. So,

$$\begin{aligned}
\mathbf{S}_i \cdot \mathbf{S}_{i+1} &= \frac{1}{2} [S_{i,i+1}^{\text{tot}}(S_{i,i+1}^{\text{tot}} + 1) - S_i(S_i + 1) - S_{i+1}(S_{i+1} + 1)] \\
&= \begin{cases} -2 & (S_{i,i+1}^{\text{tot}} = 0) \\ -1 & (S_{i,i+1}^{\text{tot}} = 1) \\ 1 & (S_{i,i+1}^{\text{tot}} = 2) \end{cases} \quad (6.13)
\end{aligned}$$

Thus,

$$\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 = \begin{cases} -\frac{2}{3} & (S_{i,i+1}^{\text{tot}} = 0) \\ -\frac{2}{3} & (S_{i,i+1}^{\text{tot}} = 1) \\ \frac{4}{3} & (S_{i,i+1}^{\text{tot}} = 2) \end{cases}, \quad (6.14)$$

and therefore, the AKLT Hamiltonian can be written as the sum of the projection onto the $S_{i,i+1}^{\text{tot}} = 2$

$$H = \sum_i P_i^{(S_{i,i+1}^{\text{tot}}=2)} \quad (6.15)$$

Remember that the AKLT state constructed in this subsection have singlets between site i and site $i + 1$ (Fig. 6.1), then we can see that the AKLT state is the ground state of (6.1).

6.1.2 AKLT state as a state with the symmetry-protected topological order

Next, let me show some properties of the AKLT state using the MPS form. First, in order to normalize the AKLT in MPS representation, we multiply $P^{(m_i)}$ by $2/\sqrt{3}$. Renewed P 's are

$$P^{[1]} = \begin{pmatrix} \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 \end{pmatrix}, \quad P^{[0]} = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ \sqrt{\frac{2}{3}} & 0 \end{pmatrix}, \quad P^{[-1]} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{2}{\sqrt{3}} \end{pmatrix}. \quad (6.16)$$

Then, the MPS tensor of the AKLT state (6.8) satisfies the canonical condition (6.9):

$$\begin{array}{c} \begin{array}{c} \boxed{P^*} \text{---} \boxed{A^*} \\ | \\ \boxed{P} \text{---} \boxed{A} \end{array} = \left[\begin{array}{c} \text{---} \\ \text{---} \end{array} \right] \end{array} \quad (6.17)$$

$$\begin{array}{c} \begin{array}{c} \text{---} \boxed{P^*} \text{---} \boxed{A^*} \\ | \\ \text{---} \boxed{P} \text{---} \boxed{A} \end{array} = \left[\begin{array}{c} \text{---} \\ \text{---} \end{array} \right] \end{array} \quad (6.18)$$

These equation also suggests that the Schmidt eigenvalue of the AKLT chain is $\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}$ for any length L .

Generally, if $|\psi\rangle$ is symmetric under some group G , then $U_g |\psi\rangle \propto |\psi\rangle$. Especially, when the U_g is the linear representation of an onsite symmetry, i.e. $U_g = \otimes_i u_g$, then this invariance of the state under the onsite symmetry leads to a symmetry constraint on the MPS tensor [102]:

$$\begin{array}{c} \text{---} \boxed{\Gamma} \text{---} \\ | \\ \text{---} \circ u_g \end{array} = e^{i\varphi_g} \times \begin{array}{c} \text{---} \boxed{\Gamma} \text{---} \\ | \\ \text{---} \end{array} \begin{array}{c} V_g^\dagger \\ \text{---} \end{array} \begin{array}{c} V_g \\ \text{---} \end{array} \quad (6.19)$$

Here, Γ is an MPS tensor of symmetric $|\psi\rangle$ that satisfies canonical condition (6.9). Under this condition, the V_g on the right-hand side is a unitary matrix. If we are given the canonical MPS tensor and linear representation of G , there is a well-established way to get V_g for every $g \in G$ [81].

Since the AKLT state has the onsite $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, the symmetry action on the spin-1 Hilbert space of each site (6.19) is

$$\begin{array}{c} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \\ | \\ \text{---} \circ u_g \end{array} = \begin{array}{c} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \\ | \\ \text{---} \end{array} \begin{array}{c} V_g^\dagger \\ \text{---} \end{array} \begin{array}{c} V_g \\ \text{---} \end{array}, \quad (6.20)$$

where $\{u_g\}$ is a linear representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$, for example, $\{1_3, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$.

Then, we can get the V_g 's as an eigenvector of the transfer matrix

$$T_{u_g} = \begin{array}{c} \text{---} \boxed{P^*} \text{---} \boxed{A^*} \text{---} \\ | \\ \textcircled{u_g} \\ | \\ \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \end{array} \quad (6.21)$$

of $|\lambda| = 1$. Consequently, $\{V_g\} = \{1_2, X, Y, Z\}$ for the AKLT state. This is a non-trivial projective representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$ because $V_g V_h = -V_{gh} \neq V_{gh}$ for $g \neq e \neq h$ and $g \neq h$ even though $u_g u_h = u_{gh}$. Note that the resulting projective representation depends on the state. For example, $\otimes_i |0\rangle_i$ is the ground state of the

$$H(D) = J \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] + D \sum_i (S_i^z)^2 \quad (6.22)$$

in the large- D limit, and in this case, V_g 's are 1×1 matrices (i.e. numbers) since the state is just the product state. For this product state, the symmetry-protected edge state does not exist, and this is the difference between the AKLT state and the trivial case. By the discussion so far, the action of the global symmetry results in nothing for the bulk but acts on the fractionalized edge states for the case of the finite chain:

$$\begin{array}{c} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \end{array} = \begin{array}{c} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \end{array} \\ = \begin{array}{c} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \boxed{P} \text{---} \boxed{A} \text{---} \textcircled{u_g} \text{---} \end{array} \quad (6.23)$$

The SPT phases in one dimensional system are classified by this projective representation of G , which is the symmetry action on the edge state [6].

This happens also when we calculate the string order parameter. The string order parameter has the form like $\lim_{|i-j| \rightarrow \infty} \left\langle O_i^l \left(\bigotimes_{k=i+1}^j u_g^k \right) O_j^r \right\rangle$. Here, O_j^l (O_j^r) is the left (right) end operator. We calculate the part of $\left\langle O_i^l \left(\bigotimes_{k=i+1}^j u_g^k \right) O_j^r \right\rangle$ as the following:

$$\begin{aligned}
\left\langle O_i^l \left(\bigotimes_{k=i+1}^j u_g^k \right) O_j^r \right\rangle &= \\
&= \\
&\rightarrow \left(\begin{array}{c} \text{Diagram with four horizontal lines. Top line: } P^* \text{---} A^* \text{---} P^* \text{---} A^* \text{---} P^* \text{---} \dots \text{---} P^* \text{---} A^* \text{---} P^* \text{---} A^* \text{---} P^*. \text{ Second line: } O^l \text{---} u_g \text{---} u_g \text{---} \dots \text{---} u_g \text{---} u_g \text{---} O^r. \text{ Third line: } P \text{---} A \text{---} P \text{---} A \text{---} P \text{---} \dots \text{---} P \text{---} A \text{---} P \text{---} A \text{---} P. \text{ Bottom line: } P^* \text{---} A^* \text{---} P^* \text{---} A^* \text{---} P^* \text{---} \dots \text{---} P^* \text{---} A^* \text{---} P^* \text{---} A^* \text{---} P^*. \text{ Vertical connections: } O^l \text{ to } P, u_g \text{ to } P \text{ and } P^*, P \text{ to } A, A \text{ to } P^*, P^* \text{ to } A^*, A^* \text{ to } P^*. \text{ End operators } V_g^\dagger \text{ and } V_g \text{ are shown on the } A \text{ and } P \text{ boxes respectively.} \end{array} \right) \\
&= \left(\begin{array}{c} \text{Diagram with two horizontal lines. Top line: } P^* \text{---} A^*. \text{ Bottom line: } P \text{---} A. \text{ Vertical connections: } P^* \text{ to } P, A^* \text{ to } A. \text{ End operators } V_g^\dagger \text{ and } V_g \text{ are shown on the } A \text{ and } P \text{ boxes respectively.} \end{array} \right) \left(\begin{array}{c} \text{Diagram with two horizontal lines. Top line: } P^* \text{---} A^*. \text{ Bottom line: } P \text{---} A. \text{ Vertical connections: } P^* \text{ to } P, A^* \text{ to } A. \text{ End operators } V_g^\dagger \text{ and } V_g \text{ are shown on the } A \text{ and } P \text{ boxes respectively.} \end{array} \right) \\
&= \left(\text{Tr} [T_{O^l}(V_g^\dagger)] \text{Tr} [T_{O^r}^\dagger(V_g)] \right)
\end{aligned} \tag{6.24}$$

At the last line, we use

$$\begin{array}{c} \text{Diagram with two horizontal lines. Top line: } P^* \text{---} A^*. \text{ Bottom line: } P \text{---} A. \text{ Vertical connections: } P^* \text{ to } P, A^* \text{ to } A. \end{array} = \left[\begin{array}{c} \text{Diagram with two horizontal lines. Top line: } P^* \text{---} A^*. \text{ Bottom line: } P \text{---} A. \text{ Vertical connections: } P^* \text{ to } P, A^* \text{ to } A. \end{array} \right] \left[\begin{array}{c} \text{Diagram with two horizontal lines. Top line: } P^* \text{---} A^*. \text{ Bottom line: } P \text{---} A. \text{ Vertical connections: } P^* \text{ to } P, A^* \text{ to } A. \end{array} \right]
\tag{6.25}$$

, which holds because of (6.17) and (6.18). So, in order for the string order parameter to remain finite, both $\text{Tr} [T_{O^l}(V_g^\dagger)]$ and $\text{Tr} [T_{O^r}^\dagger(V_g)]$ are non-zero. For example, if $O^l = O^r = S^z$ and $u_g = e^{i\pi S^z}$, then these are finite for the AKLT state and 0 for the trivial phase. The generalization of this leads us to the "selection rule" or "pattern of zeros" of the string order parameter [81]. The selection rule is the condition of the combination of the u_g and the end operator $O^{l(r)}$ for the string order parameter not to vanish. The string order parameter detects a long-range order and was originally introduced in Ref [5]. for the sake of the investigating the hidden (or diluted) antiferromagnetic order of antiferromagnetic Heisenberg chain with odd-integer spin. Heisenberg chain has a peculiar property that the energy spectrum is gapped or gapless depending on whether the spin is respectively integer or half-odd. So, for example, the spin-1/2 antiferromagnetic Heisenberg chain has the quasi-long range antiferromagnetic order,

and on the other hand the spin-1 Heisenberg chain does not have that. Instead, the antiferromagnetic spin-1 Heisenberg chain has another long-range order. Later it turned out that this non-local order is related to SPT order protected by the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

6.1.3 AKLT state coupled to the spin-1/2's on each end

Now, let us consider the Hamiltonian of AKLT model coupled to the spin-1/2's on each end:

$$H = \frac{4}{3} J \mathbf{s}_{\text{in}} \cdot \mathbf{S}_1 + J \sum_{i=1}^{N-1} \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right] + \frac{4}{3} J \mathbf{S}_N \cdot \mathbf{s}_{\text{out}}. \quad (6.26)$$

In the similar way as the previous subsection, the (normalized and canonical) MPS [79, 21] form of the ground state of this Hamiltonian is

$$\begin{aligned} & |\psi_{\text{AKLT}}\rangle \\ &= \sum_{\sigma_{\text{in/out}}} \sum_{\{m_i\}} (A^{[\sigma_{\text{in}}]} P^{[m_1]} A \dots P^{[m_N]} A^{T[\sigma_{\text{out}}]}) |\sigma_{\text{in}}\rangle |m_1 \dots m_N\rangle |\sigma_{\text{out}}\rangle, \end{aligned} \quad (6.27)$$

where the matrix

$$A = \begin{pmatrix} 0 & -1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{pmatrix} \quad (6.28)$$

describes the singlet bond in Fig. 6.4, and

$$P^{[1]} = \begin{pmatrix} \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 \end{pmatrix}, \quad P^{[0]} = \begin{pmatrix} 0 & \sqrt{\frac{2}{3}} \\ \sqrt{\frac{2}{3}} & 0 \end{pmatrix}, \quad P^{[-1]} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{2}{\sqrt{3}} \end{pmatrix} \quad (6.29)$$

projects two spin-1/2 states onto the spin-1 state on each site. These are proportional to those of the ordinary AKLT state in the previous subsection, so the additional two spin-1/2's do not change the physics of the bulk system. The exceptional matrix $A^{[\sigma]}$ ($A^{T[\sigma]}$) on the edge is the row (column) vector sliced from the matrix A . The MPS form of this state (6.27) is diagrammatically pictured as Fig. 6.5. It is known that the AKLT state has the four-fold degeneracy due to the free spin-1/2 degree of freedoms on both ends in the open boundary condition, so these two extra spin-1/2's make the ground state of Eq. (6.26) unique even in this boundary condition [104]. There is another reason we added two spin-1/2's motivated by the quantum informational perspective. This will be discussed in section 6.3.

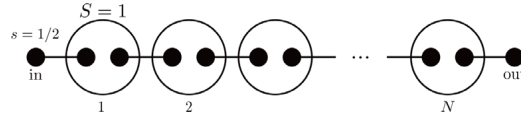


Figure 6.4: A schematic diagram of AKLT state coupled with two extra one-half spins. Dots and line segments between them describe spin-1/2 degrees of freedom and their singlet bonds, respectively. Circles including two adjacent dots means the projection onto the spin-1 degree of freedom. (Reproduced from Ref. [105])

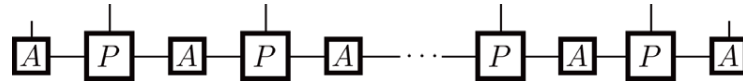


Figure 6.5: Diagram of MPS form of AKLT state with two additional spin-1/2's. Each square corresponds to the MPS tensor of (6.27). Horizontal lines connecting the adjacent squares means entanglement bond, and the connection does the matrix product in (6.27). Vertical lines denotes physical degrees of freedom on each site, which are labeled as $\sigma_{\text{in}}, m_i, \sigma_{\text{out}}$. Here, the exceptional spin-1/2 degrees of freedom on edges are described as short vertical lines. (Reproduced from Ref. [105])

6.2 The SPT order in open quantum system

Extensive research has been conducted on the SPT order of pure states, and methods for detecting the non-triviality of states with SPT order have been well-established. In contrast, the study of open quantum systems in this context can be said to be largely unexplored. Our primary research focus is on this area, and the purpose of this chapter is to briefly introduce the research that has been made so far before detailing our research results in the following chapter.

6.2.1 symmetry condition of quantum channels

Now let us consider systems coupled to environment. In those systems, states are generally represented by a density operator ρ and its time evolution is described by a completely positive trace-preserving (CPTP) map or a quantum channel $\mathcal{E}$ (see, e.g., Refs. [106, 107] for reviews):

$$\rho \rightarrow \rho' = \mathcal{E}[\rho]. \quad (6.30)$$

$$U_g \rho U_g^\dagger = \rho \quad \implies \quad U_g \mathcal{E}(\rho) U_g^\dagger = \mathcal{E}(\rho) \quad (6.31)$$
$$\mathcal{E}(\rho) = \sum_{\alpha} K_{\alpha} \rho K_{\alpha}^{\dagger} \quad \left(\sum_{\alpha} K_{\alpha}^{\dagger} K_{\alpha} = 1 \right) \quad (6.32)$$
$$\sum_{\alpha} (U_g K_{\alpha} U_g^{\dagger}) \rho (U_g K_{\alpha} U_g^{\dagger})^{\dagger} = \sum_{\alpha} K_{\alpha} \rho K_{\alpha}^{\dagger}, \quad (6.33)$$
$$U_g \mathcal{E}(\rho) U_g^\dagger = \sum_{\alpha} U_g K_{\alpha} \rho K_{\alpha}^\dagger U_g^\dagger \quad (6.34)$$

$$= \sum_{\alpha} U_g K_{\alpha} (U_g^{\dagger} U_g) \rho (U_g^{\dagger} U_g) K_{\alpha}^{\dagger} U_g^{\dagger} \quad (6.35)$$

$$= \sum_{\alpha} (U_g K_{\alpha} U_g^{\dagger}) \rho (U_g K_{\alpha}^{\dagger} U_g^{\dagger}) . \quad (6.36)$$

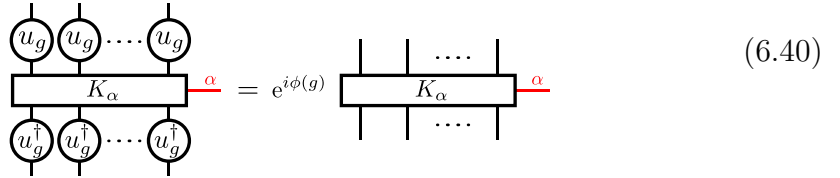
$$U_g K_\alpha^g U_g^\dagger = e^{i\theta_\alpha(g)} K_\alpha^g \quad \text{for } \forall \alpha \quad (6.37)$$
$$\begin{array}{c}
\textcircled{u_g} \quad \textcircled{u_g} \quad \dots \quad \textcircled{u_g} \\
\hline
\text{---} K_\alpha \text{---} \\
\hline
\textcircled{u_g^\dagger} \quad \textcircled{u_g^\dagger} \quad \dots \quad \textcircled{u_g^\dagger}
\end{array}
\begin{array}{c}
\text{---} \alpha \text{---}
\end{array}
= e^{i\phi_\alpha(g)}
\begin{array}{c}
\text{---} \text{---} \text{---} \text{---} \text{---} \\
\hline
\text{---} K_\alpha \text{---} \\
\hline
\text{---} \text{---} \text{---} \text{---} \text{---}
\end{array}
\begin{array}{c}
\text{---} \alpha \text{---}
\end{array}
\quad (6.38)$$

This is also the weak symmetry condition.

