ASPECTS OF CRITICAL SPIN 1 CHAINS AND 2 DIMENSIONAL SYMMETRY PROTECTED TOPOLOGICAL PHASES OF MATTER

BY

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DISSERTATION

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Abstract

Effective field theory is a very useful technique for understanding quantum many body systems. We use this approach to study a certain class of critical quantum spin-1 chains and symmetry protected topological phases of matter in two spatial dimensions.

In the first context we consider the SU(3) symmetric spin-1 chain with additional interactions. We use bosonization to demonstrate that the effective field theories describing the critical behaviour of these spin chains can be mapped to free compact boson conformal field theories (CFTs) with central charge $c = 2$. We also describe how some predictions from field theory can be verified in numerical calculations using exact diagonalization (ED) and the density matrix renormalization group (DMRG) algorithm. In particular, the bosonization method gives a formula for the evolution of four Tomonaga-Luttinger liquid (TLL) parameters as a function of the lattice parameters. Using the analytic formulae for the scaling dimensions in terms of the TLL parameters and matching of lowest scaling dimensions, we numerically calculate these field-theoretic parameters and confirm that their evolution agrees with the prediction using bosonization.

We also tackle aspects of the challenging problem of understanding interacting topological phases. In this context, we aim to understand the effects if interactions in certain classes of symmetry protected topological (SPT) phases of matter. We consider non-chiral SPT phases in two spatial dimensions protected by a discrete symmetry such as $\mathbb{Z}_K$ or $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry. We argue that modular invariance/noninvariance of the partition function of the one-dimensional edge theory can be used to diagnose whether, by adding

a suitable potential, the edge theory can be gapped or not without breaking the symmetry. By taking bosonic phases described by Chern-Simons K-matrix theories and fermionic phases relevant to topological superconductors as examples, we demonstrate explicitly that when modular invariance is achieved, we can construct an interaction potential that is consistent with the symmetry and can completely gap out the edge.

We also briefly discuss preliminary results of a numerical approach for simulating the 3 dimensional Landau Level problem. This includes a brief description of a potential application of variational Monte Carlo to spin-orbit coupled ab initio systems.

"To my parents."

Acknowledgments

My time at the University of Illinois has been quite remarkable. It has been such a great honor to be part of a vibrant intellectual community full of wonderful people. My experience here will no doubt remain crucial to my personal and professional development. When I enrolled in the physics department I was filled with excitement and eagerness to contribute to the ideas developed over the years to understand fundamental aspects of nature. Initially my excitement hardly translated into any productivity in research. Things took a turn for the better when I started interacting with my research adviser professor Shinsei Ryu. I am very grateful to him for providing me with the guidance I needed to ask useful questions and frame the answers in the context of scientific research.

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Chapter 1

Introduction

Given a strongly correlated quantum system, some basic properties that are important to understand include the presence or absence of an energy gap, the presence of spontaneous symmetry breaking etc. One then asks for more specific information, and ultimately, the complete description of the underlying low energy physics. Quite often, this involves determining an effective field theory and using the properties of the deduced field theory. Examples include conformal field theories (CFT), describing the set of independent critical exponents in gapless systems and topological field theories describing the full braiding statistics in gapped quantum systems. The main goal of this thesis is to describe original contributions to the study of critical spin-1 chains [72] and SPT Phases of matter in 2-d (two spatial dimensions) [73]. We also include a brief description of preliminary results of application of variational Monte Carlo (VMC) to the 3d Landau level (LL) problem.

Critical spin chains and SPT phases in 2-d are quite different physical systems who do not seem to have anything in common since the former are gapless and the latter are gapped (in the bulk). However one of the usual signatures of gapped topological phases of matter is the existence of boundary modes. In the field theory language these boundary modes are necessary to define the full topological quantum field theory for the system on

a manifold with a boundary. These boundary modes provide a way for us to theoretically understand what is non-trivial about the physics of gapped topological phases whenever there is a symmetry we would like to preserve. In this way one can think of the boundary theory as encoding some aspects of non-triviality of the bulk.

For the type of gapped SPT phases that we consider in 2-d, the boundary modes are gappless and can be described using 1+1-D CFT. Therefore in both problems that we tackle we will encounter gapless degrees of freedoms described at long distances by 1+1-D CFT. We provide some description of the results from CFT used as they come up. In the next two sections we give a broader background and dicuss the specific issues that are addressed in this thesis.

1.1 1-d Critical Systems

It is widely accepted that the critical physics of any 1-d quantum system at a continous phase transition can be described by a 1+1 D CFT, this is reviewed for example in [15]. An interesting challenge is to deduce the CFT governing any given 1-d critical lattice system. In this context, the entanglement entropy (EE), Renyi entropies and entanglement spectrum [12,37,38,49,52,55,66,67,75] have proved to be useful probes. For example, the finite-size scaling of the EE in one-dimensional critical systems, provides a precise estimate of the central charge c of the corresponding CFT. Recent studies have also developed other ways of using reduced density matrices [1,20,30,39,56,59] which reveal information about complementary aspects of the low-energy theory (such as scaling dimensions and operators).

Tomonaga-Luttinger liquids (TLL) in one dimension [2, 21, 30, 42, 43] arise in the description of electrons moving in one spatial dimension. The suprising result is that the low energy excitations of a large class of gapless one dimensional systems are not fermionic but bosonic quasiparticles. Therefore correlation functions exhibit anomalous power laws

in space and time with interaction independent exponents. To demonstrate TLL physics, one linearizes the dispersion close to the Fermi momentum k_F. In the absence of any spin degrees of freedom, the low-energy physics is summarized in terms of a scalar boson ϕ and its canonical conjugate π as

$$H = \frac{v_F}{2} \int dx\, K\pi(x)^2 + K^{-1} \left(\partial_x \phi(x)\right)^2 . \tag{1.1}$$

The bosonic field ϕ is compactified on a circle of radius R with the relationship $K = 1/2\pi R^2$. K is called the TLL parameter and once it has been specified, it is an exercise in CFT to write down the spectrum of operators, scaling dimensions etc. Therefore the TLL parameter gives a complete characterization of the critical physics of an TLL liquid. The TLL parameter can be directly calculated from the Renyi entropy [30] and other methods involving reduced density matrices [43].

1.1.1 Quantum Spin-1 Chain

As described above the physics of a TLL with one parameter is quite well developed and understood. An important quantity in a CFT is the central charge c, which roughly accounts for the number of degrees of freedom. More precisely it arises as a central extension of the classical conformal algebra, the Witt algebra to the Virasoro algebra with an extension parameter which is $c > 0$. To have a unitary CFT one requires $c >= 1$ or a discrete set of possibilities with $c < 1$. The discrete possibilities with $c < 1$ have been classified and are known as minimal models. The field theory in equation (1.1) has $c = 1$, and one reason why the TLL theory is well understood is that the moduli space of $c = 1$ theories is well understood. This is discussed further in section (2.2.4). However the landscape of CFTs is abound with many theories with $c > 1$, and since there exist real physical systems with this property [53, 69], it is important to extend our understanding to these

cases. In this thesis, we will consider examples of systems described by $c = 2$ CFTs, these theories require four dimensionless parameters for their complete description.

In some special cases, a $c = 2$ CFT can be understood as a tensor product of two $c = 1$ CFTs: for example, the 1D Hubbard model has two TLL parameters, one for spin and the other for charge. In general such a factorization is not possible. As an example, we concentrate on studying the spin-1 lattice model whose Hamiltonian is,

$$H = \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij \rangle} \left(\mathbf{S}_i \cdot \mathbf{S}_j \right)^2 + Q_x \tag{1.2a}$$

$$Q_x = q_x \sum_i U_x^{\dagger i} U_x^{i+1} + \text{h.c.} \tag{1.2b}$$

where $\mathbf{S}_i$ is a spin-1 operator living on site i, while q_x is a scalar constant. U_x is a 3×3 matrix which in the S_z basis $(-1, 0, 1)$ is given by,

$$U_x = \begin{pmatrix} \omega^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \omega \end{pmatrix}, \tag{1.3}$$

where $\omega = \exp(i2\pi/3)$. For $q_x = 0$, this model is the analytically solvable Lai-Sutherland model [40, 45, 74], which serves as a useful guide for checking our calculations.

This model is of interest in the context of exotic phases such as Bose metals [58] on three leg ladders, and the recently proposed quantum torus chain [65]. In section 2.1 we describe how this type of model arises in a Bose model on a three leg ladder at one third filling. This family of models may also share common low-energy properties with spin-1/2 quantum spin-tubes [17, 69]. A generalized version is the bilinear-biquadratic model [60], whose phase-diagram includes a gapless phase and the gapped Haldane phase [5, 35] and which has been experimentally realized in $LiVGe_2O_6$ [57].

1.1.2 Specific Issues Addressed

In the first part of this thesis we describe a TLL parameter extraction procedure for a $c = 2$ CFT that does not necessarily factorize as a product of two $c = 1$ theories. This is explained in detail in chapter 2. In particular we deduce the evolution of the dimensionless parameters which are a generalization of the TLL parameter as a function of q_x that appears in equation (1.2a). Our analysis depends on an expansion in terms of effective fields close to the $SU(3)$ point. We give some numerical evidence for why we believe our results are correct in particular for $q_x < 0.5$.

1.2 SPT Phases in 2-d

Since the discovery of the quantum Hall effects (QHEs) [62] a major problem of interest in the study of many body systems is to understand and characterize different phases of matter that are beyond the symmetry breaking paradigm pioneered by Landau. Distinct quantum Hall systems have the same charge conservation $\mathrm{U}(1)$ symmetry but are different phases of matter as characterized by different values of the Hall conductivity. In fractional quantum Hall systems there are no local order parameters that can be defined to characterize the different phases that occur [79]. More recently the theoretical prediction and experimental discovery of topological insulators (TIs) [36] in 2 and 3 spatial dimensions (2d and 3d) provide more examples of systems where the symmetry breaking notion of Landau alone is not very useful for understanding the different phases. TIs are gapped phases of matter (usually free electrons although bosonic versions have been predicted to occur) which are insulating in the bulk but have gapless Dirac modes at their boundary protected by symmetry (e.g time reversal symmetry for conventional TIs and mirror symmetry for crystalline TIs). Topological insulators are an example of symmetry protected topological (SPT) phases [18] which would be the focus in the second part

of this thesis. The gapless edge modes in topological insulators are protected in the absence of interactions by symmetry. Another example of SPTs which feature in this thesis are 2d topological superconductors (TSCs) [11] which host Majorana modes at their edge protected by time reversal symmetry.

More generally a SPT phase of matter is a quantum system invariant under symmetry group G, and has a gapped ground state which does not spontaneously break G. Furthermore, the ground state cannot be adiabatically connected to a direct product state without breaking G or closing the bulk gap. A final property is that the ground state can be connected to a trivial direct product state without closing the bulk gap if G is allowed to be broken. The classification of non-interacting SPT phases of free fermions has been worked out in several related contexts using disorder properties of fermions on the boundary [71], K-theory [44] etc. In some cases it has been explicitly shown that this classification is unstable to interactions [26]. Accordingly, an outstanding open problem is to understand the classification of interacting SPT phases of matter.

1.2.1 Specific Questions and Techniques

Following the idea in Ref. [68] we demonstrate how modular invariance can be used to understand interacting SPT phases in 2d systems protected by a finite unitary symmetry group. Modular invariance is a basic constraint imposed on a CFTs derived from 1d lattice systems [16]. At the basic level, if one considers thermal physics at finite temperature on a periodic lattice so that Euclidean spacetime is a torus, modular invariance means that the CFT is independent of what choice of basis is used to describe the torus viewed as the unit cell of a lattice. A non modular invariant theory cannot exist on its own but can be viewed as the boundary of a system in 2d. In the context we explore here, the 2d system is a cylinder. It is known [19] that SPT phases in 2d systems with a boundary have gapless excitations localized on the boundary. We focus on non-chiral systems and consider the non-chiral CFT describing gapless modes on one of the edges of the cylinder.

After enforcing the symmetry, if modular invariance cannot be achieved we claim that this implies that the edge must be viewed as the boundary of a non-trivial bulk SPT which couples one edge to another so that the combined edges are modular invariant. On the other hand, if modular invariance can be achieved then the edge can exist on its own independently of the bulk and hence the other edge, and we view this as a trivial SPT phase. Since a non-trivial SPT phase has a symmetry protected gapless edge, our method may also be considered as a tool which can be applied to check if a 1+1 D CFT can be gapped or not under a set of symmetry constraints. For the cases where modular invariance can be achieved after enforcing symmetry we explicitly construct potentials that can gap out the edge. This procedure is described fully in chapter 4.

1.3 SPT Phases in 3-d

In chapter 5 we briefly introduce numerical methods that may be useful for quantum Monte Carlo simulations of spin-orbit coupled ab-initio system. In particular we discuss variational Monte Carlo simulation of the 3 dimensional Landau Level problem. This is an important problem because it is believed to be an example of a 3 dimensional topological insulating system [50]. Therefore being able to simulate in correctly would be a good first step to understanding what role interactions play. We discuss some preliminary results in this direction.

Chapter 2

Spin-1 Chains

Many of the contents of this chapter are taken from what was reported in [72], however, in some areas we try to provide some more details.

2.1 Boson Model On A Three Leg Ladder

To demonstrate how a system described by a Hamiltonian $(1.2a)$ might arise in a real setting. We consider a model that realizes a mulicomponent TLL. The most natural geometry for doing this is a ladder (or tube), a quasi-one dimensional system made up of one dimensional legs which are additionally coupled in the transverse or rung direction, with open (or periodic) boundary conditions. Fig. 2.1 shows an example with three legs, relevant for modelling quasi one-dimensional compounds such as $[(CuCl_2tachH)_3Cl]Cl_2$ [70] and $CsCrF_4$ [54], and to which recent theoretical works [17, 58, 69] have been devoted.

Following the work of Mishmash et al. [58] we consider a system governed by the

Hamiltonian,

$$
\begin{aligned}
H &= H_{\text{hop}} + H_K && \text{(2.1a)}\\
H_{\text{hop}} &= -t_x \sum_{\mathbf{r}} b^\dagger_{\mathbf{r}} b_{\mathbf{r}+\hat{x}} + \text{h.c.} - t_y \sum_{\mathbf{r}} b^\dagger_{\mathbf{r}} b_{\mathbf{r}+\hat{y}} + \text{h.c.} && \text{(2.1b)}\\
H_K &= K \sum_{\mathbf{r}} b^\dagger_{\mathbf{r}} b_{\mathbf{r}+\hat{x}} b^\dagger_{\mathbf{r}+\hat{x}+\hat{y}} b_{\mathbf{r}+\hat{y}} + \text{h.c.} && \text{(2.1c)}
\end{aligned}
$$

where t_y and t_x are the hoppings along the transverse (y) and length (x) directions respectively, K is a correlated exchange on a square plaquette. The phase diagram of this model is expected to be quite rich; here we only consider the case of $t_x, t_y \to 0$ with $1/3$ filling of bosons. In this parameter regime, the low-energy theory of this model involves only one boson per rung (column) allowing three distinct states on it. The number of bosons per rung can not change because of the absence of hopping in the x direction.

On making a change of basis of the bosonic creation operators along the y direction, a new basis at every x location is defined as,

$$
\begin{aligned}
|0\rangle_x &\equiv \frac{1}{\sqrt{3}} \left(b^\dagger_{x,0} + b^\dagger_{x,1} + b^\dagger_{x,-1} \right) \\
|\pm\rangle_x &\equiv \frac{1}{\sqrt{3}} \left(b^\dagger_{x,0} + \omega b^\dagger_{x,\pm 1} + \omega^2 b^\dagger_{x,\mp 1} \right) && \text{(2.2)}
\end{aligned}
$$

where $\omega = \exp(i2\pi/3)$ is the same value as appearing in Eq. 1.3. The three components can be thought of as those corresponding to a pseudospin-1 object, leading to the effective spin-Hamiltonian. In the boson occupation number basis at $1/3$ filling which we order as $\{y = -1, y = 1, y = 0\}$ (so that for example occupation on the -1 cite is given by a three component vector with one in the first column and zero everywhere else), the Hamiltonian on a neighboring pair of x lattice sites is represented by

$$
H_K = K \left(U_{-1,0} \otimes U^\dagger_{-1,0} + U_{0,1} \otimes U^\dagger_{0,1} + U_{1,-1} \otimes U^\dagger_{1,-1} \right), \qquad \text{(2.3)}
$$

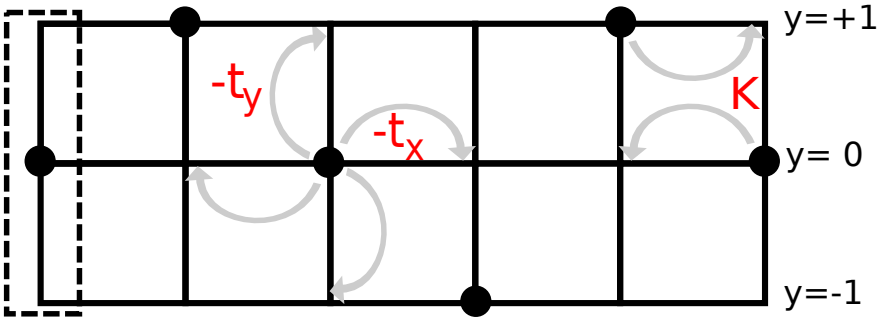

Figure 2.1: A representative configuration of hard-core bosons on a three leg ladder with periodic boundary conditions in the transverse or rung direction, with Hamiltonian given by Eq. 2.1a. The hopping in the length (t_x) and transverse (t_y) directions respectively and the correlated hop (K) on the square plaquette have been indicated by arrows. For $t_x = 0$ and at 1/3 filling, the low energy model involves configurations with only with exactly one boson per rung. The three configurations per rung, one of which has been enclosed in a dotted rectangle, after an appropriate change of basis, are mapped to a spin-1 basis. the form Eq. 1.2a

where $U_{-1,0}$ represents $b_0^\dagger b_{-1}$ and is given by

$$U_{-1,0} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.4}$$

The other terms appearing in (2.3) can de deduced similarly based on the ordering of the basis. A calculation of tensor products, for example in any convenient software package reveals that under the change of basis (2.2),

$$H_K \to K \left(H_{SU(3)} - \frac{Q_y}{3} - \frac{4}{3} \right), \tag{2.5}$$

where the term Q_x which appears in $(1.2a)$ transforms as $Q_x \to Q_y$ after applying this change of basis globally on all lattice sites. To derive this result it may be useful to start from the right hand side and note that $H_{SU(3)}$ is invariant. From this invariance it is clear that the model on the right of (2.5) is equivalent to a model with Q_y replaced by Q_x, which is the model (1.2a) with q_x tuned to a particular value. We are going to work mostly in

the spin-1 basis but the bosonic theme of the physics would be inherent in our treatment in the next subsections.

2.2 Bosonizing the Chain at Criticality

2.2.1 Symmetries

In this section, we develop a continuum field theory description for the lattice Hamiltonian (1.2a), by closely following the treatment of the SU(3) point developed in Refs. [3,40]. First we consider the symmetry properties of the Hamiltonian (1.2a). We note that the spin-1 part of the Hamiltonian (1.2a) can be written (up to a constant factor) in a manifestly SU(3) symmetric way in terms of 3×3 elementary matrices L^{α}_{β} with one on row α and column β, and zero everywhere else as

$$H_{\mathrm{SU(3)}} = \sum_{\langle ij \rangle} \sum_{\alpha,\beta=0,1,2} L^{\alpha}_{\beta\, i} L^{\beta}_{\alpha\, j}. \tag{2.6}$$

We can write this Hamiltonian in terms of fermionic operators by expressing $L^{\alpha}_{\beta\, i} = c_i^{\alpha\dagger} c_{\beta\, i}$, with the constraint

$$\sum_{\alpha=0,1,2} c_i^{\alpha\dagger} c_{\alpha\, i} = \sum_{\alpha=0,1,2} n_{\alpha i} = 1, \tag{2.7}$$

at each site i. The constraint prevents zero, double or triple occupancy on each lattice site. It ensures that the fermionic operators like the spin operators act on a three dimensional Hilbert space. The Hamiltonian $H_{\mathrm{SU(3)}}$ conserves the particle numbers $N_1 - N_0$ and $N_2 - N_0$, where $N_\alpha = \sum_i c_i^{\alpha\dagger} c_{\alpha i}$. Defining the dual basis by $\tilde{c}_n = 3^{-1/2} \sum_{\alpha=0}^{2} c_\alpha w^n$ for $n = 0, 1, 2$, and the corresponding particle numbers as $\tilde{N}_n = \sum_i \tilde{c}_i^{n\dagger} \tilde{c}_{ni}$, the Hamiltonian $H_{\mathrm{SU(3)}}$ also conserves the dual particle numbers $\tilde{N}_1 - \tilde{N}_0$ and $\tilde{N}_2 - \tilde{N}_0$.

