Entanglement properties and correlations of certain one-dimensional magnets out of equilibrium using Matrix Product States

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Entanglement properties and correlations of certain one-dimensional magnets out of equilibrium, using Matrix Product States

by

Richard Cole

A Doctoral Thesis

Submitted in partial fulfilment of the requirements for the award of Doctor of Philosophy of Loughborough University

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Abstract

This thesis is devoted to the study of one-dimensional quantum spin chains using matrix product state-based techniques known. We deal mostly with the transverse field Ising model and perturbations. Firstly, we consider an out of equilibrium steady state by applying an energy current. We confirm the phase diagram, the correlations and the entanglement scaling. Subsequently, we introduce two kinds of perturbations. Firstly, we add an interaction that takes the system away from integrability and we study the correlations and the entanglement scaling, determining its phase diagram. Secondly, we weaken the strength of the interaction every $n$th pair with focus on the simplest case $n=2$. In every case we compute correlations and central charge (entanglement scaling) and we show that in the presence of an energy current, there is no conservation of energy. Finally, we motivate briefly work on a system that exhibits the Haldane phase.
Acknowledgements

Firstly, I would like to express my sincerest gratitude to Dr. Joseph Betouras. His supervision has been an essential part in producing the final state of this work. I appreciate all his time and patience, motivating me through the struggles and successes in this work. He inspired me to continue learning beyond my undergraduate studies and I am extremely grateful for the opportunity extended to me to follow this research project advised by him.

I am in debt to Dr. Frank Pollmann for his help with the technical aspects of the project. The numerical code is based on his previous efforts and communications via e-mail and Skype helped me overcome any issues I faced. Also, allowing me to visit him at the Max Planck Institute in Dresden provided an invaluable intensive instruction into the method and the physics behind entanglement scaling.

Finally, I want to express thanks to the Loughborough Graduate School for awarding me the research studentship making this all possible.
Contents

Abstract i
Acknowledgements ii
List of Figures x
List of Abbreviations xi

1 Introduction 1

2 Quantum phase transitions 7
  2.1 Quantum criticality ........................................ 9
  2.2 Critical entanglement properties .......................... 13
    2.2.1 Entropy of entanglement .............................. 13
    2.2.2 Area laws and entanglement scaling .................. 14

3 Numerical technique 16
  3.1 Density Matrix Renormalisation Group ................... 17
  3.2 Matrix Product States ..................................... 19
    3.2.1 Schmidt decomposition ............................... 19
    3.2.2 Decomposition into a Matrix Product State .......... 21
  3.3 Infinite Time Evolving Block Decimation .................. 23
    3.3.1 Vidal’s decomposition ............................... 23
    3.3.2 Graphical representation ............................. 24
List of Figures

2.1 Example phase diagrams near a quantum critical point. (a) The absence of order at $T > 0$ in systems obeying the Mermin-Wagner theorem. (b) Otherwise, order at finite temperature extends over a region with a boundary of second-order phase transitions.

3.1 Redesigned from [1]. Left: Infinite DMRG. The system is split into blocks A (blue) and B (red). Two sites are added and the blocks renormalised into subsystems A and B (the superblock). The decision can be made to continue this process iteratively until a desired size is reached (1), an extrapolation technique may be used to form the chain for $N \to \infty$, or the finite algorithm commences (2). Right: From this point we can take the block to be a finite chain of length $N$. Instead of adding sites, the current ones are extracted from the blocks in pairs and refined in sweeps.

3.2 (a) Tensors $\Gamma$ are represented by a circle with three legs for each index with conjugate inverse. (b) Bonds $\lambda$ have one index joining the chain together. (c) Two-site MPS formed from the combination of (a) and (b) parts.