On the other hand, the strong symmetry condition is more strict condition than (6.37) or (6.38). The strong symmetry condition is defined as the condition where the each Kraus operator is invariant under the conjugate action of the symmetry group G up to a phase depending on the $g \in G$ (and independent of α)

$$U_g K_\alpha^g U_g^\dagger = e^{i\theta(g)} K_\alpha^g \quad \text{for } \forall \alpha \quad (6.39)$$

i.e.

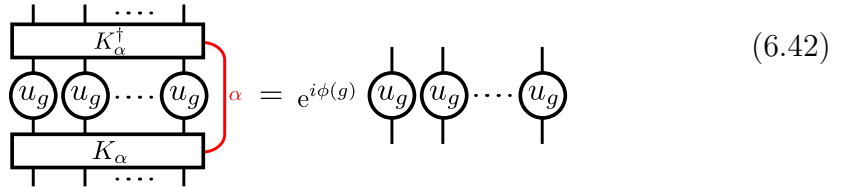


$$(6.40)$$

For the case of $\mathbb{Z}_2 \times \mathbb{Z}_2$, since $U_g = U_g^\dagger$, applying U_g from both left and right of each side of Eq. (6.39) leads to $e^{i\theta(g)} = \pm 1$. Note that if a certain set of the Kraus operators satisfies (6.39), so do *all* the others that are related by unitaries. Therefore, the strong-symmetry condition (6.39) does not depend on the particular choice of the Kraus operators. With the help of the completeness condition, this strong symmetry condition (6.40) can be rephrased as [101]:

$$\mathcal{E}^\dagger(U_g) := \sum_\alpha K_\alpha^\dagger U_g K_\alpha = e^{i\phi(g)} U_g, \quad (6.41)$$

i.e.



$$(6.42)$$

which means, in the Heisenberg picture, that after the time-evolution under $\mathcal{E}$, U_g is kept invariant up to a (g -dependent) phase.

Here, an important remark is in order about the relation between the symmetry conditions [Eqs. (6.37) and (6.39)] and the choice of a (linear) representation of the on-site symmetry group G . The symmetry conditions have the definite meanings only after a particular representation of G is given; even if a Kraus representation satisfies the strong symmetry condition for a certain representation of G , it may not for other representations. In Ref. [101], they defined the SPT order in the open quantum system based on the pattern of zeros of the string order parameter. That is, they defined a

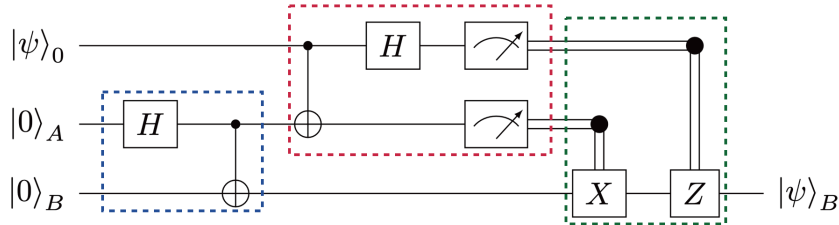
mixed state originated from the pure SPT state has the SPT order if the decohered state has the same pattern of zeros of the string order parameter as the pure case. They assert that this strong symmetry condition of the quantum noises rather than weak one is necessary for the SPT order to survive in open quantum system. In addition, the strong symmetry condition is sufficient condition if the quantum noise is uncorrelated, which means that the quantum noise is composite of the local noise: $\mathcal{E} = \circ_i \mathcal{E}_i$.

6.3 Measurement-Based Quantum computation

In this section, we review measurement-based quantum computation (MBQC). In subsection 6.3.1, we review the quantum teleportation, which is followed by the introduction of the gate teleportation in subsection 6.3.2 as the generalization of the quantum teleportation. Next, we see that MBQC is grounded in the principles of quantum teleportation.

6.3.1 quantum teleportation

In this subsection, as a preparation to explain the measurement-based quantum computing, we will briefly review the quantum teleportation. The quantum teleportation is a way to send a quantum state from one to another. In this method, generally, the sender has no information about the quantum state being sent, but it is possible to transmit it by sharing another entangled state between the sender and the receiver and by appropriately measuring the state at sender's side. Below, for simplicity, we consider quantum teleportation of a single qubit. The quantum circuit of the quantum teleportation looks like the following diagram:



Now, we quickly check the fact that the sender can transit one qubit state to the receiver by this quantum circuit. Let us define the state to be sent as $|\psi\rangle_0 = \alpha|0\rangle + \beta|1\rangle$. First,

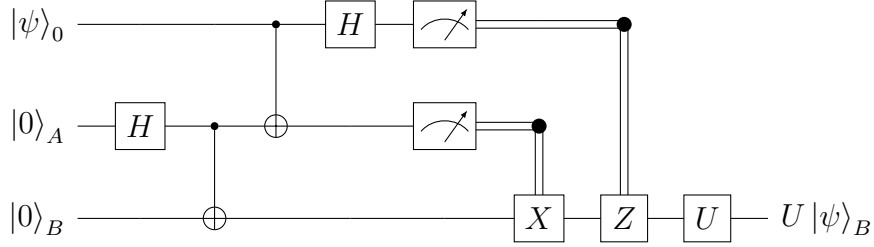
the portion enclosed by the blue dashed lines in this circuit diagram represents the stage of generating entanglement. Here, after applying Hadamard gate and controlled-X gate to $|00\rangle_{AB}$, the sender and the receiver share the maximally entangled pair $|\phi\rangle_{AB} := (|0\rangle_A |0\rangle_B + |1\rangle_A |1\rangle_B)/\sqrt{2}$. Next, the portion enclosed by red dashed lines corresponds to the stage of performing Bell measurements. The meter symbols in this quantum circuit describe the measurements in the computational basis $|0\rangle, |1\rangle$, so Bell measurement is a two-qubit projective measurement in the basis of $\{(|00\rangle + |11\rangle)/\sqrt{2}, (|00\rangle - |11\rangle)/\sqrt{2}, (|01\rangle + |10\rangle)/\sqrt{2}, (|01\rangle - |10\rangle)/\sqrt{2}\}$. Before the meter symbol, the entire system is

$$\begin{aligned}
H_0 CZ_{0A}(|\psi\rangle_0 \otimes |\phi\rangle_{AB}) &= H_0 \frac{1}{\sqrt{2}} (\alpha |0\rangle_0 |\phi\rangle_{AB} + \beta |1\rangle_0 (|01\rangle_{AB} + |10\rangle_{AB})) \\
&= \frac{1}{2} \left(|00\rangle_{0A} (\alpha |0\rangle_B + \beta |1\rangle_B) + |01\rangle_{0A} (\alpha |1\rangle_B + \beta |0\rangle_B) \right. \\
&\quad \left. + |10\rangle_{0A} (\alpha |0\rangle_B - \beta |1\rangle_B) + |11\rangle_{0A} (\alpha |1\rangle_B - \beta |0\rangle_B) \right) \\
&= \frac{1}{2} \left(|00\rangle_{0A} |\psi\rangle_B + |01\rangle_{0A} X_B |\psi\rangle_B \right. \\
&\quad \left. + |10\rangle_{0A} Z_B |\psi\rangle_B + |11\rangle_{0A} X_B Z_B |\psi\rangle_B \right) \\
&= \frac{1}{2} \sum_{x,z=0,1} |zx\rangle_{0A} \left(X_B^x Z_B^z |\psi\rangle_B \right) \tag{6.43}
\end{aligned}$$

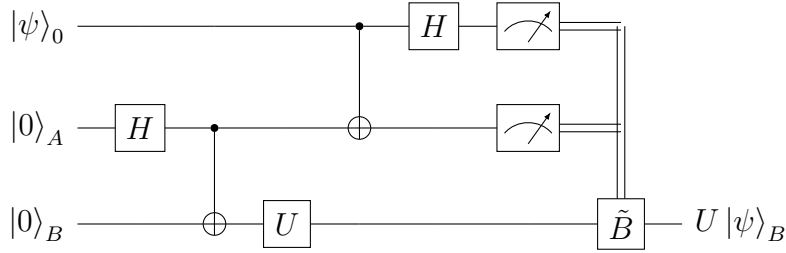
So, after the meter symbol, the whole system is projected onto $|zx\rangle_{0A} \left(X_B^x Z_B^z |\psi\rangle_B \right)$ ($x, z = 0, 1$) with the same probability $1/4$. Therefore, after the two-qubit measurement, the sender tell the result (two classical bits (x, z)) to the receiver via classical communication, and then, depending on the measurement result, the receiver apply $Z_B^z X_B^x$ to the one-qubit state on the receiver's side (the green dashed line in the quantum circuit above). In the end, the receiver has $|\psi\rangle$ in the receiver's hand. As shown here, the important thing is that we utilize the entanglement in order to transmit the quantum state.

6.3.2 gate teleportation

In this subsection, we generalize the quantum teleportation. This section considers the situation where the sender has $|\psi\rangle$ at first and then receiver has $U|\psi\rangle$ after the transmission. Trivially, we realize this by applying U after the teleportation:



Here, for simplicity, we consider the case where U is a Clifford operator, which transforms Pauli group to itself by the conjugate action. Under this condition, U can commute with the Pauli byproducts:



$\tilde{B}$ denotes the product of Pauli operators such that $BU = U\tilde{B}$, where the $B = Z_B^z X_B^x$ is the byproduct operator for the ordinary quantum teleportation in the last subsection. This circuit indicates that if we can prepare state $|\psi_U\rangle := \frac{1}{\sqrt{2}}(I \otimes U)(|00\rangle + |11\rangle)$ using a method other than directly implementing the gate U , it is possible to send the state $U|\psi\rangle$ instead of $|\psi\rangle$. Indeed, MBQC is based on this fact. There, we just only utilize measurements on some many-body state to create state $|\psi_U\rangle$ and ultimately perform quantum computations using measurements alone.

6.3.3 MBQC on the pure AKLT state and its one-qubit universality

Let us implement the MBQC on the AKLT state (with two additional spin-1/2's) (6.27),

$$|\psi\rangle = \sum_{\sigma_{\text{in/out}}} \sum_{\{m_i\}} (AP^{[m_1]}A \dots P^{[m_N]}A)_{\sigma_{\text{in}}\sigma_{\text{out}}} |\sigma_{\text{in}}\rangle |m_1 \dots m_N\rangle |\sigma_{\text{out}}\rangle \quad (6.44)$$

As already seen, the AKLT state has topologically protected edge states on the both ends, and we utilize this edge state as a qubit in the MBQC. The two additional spin-1/2's at both ends serve not only to obtain non-degenerate ground states, but also to initialize and read out qubits in MBQC. On the other hand, we realize literally the unitary gate by measurements.

Here, we realize Z -rotation $e^{-i\theta Z/2}$ with the MBQC on the AKLT state by measuring in the basis of $|\alpha_\theta\rangle_i$, $|\beta_\theta\rangle_i$, and $|\gamma\rangle_i$, which are respectively zero-eigenvectors of $S_i^x \cos(\theta/2) + S_i^y \sin(\theta/2)$ ($=: \tilde{S}_i^1$), $-S_i^x \sin(\theta/2) + S_i^y \cos(\theta/2)$ ($=: \tilde{S}_i^2$), and S_i^z :

$$|\alpha_\theta\rangle_i := \frac{1}{\sqrt{2}} \left\{ -e^{-i\frac{\theta}{2}} |1\rangle_i + e^{i\frac{\theta}{2}} |-1\rangle_i \right\}, \quad (6.45a)$$

$$|\beta_\theta\rangle_i := \frac{1}{\sqrt{2}} \left\{ e^{-i\frac{\theta}{2}} |1\rangle_i + e^{i\frac{\theta}{2}} |-1\rangle_i \right\}, \quad (6.45b)$$

$$|\gamma\rangle_i := |0\rangle_i. \quad (6.45c)$$

It is known that single measurement in this basis

$$\mathcal{P}(m) := \begin{cases} |\alpha_\theta\rangle\langle\alpha_\theta| & \text{when } m = \alpha_\theta \\ |\beta_\theta\rangle\langle\beta_\theta| & \text{when } m = \beta_\theta \\ |\gamma\rangle\langle\gamma| & \text{when } m = \gamma \end{cases} \quad (6.46)$$

realizes in the Z -rotation gate $U_Z(\theta) = e^{-i\theta Z/2}$ or identity gate probabilistically [84] except for $\theta = 0, 2\pi$. We quickly review this fact. Single measurement on site- i results in $|\alpha_\theta\rangle_i$, $|\beta_\theta\rangle_i$, or $|\gamma\rangle_i$. If we get the result $|\alpha_\theta\rangle$, the remaining state after the measurement will be

$$\begin{aligned} |\alpha_\theta\rangle\langle\alpha_\theta| |\psi_{\text{AKLT}}\rangle &= \sum_{\sigma_{\text{in/out}}} \sum_{\{m_k | k \neq i\}} A^{[\sigma_{\text{in}}]} P^{[m_1]} \dots A \left(\sum_{m_i} \langle\alpha_\theta | m_i\rangle P^{[m_i]} A \right) \\ &\dots P^{[m_N]} A^{T[\sigma_{\text{out}}]} |\sigma_{\text{in}}\rangle |m_1 \dots m_{i-1} \alpha_\theta m_{i+1} \dots m_N\rangle |\sigma_{\text{out}}\rangle. \end{aligned} \quad (6.47)$$

If we compile the results obtained now with those for the case of $|\beta\rangle$ and $|\gamma\rangle$,

$$\begin{array}{c} \text{III} \\ \text{---} \square \text{---} \square \text{---} \\ \text{---} \square \text{---} \square \text{---} \end{array} = \begin{cases} \sum_{m_i} \langle\alpha_\theta | m_i\rangle P^{[m_i]} A \propto X e^{-i\theta Z/2} \\ \sum_{m_i} \langle\beta_\theta | m_i\rangle P^{[m_i]} A \propto X Z e^{-i\theta Z/2} \\ \sum_{m_i} \langle\gamma | m_i\rangle P^{[m_i]} A \propto Z \end{cases} \quad (6.48)$$

Therefore, for a given AKLT state on a length- N spin-1 chain, the implementation of the Z -rotation gate proceeds as follows: First, we perform measurements in the

basis $|\alpha_\theta\rangle_i$, $|\beta_\theta\rangle_i$, and $|\gamma\rangle_i$ with the measurement angle θ until either the result $|\alpha_\theta\rangle$ or $|\beta_\theta\rangle$ (“desired” results) is obtained. When we obtain either of these two at a certain site, we set θ to 0, and measure the remaining sites with $\theta = 0$. This ensures that the probability of successfully implementing the Z -rotation gate is generally given by $1 - (1/3)^N$. Moreover, the obtained Z -rotation gate $e^{-i\theta Z/2}$ includes (i) I ($\theta = 0$), (ii) Z ($\theta = \pi$), (iii) S ($\theta = \pi/2$), (iv) T ($\theta = \pi/4$) gates, and as already noted, if $\theta = 0$, the MBQC on the pure AKLT state is deterministic. So, we can deterministically implement the identity gate by measuring in the basis of the zero-eigenstates of S^x, S^y, S^z .

In the same way, we can also implement the X -rotation gate $e^{-i\theta X/2}$. So, we can realize any one-qubit unitary gate by combining X -rotation gates and Z -rotation gates. As a result, the pure AKLT state is one-qubit universal resource.

6.3.4 MBQC on general ground states in Haldane phase and their computational power

In the last subsection, we saw that we can utilize the pure AKLT state as a one-qubit universal resource of the MBQC, which means that we can implement any one-qubit gate by the measurement on the pure AKLT state. In this subsection, we briefly describe how to evaluate the computational power of general ground states in Haldane phase. In the next subsection, we will introduce another way to quantify the computational power. In the Ref. [88], they found out the way to extract the ability to implement the identity gate from the MPS form of the general ground state in the Haldane phase, and the condition that the MPS tensor of the state with non-trivial SPT order should satisfies. MPS tensor in the basis of the zero-eigenstates of S^x, S^y, S^z can be decomposed as the following:

$$A[\alpha] = B_\alpha \otimes C_{\text{junk}}[\alpha], \quad (6.49)$$

where the B_α is an irreducible projective representation of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ and independent of the state in the Haldane phase, and the C_{junk} contains the information of the individual member of the Haldane phase. This equation means that MPS tensor in some special basis has the tensor product decomposition into the logical part, which is common throughout the Haldane phase and the junk part, and the former is the identity gate with Pauli byproduct operators acting on the logical qubits. This guarantees that we can implement the identity gate by measurement on any ground states in the Haldane phase in the basis (zero-eigenvectors of S^x, S^y, S^z), which is the common basis

throughout the phase.

This decomposition in Haldane phase guarantees that the ground state with SPT order can be utilized as the quantum wire, in other words, we can implement the identity gate in the common basis of measurement. In this sense, we can say that the identity gate is protected by the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

Later, it has been also revealed that any ground states in the Haldane phase are one-qubit universal resource [90]. The details of proof that the Haldane phase has uniform computational power throughout the phase go beyond the scope of this thesis, so we do not deal with it. However we should emphasize that any ground state in the Haldane phase has symmetry-protected qubit in their correlation space, and we can manipulate that in the proper manner.