On the other hand, the Q_x perturbation in (1.2a) can be written as

$$Q_x = 3q_x \sum_{i,\alpha} L^{\alpha}_{\alpha\, i} L^{\alpha}_{\alpha\, i+1}. \tag{2.8}$$

The Hamiltonian $H_{\mathrm{SU}(3)} + Q_x$ conserves the particle numbers $N_1 - N_0$ and $N_2 - N_0$, and it conserves the dual particle numbers $\tilde{N}_1 - \tilde{N}_0$ and $\tilde{N}_2 - \tilde{N}_0$ both (mod 3).

2.2.2 Continuum theory

The low-energy effective field theory for the Hamiltonian $H_{\mathrm{SU}(3)}$ can be developed by noting that at low energies, only excitations close to the Fermi points propagate. The Fermi point can be deduced for lattice fermions in the usual way by filling up states with negative energies. The disperison relation in this case is $E = -R_0 \cos ka_0$, (where a_0 is the lattice constant) and R_0 is a positive constant which represents the expectation value of lattice four fermion interactions in the mean field approximation [40]. The negative energy states in the Brilloin zone $|k| \leq \pi$ satisfy $|k| < \pi/a_0$, however, because of the constraint (2.7), only one third of these states can be filled, therefore, $k_F = \pi/3a_0$. Thus at low energies, we can approximate,

$$c_{\alpha\, i} \approx \sqrt{a_0}[e^{ik_F x_i}\psi_{R\alpha}(x_i) + e^{-ik_F x_i}\psi_{L\alpha}(x_i)]. \tag{2.9}$$

Substituting this in the Hamiltonian and dropping oscillatory terms, the low energy theory can be written in terms of the $U(3)$ currents,

$$J^{\alpha}_{R,L\,\beta} = \psi^{\alpha\dagger}_{R,L}\psi_{R,L\,\beta}, \tag{2.10}$$

as

$$H_{\mathrm{SU(3)}} = \pi v_F \int dx \sum_{\alpha,\beta} [J^{\alpha}_{R\,\beta} J^{\beta}_{R\,\alpha} + J^{\alpha}_{L\,\beta} J^{\beta}_{L\,\alpha} + 2 J^{\alpha}_{R\,\beta} J^{\beta}_{L\,\alpha} - 2\cos(2k_F a_0) J^{\alpha}_{R\,\alpha} J^{\beta}_{L\,\beta}], \tag{2.11}$$

where v_F is the Fermi velocity, which will be set to 1 henceforth. Beyond the mean field approximation, it can be shown that the last term in Eq. 2.11 which only depends on the charged modes is dynamically gapped. Also the third term is marginally irrelevant in the renormalization group sense [40]. Thus the critical theory in the long distance limit is

$$H_{\mathrm{SU(3)}} \approx H_{\mathrm{WZW}} = \pi \int dx \sum_{\alpha,\beta} [J^{\alpha}_{R\,\beta} J^{\beta}_{R\,\alpha} + J^{\alpha}_{L\,\beta} J^{\beta}_{L\,\alpha}]. \tag{2.12}$$

We note that this is a $U(3)$ Wess-Zumino-Witten (WZW) model and thus contains an $\mathrm{SU}(3)_1$ and $U(1)$ part [28]. The $U(1)$ piece is precisely the charged mode which is gapped and will be dropped later. (N.B. the above procedure can also be described instead of dealing with the SU(3) Lai-Sutherland model, by starting with the Hubbard type model $H = -t \sum_{\langle ij \rangle \alpha} [c^{\dagger}_{i\alpha} c_{j\alpha} + h.c.] + U \sum_{i,\alpha \neq \beta} n_{i\alpha} n_{i\beta}$ without constraint $\sum_{\alpha} n_{\alpha i} = 1$. This constraint is in fact generated dynamically and this model reduces to the SU(3) symmetric spin model when expanded in t/U.)

Applying the same reasoning above which is valid close to SU(3) point, one deduces the continuum approximation

$$Q_x \approx 3 q_x \int dx \sum_{\alpha} \left[(J^{\alpha}_{R\,\alpha})^2 + (J^{\alpha}_{L\,\alpha})^2 \right], \tag{2.13}$$

where again we have dropped the terms that only depend on the charged mode. Thus we are considering Q_x as a deformation of the Lai-Sutherland model which becomes (after ignoring gapped degrees of freedom) in the continuum theory a marginal deformation of

the $SU(3)_1$ CFT.

2.2.3 Bosonization

Bosonization is a fascinating result in 1+1 D physics that relates fermions to bosons. The general situation can be understood by appealing to the theory of affine Kac Moody algebras [32, 80]. Physically, this kind of operator algebra are realized as the Laurent series modes of conserved currents that appear in a CFT with global symmetry H, where H is a Lie group. One can explicitly construct a representation of the theory where the fundamental field lives in H. This is the Wess Zumino Witten(WZW) [80] model denoted H_k where k is an integer parameter knows as the level. In the case where the theory is a WZW model with simply connected H, the theory factorizes into a holomorphic and anitiholomorphic parts. The affine currents on both parts generate the whole spectrum and the theory is integrable.

In this section we will see aspects of this structure arise in the case where the Lie group H is $U(3)$, although we will eventually be interested in the $SU(3)$ subgroup obtained after ignoring the diagonal $U(1)$ generator which represents the charge mode.

One can introduce complex coordinates for 1+1 D space-time $z = -i(x - t)$, and $\bar{z} = i(x + t)$. These coordinates are complex conjugates in terms of imaginary time $\tau = it$, and time evolution factorizes nicely so that the fields with an $R(L)$ subscript depend only on $z(\bar{z})$ respectively and are holomorphic(anti-holomorphic). The continuum fermi fields in Eq. (2.9) can be bosonized as follows

$$\psi_{\beta L} = \frac{1}{\sqrt{2\pi a_0}} : e^{-i\sqrt{4\pi}\phi_{\beta L}} :, \quad \psi_L^{\beta\dagger} = \frac{1}{\sqrt{2\pi a_0}} : e^{i\sqrt{4\pi}\phi_{\beta L}} :, \tag{2.14}$$

where ϕ_L represents the holomorphic (left-moving) part of a free boson field. We focus on the holomorphic parts of the theory (dropping the L subscript) with similar formulae for the right moving fermions in terms of the anti-holomorphic part of the free boson field.

We have introduced normal ordering of an operator O, denoted by $:O:$, which must be used when two fields at the same point are multiplied together. We shall specify a prescription for normal ordering below. Usually when bosonizing more that one species of fermions, one introduces Klein factors to ensure that different fermi fields anticommute. These Klein factors have been ignored here since they are not dynamical and do not play a role in the Hamiltonian which is mainly what we are interested in here. The ground state expectation value of the holomorphic part of the free boson fields satisfies

$$\langle 0|\phi^\alpha(z)\phi^\beta(w)|0\rangle = -\frac{\delta^{\alpha\beta}}{4\pi}\log\left|\frac{z-w}{a_0}\right|, \tag{2.15}$$

where we have picked the lattice constant a_0 as a short distance regulator. The kernel appearing on the right of equation (2.15) is the holomorphic part inverse of the laplacian operator in 1+1D. The normal ordered product is defined by

$$:\phi^\alpha(z)\phi^\beta(w): = \phi^\alpha(z)\phi^\beta(w) - \langle 0|\phi^\alpha(z)\phi^\beta(w)|0\rangle\,, \tag{2.16}$$

With an implicit time or radial ordering in the first term. The normal ordered product is holomorphic and non-singular as $z \to w$ and we define the product

$$:\phi^\alpha\phi^\beta:(z) = \lim_{w\to z} :\phi^\alpha(z)\phi^\beta(w):\,. \tag{2.17}$$

To define the normal ordered product with more than two terms in the product one substracts all singularities as any two field positions approach each other. This results in the famous Wick's theorem for free fields. For us it is convenient to use Wick's theorem in the form

$$:F[\phi]G[\phi]: = \exp\left(\sum_{\alpha\beta}\frac{\delta^{\alpha\beta}}{4\pi}\int dz_1 dz_2 \log\left|\frac{z_1-z_2}{a_0}\right|\frac{\delta_F}{\delta\phi^\alpha(z_1)}\frac{\delta_G}{\delta\phi^\beta(z_2)}\right)F[\phi]G[\phi], \tag{2.18}$$

where the F and G are any functionals of the bosonic fields. The subscript in a functional derivative indicate what functional it acts on. The functional differentiation represent contractions and exponentiation takes care of all possible contractions. The inverse of Eq. 2.18 is

$$F[\phi]G[\phi] = \exp\left(-\sum_{\alpha\beta}\frac{\delta^{\alpha\beta}}{4\pi}\int dz_1 dz_2 \log|\frac{z_1-z_2}{a_0}|\frac{\delta_F}{\delta\phi^\alpha(z_1)}\frac{\delta_G}{\delta\phi^\beta(z_2)}\right) : F[\phi]G[\phi] :, \quad (2.19)$$

Applying this to (2.14) we obtain

$$\psi^{\alpha\dagger}(z)\psi_\alpha(w) = \frac{1}{2\pi|z-w|} : e^{i\sqrt{4\pi}(\phi_\alpha(z)-\phi_\alpha(w))} : . \quad (2.20)$$

Taylor expanding inside the normal ordered product on the right, taking the limit as $z \to w$, and keeping only non-singular terms leads to a key identity, which can be regarded as the inverse of Eq. 2.14:

$$: \psi^{\alpha\dagger}\psi_\alpha : (z) = \frac{-i}{\sqrt{\pi}}\partial\phi_\alpha(z), \quad (2.21)$$

where ∂ denotes a derivative with respect to z. To understand the split into SU(3) and U(1) WZW theories mentioned above we introduce the SU(3) and U(1) currents given by

$$J^a = \sum_{\alpha,\beta}\psi^{\alpha\dagger}T^a_{\alpha\beta}\psi_\beta, \quad J = \sum_\alpha \psi^{\alpha\dagger}\psi_\alpha, \quad (2.22)$$

where T^a are generators of the SU(3) algebra. See [31] for a description of this algebra. The $U(1)$ piece in the boson language satisfies

$$J = \frac{-i}{\sqrt{\pi}}\left(\partial\phi_0 + \partial\phi_1 + \partial\phi_2\right). \quad (2.23)$$

The SU(3) currents associated to the Cartan sub-algebra are

$$H^1 \propto \psi^{0\dagger}\psi_0 - \psi^{1\dagger}\psi_1 \propto \partial\phi_0 - \partial\phi_1,$$
$$H^2 \propto \psi^{0\dagger}\psi_0 + \psi^{1\dagger}\psi_1 - 2\psi^{2\dagger}\psi_2 \propto \partial\phi_0 + \partial\phi_1 - 2\partial\phi_2. \tag{2.24}$$

So we can make an OPE preserving orthogonal change of basis to introduce $\tilde{\phi}_{0,1,2}$ as

$$\tilde{\phi}_0 = (\phi_0 + \phi_1 + \phi_2)/\sqrt{3}, \tag{2.25}$$
$$\tilde{\phi}_1 = (\phi_0 - \phi_1)/\sqrt{2},$$
$$\tilde{\phi}_2 = (\phi_0 + \phi_1 - 2\phi_2)/\sqrt{6}.$$

In this basis the dynamics of the charged mode is now encoded in the single boson field $\tilde{\phi}_0$. Thefore dropping the charged mode corresponds to setting $\tilde{\phi}_0 = 0$. This is indicated with an arrow in the equations below. In this basis some of the SU(3) currents associated with the Cartan subalgebra are simply (up to a constant factor) $\partial\tilde{\phi}_1$, $\partial\tilde{\phi}_2$, while those associated with a choice of simple roots for SU(3) are

$$J^{\boldsymbol{\alpha}_1} \propto \psi_0^\dagger\psi_1 \propto e^{i\sqrt{4\pi}(\phi_1-\phi_0)} \to e^{i\sqrt{8\pi}\boldsymbol{\alpha}_1\cdot\tilde{\boldsymbol{\phi}}},$$
$$J^{\boldsymbol{\alpha}_2} \propto \psi_0^\dagger\psi_2 \propto e^{i\sqrt{4\pi}(\phi_2-\phi_0)} \to e^{i\sqrt{8\pi}\boldsymbol{\alpha}_2\cdot\tilde{\boldsymbol{\phi}}}.$$

$\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$ together with a third root $\boldsymbol{\alpha}_3$ are given by,

$$\boldsymbol{\alpha}_1 = (1,0),\ \boldsymbol{\alpha}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right),\ \boldsymbol{\alpha}_3 = \left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right). \tag{2.26}$$

All other roots of SU(3) can be obtained as integer linear combinations of $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_2$, for example $\boldsymbol{\alpha}_3 = \boldsymbol{\alpha}_1 - \boldsymbol{\alpha}_2$. Similarly, the vertex operators associated with all other roots can be obtained from operator products of $J^{\boldsymbol{\alpha}_1}$ and $J^{\boldsymbol{\alpha}_2}$. These construction gives precisely the vertex operators obtained in the purely bosonic construction of $\mathrm{SU}(3)_1$ where the boson

fields $\tilde{\phi}_1$ and $\tilde{\phi}_2$ are compactifield on the root lattice of the SU(3) algebra [34]. All proportionality constants can be fixed by a choice of normalization of the SU(3) generators.

We now obtain the purely bosonic description of the gapless degrees of freedom of the spin-1 chain at criticality. The key identities are

$$\begin{aligned}\sum_{\alpha} J^{\alpha}_{\alpha} J^{\alpha}_{\alpha} &= -\sum_{\alpha} \partial\phi_{\alpha}\partial\phi_{\alpha} \\ &\to -(\partial\tilde{\phi}_1\partial\tilde{\phi}_1 + \partial\tilde{\phi}_2\partial\tilde{\phi}_2), \qquad (2.27)\\ \sum_{\alpha\neq\beta} J^{\alpha}_{\beta} J^{\beta}_{\alpha} &= \sum_{\alpha\neq\beta} \partial\phi_{\alpha}\partial\phi_{\beta} \\ &\to -(\partial\tilde{\phi}_1\partial\tilde{\phi}_1 + \partial\tilde{\phi}_2\partial\tilde{\phi}_2). \qquad (2.28)\end{aligned}$$

The first of these is the square of the result obtained in Eq. 2.21. The second can be obtained similarly, and by noting that when $\alpha \neq \beta$ there is no singularity in the products of exponentials. Therefore we obtain the main result of this section,

$$\begin{aligned} H_{\mathrm{SU}(3)} &\approx -2\int dx(\partial\phi_1\partial\phi_1 + \partial\phi_2\partial\phi_2 + \text{antilhol}), \\ Q_x &\approx -3q_x\int dx(\partial\phi_1\partial\phi_1 + \partial\phi_2\partial\phi_2 + \text{antilhol}). \qquad (2.29)\end{aligned}$$

where antihol denotes the antiholomorphic part. Note that the tildes have now been dropped: the effective Hamiltonian of the spin-1 chain is now written in terms of $\mathrm{SU}(3)_1$ boson fields ϕ_1 and ϕ_2. We note that these quantities are all non-negative since we have for any field ϕ,

$$\partial\phi\partial\phi + \bar{\partial}\phi\bar{\partial}\phi = -\frac{1}{2}\left(\partial_x\phi\partial_x\phi + \partial_t\phi\partial_t\phi\right). \qquad (2.30)$$

In the next section we rewrite the $SU(3)_1$ bosonic theory in a more standard form and we explore a certain landcape of $c = 2$ CFTs.

2.2.4 General $c = 2$ Two component Boson theories

In the previous section, we derived the low-energy effective Hamiltonian that should capture the critical dynamics of the spin-1 chain with the Q_x perturbation. The low-energy effective theory consists of two compactified boson fields and has central charge $c = 2$. To put the effective theory in a general context, we discuss in this subsection a generic two-component boson theory with $c = 2$.

For the case of the single-component Tomonaga-Luttinger liquid, the landscape of the theory (often called "moduli space") is well understood. Theory space is characterized solely by a single parameter, the Luttinger parameter K or equivalently the compactification radius R of the boson field. There is a boson-vortex duality in (1+1)d (also known as "T-duality") which relates the two regions $K > 1$ and $K < 1$. These regions are separated by the self-dual point $K = 1$ where $\mathrm{SU}(2)$ symmetry is realized. With orbifolding, theory space for $c = 1$ is described in terms of two axis, each describing the ordinary free boson theory (the single-component Tomonaga-Luttinger liquid) and its orbifolded counterpart, together with a few "exceptional cases" [4].

On the other hand, the moduli space for the $c = 2$ theories is more complicated. Consider the action in 1+1 d space-time for two bosonic fields $X^{1,2}$,

$$S = \frac{1}{4\pi} \int dxdt \, (G_{ab} \partial_\mu X^a \partial_\mu X^b + B_{ab} \epsilon_{\mu\nu} \partial_\mu X^a \partial_\nu X^b), \tag{2.31}$$

where $\mu, \nu = 0, 1$, for time and space, and G and B are a symmetric (non degenerate) and antisymmetric 2 by 2 real matrix, respectively. Also the boson fields live on a unit torus i.e.

$$X^a \sim X^a + 2\pi. \tag{2.32}$$

The corresponding Hamiltonian is given by,

$$H = -\frac{1}{2\pi}\int dx\, G_{ab}(\partial X^a \partial X^b + \text{antihol}), \tag{2.33}$$

Observe that the parameter B does not enter into the Hamiltonian: it is a topological term. However, it affects the canonical commutation relations and hence the spectrum.

There are thus four independent parameters, G_{11}, G_{12}, G_{22} and B_{12}, characterizing the $c = 2$ action (2.31), as opposed to the $c = 1$ Tomonaga-Luttinger liquid parameterized by a single parameter. (As in the case of $c = 1$, one can consider various orbifolds of the two-component boson theory (2.31), leading to an even richer moduli space or phase diagram [24].)

For the case of $c = 1$ Tomonaga-Luttinger liquid, the duality relates the large and small compactification radius (the Luttinger parameter). Similarly, there is a group of duality transformations acting on the four parameters, and different values of G and B do not necessarily correspond to different spectra [10, 33]. To unveil this duality group, it is convenient to trade the four real parameters in G and B for two complex parameters ξ and ρ as follows

$$\begin{aligned} \xi &\equiv \frac{G_{12}}{G_{22}} + i\frac{\sqrt{\det G}}{G_{22}}, \\ \rho &\equiv B_{12} + i\sqrt{\det\, G}. \end{aligned} \tag{2.34}$$

These two parameters can be acted upon by independent $SL(2,\mathbb{Z})$ transformations which for ξ is given by

$$\xi \to \frac{a\xi + b}{c\xi + d}, \tag{2.35}$$

where $a, b, c, d \in \mathbb{Z}$ and $ad - bc = 1$. There is a similar independent transformation for ρ. These transformations change the parameters G and B but lead to the same spectrum.