3.3 Non-commuting parts of a general Hamiltonian applied to an MPS in Vidal form.
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4</td>
<td>Update procedure of an MPS in iTEBD with unitary two-site operator.</td>
</tr>
<tr>
<td>3.5</td>
<td>Expectation values $\langle \Psi</td>
</tr>
<tr>
<td>3.6</td>
<td>MPS with one-site operators $O_1$ at site 1 and $O_r$ at site $r$. The quantum transfer matrix (shaded) inserted $r-1$ times is used to build the central part of the chain. This generates distance between correlations.</td>
</tr>
<tr>
<td>4.1</td>
<td>(a) Exact ground state energy for TFIM compared to numerical iTEBD. (b) Relative error: $</td>
</tr>
<tr>
<td>4.2</td>
<td>Transverse Ising model exact result compared with numerical iTEBD.</td>
</tr>
<tr>
<td>4.3</td>
<td>Ising model spin-spin correlation functions (a) $\rho_{zz}(R)$ and (b) $\rho_{xx}(R)$ with site distance $R =</td>
</tr>
<tr>
<td>4.4</td>
<td>iTEBD: singular values for $\lambda^{[1]}$ decay rapidly as a function of alpha (log-linear).</td>
</tr>
<tr>
<td>4.5</td>
<td>Effective correlation length $\xi$ in the TFIM near the quantum critical point at $h=1$.</td>
</tr>
<tr>
<td>4.6</td>
<td>The scaling behaviour of the effective correlation length $\xi$ with $\chi$ using iTEBD in the TFIM.</td>
</tr>
<tr>
<td>4.7</td>
<td>Half-chain entanglement properties for the TFIM at the critical point $h=1.0$. The entropy scales with correlation length with a gradient of $1/12$ equivalent to a central charge $c = 1/2$.</td>
</tr>
<tr>
<td>4.8</td>
<td>Sketch of the Dzyaloshinskii-Moriya interaction applied to the Transverse Field Ising model.</td>
</tr>
<tr>
<td>4.9</td>
<td>Energy dispersion relation for the TFIM with energy current. Values of energy current $L = 0 - 2$ and magnetic field $h = 0 - 2$.</td>
</tr>
</tbody>
</table>
LIST OFFIGURES

4.10 Schematic diagram of the Transverse Field Ising model with energy current. A new current carrying (CC) phase exists as the energy current flows beyond a critical value. 52

4.11 TFIM with energy current $L$ in range $\{0, 0.2, ..., 1.8, 2.0\}$ and magnetic field $h = 0.5$ below the critical value $h_c = 1$. The oscillatory behaviour of the $zz$-correlation function is shown above critical value of the energy current $L_c = 1$. In the region $L \leq 1$ normal FM correlations are observed. Inset: A Fast Fourier transform (FFT) is used to calculate the period as it shifts with $L$. 54

4.12 Chiral order parameter of the TFIM at $h = 0.5$. 56

4.13 The behaviour of a chiral order parameter $C_{zy}$ as a function of magnetic field in the TFIM with energy current $L = 2.0$. 56

4.14 Central charge $c = 1$ in the current-carrying TFIM ($h = 0.5$ and $L = 1.2$). $S = \frac{c}{6} \log(\xi)$. 58

4.15 The central charge as a function of the transverse field $h$ in the current-carrying TFIM at $L = 1.2$. Left inset: Central charge $c = 1$ is determined in the current-carrying region from the calculation of $S = \frac{c}{6} \log(\xi)$. Right inset: The scaling disappears crossing into the paramagnetic phase and $S$ is constant or zero. 59

5.1 Correlations of the non-integrable TFIM at $h = 0.5$ with integrability breaking parameter $D$. Triangles (blue) denote long-range order, stars (colourless) critical correlations and circles (red) exponential decay. 62

5.2 Effective correlation length at $D = 0.25$, critical $h \approx 0.607$. 64

5.3 Entanglement entropy scaling of the non-integrable critical line. The XY point is shown on the left with central charge $c \approx 1.0$. The remaining lines starting with the TFIM on the right have central charges $c \approx 0.5$ with the rest lines falling in between these two points. 65
5.4 Phase diagram of the TFIM with integrability breaking term $D/J$ as function of the transverse field $h/J$. ................. 66

5.5 The central charge of the TFIM with a non-integrability breaking term and energy current, $L=2$. ......................... 69

6.1 The susceptibility to bond weakening, $d^2E_0/dJ'^2$, describes the response of the weak bond transverse field Ising model to reducing $J'$. The divergence of the lines, $d^2E_0/dJ'^2 \to \infty$, indicates quantum critical points. The numerical iTEBD solutions are pictured as vertical dashed lines at the peaks. The critical points are $J'/J = (h/J)^2$. The peaks are normalised for clarity since their magnitudes decay with increasing field ................ 73

6.2 The magnetisation $M_z$ and $M_x$ for the transverse field Ising model with periodic odd bond $J'$. The choice of order parameter $M_z$ shows a continuous transition to zero in the upper Figure. The magnetic field $h=0.5$ and a FM-PM transition is seen at $J'_c/J = (h/J)^2 = 0.25$ as $J'$ is weakened. ................. 74

6.3 Correlations for the TFIM with weakened bond at $h=0.5$. ... 75

6.4 Central charge as a function of $(h/J)^2$ in the weakened bond transverse field Ising model at critical $J'$. Inset is the entanglement scaling where the central charge of $c=0.5$ is extracted from. .................. 76

6.5 Illustration of the sites, the corresponding interactions, the energy currents and the bonds that are involved. Due to the symmetry of the problem, the energy current $j_{2n}$ and $j_{2n+1}$ need to be considered in the continuity equation. .................. 77