6.3.5 the gate fidelity

Now, we introduce the gate fidelity, which quantifies the performance of a quantum state as the resource of the MBQC. The gate fidelity is defined the fidelity between two states as following:

$$F = \text{Tr}_{\text{in, out}} (\rho_U |\Phi_U\rangle\langle\Phi_U|) \quad (6.50)$$

Here, $|\Phi_U\rangle = \frac{1}{\sqrt{2}}(I \otimes U)(|00\rangle + |11\rangle)$ denotes the ideal resource state for gate U teleportation [86]. We have already seen that if we have $|\Phi_U\rangle$ we can implement gate U (§6.3.2). On the other hand, ρ_U is the resource state which may have been decohered by some noise, and this is defined as the mixed state we get after consecutive measurements:

$$\rho_U = \text{Tr}_{\text{in, out}} \left[\sum_{\mathbf{m}} B_{\text{out}}^{(\mathbf{m})} \mathbf{P}(\mathbf{m}) \rho \mathbf{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} \right] \quad (6.51)$$

Here, we abbreviate the consecutive projection operators $P_N(m_N)P_{N-1}(m_{N-1}) \cdots P_1(m_1)$ as $\mathbf{P}(\mathbf{m})$, and the measurement basis is the same as the case of the pure AKLT state. The fidelity between two quantum states is nothing but the inner product between them in the case where one of them is pure state. The ideal resource state of the Z -rotation gate is $|\psi_{U_Z(\theta)}\rangle = \frac{1}{\sqrt{2}}(|0\rangle_{\text{in}}|0\rangle_{\text{out}} + e^{i\theta}|1\rangle_{\text{in}}|1\rangle_{\text{out}})$. Therefore, using its stabilizer form, we can write the gate fidelity of $U_Z(\theta)$ gate as

$$F_{U_Z(\theta)} = \text{Tr}_{\text{in, out}} \left[\rho_{U_Z(\theta)} \left(\frac{I_{\text{in}}I_{\text{out}} + Z_{\text{in}}Z_{\text{out}}}{2} \right) \left(\frac{I_{\text{in}}I_{\text{out}} + X_{\text{in}}e^{-i\theta Z_{\text{out}}/2}X_{\text{out}}e^{i\theta Z_{\text{out}}/2}}{2} \right) \right]. \quad (6.52)$$

Chapter 7

The fidelity of Z -rotation gate on noisy AKLT states

In the last chapter, we have defined the gate fidelity of the MBQC on the noisy AKLT state, and in this chapter, we specifically examine the fidelity of Z -rotation gate.

$$\begin{aligned} F_{U_Z(\theta)} &= \text{Tr}_{\text{in, out}} \left[\rho_{U_Z(\theta)} \left(\frac{I_{\text{in}} I_{\text{out}} + Z_{\text{in}} Z_{\text{out}}}{2} \right) \left(\frac{I_{\text{in}} I_{\text{out}} + X_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}}{2} \right) \right] \\ &= \frac{1}{4} \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)}] + \frac{1}{4} \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}] + \frac{1}{4} \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\ &\quad + \frac{1}{4} \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} Z_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} Z_{\text{out}} e^{i\theta Z_{\text{out}}/2}] . \end{aligned} \tag{7.1}$$

We will see that this quantum-information-originated quantity is closely related to the physical string-order parameters (4).

7.1 Calculation of the gate fidelity of Z -rotation

7.1.1 ZZ -term

The gate fidelity (7.1) consists of four terms, each of which can be calculated exactly. The first of them which does not contain the Pauli operators just yields a trivial constant term $\frac{1}{4} \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)}] = 1/4$ in the gate fidelity. Therefore, all the non-trivial contributions come from the other three terms which we focus on in the following.

First, we calculate the second term $\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}]$. Now we show that this

term will be related to $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, more precisely, to the string order parameter:

$$\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}] = -\text{Tr} \left[\rho_{Z_{\text{in}}} \left(\prod_{j=1}^N e^{i\pi S_j^z} \right) Z_{\text{out}} \right]. \quad (7.2)$$

The calculation of the $Z_{\text{in}} Z_{\text{out}}$ -term in the gate fidelity (7.1) goes as in the case of the MBQC with the cluster state [108]. First, by the definition (6.51) of ρ_U and the cyclic property of the trace, the original expression can be recast as:

$$\begin{aligned} & \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}] \\ &= \text{Tr}_{\text{in, out}} \text{Tr} \sum_{\mathbf{m}} \left[B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \rho \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} Z_{\text{in}} Z_{\text{out}} \right] \\ &= \widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho Z_{\text{in}} \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} Z_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \right] \end{aligned} \quad (7.3)$$

with the trace $\widetilde{\text{Tr}} := \text{Tr}_{\text{in, out}} \text{Tr}$ taken over the composite system made of the spin-1 bulk and the two spin-1/2s at the edges. Without loss of generality, we can postulate the by-product operator $B_{\text{out}}^{(\mathbf{m})}$ as:

$$B_{\text{out}}^{(\mathbf{m})} = X_{\text{out}}^{r_X^{(\mathbf{m})}+1} Z_{\text{out}}^{r_Z^{(\mathbf{m})}+1}, \quad (7.4)$$

where $r_X^{(\mathbf{m})}$ is the number of times we get one of the results $\{|\alpha_\theta\rangle, |\beta_\theta\rangle, |\alpha_0\rangle, |\beta_0\rangle\}$ in successive measurements, and $r_Z^{(\mathbf{m})}$ is that for $\{|\beta_\theta\rangle, |\beta_0\rangle, |\gamma\rangle\}$. For later convenience, we also introduce $r_Y^{(\mathbf{m})}$ which counts how many times we obtain one of $\{|\alpha_\theta\rangle, |\alpha_0\rangle, |\gamma\rangle\}$. By definition, these three integers sum to an even integer, i.e.,

$$(-1)^{r_X^{(\mathbf{m})}+r_Y^{(\mathbf{m})}+r_Z^{(\mathbf{m})}} = 1. \quad (7.5)$$

Then, we can move one of the by-product operators to annihilate them leaving a sign factor $(-1)^{r_X^{(\mathbf{m})}+1}$:

$$B_{\text{out}}^{(\mathbf{m})\dagger} Z_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) = (-1)^{r_X^{(\mathbf{m})}+1} Z_{\text{out}} \mathcal{P}(\mathbf{m}). \quad (7.6)$$

To rewrite the sign factor $(-1)^{r_X^{(\mathbf{m})}}$ in terms of the string operator, we note that the states $\{|\alpha_\theta\rangle, |\beta_\theta\rangle, |\gamma\rangle\}$ are the eigenstates of $e^{i\pi S^z}$ for *any* θ (including $\theta = 0$). Specifi-

cally, we use the following relations:

$$\begin{aligned} \mathcal{P}_j(m_j)e^{i\pi S_j^z} &= \begin{cases} -|\alpha_\theta\rangle\langle\alpha_\theta|_j & m_j = \alpha_\theta \\ -|\beta_\theta\rangle\langle\beta_\theta|_j & m_j = \beta_\theta \\ |\gamma\rangle\langle\gamma|_j & m_j = \gamma \end{cases} \\ &= e^{i\pi S_j^z} \mathcal{P}_j(m_j) , \end{aligned} \quad (7.7a)$$

$$\begin{aligned} \mathcal{P}'_j(m_j)e^{i\pi S_j^z} &= \begin{cases} -|\alpha_{\theta=0}\rangle\langle\alpha_{\theta=0}|_j & m_j = \alpha_{\theta=0} \\ -|\beta_{\theta=0}\rangle\langle\beta_{\theta=0}|_j & m_j = \beta_{\theta=0} \\ |\gamma\rangle\langle\gamma|_j & m_j = \gamma \end{cases} \\ &= e^{i\pi S_j^z} \mathcal{P}'_j(m_j) . \end{aligned} \quad (7.7b)$$

From Eqs. (7.7), we immediately see that the sign factor originating from $X_{\text{out}}^{r_X^{(m)}+1}$ in the by-product operator is now replaced with the action of the string operator:

$$(-1)^{r_X^{(m)}+1} Z_{\text{out}} \mathcal{P}(\mathbf{m}) = -\mathcal{P}(\mathbf{m}) \left(\prod_{j=1}^N e^{i\pi S_j^z} \right) Z_{\text{out}} . \quad (7.8)$$

As the $\mathbf{m}$ -dependence appears only in $\mathcal{P}(\mathbf{m})$, we can explicitly carry out the summation over all the possible measurement outcomes $\{\mathbf{m}\}$ to obtain the final result (7.2):

$$\begin{aligned} &\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}] \\ &= -\widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho Z_{\text{in}} \mathcal{P}(\mathbf{m})^2 \left(\prod_{j=1}^N e^{i\pi S_j^z} \right) Z_{\text{out}} \right] \\ &= -\widetilde{\text{Tr}} \left[\rho Z_{\text{in}} \left(\sum_{\mathbf{m}} \mathcal{P}(\mathbf{m}) \right) \left(\prod_{j=1}^N e^{i\pi S_j^z} \right) Z_{\text{out}} \right] \\ &= -\widetilde{\text{Tr}} \left[\rho Z_{\text{in}} \left(\prod_{j=1}^N e^{i\pi S_j^z} \right) Z_{\text{out}} \right] , \end{aligned} \quad (7.9)$$

where we have utilized:

$$\begin{aligned} &\sum_{\mathbf{m}} \mathcal{P}(\mathbf{m}) \\ &= \sum_{\mathbf{m}} P'_N(m_N) \cdots P'_{l(\mathbf{m})+1}(m_{l(\mathbf{m})+1}) P_{l(\mathbf{m})}(m_{l(\mathbf{m})}) \cdots P_1(m_1) = I_3 . \end{aligned} \quad (7.10)$$

7.1.2 other two terms

The other two terms can be calculated similarly. The difference is that now we need two different string operators and that each term has dependence of the measurement outcome.

The third and fourth terms are calculated as:

$$\begin{aligned}
& \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\
&= \cos \theta \widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho X_{\text{in}} \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} X_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \right] \\
&+ \sin \theta \widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho X_{\text{in}} \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} Y_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \right]
\end{aligned} \tag{7.11a}$$

and

$$\begin{aligned}
& \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} Z_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} Z_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\
&= -\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Y_{\text{in}} e^{-i\theta Z_{\text{out}}/2} Y_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\
&= \sin \theta \widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho Y_{\text{in}} \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} X_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \right] \\
&- \cos \theta \widetilde{\text{Tr}} \sum_{\mathbf{m}} \left[\rho Y_{\text{in}} \mathcal{P}(\mathbf{m}) B_{\text{out}}^{(\mathbf{m})\dagger} Y_{\text{out}} B_{\text{out}}^{(\mathbf{m})} \mathcal{P}(\mathbf{m}) \right].
\end{aligned} \tag{7.11b}$$

As before, we move one of the by-product operators $B_{\text{out}}^{(\mathbf{m})}$ and $B_{\text{out}}^{(\mathbf{m})\dagger}$ [see Eq. (7.4)] to make them pair-annihilate:

$$\begin{aligned}
B_{\text{out}}^{(\mathbf{m})\dagger} X_{\text{out}} B_{\text{out}}^{(\mathbf{m})} &= (-1)^{r_Z^{(\mathbf{m})}+1} X_{\text{out}} \\
B_{\text{out}}^{(\mathbf{m})\dagger} Y_{\text{out}} B_{\text{out}}^{(\mathbf{m})} &= (-1)^{r_X^{(\mathbf{m})}+r_Z^{(\mathbf{m})}} Y_{\text{out}} = (-1)^{r_Y^{(\mathbf{m})}} Y_{\text{out}},
\end{aligned} \tag{7.12}$$

where we have used Eq. (7.5). Now we use the same trick as in (7.8). Specifically, we use the followings to rewrite the sign factors appearing when the by-product operator and the Pauli operators are exchanged:

$$\mathcal{P}_j(m_j) e^{i\pi \tilde{S}_i^x(\theta)} = \begin{cases} |\alpha_\theta\rangle \langle \alpha_\theta|_j & m_j = \alpha_\theta \\ -|\beta_\theta\rangle \langle \beta_\theta|_j & m_j = \beta_\theta \\ -|\gamma\rangle \langle \gamma|_j & m_j = \gamma \end{cases} \tag{7.13a}$$

$$\mathcal{P}'_j(m_j) e^{i\pi S_j^x} = \begin{cases} |\alpha_{\theta=0}\rangle \langle \alpha_{\theta=0}|_j & m_j = \alpha_{\theta=0} \\ -|\beta_{\theta=0}\rangle \langle \beta_{\theta=0}|_j & m_j = \beta_{\theta=0} \\ -|\gamma\rangle \langle \gamma|_j & m_j = \gamma. \end{cases} \tag{7.13b}$$

and similar relations for $\tilde{S}_i^y(\theta)$ and S_i^y :

$$\mathcal{P}_j(m_j)e^{i\pi\tilde{S}_i^y(\theta)} = \begin{cases} -|\alpha_\theta\rangle\langle\alpha_\theta|_j & m_j = \alpha_\theta \\ |\beta_\theta\rangle\langle\beta_\theta|_j & m_j = \beta_\theta \\ -|\gamma\rangle\langle\gamma|_j & m_j = \gamma \end{cases} \quad (7.14a)$$

$$\mathcal{P}'_j(m_j)e^{i\pi S_j^y} = \begin{cases} -|\alpha_{\theta=0}\rangle\langle\alpha_{\theta=0}|_j & m_j = \alpha_{\theta=0} \\ |\beta_{\theta=0}\rangle\langle\beta_{\theta=0}|_j & m_j = \beta_{\theta=0} \\ -|\gamma\rangle\langle\gamma|_j & m_j = \gamma . \end{cases} \quad (7.14b)$$

Note that $|\alpha_\theta\rangle$ and $|\beta_\theta\rangle$ are no longer the eigenstates of $e^{i\pi S_i^{x,y}}$. Therefore, in contrast to the case of the $Z_{\text{in}}Z_{\text{out}}$ -term, we must use two different operators $e^{i\pi\tilde{S}_i^{x,y}(\theta)}$ (twisted) and $e^{i\pi S_i^{x,y}}$ (untwisted) respectively for $\mathcal{P}_j$ and $\mathcal{P}'_j$ in order to have the correct sign factors [see Eq. (7.7)]. To be specific, we have the following expressions:

$$\begin{aligned} B_{\text{out}}^{(\mathbf{m})\dagger} X_{\text{out}} B_{\text{out}}^{(\mathbf{m})} &= (-1)^{r_Z^{(\mathbf{m})}+1} X_{\text{out}} \mathcal{P}(\mathbf{m}) \\ &= -\mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(x)}(\theta; l(\mathbf{m})) X_{\text{out}} \end{aligned} \quad (7.15a)$$

and

$$\begin{aligned} B_{\text{out}}^{(\mathbf{m})\dagger} Y_{\text{out}} B_{\text{out}}^{(\mathbf{m})} &= (-1)^{r_Y^{(\mathbf{m})}} Y_{\text{out}} \mathcal{P}(\mathbf{m}) \\ &= \mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(y)}(\theta; l(\mathbf{m})) Y_{\text{out}} , \end{aligned} \quad (7.15b)$$

where we have introduced the following generalized string operator:

$$\mathcal{O}_{\text{str}}^{(a)}(\theta; l) := \left(\prod_{j=1}^l e^{i\pi\tilde{S}_j^a(\theta)} \right) \left(\prod_{k=l+1}^N e^{i\pi S_k^a} \right) \quad (a = x, y) . \quad (7.15c)$$

Note that the string operator is switched from the twisted one to the untwisted one at the site $l(\mathbf{m})$. Plugging Eqs. (7.15a) and (7.15b) into (7.11a) and (7.11b), we obtain:

$$\begin{aligned} &\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\ &= -\text{Tr} \sum_{\mathbf{m}} \left[\rho X_{\text{in}} \mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(x)}(\theta; l(\mathbf{m})) X_{\text{out}} \right] \cos\theta + \text{Tr} \sum_{\mathbf{m}} \left[\rho X_{\text{in}} \mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(y)}(\theta; l(\mathbf{m})) Y_{\text{out}} \right] \sin\theta \end{aligned} \quad (7.16a)$$

and

$$\begin{aligned} &\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} Z_{\text{in}} e^{-i\theta Z_{\text{out}}/2} Z_{\text{out}} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\ &= -\text{Tr} \sum_{\mathbf{m}} \left[\rho Y_{\text{in}} \mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(x)}(\theta; l(\mathbf{m})) X_{\text{out}} \right] \sin\theta - \text{Tr} \sum_{\mathbf{m}} \left[\rho Y_{\text{in}} \mathcal{P}(\mathbf{m}) \mathcal{O}_{\text{str}}^{(y)}(\theta; l(\mathbf{m})) Y_{\text{out}} \right] \cos\theta . \end{aligned} \quad (7.16b)$$

$\left(\prod_{j=1}^{l(\mathbf{m})} e^{i\pi\tilde{S}_j^{x,y}(\theta)}\right)$ (*twisted*) and $\left(\prod_{j=l(\mathbf{m})+1}^N e^{i\pi S_j^{x,y}}\right)$ (*untwisted*) to write down the expressions similar to Eq. (7.8). As a result, we obtain:

$$\begin{aligned} & \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} e^{i\theta Z_{\text{out}}/2}] + \text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} X_{\text{in}} Z_{\text{in}} e^{-i\theta Z_{\text{out}}/2} X_{\text{out}} Z_{\text{out}} e^{i\theta Z_{\text{out}}/2}] \\ &= -\text{Tr} \sum_{\mathbf{m}} \left[\rho(X_{\text{in}} \cos \theta + Y_{\text{in}} \sin \theta) \mathcal{P}(\mathbf{m}) \left(\prod_{j=1}^{l(\mathbf{m})} e^{i\pi\tilde{S}_j^x(\theta)} \right) \left(\prod_{j=l(\mathbf{m})+1}^N e^{i\pi S_j^x} \right) X_{\text{out}} \right] \\ & \quad - \text{Tr} \sum_{\mathbf{m}} \left[\rho(-X_{\text{in}} \sin \theta + Y_{\text{in}} \cos \theta) \mathcal{P}(\mathbf{m}) \left(\prod_{j=1}^{l(\mathbf{m})} e^{i\pi\tilde{S}_j^y(\theta)} \right) \left(\prod_{j=l(\mathbf{m})+1}^N e^{i\pi S_j^y} \right) Y_{\text{out}} \right]. \end{aligned} \quad (7.17)$$

It is important to note that, in contrast to the term $\text{Tr}_{\text{in, out}} [\rho_{U_Z(\theta)} Z_{\text{in}} Z_{\text{out}}]$, this is not of the form of the *ordinary* string order parameter in the sense that the operator strings consist of the two different elements of $\mathbb{Z}_2$ [i.e., the twisted ($e^{i\pi\tilde{S}_j^a(\theta)}$) and untwisted ($e^{i\pi S_j^a}$) ones]. Only for $\theta = 0$ at which $\tilde{S}_i^x(0) = S_i^x$ and $\tilde{S}_i^y(0) = S_i^y$, the twist is absent and the fidelity for the identity gate $U_Z(\theta = 0) = I$ reduces to the sum of the three string order parameters:

$$F_I = \frac{1}{4} - \frac{1}{4} \sum_{a=1,2,3} \text{Tr} \left[\rho \mathcal{X}_{\text{in}}^{(a)} \left(\prod_{j=1}^N e^{i\pi S_j^a} \right) \mathcal{X}_{\text{out}}^{(a)} \right] \quad (7.18a)$$

with $\mathcal{X}_{\text{in/out}}^{(a)}$ and S_j^a defined by:

$$(\mathcal{X}_{\text{in/out}}^{(a)}, S_j^a) = \begin{cases} (X_{\text{in/out}}, S_j^x) & \text{for } a = 1 \\ (Y_{\text{in/out}}, S_j^y) & \text{for } a = 2 \\ (Z_{\text{in/out}}, S_j^z) & \text{for } a = 3. \end{cases} \quad (7.18b)$$

In summary, the fidelity for the Z -rotation gate $U_Z(\theta) = e^{-i\theta Z/2}$ contains the string order parameter as well as other non-local string-like operators, and especially for the identity gate $I = U_Z(\theta = 0)$, the gate fidelity coincides with the sum of the string order parameters corresponding to the representation $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ of $\mathbb{Z}_2 \times \mathbb{Z}_2$.