Effectively the target space of the boson fields corresponds to two tori, which are left invariant by $SL(2,\mathbb{Z}) \times SL(2,\mathbb{Z})$ transformations. There are two further discrete transformations that leave the spectrum invariant:

$$(\xi, \rho) \to (\rho, \xi), \quad (\xi, \rho) \to (-\bar{\rho}, -\bar{\xi}). \tag{2.36}$$

When $B_{12} = G_{12} = 0$, we have a product of two $c = 1$ theories. In this case, the first transformation sends $G \to G^{-1}$, which corresponds to two independent duality transformations for each $c = 1$ theory. Fig. 2.2 depicts a portion of the space of theories in the $\xi = \rho$ plane together with some points of enhanced symmetry. We anticipate that these theories capture the critical behavior of the gapless degrees of freedom of spin-1 chains such as the model in Eq. (1.2a).

To deduce the spectrum of these bosonic theories we switch to Euclidean signature $t \to -it$. We take space-time to be a torus of modulus $\tau = \tau_1 + i\tau_2$ i.e we compactify Euclidean space-time as $x \sim x + 2\pi$ and $(x,t) \sim (x,t) + (2\pi\tau_1, 2\pi\tau_2)$. One can quantize using path integrals, the path integral yields a sum over instanton sectors. We can write in each instanton sector

$$X^a_{n,w} = X^a_{n,w,\,\mathrm{cl}} + X^a_q \tag{2.37}$$

where

$$X^a_{n,w,\,\mathrm{cl}}(x,t) = w^a x + \frac{(n^a - w^a\tau_1)t}{\tau_2} \tag{2.38}$$

is a classical solution that winds n and w times along the two non trivial cycles on the

torus. The partition function is

$$Z = \sum_{n,w} e^{-S^{cl}_{n,w}} \int [DX_q] e^{-S[X_q]}, \tag{2.39}$$

where $S^{cl}_{n,w}$ is the classical action evaluated on shell for Eq. (2.38), and the quantum path integral is over a continuous uncompactified variable X_q. The second term in Eq. (2.31) is a total derivative for periodic functions X_q and can be neglected. Thus the integral over X_q yields the determinant of the quadratic differential operator appearing in Eq. (2.31) which is just the Laplacian in the spacetime index times the G matrix in the internal index a. After applying a Poisson resummation in n for the classical contribution one finds

$$Z = \frac{1}{\det G^{1/2}} \left(\frac{\tau_2}{\det{}' \nabla^2} \right)^{c/2} \sum_{p_L, p_R} e^{2\pi i \tau_1 (p \circ p) - 2\pi \tau_2 (p \cdot p)}, \tag{2.40}$$

where $c = 2$,

$$\begin{aligned} p \circ p &= p_L^T G p_L - p_R^T G p_R, \\ p \cdot p &= p_L^T G p_L + p_R^T G p_R, \end{aligned} \tag{2.41}$$

and

$$\begin{aligned} p_L &= \frac{1}{2} \left(G^{-1}(n - Bw) + w \right), \\ p_R &= \frac{1}{2} \left(G^{-1}(n - Bw) - w \right). \end{aligned} \tag{2.42}$$

The Laplacian determinant can be regularized as $\det{}' \nabla^2 = \tau_2 |\eta(\tau)|^{-4}$, where the prime superscript indicates that the zero modes have been removed and $\eta(\tau)$ is the Dedekind eta function.

Comparing with the standard formula for a CFT partition function on the torus [28],

one can read off the spectrum of scaling dimensions

$$\Delta = p_L^T G p_L + p_R^T G p_R + \sum_{n_L>0} n_L N_n^L + \sum_{n_R>0} n_R N_n^R, \tag{2.43}$$

where the last two terms corresponds to the determinant of the Laplacian and represents in canonical quantization harmonic oscillators indexed by a positive integer $n_{L,R}$ and $N_n^{L,R}$ is the occupation number of oscillator $n_{L,R}$.

In the representation (2.31), the $\mathrm{SU}(3)_1$ WZW theory can be obtained by choosing G and B to be,

$$G = \frac{1}{2}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, \quad B = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \tag{2.44}$$

Here G is proportional to the inverse of the Cartan matrix of $\mathrm{SU}(3)$. The above choice of parameters at the $\mathrm{SU}(3)$ point is consistent with that used in the numerical sections below. The relationship to the fields used in the previous section (note they were tilded) is simply a change of basis that diagonalizes G and rescales the diagonal elements to 1 i.e

$$\phi_1 = \frac{1}{\sqrt{8\pi}}(X_1 - X_2), \quad \phi_2 = \sqrt{\frac{3}{8\pi}}(X_1 + X_2). \tag{2.45}$$

Since the terms in Eq. (2.29) correspond to the G term in the Hamiltonian (2.32) we deduce that the continuum version of the transformation $H_{\mathrm{SU}(3)} \to H_{\mathrm{SU}(3)} + q_x Q_x$ is

$$G_{SU(3)} \to G_{SU(3)} + q_x \frac{3}{2} G_{SU(3)}. \tag{2.46}$$

This prediction will be tested with the help of accurate numerical calculations, discussed at length in the next section. Fig. 2.3 depicts the portion of the space that we traverse starting with our choice of parameters for the $\mathrm{SU}(3)$ model and varying G as a function

of q_x. The form of the G matrix in Eq. (2.46) is consistent with and expected from the $\mathbb{Z}_3$ symmetry, i.e., the conservation of $\tilde{N}_1 - \tilde{N}_0$ and $\tilde{N}_2 - \tilde{N}_0$ mod 3 – see Sec. 2.2.1. The $\mathbb{Z}_3$ symmetry can be thought of as a $\frac{2\pi}{3}$ rotation in the root space of SU(3). In the effective field theory this is represented by the transformation on the currents $(J^{\boldsymbol{\alpha}_1}, J^{\boldsymbol{\alpha}_2}, J^{\boldsymbol{\alpha}_2})$ (with superscripts defined in Eq. (2.26)) as $(J^{\boldsymbol{\alpha}_1}, J^{\boldsymbol{\alpha}_2}, J^{\boldsymbol{\alpha}_3}) \rightarrow (J^{-\boldsymbol{\alpha}_2}, J^{\boldsymbol{\alpha}_3}, J^{-\boldsymbol{\alpha}_1})$. In terms of the boson fields ϕ_1 and ϕ_2 which live on the SU(3) root lattice, this amounts to

$$\boldsymbol{\phi} \rightarrow M \cdot \boldsymbol{\phi}, \quad M = \begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}. \tag{2.47}$$

In the $\boldsymbol{X}$ basis the $\mathbb{Z}_3$ symmetry is represented by

$$\boldsymbol{X} \rightarrow M' \cdot \boldsymbol{X}, \quad M' = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}. \tag{2.48}$$

The G matrix in Eq. (2.46) is left invariant under the $\mathbb{Z}_3$ transformation. i.e. we have $M'^T G M' = G$. One can show generally that any symmetric matrix left invariant by M' is proportional to $G_{SU(3)}$.

2.3 Some numerical Techniques

In this section we discuss some numerical techniques [1] that complements the above study of the perturbed SU(3) symmetric spin chain. Having described the field theory for $c = 2$ spin chains, we provide numerical evidence for the proposed correspondence. Our dicussion first focus on various ways of calculating scaling dimensions (2.43), after which we discuss the procedure for extraction of the TLL parameters G_{ab} and B_{ab} for $a, b = 1, 2$. We numerically confirm an important prediction of the field theory, namely Eq. (2.46).

We carried out exact diagonalization (ED) and density matrix renormalization group

[1] The numerical results and figures were produced by Hitesh J. Changlani.

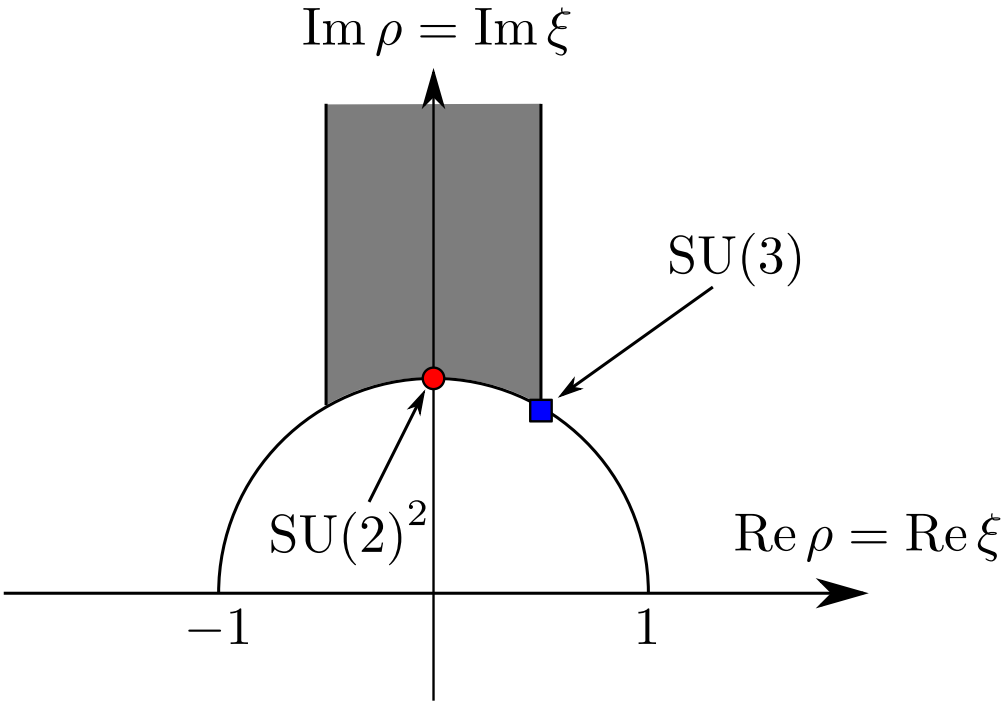

Figure 2.2: Theory space of the two-component Tomonaga-Luttinger liquid with $\rho = \xi$. The shaded region represents the "fundamental domain"; Because of the duality, different points in the theory space that are related by the duality are isospectral. The fundamental region is a set of representatives for all points related by the duality. I.e., starting from points in the shaded region, by mapping these points by the duality group, the entire theory space is covered. Some spectial points in the theory space are also marked: "SU(3)" represents the SU(3) WZW theory, and "$\mathrm{SU}(2)^2$" consists of two copies of SU(2) WZW theories, which may be realzed, e.g, as two copies of the XXX spin chain.

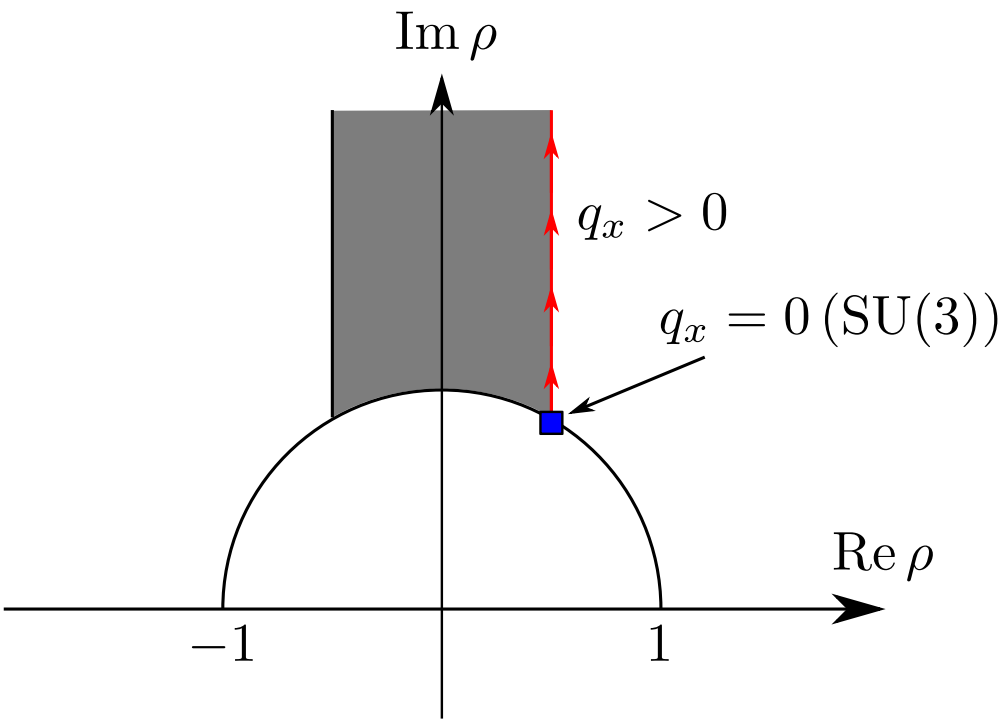

Figure 2.3: Theory space of the two-component Tomonaga-Luttinger liquid with $\xi = 1/2 + \sqrt{3}/2i$. The point "$q_x = 0(\mathrm{SU}(3))$" corresponds to the SU(3) symmetric Lai-Sutherland model. The red line with arrows represents the points in theory space traversed as q_x is increased from 0. (The arrows here do not indicate the renormalization group flow.)

(DMRG) calculations for periodic chains: finite size scaling of the energy gaps provides estimates of the lowest scaling dimensions. For bigger open chains, we calculate the same information from the mutual information for spatially disjoint blocks. The mutual information measure is completely determined from the ground state wavefunction, making it useful for situations where obtaining excited states is difficult.

The numerical calculations in this section were performed with a combination of our own codes and the ALPS libraries [9].

2.3.1 Inferences from Exact Diagonalization and Density Matrix Renormalization Group

For a one dimensional periodic chain of length L, the scaling dimensions x_j, corresponding to the j^{th} excited state with energy E_j, are given by (to leading order),

$$E_j - E_0 = \frac{2\pi v x_j}{L} + \frac{a}{L \log L} \tag{2.49}$$

where a is a model specific constant, v is the TLL velocity obtained from the finite size scaling of the ground state energy E_0,

$$\frac{E_0}{L} = e_\infty - \frac{\pi c v}{6L^2} + \frac{b}{L^2 (\log L)^3} \tag{2.50}$$

where e_∞ is the energy per site in the thermodynamic limit and c is the central charge and b is a constant. We note that the above formulae assume all excitations propagate with the same velocity v, while for multi-component TLL, more than one velocity may appear in general. (For more generic models, these formulae need modifications: for example see the work of Itoi et al. [41] on a $\mathrm{SU}(2) \times \mathrm{SU}(2)$ model.) In our model, a naive continuum limit and the bosonization analysis, (2.13) and (2.29), suggests that the excitations of the system, even when $q_x \neq 0$, should be described by a single velocity. We will take this

as our working hypothesis. While our spectral analysis by ED/DMRG depends on this assumption, our analyses based on the entanglement entropy and the mutual information do not.

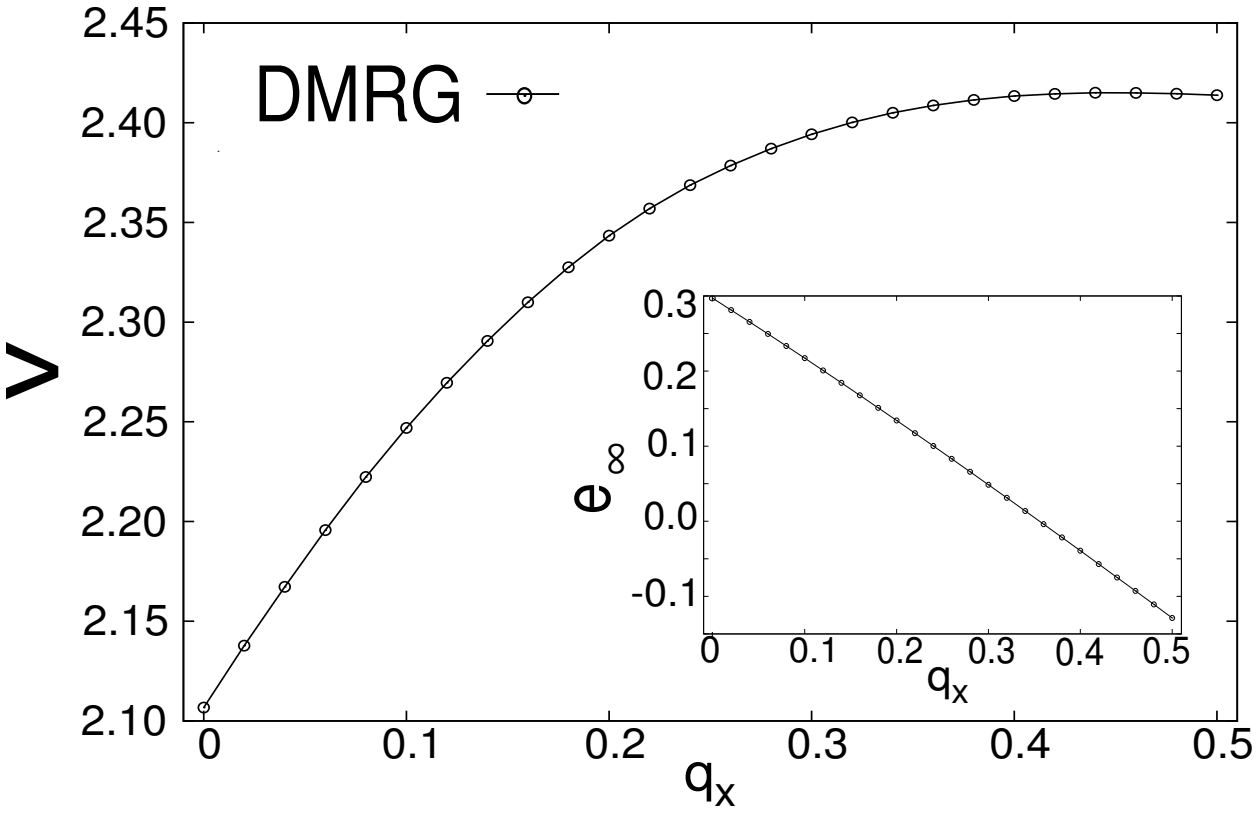

Figure 2.4: Velocity of the coupled TLLs as a function of q_x. The inset shows the energy per unit length in the thermodynamic limit as a function of q_x. The lines are guides to the eye.

Fig. 2.4 shows the TLL velocity v and ground state energy per site (in the thermodynamic limit) e_∞ as a function of q_x obtained by fitting our data to Eq. (2.50). Our results for the SU(3) symmetric point are in excellent agreement with analytic results [25] and previous numerical studies [6,25,29,46]. For example, we get $e_\infty = 0.29679$ and $v = 2.107(1)$ (close to the exact results of $2 - \ln 3 - \frac{\pi}{3\sqrt{3}}$ and $2\pi/3$ respectively). Care must be taken in comparing our results with studies which parameterize the bilinear and biquadratic terms in the Hamiltonian 1.2a to be $J\cos\theta$ and $J\sin\theta$ with $\theta = \frac{\pi}{4}$, thus requiring an additional factor of $1/\sqrt{2}$. We have used the value of the central charge $c = 2$, which we

established independently from the scaling of the entanglement entropy (EE), discussed next.

Before we proceed, we mention an important subtlety associated with the choice of system sizes used in finite-size scaling. In a previous DMRG study on the SU(3) symmetric model, Aguado et al. [6] showed the absence of the singlet ground state (scaling dimension 0 in the CFT) for chains with lengths $6M+2$ and $6M+4$, where M is a positive integer. [2] Thus, we restrict ourselves to analyzing chains with lengths that are multiples of 6.

Central charge

We establish the relevant region in parameter space where the TLL physics is expected to hold. For this purpose, we extract the central charge c, obtained from the scaling of the EE of a subsystem or "block" (readily available in DMRG) as a function of its size l. For open chains, the analytic form for the EE, denoted by $S(l)$, is,

$$S(l) = \frac{c}{6} \log\left(\frac{L}{\pi} \sin\left(\frac{\pi l}{L}\right)\right) + S_0, \tag{2.51}$$

where S_0 is a subleading correction. In Fig. 2.5 we show the profile of the EE and verify that the $c = 2$ fit to it is very accurate for all $q_x > 0$ [3] (However, the EE profile has local structure occurring on the scale of three sites, that arise due to open boundaries. These are not captured by the leading term in Eq. (2.51). Other similar quality fits are possible with a lower value of c: we estimate $c = 1.96 \pm 0.05$). Also note that S_0 is non-universal: in this case dependent on q_x alone. This explains why the various curves in Fig. 2.5 differ despite having the same central charge.