6.6 Critical boundary for transverse Ising model with weakened bond over $n$-sites, $(J'_c/J) = (h/J)^n$. Second-order phase transition occurs crossing the line from above (ordered to disordered). 78
7.1 Detection of the Haldane phase using degeneracy of the first two Schmidt coefficients $\lambda_1 - \lambda_2$. The on-site anisotropy is tuned in and out of the Haldane phase. . . . . . . . . . . . . . . . . . . . . . . . 83
LIST OF ABBREVIATIONS

List of Abbreviations

DMRG  Density Matrix Renormalisation Group
iTEBD  Infinite Time Evolving Block Decimation
TFIM  Transverse Field Ising Model
MPS  Matrix Product State
SVD  Singular Value Decomposition
NESS  Non-equilibrium steady-state
DM  Dzyaloshinskii-Moriya
FM  Ferromagnetic
AFM  Antiferromagnetic
PM  Paramagnetic
CC  Current-carrying
Chapter 1

Introduction

The study of strongly correlated electron systems presents many exciting challenges in condensed matter physics [2]. Numerous new phases emerge due to the strong interactions and novel physical properties require deep understanding and, very often, new physics to explain the observations [3]. Successes in experimental and theoretical work have developed a basis to explain important properties in materials science [4]. Semiconductors, magnetic alloys, dielectrics, nanoscale materials, and photonic materials all exhibit different chemical, physical, electronic, and optical properties. This, in turn, has lead to new technological discoveries ranging from the development of transistors, detectors and emitters, nanodevices, and energy storage materials like fuel cells or photovoltaics. The prospect for more efficient and better performing devices is bright, and this field continues to be an immensely active area of research.

Theoretical work offers explanations to new phenomena or pioneers new areas of research, enabling and supporting novel breakthroughs. Strong interactions among the constituent units in materials are responsible for new phenomena that require theoretical attention. High-temperature superconductivity, metal-insulator transitions, spin-charge separation, quantum Hall effect, multiferroic materials, colossal magnetoresistance, are just a subset of the most important. Strong correlations also play an important role in mag-
netism. Most recognisable from our everyday experience are permanent magnets which exhibit ferromagnetism but a wealth of magnetic phenomena are associated with strong correlations.

The origin of strong magnetic effects in condensed matter systems is quantum mechanical. In practice the physics of these effects is difficult to study in a general way. A crucial strategy involves writing down simpler models of reality that capture the main features of the real system but they are still tractable in some ways. Then most of the physics is retained but the complexity of the problem is reduced. The Hubbard and Heisenberg models are two very effective examples in this direction, which accurately describe the properties of magnetic metals and insulators [5–8] respectively, with relatively simple Hamiltonians. The literature is full of methods to exactly solve variants of these models with different methods appropriate under different circumstances [9–11]. There are numerous tools available currently to treat those systems, both analytically and numerically, some of them only applicable in one dimension. These, specific to one dimension, include the Bethe ansatz and fermionisation (e.g. using Jordan-Wigner and Majorana representations). In general there are quantum field theory approaches (e.g. nonlinear sigma models), or approximations using perturbation theory etc. To a good extent, analytical techniques can give us a good understanding of the physics, but numerical techniques have been developed in parallel to work in conjunction guiding or opening the situation to a wider range of problems in strongly correlated systems. Well known numerical tools include exact diagonalisation, Quantum Monte Carlo, numerical renormalisation group, density matrix renormalisation group (DMRG) and its derivatives like time evolving block decimation (TEBD) considered in this work. Most are limited by some finite-scale of the system, for example number of constituents or the amount of entanglement in the system.

Strong interactions in materials provide the following microscopic picture of the physics. Strongly-correlated electrons loosely bound to lattice sites where the ions are in close proximity to each other. In the crystal lattice they have quantum states which overlap. Their wave-functions extend over all space.
with prominence at lattice sites. Those closest, separated by a single lattice spacing, have the greatest overlap and as a consequence of the Pauli exclusion principle are subject to fermion statistics. The interchange of two electrons is indistinguishable resulting in an exchange integral. The sign of which is vital in determining magnetic phases. It is an energy term which tends to hold neighbouring spins parallel or anti-parallel, depending on the sign of the interaction term as we will explain below. This is the basic theory leading to the Heisenberg model. A prototypical and fundamental model for magnetism, the study of which provides an understanding of coupled spin systems. A useful visualisation is of an arrangement of localised electron spins bound to ion sites individually possessing a magnetic dipole moment. As we will be dealing with insulating magnetic systems, contributions from conduction electrons, in the form of itinerant magnetism is neglected taking the material to be an insulator, and any orbital moment coupling to the spin (L-S coupling) is generally weak, except in a special case involving weak ferromagnetism discussed later in the context of Dzyaloshinskii-Moriya interaction. Therefore the total angular momentum is mostly spin with the density of magnetic moments contributing to the bulk magnetisation.