7.1.3 Ground-state gate fidelity

In this subsection, we proceed with the calculation in the previous subsections when ρ is pure: $\rho = |\psi\rangle\langle\psi|$ with $|\psi\rangle$ being a G -symmetric AKLT state $|\psi_{\text{AKLT}}\rangle$ satisfying

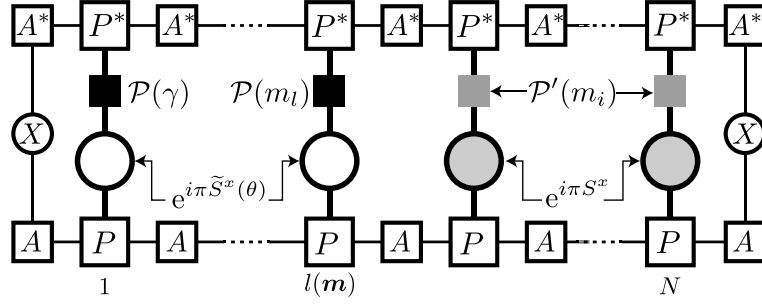


Figure 7.1: A typical term that appears in the first line on the right-hand side of Eq. (7.16a). The symbols $\blacksquare$ and $\blacksquare$ denote the application of the projective measurement (6.48) with generic θ and $\theta = 0$, respectively. (Reproduced from Ref. [105])

The first equality of Eq. (7.20) holds since both transfer matrices

$$\begin{array}{c}
 \begin{array}{c} \text{---} A^* \text{---} P^* \text{---} \\ \blacksquare \mathcal{P}(\gamma) \\ \text{---} A \text{---} P \text{---} \end{array} \quad \text{and} \quad \begin{array}{c} \text{---} P^* \text{---} A^* \text{---} \\ \blacksquare \mathcal{P}'(m_i) \\ \text{---} P \text{---} A \text{---} \end{array} \\
 e^{i\pi \tilde{S}^x(\theta)} \quad \quad \quad e^{i\pi S^x}
 \end{array} \quad (7.21)$$

respectively have the left and right eigenvectors $\begin{array}{c} \text{---} X \end{array}$ and $\begin{array}{c} \text{---} Y \end{array}$ with the same eigenvalue $1/3$, while the second equality holds since

$$\begin{array}{c} \text{---} A^* \text{---} P^* \text{---} \\ \blacksquare \mathcal{P}(\alpha_\theta), \\ \blacksquare \mathcal{P}(\beta_\theta) \\ \text{---} A \text{---} P \text{---} \end{array} e^{i\pi \tilde{S}^x(\theta)} = \frac{\cos \theta}{3} \begin{array}{c} \text{---} X \end{array} - \frac{\sin \theta}{3} \begin{array}{c} \text{---} Y \end{array}. \quad (7.22)$$

On the other hand, when we obtain the result $\mathbf{m} = (\gamma, \gamma, \dots, \gamma)$,

$$\begin{array}{c} \text{---} A^* \text{---} P^* \text{---} A^* \text{---} \dots \text{---} P^* \text{---} A^* \text{---} \\ \blacksquare \mathcal{P}(\gamma) \quad \mathcal{P}(\gamma) \blacksquare \\ \text{---} X \end{array} e^{i\pi \tilde{S}^x(\theta)} = \left(\frac{1}{3} \right)^N. \quad (7.23)$$

Therefore, when the summation over $\mathbf{m}$ is carried out, the first line of the right-hand side of Eq. (7.16a) is $\{(1 - \frac{1}{3^N}) \cos \theta + \frac{1}{3^N}\} \cos \theta$. Then, the sum of (7.16a) and (7.16b) is given by:

$$2 \left(1 - \frac{1}{3^N} \right) + \frac{2}{3^N} \cos \theta. \quad (7.24)$$

Consequently, the fidelity (7.1) for the Z -rotation gate on the pure AKLT state $\rho = |\psi_{\text{AKLT}}\rangle\langle\psi_{\text{AKLT}}|$ reads:

$$F_{U_Z(\theta)} = 1 - \frac{1}{2 \cdot 3^N} (1 - \cos\theta) . \quad (7.25)$$

Alternatively, the same result could have been obtained in another simpler way. We first note

$$\rho_U = \left(1 - \frac{1}{3^N}\right) |\psi_U\rangle\langle\psi_U| + \frac{1}{3^N} |\psi_I\rangle\langle\psi_I| \quad (7.26)$$

for $\rho = |\psi_{\text{AKLT}}\rangle\langle\psi_{\text{AKLT}}|$, since always the ideal resource state $|\psi_U\rangle$ is obtained except for the case $\mathbf{m} = (\gamma, \gamma, \dots, \gamma)$ which occurs with a probability $1/3^N$. By substituting this into the definition of the gate fidelity (6.50), we reproduce the result Eq. (7.25). Therefore, the fidelity of the MBQC on the pure AKLT state in general is smaller than 1 when the system size N is finite, and in the limit $N \rightarrow \infty$, it approaches 1 for any gate U since, for any U , $\rho_U \rightarrow |\psi_U\rangle\langle\psi_U|$ in this limit. The fact that the gate fidelity of the MBQC on the pure AKLT state can generally be less than 1 for finite system sizes reflects that the MBQC is not deterministic but probabilistic (as is suggested by the term $1/3^N$) except for $\theta = 0, \pi$. However, that we have obtained F_U smaller than 1 here must be distinguished from the reduction due to external noises, since we can completely trace the probabilistic failures in the MBQC on the pure AKLT state.

Chapter 8

Effects of noise on gate fidelity

In the previous chapter, we calculated the fidelity of Z -rotation gate with respect to a general state, and specifically, we thoroughly discussed the gate fidelity in the ground state i.e. in the case without noises. In this chapter, we examine the behavior of the fidelity under various specific noises to show that our results are consistent with the known ones [101]. Furthermore, the gate fidelity gives us more detailed information on the structure of decohered SPT phases, compared to the existing methods based on (non-local) order parameters. We focus on the site-wise uncorrelated noise $\mathcal{E} = \circ_i \mathcal{E}_i$ below. Our numerical calculations used the ITensor library [64].

8.1 Symmetry condition and gate fidelity

Before discussing the open quantum systems subject to some specific noises, we introduce a very useful proposition that relates the performance of MBQC to the strong symmetry condition:

Proposition 1. *The fidelity of the identity gate does not decay by an uncorrelated noise, i.e., $F_I = 1$ on the noisy AKLT state if and only if the noise $\mathcal{E}$ satisfies the strong symmetry condition (6.39) for the canonical (linear) representation $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ of the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetry.*

A remark is on order here about the choice of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ representation. Since the AKLT state is isotropic, one may think that the same statement holds for any other representations that are related to the canonical one by rotation after due modification of the Kraus operators. However, the measurement basis (6.45a)-(6.45c) already fix the directions and the canonical representation is crucial for the statement.

We can easily check the above statement. By Eqs. (6.42) and (7.18a), if a quantum noise satisfies the strong symmetry condition, then the gate fidelity does not decay. Conversely, if $F_I = 1$ on a noisy AKLT state, each of the four terms in Eq. (7.18a) must take its maximal value, which is possible only when the strong symmetry condition holds. The fact that we can perfectly perform the identity gate even on the noisy AKLT state under the strongly symmetric channel can be checked by directly probing the MPO tensor of the mixed state. (See Sec. 8.3)

The Prop. 1 suggests that the strong symmetry condition is not sufficient for the noisy AKLT state to be a one-qubit universal resource of MBQC necessitating stronger conditions for this purpose. In the following section, by demonstrating the numerical results, we will see that the strong $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry of quantum noises is not sufficient for the one-qubit universal computation.

8.2 Discrete time-evolution of the fidelity of Z -rotation gate under some symmetric noises

In this section, we consider the discrete time-evolution of the SPT states under the repeated application of quantum noises described by (6.32).

Precisely, we calculate the gate fidelity F_U at each time step by replacing $\tilde{\rho}$ in (6.51) with the one obtained after the step. First, by calculating the gate fidelities against noises shown in Table 8.1, we numerically show that time-reversal symmetry of the decohered state does not affect the fidelity of the Z -rotation gate. Then, we will see, as mentioned in the previous section, that the strong symmetry condition (6.39) or (6.42) alone is not sufficient for the implementation of the Z -rotation gate, not to mention, realization of the one-qubit universal computation. We will derive the condition to implement the Z -rotation gate and prove that any non-trivial quantum channel disables the one-qubit universal computation in our MBQC scheme.

To be specific, we restrict ourselves to uncorrelated quantum channels of the following form:

$$\begin{aligned} \mathcal{E} &= \mathcal{E}_1 \circ \mathcal{E}_2 \circ \cdots \circ \mathcal{E}_N, \\ \mathcal{E}_i(\rho) &= (1-p)\rho + \frac{p}{n} \sum_{\alpha=1}^n \mathcal{K}_\alpha \rho \mathcal{K}_\alpha^\dagger. \end{aligned} \tag{8.1}$$

Note that $\mathcal{E}_i$ acts only on the spin-1 Hilbert space at site- i . With a slight abuse of terminologies, we call the operators $\{\mathcal{K}_\alpha\}$ appearing here the Kraus operators as well

	Kraus op. $\{\mathcal{K}_\alpha\}$	$\mathbb{Z}_2 \times \mathbb{Z}_2$	time-reversal
Noise 1	$\{1, e^{i\pi S_x}, e^{i\pi S_y}, e^{i\pi S_z}\}$	S.S.	S.S.
Noise 2	$\{1, S_x S_y S_z, \text{ and perm.}\}$	S.S.	W.S.
Noise 3	$\{1, S_x S_y, S_y S_z, S_z S_x\}$	W.S.	S.S.
Noise 4	$\{1, e^{i\pi S_z}\}$	S.S.	S.S.

Table 8.1: Several quantum noises considered and the corresponding Kraus operators $\{\mathcal{K}_\alpha\}$ [see Eq. (8.1)]. These noises are either weakly symmetric [W.S.; see Eq. (6.38) for the definition] or strongly symmetric [S.S.; (6.39)] under the symmetry operations $\mathbb{Z}_2 \times \mathbb{Z}_2$ and time-reversal. “Noise 1” is called “dephasing” in Ref. [101].

although they do not satisfy the usual completeness relation. Below, we consider the AKLT states subject to the four types of quantum noises shown in Table 8.1.

Let us begin with Noise 1 defined by the Kraus operators $\{1, e^{i\pi S_x}, e^{i\pi S_y}, e^{i\pi S_z}\}$ (see Table 8.1). Below, all the numerical simulations were done for the AKLT chain with $N = 7$ $S = 1$ spins (and two spin-1/2s at the ends) and for the error rate $p = 0.25$. The discrete time-evolution of the fidelity F_U for the Z -rotation gate $U = e^{-i\theta Z/2}$ is shown in Fig. 8.1 for several values of θ . Since Noise 1 satisfies the strong symmetry condition (6.39) for a particular representation $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ of the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$, the fidelity F_U of the identity gate ($\theta = 0$) stays at unity as guaranteed by Prop. 1. However, the fidelity of the Z -rotation gate $e^{-i\theta Z/2}$ decays for $\theta \neq 0$, which means that we cannot “practically” implement the generic Z -rotation under this noise, that is, the noisy AKLT state is no longer a one-qubit universal resource.

For Noise 2 in Table 8.1, we obtained essentially the same results (see Fig. 8.2). The only difference between the two cases is that Noise 1 respects the strong time-reversal symmetry, while Noise 2 does not. Therefore, we can conclude that the strong symmetry condition with respect to time-reversal symmetry does not affect the gate fidelity essentially. This is expected from the fact that the gate fidelity is given by a sum of string-like operators associated to the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry as we have shown in Sec. 7.1.

As is seen in Fig. 8.3, the situation is drastically different for Noise 3 which respects the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetry only weakly (see Table 8.1). Now the gate fidelity F_U quickly damped to its lowest possible value 1/4 for *all* θ (including $\theta = 0$). This is to be contrasted to the behavior under Noise 4 (see Fig. 8.4) which is strongly symmetric

under $\mathbb{Z}_2 \times \mathbb{Z}_2$; there F_U never decays and stays at a constant (7.25) determined by the system size N as well as θ . Since the value $1/4$ is equal to F_U for the maximally mixed state, it is clear that under noises that are strongly symmetric with respect to time reversal but not to the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$, the AKLT state totally loses its computational power.

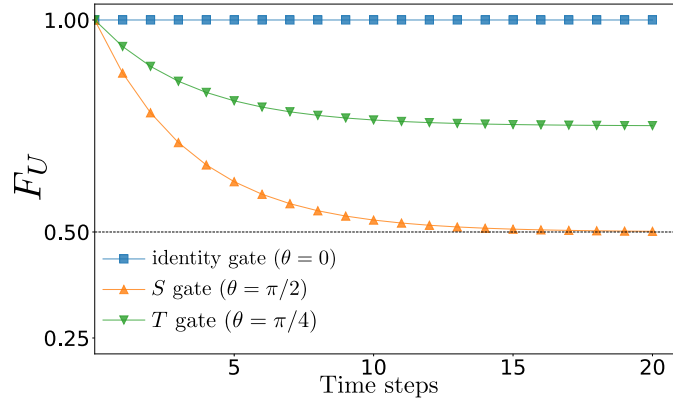


Figure 8.1: Discrete time-evolution of the gate fidelity F_U for $U = e^{-i\theta Z/2}$ under Noise 1 (called “dephasing” in Ref. [101]) in Table 8.1. The asymptotic value for the gate $e^{-i\theta Z/2}$ is given by $(1 + \cos^2\theta)/2$. (Reproduced from Ref. [105])

The weak symmetry condition (6.33) guarantees that if the initial ρ has the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, then the decohered $\mathcal{E}(\rho)$ respects the same symmetry: $U_g \mathcal{E}[\rho] U_g^\dagger = \mathcal{E}[U_g \rho U_g^\dagger] = \mathcal{E}[\rho]$. Therefore, the fact that we are not able to implement the MBQC on the state decohered by a weakly symmetric noise suggests the following two possibilities. The first is that the preservation of the protecting symmetry ($\mathbb{Z}_2 \times \mathbb{Z}_2$, here) alone does not ensure the existence of the symmetry-protected edge states unlike in the case of the pure state. In fact, it has been demonstrated recently [109] that the strong symmetry condition is necessary for the well-defined edge states to exist in the steady states of the Lindbladian dynamics. The second possibility is that the protected edge states still exist, whereas we cannot accurately manipulate them. Unfortunately, however, we are not able to determine which of the two is the case based on our present numerical results.