We motivate an understanding of the TLL behavior for all $q_x > 0$ by considering the

[2] This observation can possibly be better understood by extracting the scaling operators from numerics (which need a coarse grained operator that spans three sites). This is a direction we will not explore in the present paper.

[3] Practically this was checked for $0 < q_x < 100$

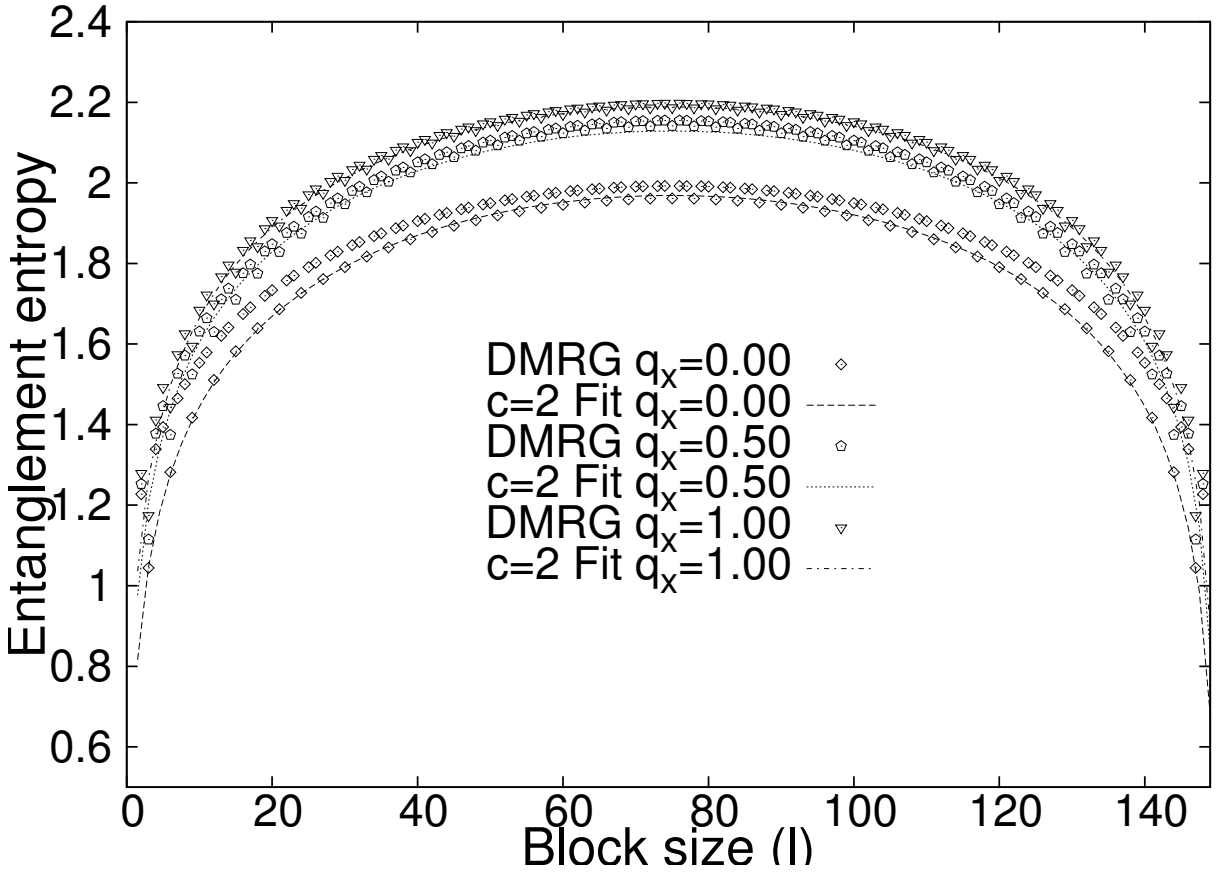

Figure 2.5: Entanglement entropy as a function of block size (l) and its fit to the formula (2.51) for $c = 2$ for a 150 site open chain for various q_x.

case $q_x \to \infty$ [65]. In this limit, the model is a purely classical one, with a macroscopically large number of ground states. To see this, we write out the Q_x term on a bond $\langle i, j \rangle$ in terms of S_z and S_z^2 operators,

$$U_x^{\dagger i} U_x^j + \text{h.c.} = 2 - 3{S_z^i}^2 - 3{S_z^j}^2 + \frac{9}{2}{S_z^i}^2{S_z^j}^2 + \frac{3}{2}S_z^i S_z^j. \tag{2.52}$$

This expression indicates that the configurations $|\mp 1 \pm 1\rangle$ and the configurations $|\pm 1\ 0\rangle$ (and $|0\ \pm 1\rangle$) are exactly degenerate and have the lowest energies possible. This means that starting from a spin-1 "Néel" state, for example $|+1-1+1-1\rangle$, one can locally replace each $|+1-1\rangle$ "dimer" by a $|+1\ 0\rangle$ without changing the total energy. Thus, there is an exponentially large number of degenerate states. Adding the SU(3) symmetric term lifts this degeneracy, but the model stays critical. Such a macroscopic degeneracy does not exist in the spin-1/2 XXZ model in the Ising limit: this is why there is a finite value of anisotropy at which the spin-1/2 XXZ model ceases to be critical.

Scaling dimensions and degeneracies

In order to obtain multiple excited states in the same symmetry sector (here sectors of definite S_z), we perform a state averaging procedure with two target states in the finite system DMRG method. A sequence of bond dimensions varying from $m = 400$ to $m = 2000$ states and periodic chains of lengths varying from 24 to 66 sites, were studied. For the ED calculations (from 6 to 18 sites), multiple excited states were calculated to give us a picture of the low energy degeneracy structure of this model.

A note about boundary conditions is now in order. Working with open boundary conditions, favorable for DMRG, can complicate the mapping of a spin chain to a conformal field theory: the notion of strict "conformal invariance" is broken. Hence we do not rely on open boundary conditions to give us a picture of the degeneracy structure of this system. (That said, scaling dimensions can still be reliably numerically estimated from open

chains.)

For the SU(3) symmetric model, it is analytically known that the first excited state is 18-fold degenerate in the "conformal limit" and the second excited state is 16-fold degenerate. However, in finite size simulations, the conformal limit is reached rather slowly as a function of system size. (The lattice model (2.6) flows into the $SU(3)_1$ WZW critical point only logarithmically fast). Thus, we rely only on trends seen in the ED results.

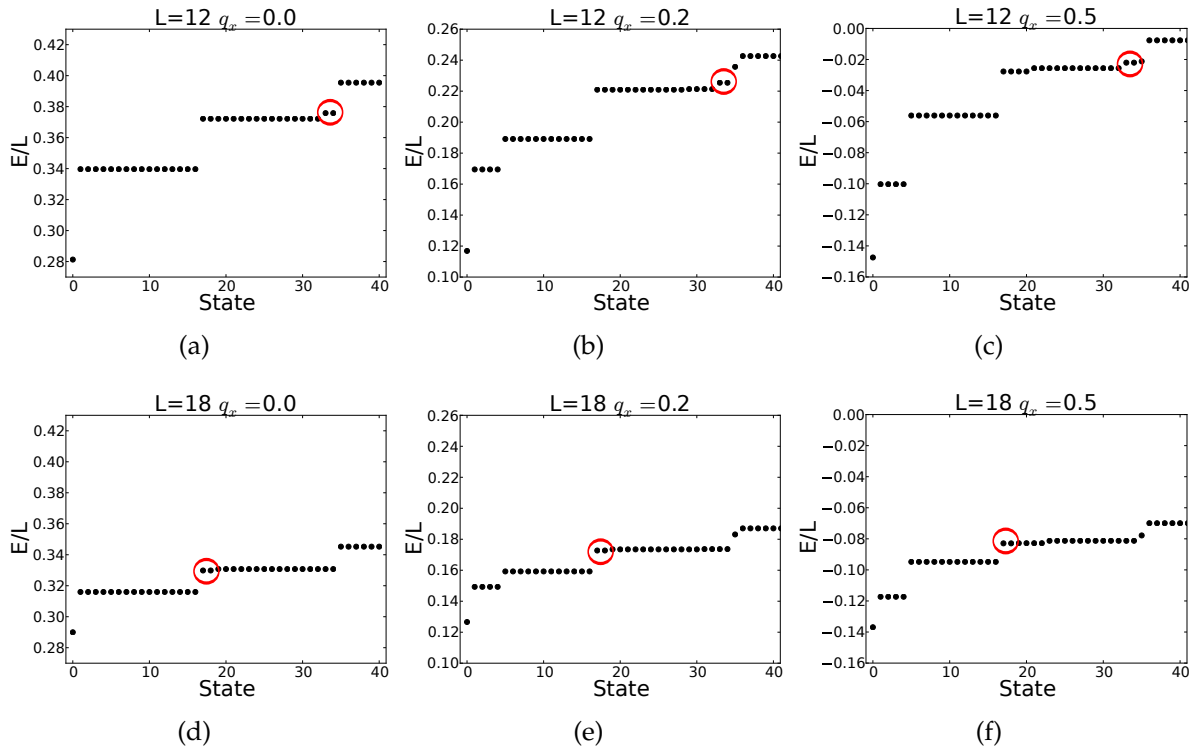

Figure 2.6: Low energy manifold of the Hamiltonian (1.2a) for $L = 12$ (upper panels) and $L = 18$ site chains (lower panels) for various values of q_x. For $q_x = 0$, shown in panels (a),(d) the first excited state is known to be 18-fold degenerate in the conformal limit. On increasing L, the inferred trend is that the two higher lying singlets (marked by circles) descend to possibly join the 16-fold exactly degenerate states. (b),(e) and (c),(f) show similar trends for $q_x = 0.2$ and $q_x = 0.5$: in these cases the degeneracy structure is narrowed down to few possibilities.

For the 12 site ED results, we observe that the low energy manifold consists of a non-degenerate singlet state, two sets of 16-fold degenerate states (a consequence of SU(3) symmetry), followed by two degenerate singlets. As can be seen in Fig. 2.6(a),(d) on

going from 12 to 18 sites, the two singlets descend below the second manifold of 16 states: it is thus conceivable (though not rigorous), that these two states will join the 16-fold degenerate first excited state resulting in a 18-fold degeneracy in the conformal limit.

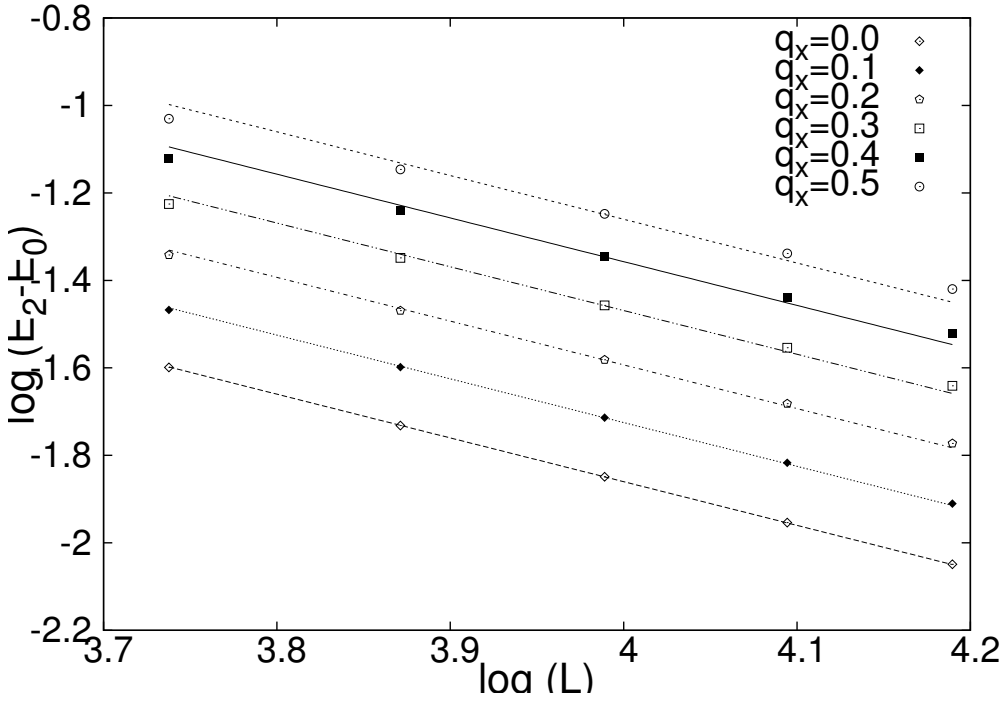

Figure 2.7: Finite size scaling of the second excited state energy gap for various q_x. Two independent DMRG calculations are performed, one each for the ground state in the $S_z = 0$ and $S_z = 1$ sectors. The fits to Eq. (2.49), along with the knowledge of the TLL velocity give the second lowest scaling dimension.

Next, consider the effect of adding the Q_x term with $q_x > 0$. From ED, we find that the (exact) 16-fold degeneracy of the first excited state splits: the first excited state is now 4-fold degenerate (all corresponding to $S_z = 0$ states) and the next excited state is 12-fold degenerate (corresponding to four sets of $S_z = \pm 1$ and two sets of $S_z = \pm 2$ states) states. Here too, the two degenerate singlets in the low energy spectrum descend to lower values on increasing the length of the chain, as can be seen in Fig. 2.6(b),(e) and (c),(f). Based on our experience with the SU(3) point, we conjecture that restoration of conformal symmetry will result in the 4-fold degeneracy being transformed to a 6-fold degeneracy (although other possibilities are not completely ruled out based on this data

alone). We expect this degeneracy structure to hold only as long as the second excited state does not become the third excited state. The field theoretic prediction (2.46) confirms these inferences: once the second scaling dimension exceeds the value of 1, there is a reorganization of energy scales. This occurs for $q_x \lesssim 0.5$: the quantum numbers denoted by $\{n_1, n_2, w_1, w_2\}$ (see Eq. 2.42) corresponding to the lowest 6 states are $\{\pm 1, \pm 1, 0, 0\}$, $\{\pm 1, 0, 0, 0\}$, $\{0, \pm 1, 0, 0\}$. and the next 12 states are $\{\mp 1, \mp 1, \pm 1, \mp 1\}$, $\{\pm 1, 0, 0, \pm 1\}$, $\{0, 0, \pm 1, 0\}$, $\{0, 0, 0, \pm 1\}$, $\{0, \pm 1, \mp 1, 0\}$, $\{0, 0, \pm 1, \mp 1\}$.

Fig. 2.7 shows fits to Eq. (2.49) (after taking logarithms) to extract the second scaling dimension x_2, for various q_x (similar trends are seen for the first scaling dimension). The corrections to scaling are found to increase on going from the $q_x = 0.0$ to $q_x = 0.5$: whether these effects are genuine deviations from the TLL physics or a lack of sufficient size to see "true scaling" can not be definitively established within our present methodology. We attribute the deviations close to $q_x \approx 0.5$ to "energy crossings" (i.e. changing multiplet structure), which can cause additional level repulsions. Thus, one may need very large sizes to get precise estimates in this region.

Despite this source of inaccuracy, the scaling dimensions vary within 10% when they are computed using Eq. (2.49) for fixed L, over the range of lengths considered ($24 - 66$ sites). The obtained values validate the correspondence between the lattice model and the CFT and the general trends of their variations with q_x support our main conclusions.

2.3.2 Extracting the lowest scaling dimensions from mutual information

It is difficult to target multiple excited states in DMRG for long chains, especially for a critical system where the entanglement entropy grows logarithmically with system size. Thus it is extremely desirable to have a method to obtain scaling dimensions that involves only the ground state.

Typically this is achieved by measuring ground state correlation functions between two distant regions. However, in the most general setting, we apriori do not know the scaling operators on the lattice i.e. the operators whose expectations are to be measured. To obtain generalized correlation functions between two regions (say A and B) we calculate their combined reduced density matrix (for varying separations) and extract the "mutual information", denoted by I_{AB} and formally defined as,

$$I_{AB} \equiv S_A + S_B - S_{AUB}, \tag{2.53}$$

where S_A,S_B, S_{AUB} is the EE of regions A, B and the union of A and B respectively. A schematic of the geometry used for this computation is shown in Fig. 2.8(a).

The mutual information, unlike the block entanglement entropy, is not directly available in DMRG and must be calculated in a matrix product state (MPS) framework. (Practically, this is achieved by reshaping all left and right optimized transformation matrices at the end of the DMRG calculation to get the MPS. Then, the reduced density matrix of disjoint regions is calculated using a partial-contraction scheme discussed in Ref. [59]. More details of our calculations will be provided elsewhere.) The mutual information can also be calculated with Monte Carlo methods in sign-problem free systems [56,78].

We now discuss extraction of the lowest scaling dimension from I_{AB}, for which we briefly present known results from the literature. To do so, we closely follow Ref. [30], whose notations we also use here.