Electrons close to the nucleus are tightly bound and only those in the outer shells are affected by interactions with other sites. This simplifies the problem by neglecting complex inter-shell electron-electron interactions. The free electron interactions can be simplified further to those between nearest neighbours since the Coulomb force between all electrons has infinite range but diminishes strongly over short distances as an inverse square law. The problem has been significantly reduced from one where a seemingly impossible amount of information about the system is required to one of a manageable size.

The realisation of bulk quasi one-dimensional systems has been known since the 1970’s. In early research organic compounds such as salts [12] were known and in more recent work inorganic materials like monatomic metal chains [13] can be made. These system are in between one and two dimensional due to
CHAPTER 1. INTRODUCTION

near isolation of the spin chain which is only weakly coupled to the environment. Experimental studies are performed using techniques such as inelastic neutron scattering, nuclear magnetic resonance, muon spectroscopy etc. These methods provide much of our understanding about the magnetic structure and dynamic properties of materials. For example, in neutron scattering, the success comes because neutron spin interacts with the electron spin magnetic moment. Relatively strong scattering is present in particular directions with intensity that depends on the angle of the detector. From this information, the lattice and spin arrangements can be deduced. Since higher order interference terms are too weak to be detected, only the low order two-particle correlations contribute to the perturbation intensity. To test this against the theory we can link the scattering cross section to spin-spin correlations by a proportionality relation. The partial differential cross section is proportional to the neutron structure factor which is in turn related to the correlation function by a Fourier transform [14, 15]. The observed magnetic moment is quite small and neutron interactions are weak. This can cause difficulties in experiment especially in low dimensional systems with low spin where this is even more apparent [16]. The exceptionally weak magnetic moment can make it hard to study, but despite this many Hamiltonians have been realised in low dimensions [17–20].

Multi-particle systems can exhibit interesting non-local behaviour. If a state is generated such that at least two parts of the system cannot be described independently it is called entangled. The study of which is a fundamental part of quantum information theory, going beyond the traditional condensed matter and materials physics, even having implications in philosophical realism [21]. The parts which make up the system are called qubits (quantum bits), they can take on two possible states just like a classical bit. In order to build a qubit register (a linked unit of controlled qubits used for computation) particles must have two distinct states which have sufficient energy gap between them. The ability to create and control a sequence of qubits is vital in all architectures of quantum computation. Simple models like the Transverse Field
Ising model (TFIM) are effective in describing a chain of qubits [22], or more complicated arrangements such as the Cayley tree geometry [23]. Exploring the bounds and optimum nature of entanglement gives context to the limit in which these systems can be exploited. Understanding measures of entanglement is the first step in quantifying a useful characterisation thereof. The selection of which is not always equally suited for all states and multitudes of special forms have been developed [24]. These measures must observe some key points: (1) an unentangled state shows no entanglement and the result is zero, and (2) the formation of entangled states cannot be generated by local operations alone. Following (2) local operations cannot increase entanglement and the action of measurement on non-local parts will decrease it instead.

The reversible nature of unitary operations can be seen as the upper limit to the effect of local operations on entanglement. Using their inversion properties ensures we can recover the original quantum state with the same entanglement properties. This means that the transformed state will have the same or reduced capacity of outcomes by local operations. This implies that entanglement is a useful resource which defines the utility of a quantum state. The von Neumann entropy satisfies these requirements. Through imaginative manipulation of entanglement the invention of novel quantum information protocols have been made possible. Exciting advancements in quantum cryptology have potential for more secure data transfer, quantum teleportation and entanglement swapping to move states between locations and the most sought after objective, algorithms to run on a quantum computer. Whether or not a universal machine can be made leads to speculation of their capability. Quantum computers might come in the form of specialist machines for solving particular problems. Obstacles hindering the development of a Universal Quantum Computing (UQC) will only be effectively tackled with a dual approach of theory and experiment.

Regarding the appearance of new phases and ordering, in low-dimensions $d \leq 2$ the Mermin-Wagner theorem [25] states that no spontaneous breaking of a continuous symmetry can occur at finite temperatures with sufficiently short-
range interactions. Strong thermal and quantum fluctuations have greater in-
fluence on symmetries in low-dimensional systems which have fewer degrees
of freedom. Order is forbidden at finite temperatures as thermal fluctuations
destroy it. This can be avoided under the assumption that there is always a
negligible coupling in other directions that makes the system effectively higher
dimensional. Under these conditions a zero temperature quantum phase tran-
sition can occur. The so-called quantum critical point (where change of phase
occurs) has implications on a nearby extended critical region and it domi-
nates the thermodynamic properties. The simplest model with spontaneous
order that exhibits a quantum critical point is the TFIM. In this thesis, I will
be focusing on the TFIM in one dimension and in various settings, exploring
mainly the entanglement properties and correlations. We focus on out of equi-
librium steady states first and then we add other perturbations asking similar
questions.