Next, let us compare the results in Fig. 8.1 (obtained for Noise 1) and in Fig. 8.4 (for Noise 4). Both of types satisfy the strong symmetry conditions for $\mathbb{Z}_2 \times \mathbb{Z}_2$ and

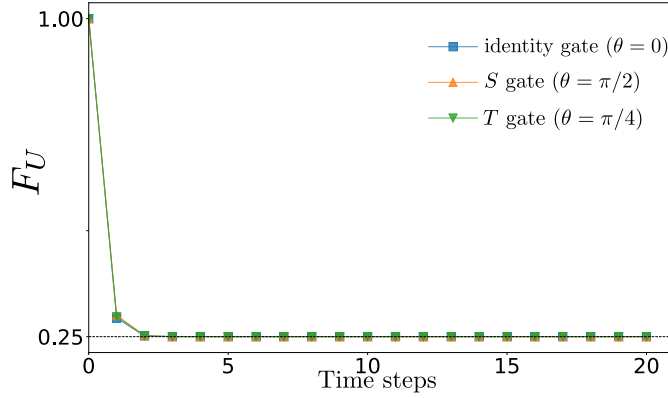


Figure 8.3: Discrete time-evolution of the gate fidelity F_U for $U = e^{-i\theta Z/2}$ under the weakly symmetric Noise 3 (see Table 8.1). For all cases (including $\theta = 0$), F_U quickly converges to its minimal value $1/4$. As noted in the main text, this value is the same as in the case of MBQC on the maximally mixed state. (Reproduced from Ref. [105])

proof of Lemma. 1

First, we prove the following Lemma 2:

Lemma 2. *If $G = \mathbb{Z}_2 \times \mathbb{Z}_2$ the phase of the right-hand side of Eq. (6.39) is $e^{i\theta(g)} = 1$ for all $g \in G$.*

Without loss of generality, we can choose $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$. By Eq. (6.39),

$$K_p = U_g(U_g K_p U_g)U_g = e^{i\theta(g)}U_g K_p U_g = (e^{i\theta(g)})^2 K_p, \quad (8.3)$$

for $\forall \alpha$ since $U_g = U_g^\dagger$. So,

$$e^{i\theta(g)} = \pm 1 \quad (\text{for } \forall g). \quad (8.4)$$

Next, we show $e^{i\theta(g)}$ can not be -1 for any g . Multiplying both sides of Eq. (6.39) by $\mathcal{P}(m)$ and $\mathcal{P}(m')$ ($m, m' = \alpha, \beta, \gamma$) respectively yields the following equation:

$$\mathcal{P}(m)(U_g K_p U_g)\mathcal{P}(m') = e^{i\theta(g)}\mathcal{P}(m)K_p\mathcal{P}(m') \quad (8.5)$$

Now, let K_p be

$$K_p = \begin{pmatrix} a_p & b_p & c_p \\ d_p & e_p & f_p \\ g_p & h_p & i_p \end{pmatrix} \quad (8.6)$$

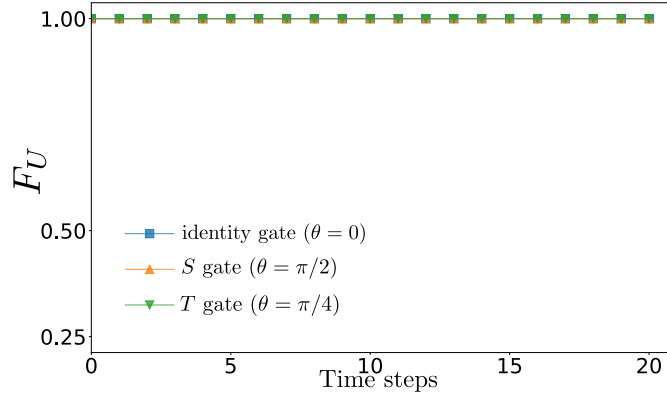


Figure 8.4: Discrete time-evolution of the gate fidelity F_U for $U = e^{-i\theta Z/2}$ under Noise 4 in Table 8.1. The F_U stays at a constant $1 - \frac{1}{2 \cdot 3^N}(1 - \cos\theta)$ ($N = 7$), which is the value for the *pure* AKLT state $\rho = |\psi_{\text{AKLT}}\rangle\langle\psi_{\text{AKLT}}|$ [see Eq. (7.25)]. (Reproduced from Ref. [105])

in the basis of α, β, γ . For each g ,

- $U_g = e^{i\pi S^x}$
When $e^{i\theta(g)} = 1$, $b_p = c_p = d_p = g_p = 0$ for $\forall p$, and otherwise $a_p = e_p = f_p = h_p = i_p = 0$.
- $U_g = e^{i\pi S^y}$
When $e^{i\theta(g)} = 1$, $b_p = d_p = f_p = h_p = 0$ for $\forall p$, and otherwise $a_p = c_p = e_p = g_p = i_p = 0$.
- $U_g = e^{i\pi S^z}$
When $e^{i\theta(g)} = 1$, $c_p = f_p = g_p = h_p = 0$ for $\forall p$, and otherwise $a_p = b_p = d_p = e_p = i_p = 0$.

Let u_g, u_h, u_{gh} respectively denote $e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}$. Then,

Case 1 $(e^{i\theta(g)}, e^{i\theta(h)}, e^{i\theta(gh)}) = (1, 1, -1)$

In this case, $K_p = O$ for $\forall p$.

Case 2 $(e^{i\theta(g)}, e^{i\theta(h)}, e^{i\theta(gh)}) = (1, -1, -1)$

In this case,

$$K_p = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & f_p \\ 0 & h_p & 0 \end{pmatrix} \quad (8.7)$$

for $\forall p$. However, these K_p 's do not satisfy $\sum_p K_p^\dagger K_p = I_3$.

Case 3 $(e^{i\theta(g)}, e^{i\theta(h)}, e^{i\theta(gh)}) = (-1, -1, -1)$

In this case, $K_p = O$ for $\forall p$.

We can easily check remaining patterns in the same manner, and neither case is suitable, so eventually $e^{i\theta(g)} = 1$ for $\forall g$.

Corollary 1. *If $\{K_p\}$ satisfies the strong symmetry condition for $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$,*

- K_p 's are diagonal in the basis of α, β, γ .
- $K_p \mathcal{P}(m) = \mathcal{P}(m) K_p$ for $\forall p, m$

Conversely, if $K_p \mathcal{P}(m) = \mathcal{P}(m) K_p$,

$$\begin{aligned} U_g K_p \mathcal{P}(m) U_g &= U_g \mathcal{P}(m) K_p U_g, \\ \implies U_g K_p \mathcal{P}(m) &= \mathcal{P}(m) K_p U_g, \\ \implies \sum_m U_g K_p \mathcal{P}(m) &= \sum_m \mathcal{P}(m) K_p U_g, \\ \implies U_g K_p &= K_p U_g, \end{aligned}$$

so $\{K_p\}$ is strongly symmetric for $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$. Therefore, $K_p \mathcal{P}(m) = \mathcal{P}(m) K_p$ for $\forall p, m$ and the statement that a quantum channel satisfies the strong symmetry condition for $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ are equivalent.

Furthermore,

$$\begin{aligned} K_p \mathcal{P}(m) &= \mathcal{P}(m) K_p \\ \implies \sum_p K_p^\dagger K_p \mathcal{P}(m) &= \sum_p K_p^\dagger \mathcal{P}(m) K_p \\ \implies \mathcal{P}(m) &= \sum_p K_p^\dagger \mathcal{P}(m) K_p. \end{aligned}$$

On the contrary, if $\sum_p K_p^\dagger \mathcal{P}(m) K_p = \mathcal{P}(m)$,

$$\begin{aligned}
& \sum_p (P(m)K_p - K_p P(m))^\dagger (P(m)K_p - K_p P(m)) \\
&= \sum_p K_p^\dagger P(m) K_p - P(m) \left(\sum_p K_p^\dagger P(m) K_p \right) \\
&\quad - \left(\sum_p K_p^\dagger P(m) K_p \right) P(m) + P(m) \left(\sum_p K_p^\dagger K_p \right) P(m) \\
&= 0,
\end{aligned} \tag{8.8}$$

and $(P(m)K_p - K_p P(m))^\dagger (P(m)K_p - K_p P(m))$ are positive, so $P(m)K_p = K_p P(m)$. Hence, Lemma 1 holds.

Finally, the proposition that the gate fidelity of $e^{-i\theta' Z/2}$ does not decay is equivalent to Eq. (8.2) for both $\theta' = 0$ and $\theta' = \theta$. So, by Lemma 1, Proposition 2 holds.

Having obtained the condition for the Z -rotation gate to be implementable on the decohered states, we now look for the condition for one-qubit universal computation. Specifically, we ask if the identity 1, the X , and Z -rotation gates can be executed. For the first two gates to be executable, the Kraus operators $\mathcal{K}_\alpha$ in Eq. (8.1) must be strongly symmetric with respect to both the canonical and rotated representations of $\mathbb{Z}_2 \times \mathbb{Z}_2$, which means $\mathcal{K}_\alpha = \text{diag}(a_\alpha, b_\alpha, a_\alpha)$ in the S^z -diagonal basis (with a constraint $\sum_\alpha |a_\alpha|^2 = \sum_\alpha |b_\alpha|^2 = 1$). For the fidelity of the X -rotation gate $e^{-i\theta X/2}$ not to decay, $\mathcal{K}_\alpha$ should have the same form $\text{diag}(a_\alpha, b_\alpha, a_\alpha)$ in the S^x -diagonal basis, which is possible only when $a_\alpha = b_\alpha$. Therefore, to implement both the Z -rotation and the X -rotation gates $e^{-i\theta Z/2}$ and $e^{-i\theta' X/2}$ with high fidelity, $\mathcal{K}_\alpha$ should be proportional to the identity I_3 for all α , i.e., the quantum channel $\mathcal{E}$ in Eq. (8.1) is identity. This may be summarized as the following statement:

Proposition 3. *When we consider the discrete time-evolution, we can realize the one-qubit universal computation on $\mathcal{E}(\rho)$ if and only if the channel is trivial: $\mathcal{E}(\rho) = \rho$.*

Of course, in the case of continuous time-evolution, the time interval can be chosen arbitrarily and we do not rule out the possibility that noisy AKLT states could work as a one-qubit universal resource for an interval sufficiently longer than the time scale for experimentally manipulating qubits.

8.3 Phase structure from computational-power perspective

Now, let us summarize what we conclude from the results in this chapter. In Sec. 8.1, we showed that quantum noise respecting the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ in the strong sense is the necessary and sufficient condition for implementing the identity gate (Prop. 1). To implement the Z -rotation gate $e^{-i\theta Z/2}$ in our MBQC scheme, we need a much stronger condition as has been shown in Sec. 8.2; if a quantum noise satisfies the strong symmetry condition for *all* the $\mathbb{Z}_2 \times \mathbb{Z}_2$ representations of the form $\{1, e^{i\pi \tilde{S}^x(\theta)}, e^{i\pi \tilde{S}^y(\theta)}, e^{i\pi S^z}\}$ (not only for $\theta = 0$), then we can implement Z -rotation gate without decay of the fidelity (Prop. 2). In general, the capability of high-fidelity one-qubit universal computation within our MBQC protocol is gone in any non-trivial quantum channel (Prop. 3).

Our initial goal was to characterize the SPT order in open quantum systems from the perspective of MBQC computational power. The method using the gate fidelity of MBQC not only yields the results consistent with those of the previous research [101] but also suggests a richer structure in the SPT order in open quantum systems. Specifically, as is seen in Fig. 8.5, we can categorize the noisy AKLT states according to what kind of unitary gates we can implement by MBQC on the decohered states. Here, we say that a given gate U can be implemented when the corresponding fidelity F_U does not decrease from its value in the pure case [e.g., Eq. (7.25)]. According to this scheme, the mixed-state SPT phase in the sense of Ref. [101] corresponds to the decohered AKLT states in which the identity gate can be implemented (see the blue region in Fig. 8.5). Among the dissipation considered here, the Noise 1 and 2, that are strongly symmetric with respect to $\mathbb{Z}_2 \times \mathbb{Z}_2$ defined by $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$, lead the initial AKLT state to this subphase.

In another phase (the green region) that results from strongly-symmetric noises (e.g., the Noise 4) satisfying the condition (6.39) both for the canonical and for *another* representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$, the Z -rotation gate is also possible. The non-local order parameter [see Eq. (7.17)] that captures this phase is not the standard string order parameter used in the previous treatment [101]. Phases capable of universal MBQC (the red point in Fig. 8.5) result only from a trivial channel. This way, the gate fidelity reveals the rich structure in the decohered AKLT states that cannot be captured by the string order parameter alone.

On the other hand, there remain delicate problems when trying to characterize the

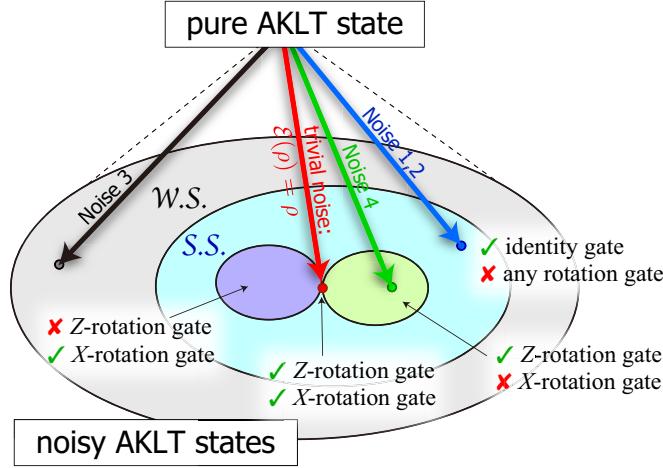


Figure 8.5: Discrete time-evolution of the pure SPT (i.e., AKLT) state by the four types of quantum noises (see Table 8.1). The “S.S.” and “W.S.” respectively mean that the corresponding noises are strongly and weakly symmetric, respectively. Even with strongly-symmetric noises, the noisy SPT (AKLT) states are further divided into several subcategories according to the ability of carrying out quantum gates. If we require that both the X and Z -rotation gates should be executable with high fidelity, only a trivial noise $\mathcal{E}(\rho) = \rho$ is allowed. (Reproduced from Ref. [105])

SPT order in open quantum systems based solely on the computational power. First of all, as we have seen in Sec. 8.2, the fidelity-based approach cannot capture the non-triviality of the SPT phases protected by symmetries (e.g., time-reversal) other than the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$, although, in the pure case, the Haldane phase is protected also by time-reversal symmetry.

Another immediate problem is related to the MBQC protocol itself. As repeatedly noted, we have only considered a simple MBQC protocol which has been originally introduced [84] for the pure AKLT state. Therefore, with more elaborated protocols (e.g., the one proposed in Ref. [90]), the one-qubit universal computation might be made possible even on the AKLT state subject to non-trivial noises. If this is the case, the picture presented in Fig. 8.5 must be modified accordingly.

To shed some light on the above issue, let us try the following strategy. In the case of pure states, the MPS-based approach to the SPT phases has been a great success; most of the important features can be understood in terms of the properties of the MPS tensor representing the non-trivial state [75, 74, 73]. Also, it is known that

the computational power of *any* ground states in the Haldane phase derives from the particular common structure of the MPS tensor [88], and the MBQC protocol improved accordingly ensures the one-qubit universal computation on all of them [90]. To apply a similar strategy to mixed states, we first need to represent a given mixed state in the form of the matrix-product operator (MPO) [110], in which the density operator is represented as a product of the MPO tensors: $\begin{array}{c} s \\ \boxed{B} \\ s' \end{array}$ (with s and s' denoting the physical states $|s\rangle$ and $\langle s'|$, respectively). Then, a natural question arises whether it is possible to extract the non-triviality directly from the MPO tensor of the mixed state. In this respect, we can rephrase Prop. 1 in the language of the MPO tensor as follows:

Proposition 4. *Let $|\psi\rangle$ be a ground state in the Haldane phase and $\mathcal{E}$ be an uncorrelated noise. Then, the diagonal elements of the MPO tensors representing the states $|\psi\rangle\langle\psi|$ and $\mathcal{E}(|\psi\rangle\langle\psi|)$ in the basis of the zero-eigenvectors of S^x, S^y , and S^z are the same, i.e., share the same computational power for the identity gate, if and only if $\mathcal{E}$ is strongly symmetric with respect to the canonical representation $\{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$ of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetry.*

Proof. For the clarity of the argument, we now prove the proposition for the case where the initial state $|\psi\rangle$ is the AKLT state. As the MPS tensors of the AKLT state in the wire basis are given by the Pauli matrices [see Eq. (6.48)], the corresponding MPO tensors are:

$$\begin{array}{c} s \\ \boxed{B} \\ s' \end{array} := \begin{array}{c} s \\ \boxed{\sigma_s} \\ \boxed{\sigma_{s'}^*} \\ s' \end{array} = \sigma_s \otimes \sigma_{s'}^* \quad (s, s' = x, y, z). \quad (8.9)$$

Then, the local MPO tensor on each site after an uncorrelated noise $\mathcal{E} = \circ_i \mathcal{E}_i$ is applied reads as:

$$\begin{array}{c} s \\ \boxed{C} \\ s' \end{array} := \begin{array}{c} s \\ \boxed{K_p} \\ \boxed{\sigma} \\ \boxed{\sigma^*} \\ \boxed{K_p^\dagger} \\ s' \end{array} \quad (s, s' = x, y, z), \quad (8.10)$$

where the K_p 's in the left-hand side are the Kraus operators of the local channel $\mathcal{E}_i$.

We now suppose that the uncorrelated noise $\mathcal{E}$ is strongly symmetric. Then, by Corollary 1, these Kraus operators are diagonal in the wire basis (in which all the $\mathbb{Z}_2 \times \mathbb{Z}_2$ generators are diagonal). Therefore, after the projective measurement, the

local tensor on the right-hand side changes to (now s' is set to s by the measurement):

$$\begin{aligned}
\begin{array}{c} s \\ \boxed{C} \\ s \end{array} &= \sum_p \sum_{t,t'} ([K_p]_{st} \sigma_t) \otimes ([K_p^\dagger]_{t's} \sigma_{t'}^*) \\
&= \sum_p ([K_p]_{ss} \sigma_s) \otimes ([K_p]_{ss}^* \sigma_s^*) \\
&= \left(\sum_p |K_{ss}^{(p)}|^2 \right) \sigma_s \otimes \sigma_s^* = \sigma_s \otimes \sigma_s^* \quad (s = x, y, z).
\end{aligned} \tag{8.11}$$

Here, the last equality arises from $\sum_p K_p^\dagger K_p = I$. Hence, on the AKLT state decohered by a strongly symmetric noise, the projective measurement in the wire basis realizes the identity gate with the same byproduct operator σ_s as the pure case.