For a CFT, Calabrese and Cardy (CC) [12] argued that the entanglement entropy of two intervals $A = [x_1, x_2]$ and $B = [x_3, x_4]$ in an infinite lattice is given by,

$$S_{AUB} = \frac{c}{3} \log \left(\frac{x_{21} x_{32} x_{43} x_{41}}{x_{31} x_{42}} \right) + 2s_1, \tag{2.54}$$

where $x_{ij} \equiv x_i - x_j$. The constant $2s_1$ is determined by demanding that $S_{AUB} \to S_A + S_B$

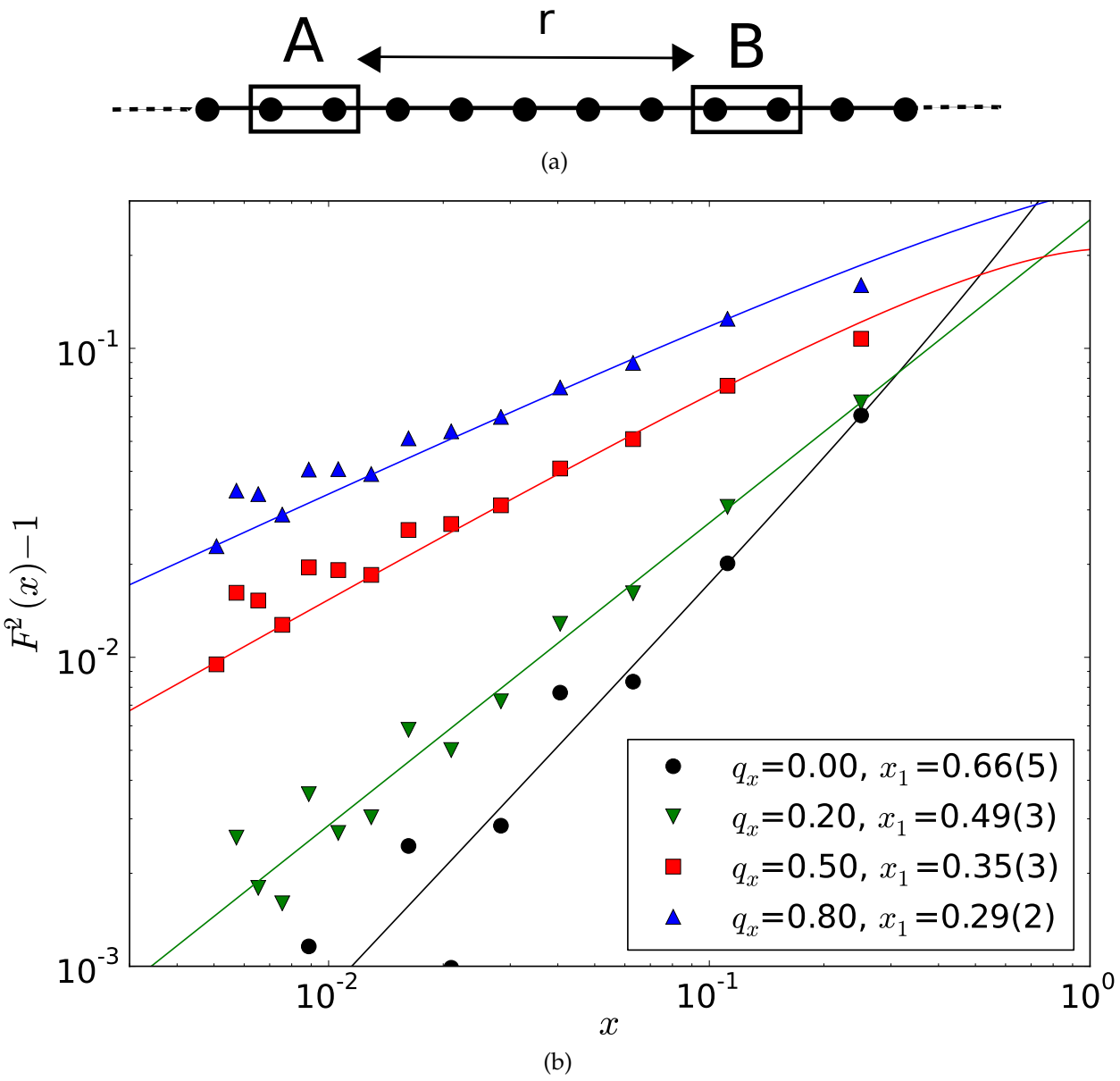

Figure 2.8: (Color online): (a) Geometry used to compute the mutual information consists of two 2-site blocks separated by distance r. The calculations were performed for a 150-site chain with $r < 30$ (larger r data was discarded to avoid edge effects). (b) $F^2(x) - 1$ (derived from the mutual information) vs the conformal ratio x calculated with DMRG and fitted to the analytic form, Eq. (2.61) in the text.

in the limit $x_{21}, x_{43} << x_{31}, x_{42}$. Rewriting this formula in terms of the mutual information (i.e. on subtracting out the single interval contributions), one gets,

$$I_{AB}^{CC} = \frac{c}{3} \log \left(\frac{x_{32} x_{41}}{x_{31} x_{42}} \right). \tag{2.55}$$

For a finite periodic chain, one replaces x_{ij} by the cord distance $L/\pi \sin\left(\pi x_{ij}/L\right)$, this results in,

$$I_{AB}^{CC} = \frac{c}{3} \log \left(\frac{\sin(\pi x_{32}/L) \sin(\pi x_{41}/L)}{\sin(\pi x_{31}/L) \sin(\pi x_{42}/L)} \right). \tag{2.56}$$

It is thus convenient to define the conformal ratio x as,

$$x \equiv \frac{\sin(\pi x_{32}/L) \sin(\pi x_{41}/L)}{\sin(\pi x_{31}/L) \sin(\pi x_{42}/L)}. \tag{2.57}$$

The notion of mutual information can be generalized beyond the von-Neumann entropy, which is assigned an index $n = 1$, and thus denoted more generally by $I_{AB}^{(n)}$. This is achieved by the following replacements in the CC formulae,

$$S_1 \to S_n, \quad c \to \frac{1+n}{6n} c. \tag{2.58}$$

Furukawa et al. [30] found that the true mutual information and the CC mutual information differ by a function $f^n(x)$,

$$I_{AB}^{(n)} - {I^{(n)}}_{AB}^{CC} = f^{(n)}(x), \tag{2.59}$$

which is reparameterized as,

$$\frac{1}{n-1} F^{(n)}(x) \equiv f^{(n)}(x). \tag{2.60}$$

Calabrese and co-workers [7,13] have shown that for $n > 1$ and in the limit of small x,

$$F^{(n)}(x) - 1 = \left(\frac{x}{4n^2}\right)^{\alpha} s_2(n) + \left(\frac{x}{4n^2}\right)^{2\alpha} s_4(n) + (\text{higher order}), \tag{2.61}$$

where α is twice the lowest scaling dimension x_1. The coefficients $s_2(n)$ and $s_4(n)$ are the contributions in the small x expansion coming from the two and four-point functions of the operator in the CFT with the lowest scaling dimension.

Two concerns when using equation (2.61) in numerical simulations are (1) it holds only for an infinite lattice and (2) it assumes that the non-zero contributions are solely from the operator with the lowest scaling dimension. However, for a finite system there are contributions from all operators. Thus the lowest scaling dimension fitted is simply an effective one trying to mimick the action of a linear combination of many (different scaling) operators. Empirically, for an open chain of 150 sites, all the errors (systematic and due to fitting) appear to be within 10%, which is roughly the error we also obtain from fitting to energies.

Our results for fits to a power law for $F^2(x) - 1$ for various q_x are shown in Fig. 2.8(b). The overall fits are reasonable, though there are local features not captured by Eq. (2.61): just like the case of the EE, these are attributed to open boundaries. Such features are also seen in the spin-1/2 XXZ model, studied independently by Barcza et al. [1].

2.3.3 Extraction of TLL parameters

Fig. 2.9 shows the lowest two scaling dimensions obtained from finite size scaling of energy gaps as a function of q_x. The inset shows the lowest scaling dimension from the mutual information method. (With this metric, we were able to explore a larger range of q_x.) The general agreement (within errors) between these independent metrics confirms our that we can reliably calculate lowest scaling dimensions. Thus we proceed to discuss

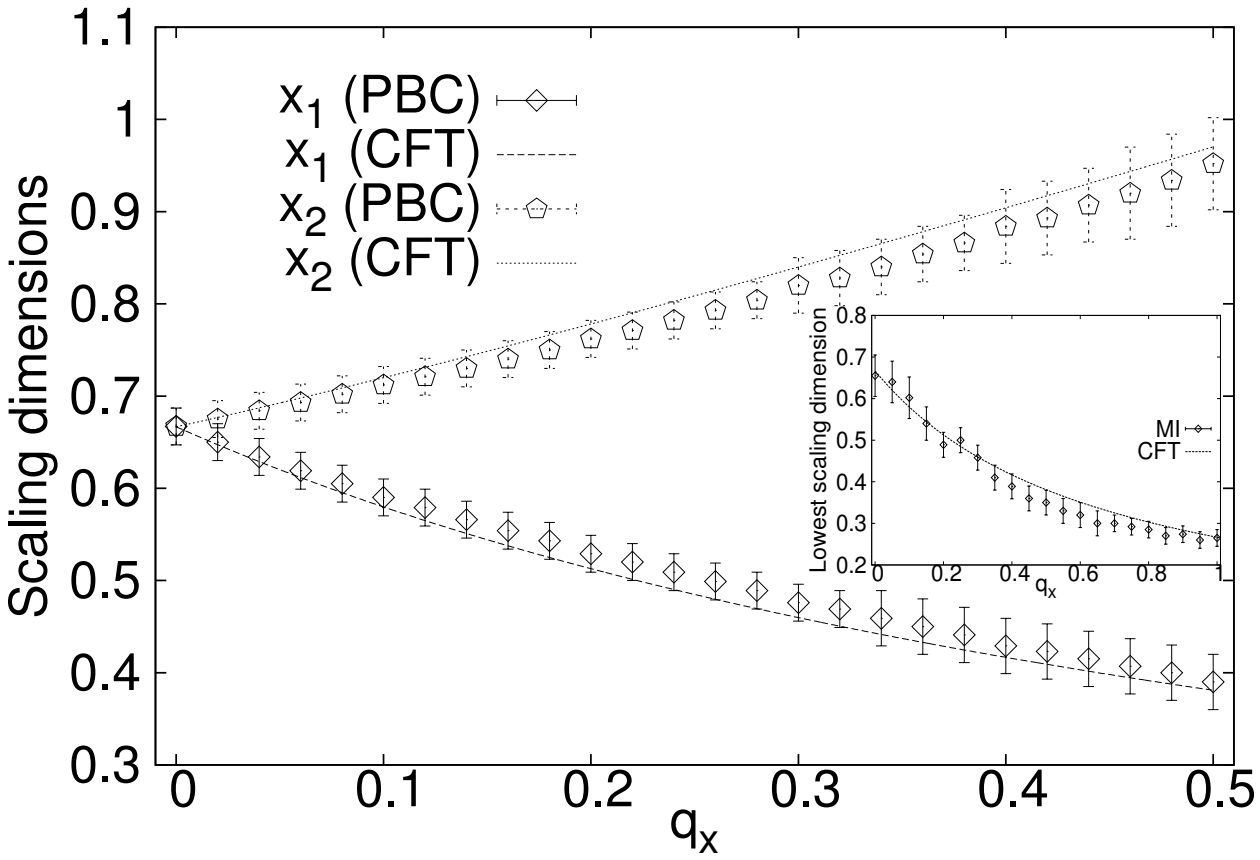

Figure 2.9: The main panel shows the first two scaling dimensions, x_1 and x_2, as a function of q_x, obtained from finite size scaling of energy gaps obtained from a combination of exact diagonalization (ED) and the density matrix renormalization group (DMRG) for periodic chains (denoted by PBC). The $c = 2$ conformal field theory (CFT) prediction is also shown. The inset shows the lowest scaling dimension obtained from the mutual information (MI) measure (see text), computed within the DMRG/Matrix product state framework for an open chain of 150 sites.

the extraction method for the four TLL parameters.

Given a trial set of G_{ab} and B_{ab}, we calculate the lowest 18 scaling dimensions (which need not be distinct), and denote them by $x_i^{\mathrm{G,B}}$. We then evaluate a cost function,

$$C(\mathrm{G,B}) \equiv \sum_i (x_i^{\mathrm{G,B}} - x_i^{\mathrm{DMRG}})^2 \tag{2.62}$$

and minimize it with respect to G_{11}, G_{12}, G_{22} and B_{12} to obtain the best fit. We used the Nelder-Mead simplex algorithm built into the GNU Scientific library for this purpose.

In order to confirm our inferences about the nature of the degeneracies in the low energy manifold, we attempted to fit to two degeneracy structures for the first and second excited states. First, we assumed that the degeneracy (denoted by g_i) of the first two distinct scaling dimensions to be $(g_1, g_2) = (6, 12)$ and in the second case $(g_1, g_2) = (4, 12)$. In all cases, for $q_x < 0.5$, we found the former gave a significantly better fit to the CFT formulae (2.43). In fact, attempts to use the $(4, 12)$ structure gave optimized solutions closer to a $(g_1, g_2, g_3) = (4, 2, 12)$ degeneracy structure, hinting that the imposed structure was incorrect. The quality of our fits are checked by how well the scaling dimensions were reproduced (for the correct degeneracy structure, these agreed to within ± 0.03).

The agreement of the values of the measured and expected scaling dimensions, shown in Fig. 2.9, strongly indicates an internally consistent scenario for the lattice model to CFT mapping. This is also equivalently seen in the extracted TLL parameters, shown in Fig. 2.10, which are consistent with Eq. (2.46): they satisfy the expected relation $G_{11} = G_{22} = 2G_{12}$. (The relative error in the scaling dimensions propagates to these parameters: for eg. the overall error in G_{11} is roughly twice the error in x_2.) As expected from the duality explained in section 2.2.4, the scaling dimensions depend on B_{12} up to an integer shift. Thus we focus on a particular representation and find that $B_{12} = 1/2$ explains our data for all q_x. Finally, even though we have shown data only for $q_x < 0.5$, the mutual information data in Fig. 2.9 (inset) suggests the validity of the theory for larger q_x.

This concludes our explanation of our results for the spin 1 chain. In chapter 6, we highlight the important points and discuss the outlook for our approach. In the next chapter we switch gears and give a brief discussion of Laughlin's argument for the integer QHE which sets the state for our discussion of SPT phases in two dimensions.

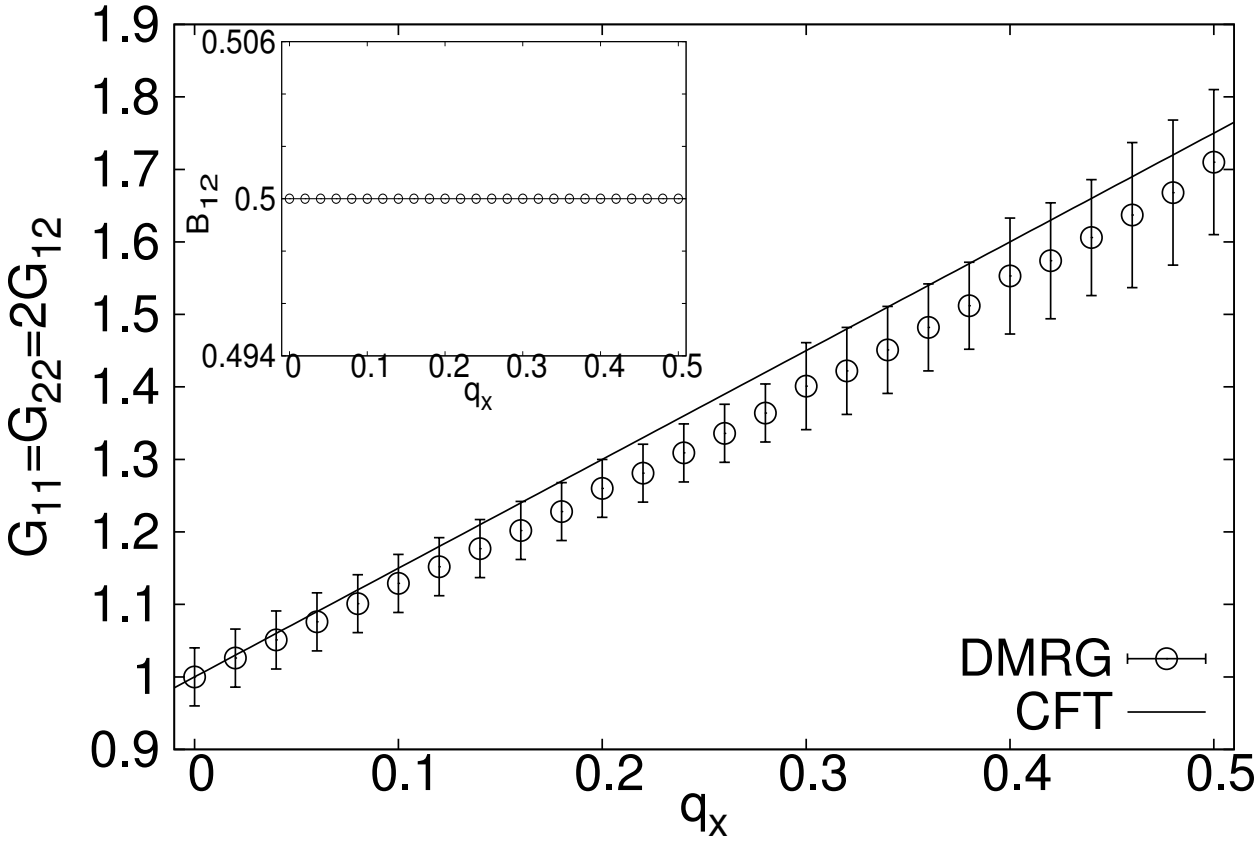

Figure 2.10: TLL parameters as a function of q_x extracted from matching scaling dimensions to a $c = 2$ CFT. The main panel shows G_{11} as a function of q_x and we find $G_{11} = G_{22} = 2G_{12}$. The inset shows B_{12} which is found to be constant. The CFT prediction is shown by the solid lines.

Chapter 3

Geometric version of Laughlin's Argument

This chapter draws extensively from what was reported in Ref. [73].

3.1 Quantum Hall Effect

3.1.1 Laughlin's argument

Consider a quantum Hall system on a finite cylinder with two edges, I and II. If magnetic flux Φ is threaded adiabatically through the cylindrical hole, as the flux is increased (adiabatically), starting from, say, zero flux, the Hamiltonian $H(\Phi)$ of the system is in general not invariant under the flux insertion. However, after an increase by an integral multiple of the flux quantum Φ_0, the Hamiltonian comes back to itself. That is, $H(\Phi + n\Phi_0) = H(\Phi)$, for any integer n. This is a symmetry of the system but it cannot be achieved by successive applications of infinitesimal gauge transformations.

In the process of increasing the flux, an integer multiple of electric charge gets pumped from one edge to the other due to the QHE. One can analyze this from the point of view of the partition function for the excitation spectrum of the system. Since the transformation

is adiabatic and the bulk spectrum is gapped it is enough to focus on the partition function of the gapless edge excitations given by

$$Z(\Phi) = \sum_{a,b} N_{ab} \chi_a^{\mathrm{I}}(\Phi) \chi_b^{\mathrm{II}}(\Phi), \tag{3.1}$$

where $\chi_a^{\mathrm{I,II}}$ is a chiral contribution to the partition function for each edge and N_{ab} are constants. Under a large gauge transformation in general, the chiral parts of the partition function are not invariant, $\chi_a(\Phi + n\Phi_0) \neq \chi_a(\Phi)$, while the total partition function is invariant.

This is to be expected for a system with non-trivial bulk and signals the non-conservation of charge [14]. In the case of the quantum spin Hall effect, a similar flux threading argument [64] can be applied to show that a flux change by $\Phi_0/2$ pumps fermion number parity and leads to spin charge separation.

In the cases we will be interested in, the total charge may not necessarily be conserved, we look for an alternative to the flux Φ. A natural thing to do is to simply replace Φ by the modular parameter of the torus τ. Let us explain this in further detail.

3.1.2 Modular Invariance

CFT's are by definition invariant under a change of distance scale which can be thought of as rescaling of the metric on spacetime. It can be shown [61] that in 1+1 D this is equivalent to global conformal transformations. A low genus surface like the 2-sphere has the special property that any two that are topologically equivalent are also conformally equivalent. However at higher genus this is not the case. For tori one finds that there is a correspondence between conformally inequivalent tori and points in the upper-half plane. Every point τ(the modular parameter) on the upper half plane represents a torus,

but under the modular transformation

$$\tau \to \frac{a\tau + b}{c\tau + d}, \quad a, b, c, d \in \mathbb{Z}, \;\; ad - bc = 1 \tag{3.2}$$

one gets a conformally equivalent torus. These transformations from the group $SL(2, \mathbb{Z})$ and are generated by the so called Dehn twists $\tau \to \tau + 1$ and $\tau \to -1/\tau$. Invariance under the former known as the T modular transformation imposes a constraint on the spectrum of dimensions of operators in a CFT [16], while the latter known as the S modular transformation exchanges the direction of space and time. Our proposal is to replace the large gauge transformation of electromagnetism by modular transformations which are large conformal gauge transformations on the torus.

The non-chiral edge theory of a SPT phase is modular invariant if symmetry conditions are not enforced – without enforcing symmetries, a SPT phase can be adiabatically connected to a trivial state. There may however be a conflict between modular invariance and symmetry conditions, as the latter may forbid particular ways of combining the left- and right-moving parts of the CFT. Our strategy to diagnose and characterize a SPT phase is then, to impose the symmetry conditions strictly and ask if the system is invariant under modular transformations or not. More specifically, we take only a single-edge theory (edge I or II in the above notation) and ask if it can be made modular invariant. (If we consider the two separate edges of the modular anomalous theories, they can be combined in a modular-invariant way.) We achieve the strict enforcement of the symmetry by considering a projection of the CFT by the symmetry group G. We now take a close look at the projection procedure.