The structure of the thesis is such that we start with Chapters 2 and 3
that present the foundations of the study. Chapter 2 discusses the theory
of quantum phase transitions more broadly. Quantum criticality and entan-
glement are defined in a general way. Chapter 3 gives the background of the
Matrix Product States (MPS) as used in infinite Time Evolving Block Decima-
tion (iTEBD) technique. After these preliminary presentation, the remaining
chapters contain the main findings. Chapter 4 introduces the Ising model,
where the energy current is introduced to study non-equilibrium properties
and an exact analytical solution is given. This model is also used as a basis
to learn how to optimise computation in order to minimise error in numerical
simulations. This code will be applied to more complicated Hamiltonians. Pe-
riodic impurities in Chapter 5, a non-integrable model in Chapter 6 and the
Heisenberg model with a topologically ordered Haldane phase in Chapter 7.
The thesis is summarised and brought to a conclusion in the final Chapter 8.
Chapter 2

Quantum phase transitions

Phase transitions are an important occurrence in the Universe. In our lives, water is the matter we are probably most familiar with demonstrating phases. It sustains life on Earth and gives humans an early encounter of the prevalence of matter which can exist in different forms. Through its physical states (ice, vapour and liquid) we learn about the transitions between phases by physical processes like freezing and evaporation. The stability of these phases under state variables such as temperature, pressure, or volume define regions on a phase diagram. Though a simple starting point the physics is far reaching with universal application to other forms of matter. Questions arise about how to predict the state in which the system will be in under particular state variables. In this respect the theory of equilibrium thermodynamics has the answers. It is a well developed area of physics with an extensive history. Using the tenants of this theory a majority of classical problems may be solved.

Classification of the transition falls into two groups. They can be first-order (discontinuous) transitions where the two phases may exist concurrently at the transition point. In the process of water freezing the solid and liquid phases coexist. This type of transition is not the main focus of this thesis and importance is placed on second-order, or more generally, continuous phase transitions. The transformation between states is different. There is an absence of coexistence. Instead the system continuously changes state beyond a
critical point. These transitions are important because they regularly occur in magnetic systems. Phenomena demonstrated by magnets are heavily dependent on spin ordering and their orientations under external influences. A control parameter, such as an external (magnetic) field, can push the system through a phase transition. Stable distinct phases at equilibrium bounded by transition lines defines a phase diagram. Areas in the phase diagram with different ordering patterns are determined from an order parameter sensitive to the control variable. For example in ferromagnetic systems the density of magnetic moments or magnetisation is a good order parameter, and similarly in antiferromagnets the staggered magnetisation is used. At the phase boundary is a critical point which upon approach from a non-ordered state increases the order parameter smoothly from zero to (in general) a saturation value. The saturated value can be a maximum ordering in the system like all spins aligned or anti-aligned.

The discussion up until now has been for general phase transitions. When temperature is lowered classical physics crosses over into quantum physics. Even at low temperature where thermal energy scales are suppressed, critical behaviour can continue to be expressed. These quantum critical points are described within the theory of quantum phase transitions.

Quantum mechanical systems are best studied in a controlled environment. Quantum physics manifests strongly away from decoherence effects in an isolated system with little interactions with the environment. In particular temperature finds itself as an ever constant obstacle as particle exchanges contribute to decoherence. Remedying this as $T \to 0$ thermal fluctuations reduce and microscopic energy scales like exchange energy $J$ become more prominent. This is important as ordering energies exceed any classical thermal energy scales $k_B T$ ($k_B$ is the Boltzmann constant) and thermal energy ceases entirely at $T = 0$. Fortunately for the study of quantum phase transitions the zero-point energy persists at the ground state maintaining quantum fluctuations. This means the system is active even in the lowest state.

The distinction between classical and quantum phase transitions is impor-
tant at different energy scales. A zero temperature $d$-dimensional quantum system can be mapped to a $d + 1$-dimensional classical system, called the quantum-classical QC mapping (explained in [26]). The correspondence examines similarity between the partition function of the classical and quantum systems. An imaginary time axis in the quantum system is remarkable in the fact that it is identical to an infinite spatial dimension in its classical counterpart. Their partition functions evaluated using a transfer matrix method are identical. This allows any continuous phase transition to be explained in terms of classical statistical mechanics. Examples of some success of this is proven in the 0- and 2-dimensional quantum Ising and 2-dimensional quantum XY models [27]. The Transverse Field Ising model in particular has been examined rigorously [28].