Conversely, if the local MPO tensor assumes the following simple form:

$$\begin{array}{c} s \\ \boxed{C} \\ s \end{array} = \sigma_s \otimes \sigma_s^* \tag{8.12}$$

for all s , then

$$\sum_p \left(\sum_l [K_p]_{sl} \sigma_l \right) \otimes \left(\sum_{l'} \sigma_{l'}^* [K_p^\dagger]_{l's} \right) = \sigma_s \otimes \sigma_s^* \tag{8.13}$$

must hold for all s . By the linear independence of the basis $\sigma_s \otimes \sigma_{s'}$, the above implies $[K_p]_{sl} = 0$ ($l \neq s$) for all p . Therefore, the Kraus operators are all diagonal in the wire basis, and, by Corollary 1, this quantum channel is strongly symmetric. This proof can be extended straightforwardly to generic ground states in the Haldane phase by replacing the MPS tensor $A^{[s]} = \sigma_s$ with $A^{[s]} = \sigma_s \otimes A_{\text{junk}}[s]$; again the diagonal element is invariant under the quantum channel if and only if it is strongly symmetric. $\square$

As the proposition implies that the logical space, which is seen in the form of the MPO tensor (8.9), is preserved by the quantum channel, the two states $|\psi\rangle\langle\psi|$ and $\mathcal{E}(|\psi\rangle\langle\psi|)$ share the same computational power for the identity gate. Thus we arrive at the statement given in Prop. 4:

Corollary 2. *The measurement in the wire basis implements the identity gate with fidelity 1 on the mixed states that result from any ground states in the Haldane phase if and only if the applied quantum channel satisfies strong symmetry condition for $\mathbb{Z}_2 \times \mathbb{Z}_2 = \{1, e^{i\pi S^x}, e^{i\pi S^y}, e^{i\pi S^z}\}$.*

This Prop. 4 guarantees that if a quantum channel satisfies the strong symmetry condition (for the canonical representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$), the identity gate can be implemented with fidelity 1 on *any* decohered states resulting from the ground states in

the Haldane phase. The scope of this Prop. 4 is limited to the mixed states originating from pure SPT ground states, whereas we believe that Prop. 4, together with other results obtained here, serves as a stepping stone in understanding interacting many-body phases in open quantum systems from the quantum-computational perspectives. Understanding the relation between the MPO-based picture presented here and the approaches based on the (super)MPS in the doubled Hilbert space [97, 98, 99] is an important open question.

Chapter 9

Summary of Part II

The gate fidelity, which is related to the stability of the edge states, is a quantitative measure in quantum information science that assesses how accurately we can execute MBQC by quantifying the ability to manipulate the qubit. In this thesis, we proposed to use the gate fidelity of the MBQC as a detector of the SPT signature in generic mixed states. We observed that, depending on the unitary gates under consideration, the gate fidelity consists of different string-like operators which are associated with the on-site $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

First, we defined the SPT order in open quantum system by the capability of executing the identity gate with the unit fidelity, thereby obtaining results consistent with those of the existing approaches. In particular, we established (Prop. 1) that the high-fidelity realization of the identity gate in the decohered state is equivalent to the (uncorrelated) quantum noise respecting the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in the strong sense. This is the translation of the symmetry condition for quantum channels that preserve the SPT order into the language of MBQC computational power. To put it another way, a quantum noise respecting the protecting (on-site) symmetry in the strong sense preserves not only the corresponding string order parameters but also the computational power of the initial SPT phase.

We then investigated the condition for the quantum noises under which we can perform the Z -rotation gate $U = U_Z(\theta) = e^{-i\theta Z/2}$ on noisy AKLT states and found that, to implement $U_Z(\theta \neq 0)$ with high fidelity, it is not sufficient that the quantum noise satisfies the strong symmetry condition only for a particular representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$ (see Prop. 2). Moreover, to realize one-qubit universal computation on the decohered state, a much stronger condition is required. In fact, we showed that, as far

as we stick to the simplest MBQC protocol used in this thesis, no non-trivial quantum noise exists that allows the implementation of one-qubit universal computation on the noisy AKLT states (see Prop. 3)¹. These may suggest that, as shown in Fig. 8.5, the decohered “SPT” phase defined by the perfect performance of the identity gate (or equivalently, by the persisting string order parameters) is further decomposed into subphases according to the capability of implementing other gates U with reasonably high fidelity.

Our MBQC-based approach to the SPT order in open quantum systems using the gate fidelity yielded a picture generally consistent with those from other order-parameter-based approaches [101, 109]. Nevertheless, there still remain a few important questions. First of all, as shown in Chaps. 7 and 8, the gate fidelity is always related to (generalized) string-order parameters associated with the on-site symmetry and the behavior of the fidelity has little to do with the presence or absence of the time-reversal symmetry. Therefore, for the moment, we do not know how to formulate the mixed-state SPT phases associated to the time-reversal symmetry by the computational power. Another problem is related to the choice of the MBQC protocol. Although Prop. 3 forbids the one-qubit universal computation in the presence of non-trivial noises, we cannot exclude the possibility that improved MBQC protocols will change the conclusion of Prop. 3 thereby modifying the global picture presented in Fig. 8.5. Finally, the relation between our formulation and other ones (e.g., the ones based on the doubled Hilbert space in Refs. [97, 98, 99]) is not fully understood, though our definition of the SPT order in open quantum systems leads to conclusions consistent with those in, e.g., Ref. [101].

A promising way to answer these questions (especially, the latter two) may be to directly extract the information on the computational power from the MPO tensor of the mixed state in a way parallel to what we did to understand the uniform computational power of the SPT phases [88, 90]. In this respect, Prop. 4 and its Corollary 2 may be the first step towards the exploration into these interesting open problems.

There are experimental realizations of the AKLT state and its application for the quantum teleportation on superconducting qubits [111] and MBQC on photonic AKLT

¹We do not exclude here the possibility that MBQC on noisy AKLT states could potentially be one-qubit universal at the practical level *for a finite duration* even in this simplest MBQC protocol. To investigate what kind of quantum channels leave the noisy AKLT states one-qubit universal would be one of the most practically important problems from the viewpoint of both condensed matter physics and quantum information.

state [112] with high fidelity in both experiments. Also, the Haldane phase has been realized [113] in a ultra-cold Fermi gas in which the real-space measurement of non-local string correlations is possible. We believe that our approach to formulate the interacting SPT order in open quantum systems from the viewpoint of the computational power holds significant importance not only in the condensed-matter-physics contexts but also in practical applications, especially in the rapidly advancing field of quantum technology.

Chapter 10

Conclusion and Outlook

In this thesis, we investigated how well a spin-1 antiferromagnetic chain can retain its properties, or how it loses them, when coupled with the environment. In Part I, we specifically considered a spin-1 antiferromagnetic chain coupled with conduction electrons through Kondo coupling and investigated the properties of the ground state of the entire system. We approached this problem by considering the spin-1 Kondo-Heisenberg model as the Hamiltonian, focusing on the parameter region with strong Kondo coupling where perturbation theory from the strong coupling limit can be applied. Based on the fact that the Hamiltonian is a generalization of the Kondo lattice model, we examined the changes in electrical and magnetic properties due to the explicit inclusion of direct interactions between adjacent localized spins in the Kondo lattice model. Our results also include the changes in the short-range antiferromagnetism of the spin-1 antiferromagnetic Heisenberg chain discussed in the overview.

Now, let us summarize the results regarding the problem presented in the Overview, which is how the magnetic properties of a spin-1 chain change when coupled with a conduction electron system: First, the filling of the conduction electrons causes significant differences. At half-filling, not only does the combined spin correlation of the conduction electrons and localized spins change, but also the correlation among localized spins alone also shifts from short-range antiferromagnetic order to quasi-long-range order. On the other hand, away from half-filling, the antiferromagnetism that adjacent localized spins attempt to establish competes with the ferromagnetism induced by the hopping of conduction electrons. Especially, for the case of the quarter-filling, we saw the interesting phenomena. As a result, when J_H/t is extremely weak, a ferromagnetic order forms between adjacent localized spins, whereas a sufficiently large J_H/t leads to

the formation of antiferromagnetic order. Interestingly, in the intermediate parameter range of J_H/t , the correlation between adjacent localized spins dimerizes, causing the conduction electrons to become insulating.

The investigation of the subsystem properties from the ground state of the entire system's Hamiltonian considered in Part I corresponds to the situation after sufficient time has passed since the spin-1 system coupled with the conduction electron system. Therefore, treating this as an open quantum system, exploring the changes in the properties of the localized spin system during the time evolution after the coupling occurred is an interesting open problem. Reflecting on Part II, as mentioned earlier, we did not deal with the ground state of the entire system but considered an antiferromagnetic spin-1 chain in an open quantum system.

In Part II, we investigated the stability of the SPT order, another property of the antiferromagnetic spin-1 chain mentioned in the Overview, in a general manner without specifying a particular environment. We utilized the fact that the non-trivial SPT order of the antiferromagnetic spin-1 chain can be used for MBQC. By examining the stability of the SPT phase from the perspective of quantum information, specifically as a resource for MBQC, we assessed its robustness. First, we demonstrated that even for noisy resources, the gate fidelity can be calculated as a string order parameter-like correlation function when using the same MBQC protocol as for the pure AKLT state. Specifically, we found that the fidelity of the identity gate matches the string order parameter, and we determined the conditions under which this does not decay. We demonstrated that these conditions, necessary for maintaining SPT order, are consistent with those introduced in previous research [101] regarding the symmetry conditions that noise must satisfy. Furthermore, we considered the implementation of a non-trivial gate, specifically Z -rotation, based on our MBQC protocol, and revealed that the previously mentioned conditions are too weak to prevent the decay of fidelity. In other words, to execute general non-trivial gates without fidelity decay, more stringent conditions than the strong symmetry condition are required. We also showed that within the scope of our protocol, one-qubit universal quantum computation cannot be realized in the presence of non-trivial noise.

Thus, gate fidelity has revealed the intricate structure of decohered SPT phases in an open quantum system. However, it remains an open problem whether this rich structure will be preserved even when employing a more refined MBQC protocol.

Moreover, our research primarily focused on the topological properties of spin-1 chains, evaluating whether SPT order can be maintained based on the fidelity not de-

caying at all. However, this might be a too strict criterion when considering applications to the quantum computation. In other words, when actually performing MBQC using a spin-1 antiferromagnetic chain, we need to consider the continuous time evolution under the specific noise of each physical implementation of the quantum computer. It is essential to investigate whether high fidelity can be maintained for a sufficiently long time, much longer than the duration of the computation itself. We believe that it is worthwhile to consider such practical issues.

Appendix A

Appendices for Part I

A.1 Effective Hamiltonian of spin sector of spin- S KH chain

In this section, we generalize our observation in Sec. 2.1 that the strong-coupling effective Hamiltonian for the spin-1 Kondo lattice model at half-filling is given by the spin-1/2 Heisenberg model to the case of localized spin- S . As already mentioned in Sec. 2.1.2, the low-energy effective Hamiltonian is the spin- $(S-1/2)$ antiferromagnetic Heisenberg model.

Basically, we follow the strategy in Sec. 2.1. The $4(2S+1)$ possible states at site- i are shown in Table A.1 together with the Kondo energy and the degeneracy. In the strong coupling limit ($J_K \rightarrow \infty$) at half-filling (i.e, one electron per site $n_i = 1$), the conduction electron and spin- S localized spin at each site form $2S$ -fold degenerate $S_{\text{tot}} = (S-1/2)$ states, in which the Kondo energy is given by: $J_K \mathbf{s}_i \cdot \mathbf{S}_i = -J_K(S+1)/2$. The remaining $(2S+2)$ states with $S_{\text{tot}} = (S+1/2)$ have higher energy $J_K S/2$.

On the other hand, the action of the creation operators is locally written as:

$$c_{i\uparrow}^\dagger = \sum_{\mathcal{M}=-S}^S \left\{ \left| \begin{array}{c} \uparrow \\ \mathcal{M} \end{array} \right\rangle_i \left\langle \begin{array}{c} \text{emp} \\ \mathcal{M} \end{array} \right|_i + \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M} \end{array} \right\rangle_i \left\langle \begin{array}{c} \downarrow \\ \mathcal{M} \end{array} \right|_i \right\} \quad (\text{A.1a})$$

$$c_{i\downarrow}^\dagger = \sum_{\mathcal{M}=-S}^S \left| \begin{array}{c} \downarrow \\ \mathcal{M} \end{array} \right\rangle_i \left\langle \begin{array}{c} \text{emp} \\ \mathcal{M} \end{array} \right|_i - \sum_{\mathcal{M}=-S}^S \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M} \end{array} \right\rangle_i \left\langle \begin{array}{c} \uparrow \\ \mathcal{M} \end{array} \right|_i, \quad (\text{A.1b})$$

where we have introduced the notations $\left| \begin{array}{c} \alpha \\ \mathcal{M} \end{array} \right\rangle_i$ similar to those used in Sec. 2, and the minus sign in the second equation comes from the definition of doubly-occupied state as

$|\uparrow\downarrow\rangle_i = c_{i,\uparrow}^\dagger c_{i,\downarrow}^\dagger |\text{emp}\rangle_i$. Let us rewrite these operator in the basis where S_{tot} is diagonal. To this end, we note that the relevant states are explicitly written as

$$\begin{aligned} & \left| S + \frac{1}{2}; \mathcal{M} + \frac{1}{2} \right\rangle_i \\ &= \sqrt{\frac{S + \mathcal{M} + 1}{2S + 1}} \left| \begin{array}{c} \uparrow \\ \mathcal{M} \end{array} \right\rangle_i + \sqrt{\frac{S - \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \downarrow \\ \mathcal{M} + 1 \end{array} \right\rangle_i \end{aligned} \quad (\text{A.2a})$$

$$\begin{aligned} & \left| S - \frac{1}{2}; \mathcal{M} + \frac{1}{2} \right\rangle_i \\ &= \sqrt{\frac{S - \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \uparrow \\ \mathcal{M} \end{array} \right\rangle_i - \sqrt{\frac{S + \mathcal{M} + 1}{2S + 1}} \left| \begin{array}{c} \downarrow \\ \mathcal{M} + 1 \end{array} \right\rangle_i \end{aligned} \quad (\text{A.2b})$$

$$(\mathcal{M} = -S, \dots, S - 1).$$

By inverting these equations, we can express $\left| \begin{array}{c} \uparrow/\downarrow \\ \mathcal{M} \end{array} \right\rangle_i$ in terms of $|S \pm \frac{1}{2}; \mathcal{M} + \frac{1}{2}\rangle_i$. Plugging those expressions into Eqs. (A.1a) and (A.1b), and dropping the states with $S_{\text{tot}} = S + 1/2$, we obtain the expressions of $c_{i,\uparrow/\downarrow}^\dagger$ and $c_{i,\uparrow/\downarrow}$ projected onto the $S_{\text{tot}} = S - 1/2$ states:

$$\begin{aligned} \mathcal{P}_d c_{i,\uparrow}^\dagger \mathcal{P}_{S-1/2} &= - \sum_{\mathcal{M}=-S}^S \sqrt{\frac{S + \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M} \end{array} \right\rangle \left\langle S - \frac{1}{2}; \mathcal{M} - \frac{1}{2} \right| \\ \mathcal{P}_e c_{i,\uparrow} \mathcal{P}_{S-1/2} &= \sum_{\mathcal{M}=-S}^S \sqrt{\frac{S - \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \text{emp} \\ \mathcal{M} \end{array} \right\rangle \left\langle S - \frac{1}{2}; \mathcal{M} + \frac{1}{2} \right| \end{aligned} \quad (\text{A.3a})$$

and

$$\begin{aligned} \mathcal{P}_d c_{i,\downarrow}^\dagger \mathcal{P}_{S-1/2} &= \sqrt{\frac{S - \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M} \end{array} \right\rangle \left\langle S - \frac{1}{2}; \mathcal{M} + \frac{1}{2} \right| \\ \mathcal{P}_e c_{i,\downarrow} \mathcal{P}_{S-1/2} &= - \sqrt{\frac{S + \mathcal{M}}{2S + 1}} \left| \begin{array}{c} \text{emp} \\ \mathcal{M} \end{array} \right\rangle \left\langle S - \frac{1}{2}; \mathcal{M} - \frac{1}{2} \right|, \end{aligned} \quad (\text{A.3b})$$

where $\mathcal{P}_{S-1/2}$ projects the state at site- i onto the space of total spin $S - 1/2$, and $\mathcal{P}_d$ and $\mathcal{P}_e$ respectively are the projectors onto the doubly-occupied and empty states. Therefore, the nearest-neighbor hopping on the two adjacent $|S - 1/2\rangle$'s are:

$$\begin{aligned} & \mathcal{P}_d^i \mathcal{P}_e^{i+1} c_{i,\uparrow}^\dagger c_{i+1,\uparrow} \mathcal{P}_{S-1/2}^i \mathcal{P}_{S-1/2}^{i+1} \\ &= \frac{1}{2S + 1} \sum_{\mathcal{M}_i} \sum_{\mathcal{M}_{i+1}} \sqrt{S + \mathcal{M}_i} \sqrt{S - \mathcal{M}_{i+1}} \\ &\times \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M}_i \end{array} \right\rangle \left| \begin{array}{c} \text{emp} \\ \mathcal{M}_{i+1} \end{array} \right\rangle \left\langle S - \frac{1}{2}; \mathcal{M}_i - \frac{1}{2} \right| \left\langle S - \frac{1}{2}; \mathcal{M}_{i+1} + \frac{1}{2} \right| \end{aligned} \quad (\text{A.4a})$$

$$\begin{aligned}
 & \mathcal{P}_d^i \mathcal{P}_e^{i+1} c_{i,\downarrow}^\dagger c_{i+1,\downarrow} \mathcal{P}_{S-1/2}^i \mathcal{P}_{S-1/2}^{i+1} \\
 &= -\frac{1}{2S+1} \sum_{\mathcal{M}_i} \sum_{\mathcal{M}_{i+1}} \sqrt{S-\mathcal{M}_i} \sqrt{S+\mathcal{M}_{i+1}} \\
 & \times \left| \begin{array}{c} \uparrow\downarrow \\ \mathcal{M}_i \end{array} \right\rangle \left| \begin{array}{c} \text{emp} \\ \mathcal{M}_{i+1} \end{array} \right\rangle \left\langle S-\frac{1}{2}; \mathcal{M}_i + \frac{1}{2} \right| \left\langle S-\frac{1}{2}; \mathcal{M}_{i+1} - \frac{1}{2} \right|
 \end{aligned} \tag{A.4b}$$

The expressions for $c_{i+1,\uparrow}^\dagger c_{i,\uparrow}$ and $c_{i+1,\downarrow}^\dagger c_{i,\downarrow}$ are obtained from the above by interchanging $i \leftrightarrow i+1$. Similarly, we can write down $\mathcal{P}_{S-1/2}^i \mathcal{P}_{S-1/2}^{i+1} c_{i,\uparrow}^\dagger c_{i+1,\uparrow} \mathcal{P}_e^i \mathcal{P}_d^{i+1}$, etc.