3.1.3 Orbifolding

We work in bosonic language (there are sign modifications for fermionic fields). Let $S[\phi]$ be the action for the effective low energy modes at the edge of an SPT phase invariant un-

der a symmetry transformation $\phi \to g \cdot \phi$, for $g \in G$ (a finite group). Enforcing the symmetry means that we want to think of ϕ and $g \cdot \phi$ as corresponding to the same physical configuration. This is also known as gauging or orbifolding [22, 23]. In the Hamiltonian formalism this means that we have to project the states of the theory onto G invariant states, so that the partition function is

$$Z = \mathrm{Tr}\, P e^{-tH}, \tag{3.3}$$

where $P = |G|^{-1} \sum_{g \in G} \hat{g}$ is a projection operator satisfying $P^2 = P$, as is easily verified. In the path integral formalism this has the interpretation as a sum over all fields twisted in the time direction of the torus i.e

$$Z = \sum_{g \in G} \int \mathcal{D}[\phi^g] e^{-S[\phi]}, \tag{3.4}$$

where the subscript g indicates that the path integral is over fields satisfying

$$\phi(x + 2\pi\tau_1, t + 2\pi\tau_2) = \hat{g}\phi(x,t)\hat{g}^{-1}. \tag{3.5}$$

This is the meaning of twisting in the time direction, where the direction of the modular parameter $\tau = \tau_1 + i\tau_2$ in the upper-half plane represents time.

Since modular invariance is a constraint for a gapless edge theory we need to ensure that that the projected partition function is modular invariant. Considering that S modular transformations interchange space and time it is clear that to achieve modular invariance we have to explicitly include sectors in the path integral twisted in the spatial direction. A general ansatz for the partition function of the orbifolded theory is given by

$$Z = \sum_{(h,g) \in G^2} \epsilon_g^h \int \mathcal{D}[\phi_g^h] e^{-S[\phi]}, \tag{3.6}$$

where the superscript and subscript (h, g) indicates that the path integral is restricted to fields twisted in the spatial and time directions by h and g respectively: In addition to the boundary condition (3.5), the field also obeys

$$\phi(x + 2\pi, t) = \hat{h}\phi(x, t)\hat{h}^{-1}. \tag{3.7}$$

where x represents spatial direction normalized to have a length of 2π. The ϵ_g^h are $U(1)$ phases which could arise since there is no a priori way to fix the relative amplitudes between the different twisted sectors and one is free to choose relative phases ϵ_g^h for the different sectors. The phase factors ϵ_g^h are also called discrete torsion [76] and can also be viewed as different ways to assign the quantum number for the ground state in each sector.

We consider the partition function orbifolded by the symmetry group of the problem, and ask if the partition function is modular invariant or not. We view this as a generalization of Laughlin's flux threading argument. It is a generalization in the following two ways: (i) it is a geometrical generalization (ii) symmetry plays an important role. We discuss some examples below.

Chapter 4

Applications to SPT phases

This chapter draws extensively from what was reported in Ref. [73].

4.1 K-matrix theory for Bosonic SPT phases

It is believed that the **K**-matrix formalism [79] of $U(1)$ Chern-Simons theory gives a complete classification of abelian fractional quantum Hall states. In this section we review the **K**-matrix formalism for quantum Hall states and then specialize to bosonic abelian SPT phases.

The low energy effective field theory for an abelian quantum hall state is given by the Langrangian (there is no distinction between upper and lower internal indices $I, J \ldots$)

$$\mathcal{L} = \frac{K_{IJ}}{4\pi}\epsilon^{\mu\nu\lambda}a^I_\mu\partial_\nu a^J_\lambda + a^I_\mu l_I j^\mu. \tag{4.1}$$

The a^I_μ are internal gauge fields which couple to quasi particle currents j^μ, and $\mathbf{K} \in GL(N,\mathbb{Z})$ is a symmetric matrix. The l_I are components of an integer vector l specifying the a_μ charge of a quasiparticle and the set of quasiparticle charges form an integral lattice. For states consisting fundamentally of bosons (e.g spins), all diagonal entries of **K** are even integers, while for those consisting fundamentally of fermions, at least one diagonal

entry is an odd integer. One can compute the self statistics and mutual statistics given by $\theta = \pi l^T \mathbf{K}^{-1} l$ and $\theta_{12} = 2\pi l_1^T \mathbf{K}^{-1} l_2$ respectively. By quantizating the theory [79] on a closed surface of genus g, one finds that the ground state degeneracy (topological order) is given by $|\det \mathbf{K}|^g$. For SPT states which have no intrinsic topological order we require $|\det \mathbf{K}| = 1$. By coupling to an electromagnetic $U(1)$ field one can also compute the quantized Hall conductance in terms of $\mathbf{K}$. A change of labels $l \to Wl$ for $W \in SL(N, \mathbb{Z})$ accompanied by the transformation $\mathbf{K} \to W^T \mathbf{K} W$ is a mere relabelling of quasiparticles (a change of basis of the charge lattice), and leaves all physical properties unchanged. We will refer to this fact as $SL(N, \mathbb{Z})$ symmetry.

The effective Lagrangian describing the gapless edge modes of a fractional quantum Hall state characterized by $\mathbf{K}$ can be derived using a gauge invariance argument on a surface with boundary is given by [79]

$$S = \frac{1}{4\pi} \int dt dx \left(K_{IJ} \partial_t \phi^I \partial_x \phi^J - V_{IJ} \partial_x \phi^I \partial_x \phi^J \right), \tag{4.2}$$

where $\phi^I \sim \phi^I + 2\pi$ and V_{IJ} is a positive definite (for positive energy) symmetric matrix that is non-universal (we will later exploit this to tune the values of the V matrix conveniently).

Symmetries in the K matrix formalism

We consider only unitary symmetries. A generic realization of a symmetry transformation g is given by [51]

$$\phi^I \to W^g_{IJ} \phi_I + \delta \phi^g_I, \tag{4.3}$$

where $\delta^g_I \in [0, 2\pi)$ are constants and the matrix $W^g \in SL(N, \mathbb{Z})$ satisfies $\mathbf{K} = (W^g)^T \mathbf{K} W^g$. To get a honest representation of the symmetry group G all the relations in the group must

be satisfied. Moreover using $SL(N,\mathbb{Z})$ symmetry one obtains a notion of equivalence on the set of symmetry transformations $\{(W^g, \delta\phi^g)\}$. The equivalence relation can be summarized by stating that the transformation

$$\begin{aligned} W^g &\to X^{-1} W^g X, \\ \delta\phi_I^g &\to X^{-1}\left(\delta\phi_I^g - \Delta\phi_I + W_{IJ}^g \Delta\phi_J\right) \end{aligned} \tag{4.4}$$

results in an equivalent symmetry transformation for arbirtrary constants $\Delta\phi_I$ and $X \in SL(N,\mathbb{Z})$ as long as $X^T \mathbf{K} X = \mathbf{K}$. The point is that this transformation is equivalent to a $SL(N,\mathbb{Z})$ relabelling of the quasiparticles and a global $U(1)$ transformation of quasiparticle operators. A trivial SPT phase is one in which a maximal set of commuting fields at the edge can be localized (hence gapped by a semiclassical argument) by adding a combination of potential terms of the form $\{C_a \cos\left(k_a^T + \alpha_a\right)\}$ that are neutral under the symmetry transformation. One can also define the notion of addition of phases by taking together multiple copies. One considers two SPT phases to be the same if they are equivalent up to addition of a trivial phase, this is the notion of stable equivalence. The inequivalent SPT phases are then the different inequivalent symmetry transformations up to stable equivalence.

For 2×2 $\mathbf{K}$ matrices using $SL(2,\mathbb{Z})$ symmetry one can always choose for a non -chiral bosonic phase $\mathbf{K} = \sigma_x$. In this case for $\mathbb{Z}_K$ symmetry a set of inequivalent symmetry transformations are given by [51],

$$\phi_1 \to \phi_1 + \frac{2\pi}{K}, \quad \phi_2 \to \phi_2 + \frac{2\pi q}{K}, \quad q = 0, 1, \ldots, K-1. \tag{4.5}$$

Also according to [51], $q = 0$ represents a trivial SPT phase while all others are non-trivial, below we recover this result from a modular invariance standpoint. For an example of how such a description could arise in a lattice system of spin $1/2$ degrees of freedom see

Ref. [48].

We will consider the even more general $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry transformation

$$\phi_1 \to \phi_1 + \frac{2\pi}{K}, \quad \phi_2 \to \phi_2 + \frac{2\pi}{K} \tag{4.6}$$

and we will introduce flavors which amounts to taking direct sums $\mathbf{K} = \sigma_x \bigoplus \sigma_x \ldots$ (N_f copies).

4.2 Time Reversal Invariant Topological Superconductors with additional $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry.

In this section we consider 2d topological superconductors with $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry and later generalize to $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry. If the microscopic details of how unconventional superconductivity comes about are ignored, i.e the superconducting pairing potential is taken as a background to which quasiparticles are coupled to. In the mean field approximation, one can write down the BdG Hamiltonian for the simplest model of a time reversal invariant topological superconductor is $2d$ is which can be viewed as a copy of a chiral p-wave superconductor together with its time reversed partner of opposite chirality [11]. This can be written as

$$H_{BdG} = \frac{1}{2}\sum_{\mathbf{p}} \Psi^\dagger_{\mathbf{p}} \begin{pmatrix} \frac{p^2}{2m} - \mu & 0 & 0 & -\Delta(p_x + ip_y) \\ 0 & \frac{p^2}{2m} - \mu & \Delta(p_x - ip_y) & 0 \\ 0 & \Delta^*(p_x + ip_y) & -\frac{p^2}{2m} + \mu & 0 \\ \Delta^*(p_x + ip_y) & 0 & 0 & -\frac{p^2}{2m} + \mu \end{pmatrix} \Psi_{\mathbf{p}}, \tag{4.7}$$

where $\Psi_{\mathbf{p}} = \begin{pmatrix} c_{\mathbf{p}\uparrow} & c_{\mathbf{p}\downarrow} & c^{\dagger}_{-\mathbf{p}\uparrow} & c^{\dagger}_{-\mathbf{p}\downarrow} \end{pmatrix}^T$, is a vector of fermion creation and annhilation operators of the subscripted momenta and spins. Thus the system is time reversal invariant and as usual in the BDG formalism particle-hole symmetric.

In the non-trivial phase a system with an edge would host gapless Majorana modes of opposite chirality localized at the edge. At the quadratic level it is impossibe to open up a gap at the edge without breaking time-reversal T (note we must preserve particle hole symmetry C since it is a redundancy). If these were the only symmetries we are interested in preserving then the classification is $\mathbb{Z}_2$ as can be seen by doubling the system and observing that T and C invariant mass terms can be constructed at the edge [11].

We can consider systems with an extra $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry where the spin up and spin down quantum numbers are conserved mod 2 [68]. This is equivalent to conserving the total fermion number and spin (in a particular direction) quantum number mod 2. With this additional symmetries the classification is $\mathbb{Z}$ at the quadratic level [68]. With interactions it is not obvious how to proceed, but it can be shown [26] that the system with 8 copies is unstable and can be gapped out due to interactions. Therefore the classification is broken to $\mathbb{Z}_8$ due to interactions. We will recover this result from the perspective of modular invariance after gauging the symmetry and later generalize to $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry.

If we work in the continuum limit, the effective low energy theory at the edge is the action:

$$H = \frac{i}{2\pi} \int dx \, \eta^a_L \partial_x \eta^a_L - \eta^a_R \partial_x \eta^a_R, \tag{4.8}$$

where the $\eta^a_{L,R}$ are Majorana-Weyl fermions moving in the direction indicated by the subscript and we have generalized to a system with several bands by adding flavor indices

a. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is generated by

$$\eta_{L,R} \to -\eta_{L,R}. \tag{4.9}$$

To uncover a larger symmetry, we assume the number of bands (copies) is even and combine the Majorana fields in complex pairs as:

$$\psi^a = \eta^{2a-1} + i\eta^{2a}. \tag{4.10}$$

The Hamiltonian in terms of the Dirac fermion fields is given by

$$H = \frac{i}{2\pi} \int dx \left[\psi_L^{a\dagger} \partial_x \psi_L^a - \psi_R^{a\dagger} \partial_x \psi_R^a \right], \tag{4.11}$$

this has a manifest $U(N_f) \times U(N_f)$($2N_f$ is the number of Majorana- Weyl fermions in any particular direction) symmetry but we will only be interested in the $\mathbb{Z}_K \times \mathbb{Z}_K$ subgroup generated by

$$\psi_L^a \to e^{-2\pi i/K} \psi_L^a, \quad \psi_R^a \to e^{2\pi i/K} \psi_R^a. \tag{4.12}$$

For $K = 2$ this is equivalent to Eq.(4.9). The $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry is generated by the operator $(-1)^{\frac{2F_L}{K}} \times (-1)^{\frac{2F_R}{K}}$. Where F_L and F_R are the left and right-moving fermion number operators respectively. In addition we impose $(-1)^{F_L} \times (-1)^{F_R}$ symmetry, combining with $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry requires K to be even.

This completes the discussion of our motivation for the systems that we consider, in the next sections we give a summary of the results obtained.

4.3 Results

4.3.1 bosonic SPTs

We rewrite the fields in Eq.(4.2) in terms of chiral modes $\phi_1 = \sqrt{\frac{r}{2}}(\phi_L + \phi_R)$ and $\phi_2 = \sqrt{\frac{1}{2r}}(\phi_L - \phi_R)$ where we set $V_{12} + V_{21} = 0$ to obtain a non-chiral theory and $r := \sqrt{\frac{V_{22}}{V_{11}}}$. The action is now written as

$$S = \frac{1}{4\pi} \int dt dx \left[\partial_t \phi_L \partial_x \phi_L - v(\partial_x \phi_L)^2 - \partial_t \phi_R \partial_x \phi_R - v(\partial_x \phi_R)^2 \right]. \tag{4.13}$$

We set the system size $L = 2\pi v$ and $v = 1$ without loss of generality.

The quantity of interest is the gauged partition function

$$Z = \frac{1}{K^2} \sum_{k_1,k_2,l_1,l_2=0}^{K-1} \epsilon_{(k_2,l_2)}^{(k_1,l_1)} Z_{(k_2,l_2)}^{(k_1,l_1)}(\tau) \tag{4.14}$$

with

$$Z_{(k_2,l_2)}^{(k_1,l_1)} = \mathrm{Tr}_{k_1,l_1} \left[(\hat{k}_2, \hat{l}_2) e^{2\pi i P \tau_1 - 2\pi \tau_2 H} \right] \tag{4.15}$$

being the partition function in the sector twisted by (k_1, l_1) and (k_2, l_2) in the spatial and time directions respectively by the $\mathbb{Z}_K \times \mathbb{Z}_K$ group action (4.6). This can be obtained by canonical quantization as detailed in [73]. The important properties are the modular transformations given by:

$$Z_{(k_2,l_2)}^{(k_1,l_1)}(\tau+1) = e^{-\frac{2\pi i k_1 l_1}{K^2}} Z_{(k_1+k_2,l_1+l_2)}^{(k_1,l_1)}(\tau), \quad Z_{(k_2,l_2)}^{(k_1,l_1)}(-1/\tau) = e^{\frac{2\pi i (l_1 k_2 + k_1 l_2)}{K^2}} Z_{(-k_1,-l_1)}^{(k_2,l_2)}(\tau). \tag{4.16}$$

We note that we have the following $\mathbb{Z}_K \times \mathbb{Z}_K$ " anomaly" under the relabelling of the

lower indices

$$Z^{(k_1,l_1)}_{(k_2\pm K,l_2)}(\tau) = e^{\frac{\pm 2\pi i l_1}{K}} Z^{(k_1,l_1)}_{(k_2,l_2)}(\tau), \quad Z^{(k_1,l_1)}_{(k_2,l_2\pm K)}(\tau) = e^{\frac{\pm 2\pi i k_1}{K}} Z^{(k_1,l_1)}_{(k_2,l_2)}(\tau), \tag{4.17}$$

while the lower indices are anomaly free. Since the modular action in equation (4.16) sometimes transforms the lower indices outside the set $\{0, 1, \ldots K-1\}$, we may have to apply equation (4.17) to land back in this set. This makes the analysis of the discrete torsion phases complicated. The total partition function with N_f flavors and $\mathbb{Z}_K \times \mathbb{Z}_K$ gauge invariance is given by

$$Z(\tau) = \sum_{k_1,l_1,k_2,l_2=0}^{K-1} \epsilon^{(k_1,l_1)}_{(k_2,l_2)} \left[Z^{(k_1,l_1)}_{(k_2,l_2)} \right]^{N_f}, \tag{4.18}$$

with $\epsilon^{(k_1,l_1)}_{(k_2,l_2)}$ having the same meaning as before. From equation (4.16) one determines the following conditions for S modular invariance

$$\epsilon^{(k_1,l_1)}_{(k_2,l_2)} = \begin{cases} e^{-\frac{2\pi i N_f (l_1 k_2 + k_1 l_2)}{K^2}} \epsilon^{(k_2,l_2)}_{(-k_1,-l_1)} & \text{if } k_1 = l_1 = 0 \\ e^{-2\pi i N_f \left[\frac{(l_1 k_2 + k_1 l_2)}{K^2} - \frac{l_2}{K} \right]} \epsilon^{(k_2,l_2)}_{(-k_1+K,-l_1)} & \text{if } l_1 = 0, k_1 > 0 \\ e^{-2\pi i N_f \left[\frac{(l_1 k_2 + k_1 l_2)}{K^2} - \frac{k_2}{K} \right]} \epsilon^{(k_2,l_2)}_{(-k_1,-l_1+K)} & \text{if } k_1 = 0, l_1 > 0 \\ e^{-2\pi i N_f \left[\frac{(l_1 k_2 + k_1 l_2)}{K^2} - \frac{k_2+l_2}{K} \right]} \epsilon^{(k_2,l_2)}_{(-k_1+K,-l_1+K)} & \\ \qquad \text{if } k_1, l_1 > 0 & \end{cases} \tag{4.19}$$

One also obtains the following conditions for T modular invariance:

$$\epsilon^{(k_1,l_1)}_{(k_2,l_2)} = \begin{cases} e^{\frac{2\pi i N_f l_1 k_1}{K^2}} \epsilon^{(k_1,l_1)}_{(k_1+k_2,l_1+l_2)} \\ \qquad \text{if } k_1+k_2, l_1+l_2 \leq K-1 \\ \\ e^{2\pi i N_f \left[\frac{l_1 k_1}{K^2} - \frac{l_1}{K}\right]} \epsilon^{(k_1,l_1)}_{(k_1+k_2-K,l_1+l_2)} \\ \qquad \text{if } k_1+k_2 > K-1, l_1+l_2 \leq K-1 \\ \\ e^{2\pi i N_f \left[\frac{l_1 k_1}{K^2} - \frac{k_1}{K}\right]} \epsilon^{(k_1,l_1)}_{(k_1+k_2,l_1+l_2-K)} \\ \qquad \text{if } k_1+k_2 \leq N-1, l_1+l_2 > K-1 \\ \\ e^{2\pi i N_f \left[\frac{l_1 k_1}{K^2} - \frac{l_1+k_1}{K}\right]} \epsilon^{(k_1,l_1)}_{(k_1+k_2-K,l-1+l_2-K)} \\ \qquad \text{if } k_1+k_2, l_1+l_2 > K-1 \end{cases} \tag{4.20}$$

Let us analyze Eqs. (4.19) and (4.20) in general. First focus on Eq. (4.19) and observe that when K is even

$$\epsilon^{(K/2,K/2)}_{(K/2,K/2)} = e^{\pi i N_f} \epsilon^{(K/2,K/2)}_{(K/2,K/2)}, \tag{4.21}$$

so this forces N_f be even. For even K this is the only condition required while for odd K there is no condition for consistency of Eq. (4.19) as is easily verified.

Now Eq. (4.20) gives after few iterations

$$\epsilon^{(1,1)}_{(0,0)} = e^{\frac{2\pi i N_f}{K^2}} \epsilon^{(1,1)}_{(1,1)} = \cdots = e^{\frac{2\pi i N_f (K-1)}{K^2}} \epsilon^{(1,1)}_{(K-1,K-1)} = e^{-\frac{2\pi i N_f}{K}} \epsilon^{(1,1)}_{(0,0)}, \tag{4.22}$$

which is consistent iff $N_f = 0 \bmod K$.