It may seem that a classical theory is adequate in the description of quantum phase transitions but there are other properties that may be missed. A quantum treatment gives an insight into certain additional subtleties hidden by the mapping inaccessible in the classical theory. Using imaginary time introduces a problem as information cannot be gained about real time dynamics without also considering the thermodynamics. This is based on the non-commutation of position and momentum affecting the calculation of the partition function. Dynamics and thermodynamics become mixed [29]. Also of importance is the phase coherence time. This is a time scale which sets a limit over which quantum interference effects may be seen. In most models it is inversely proportional to temperature as $\tau \propto 1/T$. Therefore in the limit of zero temperature $\tau$ diverges as the coherence time is large. This leads to perfect phase coherence over all space including disordered states. This contrasts with the classical interpretation where all correlations in disorder decay rapidly.
CHAPTER 2. QUANTUM PHASE TRANSITIONS

2.1 Quantum criticality

To induce a phase transition a physical parameter is varied through a critical point. If we consider the Hamiltonian \( H(g) = H_0 + gH_1 \), the tunable parameter \( g \) couples \( H_1 \) to \( H_0 \). The operator \( H_1 \) has a competing quantum ground state to \( H_0 \) and they describe the operators for the total energy of their respective ground states. The overall ground state is determined from \( H(g) \) and in general on a finite lattice is analytic. If \( H_1 \) commutes with \( H_0 \) then its expectation value is a conserved quantity for the system. The eigenvalues of \( H_1 \) can be obtained independently and vary with \( g \). At a particular tuning parameter \( g_c \) the first excited state mixes with the ground state i.e. the gap between states vanishes. Likewise for increasing lattice sizes the gap can gradually disappear, until in the thermodynamic limit where it is effectively zero. Therefore a quantum phase transition is expected to be observed at the critical value \( g_c \) [26].

Quantum fluctuations have increasing influence on minimising the order parameter up to the critical point, and significant influence above \( g_c \). Keeping any coupling constants unity, the fluctuations on approach to the critical point have long-ranged correlations. A characteristic length scale, the correlation length, gives a measure of the distance over which parts of the system behave similarly in a correlated way, given by

\[
\xi \propto |g - g_c|^{-\nu} \tag{2.1}
\]

which diverges as \( g \to g_c \) [26]. The critical exponent \( \nu \) is one in a set of important exponents believed to define a universality class. Models may belong to the same class under scale invariance at some large limit and consequently share exponent values and have the same critical properties and scaling functions [30,31]. For example the Heisenberg \( O(3) \) universality class [32]. Four exponents involved in the thermodynamics of the system \( \alpha, \beta, \gamma \) and \( \delta \) are derived from the free energy and define physical properties near the phase transition. They define the scaling of the specific heat, order parameter, susceptibility and critical isotherm respectively. These exponents have dependence on each
other expressed by the scaling relations

\[ 2 - \alpha = 2\beta + \gamma, \quad 2 - \alpha = \beta(\delta + 1) \] (2.2)

These relations are then conveniently used in the hyperscaling relations

\[ 2 - \alpha = d\nu, \quad \gamma = (2 - \eta)\nu \] (2.3)

to relate the exponents of the correlation length (\( \nu \)) and correlation function

\[ (-d + 2 - \eta) \] [33].

The models have an associated energy gap \( \Delta \), which is nonzero for \( g \neq g_c \) and approaches zero as \( g \to g_c \)

\[ \Delta \propto \xi^{-z} \propto |g - g_c|^{-\nu z} \] (2.4)

\( z \) is a dynamic exponent differing from the static \( \nu \) exponent. It relates to the dynamic properties of the system, in particular the characteristic time.

To give a clearer understanding of the phase transition, the two phase diagrams in Fig. 2.1 are discussed. They are divided into three key regions, which are typical of models with a quantum critical point.

In the thermally disordered region classical behaviour prevails. Finite temperature reduces the de Broglie wavelength of the constituent particles, such as electrons. As their mean separation increases beyond the lattice spacing \( a \) transport becomes classical ballistic motion. Thermal fluctuations subsequently destroy long-range order as they destabilize the order parameter and correlation function [34,35].

The quantum disordered region has fluctuations governed by the Heisenberg uncertainty principle. This makes the system disordered even at the ground state due to fluctuations imparted from the zero-point energy.