Combining all these, we can calculate the matrix elements of the second-order processes shown in Fig. A.1. For example, the matrix element of the process (i) $\rightarrow$ (ii) $\rightarrow$ (iii-a) is:

$$\begin{aligned}
 & \frac{(-t)^2}{-J_K(S+1)} \\
 & \times \mathcal{P}_{S-1/2}^i \mathcal{P}_{S-1/2}^{i+1} c_{i,\downarrow}^\dagger c_{i+1,\downarrow} \mathcal{P}_e^i \mathcal{P}_d^{i+1} c_{i+1,\uparrow}^\dagger c_{i,\uparrow} \mathcal{P}_{S-1/2}^i \mathcal{P}_{S-1/2}^{i+1} \\
 &= \frac{t^2}{J_K(S+1)(2S+1)^2} \mathfrak{S}_i^- \mathfrak{S}_{i+1}^+,
 \end{aligned} \tag{A.5}$$

where $\mathfrak{S}$ are the spin- $(S-1/2)$ operators and we have used

$$\begin{aligned}
 \mathfrak{S}_i^- &= \sum_{\mathcal{M}=-(S-1/2)}^{S-1/2} \sqrt{\{(S-1/2)+\mathcal{M}_i\} \{(S-1/2)-\mathcal{M}_i+1\}} \\
 & \times |S-1/2; \mathcal{M}_i-1\rangle_2 \langle S-1/2; \mathcal{M}_i|_2,
 \end{aligned}$$

etc. in obtaining the final expression. Similarly, the process (i) $\rightarrow$ (ii) $\rightarrow$ (iii-b) gives the diagonal term:

$$\begin{aligned}
 & \frac{t^2}{J_K(S+1)(2S+1)^2} \left\{ \mathfrak{S}_i^z \mathfrak{S}_{i+1}^z - \frac{2S+1}{2} (\mathfrak{S}_i^z - \mathfrak{S}_{i+1}^z) \right\} \\
 & - \frac{t^2}{4J_K(S+1)}.
 \end{aligned} \tag{A.6}$$

If we collect all the possible processes, the terms proportional to $(\mathfrak{S}_i^z - \mathfrak{S}_{i+1}^z)$ cancel out and we obtain the following effective Hamiltonian:

$$H_{\text{eff}} = \frac{4t^2}{(2S+1)^2(S+1)J_K} \sum_i \mathfrak{S}_i \cdot \mathfrak{S}_{i+1} + \text{const}. \tag{A.7}$$

Putting $S=1$ in this equation, we recover Eq. (A.9) in Sec. 2.1. This effective Hamiltonian indicates that the spin- S Kondo lattice model with $J_K > 0$ in the strong-coupling

region is an insulator whose spin sector is described by the spin- $(S-1/2)$ Heisenberg model; according to the Haldane conjecture [2, 3], the spin correlation is qualitatively different when S is integer and when S is half-odd-integer. If S is integer, then the spin sector exhibits antiferromagnetic quasi-long-range order, while the ground state is disordered if S is half-odd. This is consistent with the prediction [56] based on field-theory mapping.

It is straightforward to take the Heisenberg term J_H into account. To this end, we follow similar steps to find the projection of the localized spin onto the ground-state subspace:

$$\mathcal{P}_{S-1/2}^i \mathbf{S}_i \mathcal{P}_{S-1/2}^i = \frac{2(S+1)}{2S+1} \mathfrak{S}_i, \quad (\text{A.8})$$

which means that, in the strong-coupling limit, the localized spin $\mathbf{S}_i$ behaves like the effective spin- $(S-1/2)$ $\mathfrak{S}_i$ except for the overall normalization factor. From this, one immediately sees that the Heisenberg term just gives the same Heisenberg model as before, leading to the total effective Hamiltonian:

$$H_{\text{eff}}^{(n=1)} = \left\{ \frac{4t^2}{(2S+1)^2(S+1)J_K} + \left(\frac{2(S+1)}{2S+1} \right)^2 J_H \right\} \sum_i \mathfrak{S}_i \cdot \mathfrak{S}_{i+1}, \quad (\text{A.9})$$

which generalizes Eq. (2.9).

conduction electron	T	Kondo energy	degeneracy
$n_i = 0$ ($ 0\rangle$)	S	0	$2S+1$
$n_i = 1$	$S+1/2$	$J_K S/2$	$2S+2$
$(c_{i,\uparrow} 0\rangle, c_{i,\downarrow} 0\rangle)$	$S-1/2$	$-J_K(S+1)/2$	$2S$
$n_i = 2$ ($c_{i,\uparrow}c_{i,\downarrow} 0\rangle$)	S	0	$2S+1$

Table A.1: Local states of spin- S KH model. Quantum number of total spin $\mathbf{T}_i = \mathbf{s}_i + \mathbf{S}_i$ is denoted by T .

A.2 Derivation of effective Hamiltonian (2.11)

Among the $4(2S+1)$ possible on-site states listed in Table A.1, the $2S$ states $|n=1, T=S-1/2; T^z\rangle$ with a single conduction electron, and the $(2S+1)$ -fold degenerate states $|n=0, T=S; T^z\rangle$ without electron are relevant in the strong-coupling limit (less

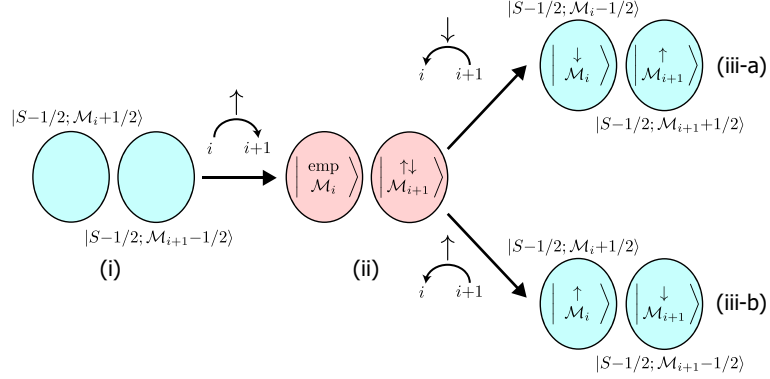


Figure A.1: Typical second-order processes in t for generic spin- S . (i) A pair of adjacent sites in the unperturbed ($t = 0$) ground state. (ii) Electron ($\uparrow$ here) hopping from the site i to $i + 1$ generates a pair of sites in excited states. (iii) Second hopping back to the site i returns the state to the ground-state subspace. Depending on the spin of the electron going back, different final states are obtained [(iii-a) and (iii-b)]. (Reproduced from Ref. [54])

than half-filling $n < 1$). As we can distinguish $|n=0, T=S; T^z\rangle$ from $|n=1, T=S-1/2; T^z\rangle$ by the value of T (S or $S-1/2$) in the strong-coupling Hilbert space, we can omit n in specifying the states, and we will abbreviate, e.g., $|n=0, T=S; T^z=\mathcal{M}\rangle_i$ as $|S; \mathcal{M}\rangle_i$ from now on. The low-energy Hilbert space is spanned by the tensor products of $|S; \mathcal{M}\rangle_i$ and $|S-1/2; \mathcal{M}\rangle_i$.

So the action of electron-creation operators on $|S; \mathcal{M}\rangle_i$ is

$$c_{i,\uparrow}^\dagger = \sum_{\mathcal{M}=-S}^S \sqrt{\frac{S-\mathcal{M}}{2S+1}} |S-1/2; \mathcal{M}+1/2\rangle_i \langle S; \mathcal{M}|_i \quad (\text{A.10a})$$

$$c_{i,\downarrow}^\dagger = - \sum_{\mathcal{M}=-S}^S \sqrt{\frac{S+\mathcal{M}}{2S+1}} |S-1/2; \mathcal{M}-1/2\rangle_i \langle S; \mathcal{M}|_i . \quad (\text{A.10b})$$

Therefore, the action of hopping operators of the conduction electron on $|S; \mathcal{M}_i\rangle \otimes |S-1/2; \mathcal{M}_{i\pm 1}\rangle_{i\pm 1}$ is

$$\begin{aligned} -tc_{i,\uparrow}^\dagger c_{i\pm 1,\uparrow} &= -\frac{t}{2S+1} \sum_{\mathcal{M}_i=-S}^S \sum_{\mathcal{M}_{i\pm 1}=-(S-1/2)}^{S-1/2} \sqrt{S-\mathcal{M}_i} \sqrt{S-\mathcal{M}_{i\pm 1}+1/2} \\ &\quad \times |S-1/2; \mathcal{M}_i+1/2\rangle_i \otimes |S; \mathcal{M}_{i\pm 1}-1/2\rangle_{i\pm 1} (\langle S; \mathcal{M}_i|_i \otimes \langle S-1/2; \mathcal{M}_{i\pm 1}|_{i\pm 1}) \end{aligned} \quad (\text{A.11a})$$

$$\begin{aligned}
-tc_{i,\downarrow}^\dagger c_{i\pm 1,\downarrow} &= -\frac{t}{2S+1} \sum_{\mathcal{M}_i=-S}^S \sum_{\mathcal{M}_{i\pm 1}=-(S-1/2)}^{S-1/2} \sqrt{S+\mathcal{M}_i} \sqrt{S+\mathcal{M}_{i\pm 1}+1/2} \\
&\times |S-1/2; \mathcal{M}_i-1/2\rangle_i \otimes |S; \mathcal{M}_{i\pm 1}+1/2\rangle_{i\pm 1} (\langle S; \mathcal{M}_i|_i \otimes \langle S-1/2; \mathcal{M}_{i\pm 1}|_{i\pm 1})
\end{aligned} \tag{A.11b}$$

If we introduce the exchange operator $X_{i,j}$ as

$$X_{i,j} |\psi\rangle_i \otimes |\varphi\rangle_j = |\varphi\rangle_i \otimes |\psi\rangle_j, \tag{A.12}$$

then (A.11a) and (A.11b) can be rewritten in the following form:

$$\begin{aligned}
-tc_{i,\uparrow}^\dagger c_{i\pm 1,\uparrow} &= -\frac{t}{2S+1} X_{i,i\pm 1} \left\{ \sum_{\mathcal{M}_i=-S}^S \sum_{\mathcal{M}_{i\pm 1}=-(S-1/2)}^{S-1/2} \sqrt{S-\mathcal{M}_i} \sqrt{S-\mathcal{M}_{i\pm 1}+1/2} \right. \\
&\times |S; \mathcal{M}_{i\pm 1}-1/2\rangle_i \otimes |S-1/2; \mathcal{M}_i+1/2\rangle_{i\pm 1} (\langle S; \mathcal{M}_i|_i \otimes \langle S-1/2; \mathcal{M}_{i\pm 1}|_{i\pm 1}) \left. \right\}
\end{aligned} \tag{A.13a}$$

$$\begin{aligned}
-tc_{i,\downarrow}^\dagger c_{i\pm 1,\downarrow} &= -\frac{t}{2S+1} X_{i,i\pm 1} \left\{ \sum_{\mathcal{M}_i=-S}^S \sum_{\mathcal{M}_{i\pm 1}=-(S-1/2)}^{S-1/2} \sqrt{S+\mathcal{M}_i} \sqrt{S+\mathcal{M}_{i\pm 1}+1/2} \right. \\
&\times |S; \mathcal{M}_{i\pm 1}+1/2\rangle_i \otimes |S-1/2; \mathcal{M}_i-1/2\rangle_{i\pm 1} (\langle S; \mathcal{M}_i|_i \otimes \langle S-1/2; \mathcal{M}_{i\pm 1}|_{i\pm 1}) \left. \right\}.
\end{aligned} \tag{A.13b}$$

If one changes the basis from $|S; \mathcal{M}_i\rangle \otimes |S-1/2; \mathcal{M}_{i\pm 1}+1/2\rangle$ to the one in which the total spin $J (= 1/2, \dots, 2S-1/2)$ is diagonal:

$$|S; \mathcal{M}_i\rangle \otimes |S-1/2; \mathcal{M}_{i\pm 1}\rangle = \sum_{J=1/2}^{2S-1/2} (\langle J; \mathcal{M}_i + \mathcal{M}_{i\pm 1} | S; \mathcal{M}_i\rangle \otimes |S-1/2; \mathcal{M}_{i\pm 1}\rangle) |J; \mathcal{M} = \mathcal{M}_i + \mathcal{M}_{i\pm 1}\rangle,$$

the above can be further recast as:

$$\begin{aligned}
-t \left(c_{i,\uparrow}^\dagger c_{i+1,\uparrow} + c_{i,\downarrow}^\dagger c_{i+1,\downarrow} \right) &= -t X_{i,i+1} \mathcal{P}_S^i \mathcal{P}_{S-\frac{1}{2}}^{i+1} \left[\frac{1}{2S+1} \sum_{k=0}^{2S-1} (-1)^k (2S-k) P_{i+1 \rightarrow i} (2S-k-1/2) \right] \\
&\mathcal{P}_S^i \mathcal{P}_{S-\frac{1}{2}}^{i+1},
\end{aligned} \tag{A.14a}$$

$$\begin{aligned}
-t \left(c_{i+1,\uparrow}^\dagger c_{i,\uparrow} + c_{i+1,\downarrow}^\dagger c_{i,\downarrow} \right) &= -t X_{i,i+1} \mathcal{P}_{S-\frac{1}{2}}^i \mathcal{P}_S^{i+1} \left[\frac{1}{2S+1} \sum_{k=0}^{2S-1} (-1)^k (2S-k) P_{i \rightarrow i+1} (2S-k-1/2) \right] \\
&\mathcal{P}_{S-\frac{1}{2}}^i \mathcal{P}_S^{i+1}.
\end{aligned} \tag{A.14b}$$

This is the generalization of the so-called double-exchange Hamiltonian [61, 114] to the case of antiferromagnetic J_K . Here we have defined another operator $P_{i \rightarrow i+1}(J)$ [$P_{i+1 \rightarrow i}(J)$] that projects the states of a pair of spins $S-1/2$ at site- i [site- $(i+1)$] and S at site- $(i+1)$ (site- i) onto the subspace with the total spin J :

$$P(J) = \sum_{\mathcal{M}=-J}^J |J; \mathcal{M}\rangle \langle J; \mathcal{M}|. \quad (\text{A.15})$$

In both expressions (A.14a) and (A.14b) of the electron hopping, the projection operator onto $J = 2S - 1/2 = S + (S - 1/2)$ (i.e., the maximal value of $\mathfrak{S}_i + \mathbf{S}_{i+1}$ or $\mathbf{S}_i + \mathfrak{S}_{i+1}$) has the largest coefficient suggesting that the ferromagnetic state optimizes the kinetic energy of the conduction electrons as in the *ferromagnetic* Kondo lattice model.

It is not difficult to write down the quantity $1/(2S+1) \sum_{k=0}^{2S-1} (-1)^k (2S-k) P_{i \rightarrow i+1}(2S-k-1/2)$ as a polynomial $f^{(S)}(\mathfrak{S}_i \cdot \mathbf{S}_{i+1})$ of $\mathfrak{S}_i \cdot \mathbf{S}_{i+1}$. The explicit forms of $f^{(S)}(X)$ are given by:

$$\begin{aligned} f^{(1/2)}(X) &= 1/2 \\ f^{(1)}(X) &= \frac{2}{3}X + \frac{1}{3} \\ f^{(3/2)}(X) &= \frac{3}{8}X + \frac{1}{4}X^2 - \frac{3}{8} \\ f^{(2)}(X) &= -\frac{1}{3}X + \frac{7}{45}X^2 + \frac{2}{45}X^3 - \frac{4}{5} \\ f^{(5/2)}(X) &= \frac{1}{6} \left\{ -\frac{305}{72}X - \frac{79}{144}X^2 + \frac{7}{36}X^3 + \frac{1}{36}X^4 - \frac{85}{48} \right\}. \end{aligned} \quad (\text{A.16})$$

The polynomial for $1/(2S+1) \sum_{k=0}^{2S-1} (-1)^k (2S-k) P_{i+1 \rightarrow i}(2S-k-1/2)$ is given simply by $f^{(S)}(\mathbf{S}_i \cdot \mathfrak{S}_{i+1})$. Setting $S = 1$ in Eqs. (A.14a) and (A.14b) and expressing $X_{i,i+1}$ and $\mathcal{P}$ with $\hat{d}_i$ and $\hat{n}_i^d$ reproduce the results (2.11) and (2.12) in Sec. 2.2.