For generic values of k_1, k_2, l_1, l_2 one obtains the following consistency condition

$$\epsilon^{(k_1,l_1)}_{(k_2,l_2)} = e^{\frac{2\pi i N_f l_1 k_1 p}{K^2}} \epsilon^{(k_1,l_1)}_{(k_2,l_2)}, \tag{4.23}$$

for some integers p, s, t such that $pk_1 - Kt = 0$ and $pl_1 - Ks = 0$. Therefore T modular invariance is possible iff $N_f = 0 \bmod K$. It is not difficult to show that with this condition on N_f and the phases, S and T modular invariance can be simultaneously achieved. Hence we conclude that modular invariance is possible iff $N_f = 0 \bmod K$.

Example: $\mathbb{Z}_2 \times \mathbb{Z}_2$

Equation (4.19) gives $\epsilon^{(1,1)}_{(1,1)} = e^{iN_f\pi} \epsilon^{(1,1)}_{(1,1)}$ which is possible, for non-zero $\epsilon^{(1,1)}_{(1,1)}$, iff $N_f = 0 \bmod 2$. With these conditions (4.19) and (4.20) give

$$\begin{aligned}
&\epsilon^{(0,0)}_{(0,1)} = \epsilon^{(0,1)}_{(0,0)} = \epsilon^{(0,1)}_{(0,1)}, \quad \epsilon^{(0,0)}_{(1,0)} = \epsilon^{(1,0)}_{(0,0)} = \epsilon^{(1,0)}_{(1,0)}, \\
&\epsilon^{(0,0)}_{(1,1)} = \epsilon^{(1,1)}_{(0,0)} = \epsilon^{(1,1)}_{(1,1)}, \\
&\epsilon^{(0,1)}_{(1,0)} = \epsilon^{(0,1)}_{(1,1)} = \epsilon^{(1,1)}_{(1,0)} = \pm\epsilon^{(1,1)}_{(0,1)} = \pm\epsilon^{(1,0)}_{(0,1)} = \pm\epsilon^{(1,0)}_{(1,1)},
\end{aligned} \tag{4.24}$$

with the minus signs when $N_f = 2 \bmod 4$ and plus signs when $N_f = 0 \bmod 4$. Therefore modular invariance can be achieved iff $N_f = 0 \bmod 2$. That is the edge theory is expected to be unstable when $N_f = 0 \bmod 2$. In Sec. 4.3.3, we will construct explicitly a potential that gaps out the edge theory.

4.3.2 $\mathbb{Z}_K$ symmetry

To compare our results to that obtained for $\mathbb{Z}_K$ SPT phases in [51], we consider the embedding $\mathbb{Z}_K \to \mathbb{Z}_K \times \mathbb{Z}_K$ given by $k \to (k, kq)$ and $N_f = 1$. To analyze this case we simply set $l_1 = k_1 q$ and $l_2 = k_2 q$ and $N_f = 1$ in the previous expressions above. Hence we can write

$$Z(\tau) = \sum_{k_1,k_2=0}^{K-1} \epsilon_{k_2}^{k_1} Z_{k_2}^{k_1}(\tau) \tag{4.25}$$

with $Z_{k_2}^{k_1} := Z_{(k_2,k_2q)}^{(k_1,k_1q)}$ and similarly for ϵ. Therefore in this case the large gauge anomaly is

$$Z_{k_2\pm K}^{k_1} = Z_{(k_2\pm K, k_2 q \pm qK)}^{(k_1,qk_1)} = e^{\pm\frac{4\pi i q k_1}{K}} Z_{k_2}^{k_1}. \tag{4.26}$$

The T modular transformation is now given by

$$Z_{k_2}^{k_1}(\tau+1) = e^{-\frac{2\pi i q k_1^2}{K^2}} Z_{k_1+k_2}^{k_1}(\tau), \tag{4.27}$$

while the S modular transformation is

$$Z_{k_2}^{k_1}(-1/\tau) = e^{\frac{4\pi i q k_1 k_2}{K^2}} Z_{-k_1}^{k_2}(\tau). \tag{4.28}$$

Thus the S modular invariance condition is

$$\epsilon_{k_2}^{k_1} = \begin{cases} e^{-\frac{4\pi i q k_1 k_2}{K^2}} \epsilon_{-k_1}^{k_2} & \text{if} \quad k_1 = 0, \\ \\ e^{-4\pi i(\frac{q k_1 k_2}{K^2} - \frac{q k_2}{N})} \epsilon_{-k_1+K}^{k_2} & \text{if} \quad k_1 > 0, \end{cases} \tag{4.29}$$

while the T modular invariance condition is

$$\epsilon_{k_2}^{k_1} = \begin{cases} e^{\frac{2\pi i q {k_1}^2}{K^2}} \epsilon_{k_1+k_2}^{k_1} & \text{if} \quad k_1 + k_2 \leq K-1, \\ \\ e^{2\pi i \left[\frac{q{k_1}^2}{K^2} - \frac{2qk_1}{K}\right]} \epsilon_{k_1+k_2-K}^{k_1} & \text{if} \quad k_1 + k_2 > K-1. \end{cases} \tag{4.30}$$

From Eq. (4.29) above, one obtains

$$\epsilon_{k_2}^0 = \epsilon_0^{k_2} = \epsilon_{-k_2+K}^0 = \epsilon_0^{-k_2+K}, \tag{4.31}$$

if $k_1 = 0$ and $k_2 \neq 0$, whereas

$$\epsilon_0^{k_1} = \epsilon_{-k_1+K}^0 = \epsilon_0^{-k_1+K} = \epsilon_{k_1}^0. \tag{4.32}$$

if $k_2 = 0$ and $k_1 \neq 0$. Similarly, for even K and $k_1 = k_2 = K/2$ one gets

$$\epsilon_{K/2}^{K/2} = e^{\pi i q} \epsilon_{K/2}^{K/2} \tag{4.33}$$

which is consistent iff $q = 0 \bmod 2$. Finally, for other values of k_1 and k_2 different from those considered above one gets

$$\begin{aligned} \epsilon_{k_2}^{k_1} &= e^{-4\pi i (\frac{qk_1k_2}{K^2} - \frac{qk_2}{K})} \epsilon_{-k_1+K}^{k_2} \\ &= e^{-\frac{4\pi i q k_1}{K}} \epsilon_{-k_2+K}^{-k_1+K} \\ &= e^{-\frac{4\pi i q k_1 k_2}{K^2}} \epsilon_{k_1}^{-k_2+K} \end{aligned} \tag{4.34}$$

where we have left out a self consistent further iteration. This shows that S modular invariance is possible for even K iff q is even and for odd K there is no condition on q.

Now we move on to analyze the T modular invariance conditions which imply

$$\epsilon_0^1 = e^{\frac{2\pi i q}{K^2}} \epsilon_1^1 = \cdots = e^{\frac{2\pi i q(K-1)}{K^2}} \epsilon_{K-1}^1 = e^{-\frac{2\pi i q}{K}} \epsilon_0^1, \tag{4.35}$$

which is self consistent iff $q = 0 \bmod K$. We now show that this condition is sufficient for T modular invariance. When $k_1 \neq 0$ after several reiterations one gets the condition

$$\epsilon_{k_2}^{k_1} = e^{\frac{2\pi i q k_1^2 p}{K^2}} \epsilon_{k_2}^{k_1}, \tag{4.36}$$

where p is an integer such that $k_1 p - Kt = 0$ for an integer t whose actual value is irrelevant to us. So that with $q = 0 \bmod K$ the phase in Eq. (4.36) is just 1.

Thus putting our results together we find that modular invariance is possible iff $q = 0 \bmod K$. I.e., the phase is trivial when $q = 0 \bmod K$ and non-trivial (i.e., SPT phase) otherwise.

4.3.3 Gapping potentials

In this section we show that there exist potentials that can fully gap our system without explicitly or spontaneously breaking the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry iff $N_f = 0 \bmod 2$. Thus we confirm that we do indeed have a SPT phase when $N_f \neq 0 \bmod 2$ and a trivial phase otherwise.

Let us first consider the case when $N_f = 1$, in this case a complete set of local operators in the field theory is given by $\partial\Phi$, $\partial\Theta$, and $\cos(m\Phi + n\Theta + \alpha)$, where ∂ denotes a generic derivative and α is a constant. Here we have switched our notation, $\phi_1 \to \Phi$ and $\phi_2 \to \Theta$, to emphasize the dual (canonical conjugate) nature of these fields, $[\Phi, \partial\Theta] \sim 2\pi i$. The most general gapping potential terms that is $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric is given by linear

combinations of the form

$$\cos(2m\Phi + 2n\Theta + \alpha). \tag{4.37}$$

Now we can do a semi-classical analysis to show that the ground state spontaneously breaks $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry once a strong enough gapping potential of the form (4.37) is added. Without loss of generality we set $\alpha = 0$, and since $[\Phi, \partial\Theta] \sim 2\pi i$ etc., we need to consider independently potentials of the form $\cos(2m\Phi)$ and $\cos(2n\Theta)$. For $\cos(2m\Phi)$ we have that classical minima correspond to $\Phi = \frac{2j+1}{2m}\pi$ (for a finite number of independent j's since $\Phi \in [0, 2\pi)$) and the $\mathbb{Z}_2$ transformation $\Phi \to \Phi + \pi$ amounts to $j \to j + m$. As one can easily see when $m = 1$, for example, these classical minima transform under $\mathbb{Z}_2$ and a choice of any one of them would spontaneously break $\mathbb{Z}_2$ symmetry. The analysis for potentials of the form $\cos(2n\Theta)$ is similar and we reach the conclusion that when $N_f = 1$ it is not possible to gap our system without breaking $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

When $N_f = 2$ we have fields $\Phi_1, \Theta_1, \Phi_2, \Theta_2$ and the most general $(\mathbb{Z}_2 \times \mathbb{Z}_2)$-invariant possible gapping potential is given by $\cos[m_1(\Phi_1 - \Phi_2) + n_1(\Theta_1 - \Theta_2) + 2l_1\Phi_1 + 2l_2\Theta_2 + \alpha]$ where $m_1, n_1, l_1, l_2 \in \mathbb{Z}$. If we focus on two mutually commuting and $(\mathbb{Z}_2 \times \mathbb{Z}_2)$-symmetric bosonic fields $\Phi_1 - \Phi_2$ we can consider a gapping potential of the form $\cos(m_1(\Phi_1 - \Phi_2) + n_1(\Theta_1 + \Theta_2))$. If we consider $-\cos(\Phi_1 - \Phi_2) - \cos(\Theta_1 + \Theta_2)$ we see that the classical minima corresponds to

$$\Phi_1 - \Phi_2 = 0, \quad \Theta_1 + \Theta_2 = 2\pi, \tag{4.38}$$

since this is invariant under $\mathbb{Z}_2 \times \mathbb{Z}_2$ and $[\Phi_1 - \Phi_2, \Theta_1 + \Theta_2] = 0$ we conclude that we can fully gap the system without spontaneously breaking the symmetry.

Most generally when $N_f = 2m$ we have fields Φ_i, Θ_i $(i = 1, \ldots, 2m)$ and the most general $(\mathbb{Z}_2 \times \mathbb{Z}_2)$ invariant possible gapping potential is given by a sum over potentials

of the form

$$\cos\Big\{\sum_{i=1}^{2m-1} m_i(\Phi_i - \Phi_{2m}) + \sum_{i=1}^{2m-1} n_i(\Theta_i - \Theta_{2m}) + 2l_1\Phi_{2m} + 2l_2\Theta_{2m} + \alpha\Big\}. \tag{4.39}$$

If we focus on two mutually commuting and $(\mathbb{Z}_2 \times \mathbb{Z}_2)$-symmetric bosonic fields then a potential of the form

$$-\sum_{i=1}^{m} [\cos(\Phi_{2i-1} - \Phi_{2i}) + \cos(\Theta_{2i-1} + \Theta_{2i})] \tag{4.40}$$

would be minimized classically by

$$\Phi_{2i-1} - \Phi_{2i} = 0, \quad \Theta_{2i-1} + \Theta_{2i} = 2\pi, \tag{4.41}$$

which is allowed since all the commutators between the different fields on the left-hand side of (4.41) are zero. On the other hand when $M = 2m + 1$, by choosing a maximal set of $2m$ commuting $(\mathbb{Z}_2 \times \mathbb{Z}_2)$-invariant fields (basically differences $\Phi_i - \Phi_j$ etc) to localize, one is always left with one field that cannot be localized and hence the system cannot be fully gapped. This concludes our analysis of bosonic SPT phases with $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

For general K the above analysis is easily generalized. For example, for $K = 3$ with $N_f = 3$ one can gap out the following independent, mutually commuting, and $(\mathbb{Z}_K \times \mathbb{Z}_K)$-invariant combinations

$$\Phi_1 - \Phi_2, \quad \Phi_2 - \Phi_3, \quad \Theta_1 + \Theta_2 + \Theta_3, \tag{4.42}$$

while for $K = 4$ with $N_f = 4$ one can gap out

$$\begin{aligned} &\Phi_1 - \Phi_2, \quad \Theta_1 + \Theta_2 - \Theta_3 - \Theta_4, \\ &\Phi_3 - \Phi_4, \quad \Theta_1 + \Theta_2 + \Theta_3 + \Theta_4. \end{aligned} \tag{4.43}$$

For generic K, one could consider, for example, a gapping potential $\sum_{i=1}^{K-1} \cos[m_i(\Phi_i - \Phi_{i-1})] + \cos[n \sum_i^K \Theta_i]$ that gaps $K = N_f$ mutually independent and $(\mathbb{Z}_K \times \mathbb{Z}_K)$ symmetric combinations of bosonic fields.

4.4 Fermionic symmetry protected topological phases

In this section, we are interested in fermionic SPT phases which are relevant to the physics of topological superconductors. We consider $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry which is a generalization of the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry discussed in Refs. [63, 68]. The relevant edge theory in the absence of interactions with several flavors is described by the free Dirac action which corresponds to the Hamiltonian in Eq.(4.11) is

$$S = \frac{i}{2\pi} \int dx dt \sum_{a=1}^{N_f} \psi_{La}^\dagger (\partial_t - \partial_x) \psi_{La} + \psi_{Ra}^\dagger (\partial_t + \partial_x) \psi_{Ra}. \tag{4.44}$$

where $\psi_L^\dagger, \psi_L, \psi_R^\dagger, \psi_R$ are creation/annihilation operators of the fermionic nonchiral edge modes that are supported by some topological bulk system. This action has a $U(1) \times U(1)$ symmetry, which contains $\mathbb{Z}_K \times \mathbb{Z}_K$ as its subgroup. As in the bosonic case we gauge this $\mathbb{Z}_K \times \mathbb{Z}_K$ subgroup to understand the corresponding SPT phases. Similar to the bosonic case, the quantity of interest is the orbifold partition function after introducing flavors,

$$Z(\tau) = \sum_{k,l,m,n} \epsilon_{(k,l,m,n)} \left[Z_l^k(\tau) \bar{Z}_n^m(\tau) \right]^{N_f}, \tag{4.45}$$

where $k, l, m, n = 0, 1, \ldots, K-1$ etc. denoting the spatial and temporal twists of ψ_L and ψ_R. This corresponds to a sum over the most general combination of left and right twistings of the spinors by the $\mathbb{Z}_K \times \mathbb{Z}_K$ group action (4.12). The modular transformations are:

$$
\begin{aligned}
Z(\tau+1) &= \sum_{k,l,m,n} \epsilon_{(k,l,m,n)} e^{-\pi i N_f (\frac{k^2-m^2}{K^2})} \left[Z^{k'}_{l'-k'}(\tau) \bar{Z}^{m'}_{n'-m'}(\tau) \right]^{N_f}, \\
Z(-1/\tau) &= \sum_{k,l,m,n} \epsilon_{(k,l,m,n)} e^{2\pi i N_f (\frac{mn-kl}{K^2} + \frac{k-m+n-l}{2K})} \left[Z^{l'}_{1-k'}(\tau) \bar{Z}^{n'}_{1-m'}(\tau) \right]^{N_f},
\end{aligned}
\tag{4.46}
$$

where the bar denotes complex conjugation.

Instead of being exhaustive, we make an ansatz that the overall partition function is holomorphically factorized so that

$$
Z(\tau) = Z_L(\tau) \bar{Z}_R(\tau) = |Z_L(\tau)|^2. \tag{4.47}
$$

In this case modular invariance is achieved as long as the left(right)-moving contribution transforms covariantly with a phase under a generic modular transformation U, $Z_L(U\tau) = e^{i\theta} Z_L(\tau)$. So we can focus on the left-moving sector,

$$
Z_L(\tau) = \sum_{k,l=0}^{K-1} \epsilon^k_l Z^{k'}_{l'}(\tau). \tag{4.48}
$$

The condition for S modular invariance is then deduced from Eq. (4.46) to be (the modular invariance conditions presented below are all up to an overall phase)

$$
\epsilon^k_l = \begin{cases} e^{2\pi i N_f (\frac{kl}{K^2} + \frac{l-k}{2K})} \epsilon^l_{K-k} & \text{if } k > 0 \\ \\ e^{2\pi i N_f (\frac{3l}{2K})} \epsilon^l_{-k} & \text{if } k = 0. \end{cases} \tag{4.49}
$$

Also from (4.46) the conditions for T modular invariance is found to be

$$\epsilon_l^k = \begin{cases} e^{\frac{\pi i N_f k^2}{K^2}} \epsilon_{l-k}^k & \text{if } 0 \leq l-k \leq K-1 \\ \\ e^{2\pi i N_f \left[\frac{k^2}{2K^2} + \frac{1}{2} - \frac{k}{K}\right]} \epsilon_{l-k+K}^k & \text{if } l-k < 0 \end{cases} \tag{4.50}$$

Let us analyze Eq. (4.49) in general. When K is even one gets

$$\epsilon_{k/2}^{k/2} = e^{\pi i N_f/2} \epsilon_{k/2}^{k/2} \tag{4.51}$$

so this requires $N_f = 0 \bmod 4$. One can check that this condition is enough for self consistency of Eq. (4.49) while for odd K, no condition on N_f is required. Equation (4.50) gives after K iterations

$$\epsilon_0^1 = e^{\pi i N_f \frac{K-1}{K}} \epsilon_0^1. \tag{4.52}$$

When K is even this requires $N_f = 0 \bmod 2K$ while for odd K this requires $N_f = 0 \bmod K$. In general several iterations of Eq. (4.50) gives

$$\epsilon_l^k = e^{\pi i N_f (\frac{k^2 p}{K^2} + t - \frac{2kt}{K})} \epsilon_l^k, \tag{4.53}$$

for some integers p and t such that

$$Kt - kp = 0. \tag{4.54}$$

For even K one sees that $N_f = 0 \bmod 2K$ is sufficient while for odd K with $N_f = 0 \bmod K$ the phase in (4.53) is $e^{\pi i N_f t \frac{k+K}{K}}$. So one needs to consider only the case when k is even. In this case (4.54) implies that t must be even. Hence the phase is one and we conclude that

modular invariance is possible for even K iff $N_f = 0$ mod $2K$ while for odd K iff $N_f = 0$ mod K.

4.4.1 $\mathbb{Z}_2 \times \mathbb{Z}_2$ Example

For the case $\mathbb{Z}_2 \times \mathbb{Z}_2$, let us check that we recover the results in Ref. [68] from our analysis. In this case Eq. (4.49) gives

$$\epsilon_1^0 = e^{\frac{3\pi i N_f}{2}} \epsilon_0^1, \quad \epsilon_0^1 = e^{-\frac{\pi i N_f}{2}} \epsilon_1^0, \quad \epsilon_1^1 = e^{\frac{\pi i N_f}{2}} \epsilon_1^1, \tag{4.55}$$

while Eq. (4.50) gives

$$\epsilon_0^1 = e^{-\frac{3\pi i N_f}{4}} \epsilon_1^1, \quad \epsilon_1^1 = e^{\frac{\pi i N_f}{4}} \epsilon_0^1. \tag{4.56}$$

Clearly Eqs. (4.55) and (4.56) are consistent iff $N_f = 0$ mod 4 which recovers the result in Ref. [68] with $N_f = 2N$ being the number of flavors of Majorana modes. This result is, of course, familiar from type II string theory [61] where the $\mathbb{Z}_2$ symmetry is generated by the fermion number current on the world sheet and the Majorana modes corresponds to directions in spacetime with two extra dimensions cancelling the ghosts modes that result from gauge fixing. Thus the GSO left right assymmetric $\mathbb{Z}_2$ projection gives rise to consistent modular invariant superstring theories in $8 + 2$ spacetime dimensions.