At \( g_c \) is a quantum critical point and the region extending upwards is a mixture of competing quantum and thermal fluctuations. The boundary of which is expressed by the competition of energies with equal magnitude

\[ k_B T \propto |g - g_c|^{\nu z}. \]
In Fig. 2.1 (a), order is only present along the blue line at $T=0$ and at any finite temperature order is forbidden. This is typical in systems obeying the Mermin-Wagner theorem i.e. no continuous symmetry can be broken in low-dimensional systems ($d \leq 2$) with short-ranged interactions, therefore no phase transition can occur. Fig. 2.1 (b) shows systems with order at finite temperatures. The classical critical line and surrounding shaded region denotes the area in which an effective classical theory of phase transitions applies. Below this line the system is ordered and a conventional second order phase transition is experienced as thermal fluctuations drive the system into disorder.

Figure 2.1: Example phase diagrams near a quantum critical point. (a) The absence of order at $T > 0$ in systems obeying the Mermin-Wagner theorem. (b) Otherwise, order at finite temperature extends over a region with a boundary of second-order phase transitions.

The singularity at $g=g_c$ only applies at $T=0$ in the ground state of the system, which is realistically unattainable in an experiment. This suggests no quantum phase transition at finite $T$. The impracticality of this situation is redeemable when studying the crossover between zero and non-zero temperatures. The singularity has influence on physical properties outside the strict critical parameter, manifested as the quantum critical region. As a consequence studies at finite temperatures are guided by this theoretical approach.
2.2 Critical entanglement properties

Entanglement occurs when two or more constituents in a system are generated such that their individual quantum states cannot be described independently. For example, a source of electron-positron pairs can be prepared with total spin zero. If one part is measured as spin-up the other has to be spin-down due to conservation of angular momentum. The wavefunction is said to collapse. Before measurement a quantum superposition of states exists and predicting the particular random outcome is impossible.

The correlation persists even after separation over large distances. The speed of light is the limiting factor for information travel but measurements affect all parts instantaneously. This demonstrates the non-local nature of entanglement and is the basis for the Einstein-Podolsky-Rosen experiment [36].

2.2.1 Entropy of entanglement

A bipartite pure state $|\psi\rangle_{AB}$ is made of the union of two systems $A$ and $B$ with Hilbert spaces $H_A$ and $H_B$ respectively. The full Hilbert space is the tensor product $H_A \otimes H_B$. The state is said to be entangled if and only if it is not separable i.e. $|\psi\rangle_{AB} \neq |i\rangle_A |j\rangle_B$, since separability implies knowing the definite quantum state of both parts. The inseparable state is entangled and the general form is

$$|\psi\rangle_{AB} = \sum_{i,j}^N c_{i,j} |i\rangle_A |j\rangle_B$$

(2.5)

where the two halves $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$ form orthonormal bases and $c_{i,j}$ are in general complex coefficients associated with each state in the linear combination and the summation is over the number of sites $N$.

The density matrix of the state is

$$\rho = |\psi\rangle_{ABAB} \langle \psi|$$

(2.6)

and the reduced density matrix for $A$ is found by taking the partial trace over
$B$

$$\rho_A = \text{Tr}_B(\rho)$$  \hspace{1cm} (2.7)

The entropy of entanglement, or von Neumann entropy, is

$$S_{EE} = -\text{Tr}(\rho_A \ln \rho_A)$$  \hspace{1cm} (2.8)

The state is maximally entangled when the reduced density matrix is a diagonal matrix with equal entries $S_{EE} = \ln(N)$. This relates to a state of maximum entropy, where in a two-qubit system there are four possibilities called Bell states.

### 2.2.2 Area laws and entanglement scaling

Entanglement is bounded in ground states of gapped systems with local interactions by area laws [37]. In non-critical conditions the area law for the entropy between a block of $L$ spins with the rest of a much larger (possibly infinite) chain $N$ is $S_L \sim L^{\text{dim}-1}$ [38]. Instead of following a volume law the power of the dimension is reduced by one. This is especially important in one dimension since the entropy $S_L \sim \text{const}$. The consequence of this limiting nature of entropy is that it allows states to be efficiently approximated by a Matrix Product State, discussed later. This is vital in the success of numerical methods for quantum many-body systems in one-dimension [1].