A.3 Rigorous proof of the ferromagnetic ground state for effective Hamiltonian (2.11)

In this section, starting from the strong-coupling effective Hamiltonian (2.11), we derive the ferromagnetic ground state of spin-1 Kondo lattice model (i.e., $J_H = 0$) with filling $0 \lesssim n \lesssim 1$. As we can follow almost the same steps to generalize the statement to the arbitrary spin- S , we describe the proof only for $S = 1$ for simplicity.

For this purpose, let $H^{(l)}$ be the Hamiltonian (2.11) of l -site system:

$$H^{(l)} = -t \sum_{i=1}^{l-1} \left\{ \hat{d}_{i+1}^\dagger \hat{d}_i f_{i \rightarrow i+1}^{(S=1)}(\mathbf{D}_i \cdot \mathbf{S}_{i+1}) \hat{n}_{d,i} (1 - \hat{n}_{d,i+1}) + \hat{d}_i^\dagger \hat{d}_{i+1} f_{i+1 \rightarrow i}^{(S=1)}(\mathbf{S}_i \cdot \mathbf{D}_{i+1}) (1 - \hat{n}_{d,i}) \hat{n}_{d,i+1} \right\},$$

which is block-diagonal in the number of doublets $N_d(l) = \sum_{i=1}^l n_{d,i}$ (which is equal to the number of conduction electrons) and the total $S_{\text{tot}}^z(l) = \sum_{i=1}^l T_i^z$:

$$H^{(l)} = \bigoplus_{N_d(l), S_{\text{tot}}^z(l)} H_{N_d(l), S_{\text{tot}}^z(l)}^{(l)}. \quad (\text{A.17})$$

The first step is to prove that, (A) for $1 \leq N_d(L) \leq L-1$ (L : the system size), the matrix representation of $H_{N_d(L), S_{\text{tot}}^z(L)}^{(L)}$ is *non-positive* and *indecomposable* in the standard basis ¹:

$$\{|T_1^z, \dots, T_L^z\rangle = \otimes_i |T_i^z\rangle\} \quad (T_i^z = \pm 1/2, 0, \pm 1). \quad (\text{A.18})$$

Note that when $T_i^z = \pm 1/2$, an electron exists at site- i forming a Kondo doublet ($|\uparrow\rangle_i$ or $|\downarrow\rangle_i$), while there is no electron if $T_i^z = 0, \pm 1$. Then, we can use the Perron-Frobenius theorem (see, e.g., Ref. [115] for a physicist-friendly exposition of the theorem and its applications) to show that the ground state within each sector is unique and that the ground-state “wave function” in this basis is strictly positive. The second step is to show that (B) the above unique ground state has a non-zero overlap with the state of maximal total spin: $S_{\text{tot}} = L - N_d/2$, which means that the unique ground state is indeed ferromagnetic.

The proposition (A) is proven by the mathematical induction in the system size L . Let us start from the simplest case $L = 2$. In this case, it suffices to consider only $N_d(2) = 1$ since $H_{N_d, S^z}^{(L=2)}$ is trivially zero for $N_d(2) = 0$ and $2(= L)$. When $N_d(2) = 1$, there are twelve states [six spin states for each of the two possible configurations of

¹We do not need to specify the local doublet (i.e., electron) number n_i^d since $T_i^z = \pm 1/2$ ($0, \pm 1$) already imply $n_i^d = 1$ (0).

$S = 1/2$ (electron) and $S = 1$ (hole)]:

$$\begin{aligned}
S_{\text{tot}}^z(2) = 3/2 : & |T_1^z, T_2^z\rangle = |1, 1/2\rangle, |1/2, 1\rangle \\
S_{\text{tot}}^z(2) = 1/2 : & \\
& |T_1^z, T_2^z\rangle = |1/2, 0\rangle, |-1/2, 1\rangle, |0, 1/2\rangle, |1, -1/2\rangle \\
S_{\text{tot}}^z(2) = -1/2 : & \\
& |T_1^z, T_2^z\rangle = |-1/2, 0\rangle, |1/2, -1\rangle, |0, -1/2\rangle, |-1, 1/2\rangle \\
S_{\text{tot}}^z(2) = -3/2 : & |T_1^z, T_2^z\rangle = |-1, -1/2\rangle, |-1/2, -1\rangle.
\end{aligned}$$

The matrix representation of the effective Hamiltonian in the above basis can be obtained readily from Eqs. (A.11a) and (A.11b). For instance, the block Hamiltonian for $S_{\text{tot}}^z(2) = 3/2$ and $S_{\text{tot}}^z(2) = 1/2$ are respectively given by:

$$H_{1,3/2}^{(2)} = -\frac{t}{3} \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}. \quad (\text{A.19})$$

and

$$H_{1,1/2}^{(2)} = -\frac{t}{3} \begin{pmatrix} 0 & 0 & 1 & \sqrt{2} \\ 0 & 0 & \sqrt{2} & 0 \\ 1 & \sqrt{2} & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 \end{pmatrix} \quad (\text{A.20})$$

(the others are: $H_{1,-1/2}^{(2)} = H_{1,1/2}^{(2)}$ and $H_{1,-3/2}^{(2)} = H_{1,3/2}^{(2)}$). Clearly, all the off-diagonal elements of these matrices are non-positive.

The connectivity of these matrices can be represented by the connected graph shown in Fig. A.2, in which the vertices represent the basis states and the edges correspond to non-zero matrix elements among them. It is easy to see that for any pair of vertices (i.e., basis states) we can go from one to the other by following the edges (i.e., non-zero matrix elements); a matrix is said to be indecomposable if the corresponding graph is connected (as in Fig. A.2). Thus, we establish that the block hamiltonians are non-positive and indecomposable for $L = 2$.

Next, suppose that the statement (A) holds for *all* the system sizes l up to L , that is, all the block Hamiltonians $\{H_{N_d(l), S_{\text{tot}}^z(l)}^{(l)}\}$ [$2 \leq l \leq L$, $2 \leq N_d(l) \leq l-1$] are non-positive and indecomposable in the basis (A.18) to prove the statement for the system size $L+1$. Consider the block $H_{N_d, S_{\text{tot}}^z}^{(L+1)}$ of the system with size $L+1$. According to the five possible values of T_{L+1}^z ($= 1, 0, -1, 1/2, -1/2$), we can decompose the subspace with (N_d, S^z) into five different sectors, and the hopping between the sites L and $L+1$

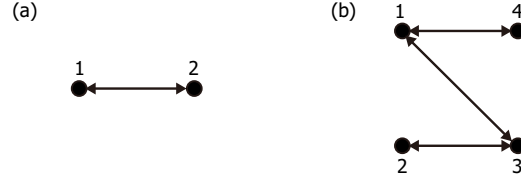


Figure A.2: Oriented graphs representing the block Hamiltonians (a) $H_{1,3/2}^{(2)}$ [Eq. (A.19)] and (b) $H_{1,1/2}^{(2)}$ [Eq. (A.20)]. The numbers on the vertices denote the matrix indices, and the arrows running from the vertex j to i mean that the (i, j) -elements are non-zero. As the Hamiltonian is represented by Hermitian matrices, all the arrows are bi-directional. (Reproduced from Ref. [54])

connects these five sectors with each other. From the explicit expressions (A.11a) and (A.11b) of the hopping term (see also Fig. A.3), we see that the Hamiltonian $H_{N_d, S_{\text{tot}}^z}^{(L+1)}$ takes the following block structure:

$$H_{N_d, S_{\text{tot}}^z}^{(L+1)} = \left(\begin{array}{ccc|cc} M_1 & \mathbf{0} & \mathbf{0} & * & \mathbf{0} \\ \mathbf{0} & M_2 & \mathbf{0} & * & * \\ \mathbf{0} & \mathbf{0} & M_3 & \mathbf{0} & * \\ \hline * & * & \mathbf{0} & M_4 & \mathbf{0} \\ \mathbf{0} & * & * & \mathbf{0} & M_5 \end{array} \right), \quad (\text{A.21})$$

where the diagonal blocks M_1 , M_2 , M_3 , M_4 , and M_5 respectively are $H_{N_d, S_{\text{tot}}^z - 1}^{(L)}$, $H_{N_d, S_{\text{tot}}^z}^{(L)}$, $H_{N_d, S_{\text{tot}}^z + 1}^{(L)}$, $H_{N_d - 1, S_{\text{tot}}^z - \frac{1}{2}}^{(L)}$, and $H_{N_d - 1, S_{\text{tot}}^z + \frac{1}{2}}^{(L)}$, and $*$ denotes non-positive matrices determined by (A.11a) and (A.11b). Since M_i ($i = 1, \dots, 5$) are all non-positive and indecomposable by the assumption, it is obvious from the corresponding graph Fig. A.4 that the entire matrix $H_{N_d, S_{\text{tot}}^z}^{(L+1)}$ itself is indecomposable, too.

A remark is in order about the exceptional cases with $N_d = 1$ (one electron in the system) and L (one hole in the system). In these cases, either (M_1, M_2, M_3) (when $N_d = L$) or (M_4, M_5) (when $N_d = 1$) are identically zero and we cannot use the indecomposability of these matrices to prove that of $H_{N_d, S_{\text{tot}}^z}^{(L+1)}$. In fact, we can treat these cases without relying on the mathematical induction. First, we note that, in the case of a single electron or hole, we can move it to an arbitrary position by the repeated action of the hopping operators (the spin configuration is modified, too). Then, we use processes in which the electron/hole moves to a certain site and comes back to the starting point to create the spin-flips of the form $T_i^+ T_j^-$, which connect between any two different spin states in the same (N_d, S^z) sector. This completes the proof

of the statement (A). Then, by the Perron-Frobenius theorem, there exists a unique lowest-energy state $|\psi_0; N_d, S_{\text{tot}}^z\rangle$ in each of the (N_d, S^z) -sectors:

$$H_{N_d, S_{\text{tot}}^z}^{(L)} |\psi_0; N_d, S_{\text{tot}}^z\rangle = E_{\text{g.s.}}(N_d, S_{\text{tot}}^z) |\psi_0; N_d, S_{\text{tot}}^z\rangle. \quad (\text{A.22})$$

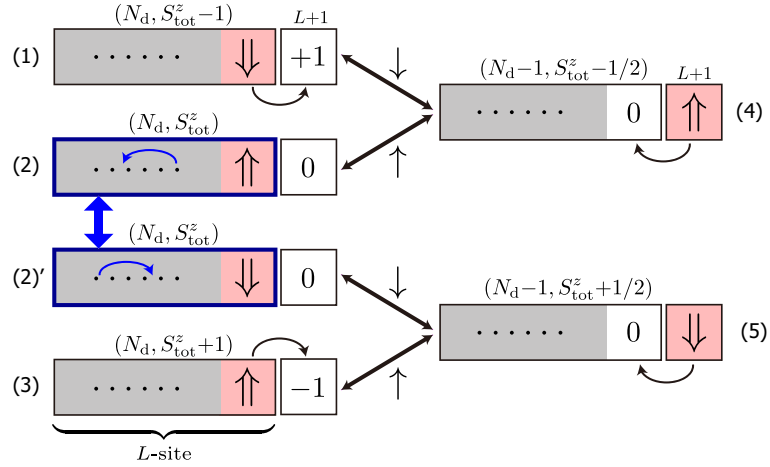


Figure A.3: Projected hopping (A.11a) and (A.11b) between the sites L and $L + 1$ connects the five different sectors (1)–(5) with each other [(1)–(5) correspond respectively to the blocks M_1 – M_5 in Eq. (A.21)]. Note that the hopping Hamiltonian of the size- L sub-system *within* each sector is indecomposable by the assumption of the induction. (Reproduced from Ref. [54])

To prove the statement (B) that the unique ground state found above indeed has the maximal total spin:

$$S_{\text{tot}} = S_{\text{max}} = (L - N_d) + (1/2)N_d = L - N_d/2,$$

we first apply the Perron-Frobenius theorem to the squared total spin: $\left(\sum_i^L \mathbf{T}_i\right)^2 = S_{\text{tot}}(S_{\text{tot}} + 1)$. As the local spin operator $\mathbf{s}_i + \mathbf{S}_i$ projected onto the ground-state subspace is of the following block-diagonal form:

$$\mathbf{T}_i = \mathbf{S}_i(S = 1) \oplus \mathbf{D}_i(S = 1/2),$$

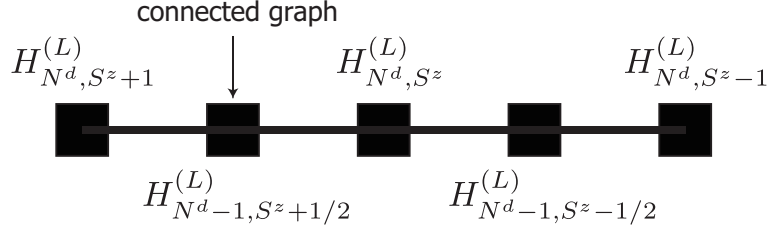


Figure A.4: Diagrammatic representation of the connectivity structure of the matrix $H_{N_d, S^z}^{(L+1)}$ in Eq. (A.21). The solid squares and the lines connecting them denote certain connected graphs (representing the diagonal blocks in $H_{N_d, S^z}^{(L+1)}$) and the non-zero (non-positive) matrices “*” in (A.21), respectively. (Reproduced from Ref. [54])

the projected total spin $\sum_i \mathbf{T}_i$ is block-diagonal with respect to the positions of the holes (i.e., spin- S) and S_{tot}^z , and so is its square². Within each block, $\left(\sum_i^L \mathbf{T}_i\right)^2$ is just a squared total spin of a mixed-spin system (with a given fixed sequence of spin- S and $S-1/2$):

$$\left(\sum_i^L \mathbf{T}_i\right)^2 = \sum_{i,j} \frac{1}{2} (T_i^+ T_j^- + T_i^- T_j^+) + \sum_{i,j} T_i^z T_j^z, \quad (\text{A.23})$$

in which $\mathbf{T}_i$ is either spin-1 $\mathbf{S}_i$ (hole) or spin-1/2 $\mathbf{D}_i$ (electron). Then, it is clear that the squared total spin (A.23) within each sector is non-negative and indecomposable [in the standard basis (A.18)], which allows us to apply the Perron-Frobenius theorem once again to show that the maximum eigenvalue of $\left(\sum_i^L \mathbf{T}_i\right)^2$ is unique. The corresponding eigenstate is a superposition of *all* the basis states allowed for the (given) hole configuration and S_{tot}^z with all-positive coefficients. Since in this S_{tot}^z -sector, S_{tot} can take any values in the range $S_{\text{tot}}^z \leq S_{\text{tot}} \leq S_{\text{max}} (= LS - N_e/2)$, the unique maximal eigenvalue is $S_{\text{max}}(S_{\text{max}} + 1)$.

Due to the peculiar property (guaranteed by the Perron-Frobenius theorem) of the unique lowest-energy state $|\psi_0; N_d, S_{\text{tot}}^z\rangle$, its overlap with the above $S_{\text{tot}} = S_{\text{max}}$ state is non-zero, i.e. $\mathcal{P}(S_{\text{max}})|\psi_0; N_d, S_{\text{tot}}^z\rangle \neq 0$ with $\mathcal{P}(S_{\text{max}})$ being the projector onto the space with $S_{\text{tot}} = S_{\text{max}}$ ³. Then, the SU(2)-symmetry of the Hamiltonian implies that

²For each S_{tot}^z value, there are $L!/[N_d!(L - N_d)!]$ sectors according to different sequences of spin- S and $(S - 1/2)$.

³Since there are $L!/[N_d!(L - N_d)!]$ different $S_{\text{tot}} = S_{\text{max}}$ states in the full S_{tot}^z -sector, $\mathcal{P}(S_{\text{max}})$ is a direct sum of the projectors onto the individual $S_{\text{tot}} = S_{\text{max}}$ states:

$$\mathcal{P}(S_{\text{max}}) = \oplus_{h \in \text{hole config.}} \mathcal{P}_h(S_{\text{max}}).$$

the $S_{\text{tot}} = S_{\text{max}}$ state $\mathcal{P}(S_{\text{max}})|\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle$ is another ground state of $H_{N_{\text{d}}, S_{\text{tot}}^z}^{(L)}$:

$$\begin{aligned} & H_{N_{\text{d}}, S_{\text{tot}}^z}^{(L)} \mathcal{P}(S_{\text{max}})|\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle \\ &= E_{\text{g.s.}}(N_{\text{d}}, S_{\text{tot}}^z) \mathcal{P}(S_{\text{max}})|\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle . \end{aligned} \tag{A.24}$$

The uniqueness of the ground state in the (full) S_{tot}^z -sector allows the only possibility

$$\mathcal{P}(S_{\text{max}})|\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle \propto |\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle ,$$

i.e., the ground state $|\psi_0; N_{\text{d}}, S_{\text{tot}}^z\rangle$ itself is ferromagnetic $S_{\text{tot}} = S_{\text{max}}$ for any values of S_{tot}^z . In particular, the above statement for $S_{\text{tot}}^z = 0$ (or $1/2$) means that the absolute ground state (i.e., the lowest-energy state in the entire Hilbert space) is unique (up to the trivial degeneracy associated with the $\text{SU}(2)$ -symmetry) and ferromagnetic. It is evident that we can readily generalize the above argument to arbitrary $S \geq 1$ by using Eqs. (A.14a) and (A.14b) instead of (2.11).

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