4.4.2 Gapping potential perspective

To analyze the stability to interactions it is convenient to bosonize the fermionic fields as follows:

$$\psi_L = A e^{i\phi_L}, \quad \psi_R = A e^{i\phi_R}, \tag{4.57}$$

where an implicit normal ordering has been omitted on the right hand side. We would also make use of

$$2\phi_L = \phi + \theta, \quad 2\phi_R = \phi - \theta, \tag{4.58}$$

so that the $\mathbb{Z}_K \times \mathbb{Z}_K$ symmetry is generated by

$$\phi_L \to \phi_L - \frac{2\pi}{K}, \quad \phi_R \to \phi_R + \frac{2\pi}{K}. \tag{4.59}$$

Let us first consider the simplest case of $\mathbb{Z}_2 \times \mathbb{Z}_2$. With four flavors one can write down the interaction term

$$\begin{aligned} V_2 = \Big(&\psi^\dagger_{R,1}\psi^\dagger_{R,2}\psi^\dagger_{L,3}\psi^\dagger_{L,4} + \psi^\dagger_{R,1}\psi^\dagger_{R,3}\psi^\dagger_{L,2}\psi^\dagger_{L,4} \\ &+\psi^\dagger_{R,1}\psi^\dagger_{R,4}\psi^\dagger_{L,2}\psi^\dagger_{L,3} + L \leftrightarrow R\Big) + c.c. \end{aligned} \tag{4.60}$$

In the bosonized form this is just

$$V_2 = 4A^4 \cos\tilde{\phi}_1 \left(\cos\tilde{\theta}_2 + \cos\tilde{\theta}_3 + \cos\tilde{\theta}_4\right) \tag{4.61}$$

where

$$\begin{aligned} 2\tilde{\phi}_1 &= \phi_1 + \phi_2 + \phi_3 + \phi_4, \\ 2\tilde{\theta}_2 &= \theta_1 + \theta_2 - \theta_3 - \theta_4, \\ 2\tilde{\theta}_3 &= \theta_1 + \theta_3 - \theta_2 - \theta_4, \\ 2\tilde{\theta}_4 &= \theta_1 + \theta_4 - \theta_2 - \theta_3, \end{aligned} \tag{4.62}$$

using $[\phi_i, \theta_j] \sim i\delta_{ij}$ one sees that all the fields in Eq. (4.62) mutually commute and can be simultaneously localized. Also one sees that there are two solutions for the classical

minima given by

$$\tilde{\phi}_1 = \pi m_1, \quad \tilde{\theta}_2 = \pi n_2, \quad \tilde{\theta}_3 = \pi n_3, \quad \tilde{\theta}_4 = \pi n_4, \tag{4.63}$$

with either m_1 odd and n_2, n_3, n_4 even or m_1 even and n_2, n_3, n_4 odd. By using the periodicity $\phi_i = \phi_i + 2\pi$ and similarly for θ_i one sees that these two solutions are equivalent and the invariance of $\tilde{\phi}_1, \tilde{\theta}_2, \tilde{\theta}_3, \tilde{\theta}_4$ implies that the system can be fully gapped without explicitly or spontaneously breaking $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry.

Let us now consider the case of $\mathbb{Z}_4 \times \mathbb{Z}_4$ symmetry as this would enable us to understand the generalization to $\mathbb{Z}_{2K} \times \mathbb{Z}_{2K}$. In this case with $N_f = 8$ one can write down the following potential

$$\begin{aligned} V_4 = {} & \psi^\dagger_{R,1}\psi^\dagger_{R,2}\psi^\dagger_{R,3}\psi^\dagger_{R,4}\psi^\dagger_{L,5}\psi^\dagger_{L,6}\psi^\dagger_{L,7}\psi^\dagger_{L,8} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,2}\psi^\dagger_{R,6}\psi^\dagger_{R,8}\psi^\dagger_{L,3}\psi^\dagger_{L,4}\psi^\dagger_{L,5}\psi^\dagger_{L,7} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,2}\psi^\dagger_{R,5}\psi^\dagger_{R,6}\psi^\dagger_{L,3}\psi^\dagger_{L,4}\psi^\dagger_{L,7}\psi^\dagger_{L,8} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,3}\psi^\dagger_{R,5}\psi^\dagger_{R,7}\psi^\dagger_{L,2}\psi^\dagger_{L,4}\psi^\dagger_{L,6}\psi^\dagger_{L,8} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,3}\psi^\dagger_{R,6}\psi^\dagger_{R,8}\psi^\dagger_{L,2}\psi^\dagger_{L,4}\psi^\dagger_{L,5}\psi^\dagger_{L,7} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,4}\psi^\dagger_{R,5}\psi^\dagger_{R,8}\psi^\dagger_{L,2}\psi^\dagger_{L,3}\psi^\dagger_{L,6}\psi^\dagger_{L,7} \\ & + \psi^\dagger_{R,1}\psi^\dagger_{R,4}\psi^\dagger_{R,6}\psi^\dagger_{R,7}\psi^\dagger_{L,2}\psi^\dagger_{L,3}\psi^\dagger_{L,5}\psi^\dagger_{L,8}. \end{aligned} \tag{4.64}$$

In terms of bosonized fields this is

$$V_4 = 4A^8 \cos\tilde{\phi}_1 \left(\sum_{i=2}^{8} \cos\tilde{\theta}_i \right) \tag{4.65}$$

where

$$
\begin{aligned}
2\tilde{\phi}_1 &= \sum_{i=1}^{8} \phi_i, \\
2\tilde{\theta}_2 &= \theta_1 + \theta_2 + \theta_3 + \theta_4 - \theta_5 - \theta_6 - \theta_7 - \theta_8, \\
2\tilde{\theta}_3 &= \theta_1 + \theta_2 + \theta_6 + \theta_8 - \theta_3 - \theta_4 - \theta_5 - \theta_7, \\
2\tilde{\theta}_4 &= \theta_1 + \theta_2 + \theta_5 + \theta_6 - \theta_3 - \theta_4 - \theta_7 - \theta_8, \\
2\tilde{\theta}_5 &= \theta_1 + \theta_3 + \theta_5 + \theta_7 - \theta_2 - \theta_4 - \theta_6 - \theta_8, \\
2\tilde{\theta}_6 &= \theta_1 + \theta_3 + \theta_6 + \theta_8 - \theta_2 - \theta_4 - \theta_5 - \theta_7, \\
2\tilde{\theta}_7 &= \theta_1 + \theta_4 + \theta_5 + \theta_8 - \theta_2 - \theta_3 - \theta_6 - \theta_7, \\
2\tilde{\theta}_8 &= \theta_1 + \theta_4 + \theta_6 + \theta_7 - \theta_2 - \theta_3 - \theta_5 - \theta_8,
\end{aligned} \tag{4.66}
$$

since the tilded fields are mutually commuting they can be simultaneously localized with $\tilde{\phi}_1 = \pi m_1$ and $\tilde{\theta}_i = \pi n_i$ with m_1 odd and n_1 even, or vice versa. Since the fields with tildes are $\mathbb{Z}_4 \times \mathbb{Z}_4$ invariant we conclude that the system can be fully gapped without breaking symmetry. It is clear that this structure can be generalized to $\mathbb{Z}_{2K} \times \mathbb{Z}_{2K}$ with $4K$ flavors, one finds the same conclusion that the system can be gapped without breaking symmetry.

Chapter 5

Towards a Quantum Monte Carlo Simulation of Interacting Spin Orbit Coupled Systems

5.1 3-D Continuum model of a Topological Insulator

Consider the many body Hamiltonian of non interacting electrons in 3-D

$$H = \sum_i -\frac{\hbar^2 \nabla_i^2}{2m} + \frac{1}{2} m\omega^2 r_i^2 - \omega \sigma_i \cdot L_i \tag{5.1}$$

This Hamiltonian (5.1) can be exactly solved. The energy eigen wavefunctions exhibit quaternionic analyticity and are a generalization of 2 dimensional Landau levels (LL). The system exhibits time reversal symmetry and the LLs are flat with an infinite degeneracy parameterized by angular momentum. On a system with a boundary each filled Landau level contributes gapless helical Dirac surface states. When there is an odd number of filled Landau levels the system is believed to be in the non-trivial $\mathbb{Z}_2$ class of the three dimensional Topological insulator [50].

When electronic interactions are turned on this system is not exactly solvable and it remains an open question what happens to the surface states. Since this is a system in the continuum a useful numerical technique to understand the interacting physics may be quantum Monte Carlo (QMC). In the next section we give a brief review of the QMC technique that is inspired by the variational principle in quantum mechanics. This is called variational Monte Carlo (VMC), and we explain how this technique may be extended to systems where the spin degree of freedom is dynamical.

5.2 Variational Monte Carlo

VMC is closely related to Monte Carlo statistical method for evaluating an integral [27], it relies on the variational principle in quantum mechanics which states that: for any system described by a Hamiltonian H, and any allowable wavefunction $|\psi\rangle$, $\langle\psi|H|\psi\rangle \geq E_0$, where E_0 is the ground state energy of the system. This imposes a lower bound on the energy expectation value on the space of wavefunctions. The VMC technique consists of writing down suitably parameterized sets of trial wavefunctions and minimizing the energy expectation value over a set of parameters.

Without spin, given a trial wavefunction ψ_T, the variational energy expectation value for a 3 dimensional system can be written as $3N$ dimensional integral

$$E_V = \frac{\int d^{3N}R \ |\psi_T(R)|^2 \psi_T(R)^{-1} \hat{H} \psi_T(R)}{\int d^{3N}R |\psi_T(R)|^2}, \tag{5.2}$$

where N is the number of particles in the sytem. By the law of large numbers this integral can be approximated as a sum $E_V \approx \sum_{j=1}^{k} F(R_j)$, where $F(R) = \psi_T(R)^{-1}\hat{H}\psi_T(R)$ is the so called local energy of the trial wavefunction and R_j are points in $3N$ dimensional real space generated independently and according to the normalized probability distribution

proportional to $|\psi_T(R)|^2$. An estimate of the size of the error bar in the approximation of the integral is σ_F^2/k, where σ_F is the variance of F which can itself be estimated as

$$\sigma_F^2 \approx \frac{1}{k-1}\sum_{j=1}^{k}\left(F(R_j) - \frac{1}{k}\sum_{l=1}^{k}F(R_l)\right)^2. \tag{5.3}$$

The R_j's are generated by Monte Carlo sampling such as the Metropolis method. The Metropolis algorithm allows one to sample random possibly unnormalized probability distributions $p(R)$. It generates a sequence of points R_j called walkers according to the follwoing rules [27]:

1. Start the walker at a random position R.

2. Make a trial move to a new position R' chosen from some probability density function $T(R \to R)$

3. Accept the trial move to R' with probability

$$A(R \to R') = Min(1, \frac{T(R' \to R)p(R')}{T(R \to R')p(R)}). \tag{5.4}$$

If the trial move is accepted then R' becomes the starting point for the next random walk. If the trial move is rejected R becomes the starting point for the next random walk. Intuitively if the point R and R' are such that $p(R) >> p(R')$ then a move to R' would be rejected most of the time.

4. Return to step 2 and repeat.

The initial points generated by this algorithm depend on the staring point and should be discarded. Eventually a diffusive equilibrium argument [27] shows that the final density of points is proportional to $p(R)$.

5.2.1 VMC with Spin 1/2 degree of freedom

With Spin $1/2$ degrees of freedom we have to evaluate 2^N sums in addition to $3N$ dimensional integral (5.2) i.e

$$E_V = \frac{\sum_{\{i_l\}} \int d^{3N}R \ \psi(R)^*_{i_1,i_2,\ldots i_N}(R)(\hat{H}\psi(R))_{i_1,i_2,\ldots i_N}}{\sum_{\{i_l\}} \int d^{3N}R \ \psi(R)^*_{i_1,i_2,\ldots i_N}(R)\psi(R)_{i_1,i_2,\ldots i_N}}, \tag{5.5}$$

where each sum is over the spin up and down component and we have ommitted the trial (T) subscript in the wavefunction. This is very inconvenient for VMC which thrives on Monte Carlo sampling of points from a continuum. It turns out that the sums appearing in (5.5) can be converted to integrals using a representation of the 2×2 identity matrix $I_{2\times 2}$ given by

$$I_{2\times 2} = \frac{1}{\pi}\int_0^{2\pi} d\theta |\theta\rangle\langle\theta|, \tag{5.6}$$

where $|\theta\rangle^T = (\sin\theta, \cos\theta)$. As an example given a 2×2 matrix M and a state $|u\rangle^T = (u_1, u_2)$, using the representation (5.6), we have

$$< u|M|u >= \sum_{i,j} u_i^* M^{ij} u_j = \int d\theta u(\theta) M \cdot u(\theta), \tag{5.7}$$

where $u(\theta) = \langle\theta|u\rangle$. This is generalized to operators acting on the tensor product space of all particles [8] so that we can write (5.5) as

$$E_V = \frac{\int d^{3N}Rd^N\Theta \ |\psi_T(R,\Theta)|^2 \psi_T(R,\Theta)^{-1}\hat{H}\psi_T(R,\theta)}{\int d^{3N}Rd^N\Theta \ |\psi_T(R,\Theta)|^2}. \tag{5.8}$$

Here $\Theta \in (0, 2\pi)^N$ is a continuum degree of freedom representing the spin degree of freedom of the N particles. In this representation random points in R, Θ space can

be generated using Monte Carlo sampling such as the Metropolis algorithm described above.

5.3 Implementing and testing VMC with Spin degrees of freedom in Qwalk

Some of the ideas discussed in the previous two sections have been implemented in Qwalk which is C++ code developed by Lucas Wagner et al. Qwalk is designed for doing large scale (up to a few hundred particles) simulations Monte Carlo on a cluster of computers. It has been developed over a few years and tested on systems where the spin degree of freedom is not dynamical [77]. Recently new modules have been added to Qwalk to simulate Monte Carlo sampling of points in spatial and spin space.

We performed some preliminary tests of the new modules by simulating the 3-D Landau level problem. We have been able to correctly reproduce the ground state energy. For example in the units $\hbar = m = \omega = 1$. The ground state energy of (5.1) is $1.5N$ where N is the number of particles. This has been calculated for up to 10 particles with an accuracy of 0.00004%. While these numbers are encouraging we should mention that exact energy eigen states where used and this greatly reduces the variance in the estimation of the integrals according to the zero variance property of exact eigen states trial wavefunctions [27]. However, our results are still interesting and indicates that the integrals over the continous spin degree of freedom is a promising idea. These trend of ideas can potentially be used to understand what happens to the 3-D Landau level system when interactions such as the Couloumb interaction $\sum_{i<j} -\frac{e^2}{|r_i - r_j}$ are added. More broadly it may be used to simulate ab initio quantum mechanical systems where spin degree of freedom cannot be ignored.

Chapter 6

Conclusion

6.1 Summary

In conclusion, we have developed an analytic correspondence between $c = 2$ free boson theories and microscopic spin-1 models, using bosonization techniques. For the particular form of Hamiltonian considered (Eq. (1.2a)), we made a prediction for the value of the Tomonaga-Luttinger liquid (TLL) parameters as a function of q_x, the parameter characterizing the lattice model.

To build evidence on the numerical front, we performed exact diagonalization (ED) and density matrix renormalization group (DMRG) calculations to obtain the lowest scaling dimensions from the energetics of the system: a scheme feasible for short periodic chains. However, our use of the mutual information entropy between disjoint blocks, calculated solely from the ground state, provides a promising route to extend these calculations to long chains.

Using this numerical data and the mapping from spin-chains to $c = 2$ theories, we deduced the value of all four TLL parameters as a function of q_x. We expect our analyses to apply to more general situations, for example the model in Eq. (1.2a) with non zero q_y. In future work, we aim to extend these ideas to calculate multiple low-lying scaling

operators and dimensions of the $c = 2$ CFT using the correlation density matrix [20, 59].

Our broader objective is an effort to develop generic methods to map lattice models to multi-component field theories. We anticipate that this multi-scale modelling approach will be useful for understanding the physics at very large length scales: sizes that may not be directly accessible in numerical simulations. Once we have built confidence in the mapping between the lattice and continuum descriptions, we can use the (often known) predictions of the latter.

We have also proposed and developed a theoretical framework that allows us to determine if a given (edge) CFT can be gapped out or not without breaking a given set of symmetries. It is based on the modular invariance/non-invariance of the CFT with symmetry projection; it makes use of a way any 2D CFT couples to the background geometry (complex structure of the torus) and hence can be applied to a wide range of systems.

There are a number of merits to our approach; It does not rely on the presence/absence of a conserved U(1) charge such as particle number. Unlike topological invariants built from single-particle electron wave functions, our method does not rely on single-particle physics and hence is applicable to strongly interacting systems. It is simpler and more convenient than actually looking for all possible perturbations that can potentially gap out the edge theory on a case -by- case basis. For 2D SPT phases that have non-abelian quasiparticles there is no K-matrix formulation but our approach can be extended to such situations. For example, one could consider orbifolds of Wess-Zumino-Witten(WZW) models with discrete torsion.

We have demonstrated that our scheme indeed works for bosonic and fermionic SPT phases with $\mathbb{Z}_K \times \mathbb{Z}_K$ or $\mathbb{Z}_K$ symmetry. In particular, we have checked explicitly that for the cases when the modular invariance is achieved, one can find an interaction potential that can gap out the edge theory without breaking symmetry.

The validity of our approach based on the modular invariance is further supported by a complementary point of view proposed in Refs. [47, 48]. In various cases, our method

based on the modular invariance and the arguments in Refs. [47,48] that makes use of the fractional statistics in the bulk also lead to the same conditions for the "gappability" of the edge theory.

One immediate generalization of our work is to apply our method to symmetry-enriched topological (SET) phases, i.e., topologically ordered phases that have a set of symmetries. For example, our calculations for Bosonic SPT phases can be directly generalized to the case with $|\det \mathrm{K}| > 1$, which has ground state degeneracy. We have checked for a few simple cases with $|\det \mathrm{K}| > 1$ that when the modular invariance is achieved we can construct an interaction potential to gap out the edge theory. Other interesting future work would be to consider SET phases with non-abelian symmetry and(or) non-Abelian statistics.

As discussed in the introduction, modular invariance is a global anomaly in CFT. On the other hand, it is interesting to note that in CFT a local anomaly associated with rescaling invariance occurs proportionately to the total central charge c. It is also instructive to note that in string theory conformal invariance is a constraint and c is cancelled by working in a critical dimension. In condensed matter and statistical physics applications conformal invariance is a real symmetry (i.e., not a constraint) and the appearance of a local anomaly is a quantum effect which does not spoil the consistency of the theory (since there is no associated dynamical gauge degree of freedom).

– We have focussed entirely on modular (non-)invariance on the torus. One may wonder if there are other constraints that come about at higher genus due to modular invariance and unitarity. Examples on torodial compactifications of string theory are explored in Ref. [76], where it is shown that modular invariance and unitarity at genus 2 enforces more constraints on the phases with the various possible ways of achieving modular invariance corresponding to elements in the second group cohomology $H^2(G, U(1))$ for a finite Abelian group G. Perhaps one can make a connection between modular non-invariance and group cohomology as well, in particular the third cohomology which is

relevant for the classification of 2D SPT phases.

Finally we gave a brief preview of using quantum monte carlo to simulate spin orbit coupled systems in particular the dimensional Landau level problem.

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