Entanglement at a critical point becomes more interesting. As $N \to \infty$ finite-size entanglement follows a scaling law dependent on $L$ as [39]

$$S_L = \frac{c}{6} \log(L) + k$$  \hspace{1cm} (2.9)

The constant $k$ is non-universal with no implications on the scaling theory. The central charge $c$ is known as the conformal anomaly from Conformal Field Theory. It describes the way a system with a particular central charge reacts to changes in macroscopic length scales, for example a finite length in some geometry of an infinite system. The values of the central charge can be non-integer and those less than one are quantised by the Virasoro algebra [40].
Relevant examples include the central charges of the TFIM where $c = 1/2$ and the critical XY model where $c = 1$. Scaling is determined by their universality classes as exact details about microscopic interactions are indistinguishable at critical points. The phase transitions are described by the more general conformal field theory and scaling behaviour of free conformal fermions and free conformal bosons corresponds directly with these two models [41]. The value of the central charge is therefore evidently important in determining the critical scaling behaviour of the entanglement entropy.
Chapter 3

Numerical technique

In quantum many-body physics, strongly correlated systems are generally very hard to study. For a chain of length $N$ and local state space dimension $d$, the system size grows as $d^N$. This exponential growth of the Hilbert space becomes numerically challenging to work with. The gradual addition of constituents shows explosive growth in the number of variables needed to describe a state. Even a seemingly small chain with a length of a few hundred particles requires impossible amounts of numerical resources to store and perform operations on. Simulation of such systems is therefore difficult on classical computers. Unfortunately, there are few exact analytical ways of finding solutions, for example via Bethe ansatz [42], so a brute force numerical solution is normally only possible. Despite difficulties from system scaling, numerical methods on manageable chain lengths have been developed to calculate eigenvalues and eigenvectors of Hamiltonians with finite Hilbert spaces. A direct numerical diagonalisation is impractical, instead iterative methods like Lanczos exact diagonalisation recursively calculate low energy states of small systems [43]. Another commonly used method is an integration scheme called Quantum Monte Carlo [44], although this technique suffers from the sign problem in frustrated or fermion problems. Both suffer from finite-sized effects, thus motivating the following sections describing an effectively infinite algorithm.
3.1 Density Matrix Renormalisation Group

In low-dimensional magnetic systems, Density Matrix Renormalisation Group (DMRG) [1] is an excellent numerical tool for calculating ground state properties of quantum systems. The performance of DMRG is limited in 2 or more dimensions, but for 1D and quasi-1D systems, such as spin ladders, simulation can be achieved provided there are relatively few rungs with weak inter-chain interactions. It is essentially a variational technique, where only a subspace of the systems full Hilbert space is considered relevant to the description of the state. The space is greatly reduced to dimensions of $\chi \ll d^N$.

To understand the technique an overview of the renormalisation procedure is presented. The initial state is constructed from a small chain (the smallest being just two sites) and a bipartition splits the chain into two blocks labelled $A$ (blue) and $B$ (red), Fig. 3.1. One takes the role of the environment and the other the system. The Hilbert spaces of these blocks have sizes $\chi^A$ and $\chi^B$ with states $\{|i\rangle_A\}$ and $\{|j\rangle_B\}$, respectively.

The chain is grown by addition of two sites in between the blocks denoted $\bullet\bullet$. The length of the chain is now $N(l) = 2l + 2$ with Hilbert space size $d^A \chi^A \chi^B$. The total structure of block-site-site-block, $A \bullet \bullet B$, is called the superblock. The next step absorbs a single spin into the blocks, $A \bullet \rightarrow A'$ and $\bullet B \rightarrow B'$. The wavefunction is represented by

$$|\psi\rangle = \sum_{a,\sigma_1,\sigma_2, b} c_{a,\sigma_1,\sigma_2, b} |a\rangle_A |\sigma_1\rangle_A |\sigma_2\rangle_B |b\rangle_B$$

The block-site-site-block structure can be seen in the mathematics, sites represented as $|\sigma_{1(2)}\rangle_{A(B)}$ and blocks as $|a\rangle_{A(B)}$, and the bipartition after absorption is presented as the equivalence on the right.

Numerical diagonalisation of the superblock Hamiltonian $\hat{H}_{A\bullet\bullet B}$ is performed, preferably by some sparse-matrix solver [45] as finding eigenpairs for large matrices is very time intensive. The corresponding eigenvectors determine the state $|\psi\rangle$ which minimises to the ground state energy found from the
CHAPTER 3. NUMERICAL TECHNIQUE

typical variational functional,
\[
E = \frac{\langle \psi | \hat{H}_{A \bullet B} | \psi \rangle - \langle \psi | \psi \rangle}{\langle \psi | \psi \rangle}.
\]  

(3.2)

Calculation of the reduced density matrices \( \hat{\rho}_A = \text{Tr}_{B} |\psi\rangle \langle \psi| \) and \( \hat{\rho}_B = \text{Tr}_{A} |\psi\rangle \langle \psi| \), represents the state of just the subsystems \( A' = A \bullet \) and \( B' = B \bullet \) respectively, as the other block is traced out. This is a key step in DMRG as the application of a truncation procedure can be applied to the reduced density matrices which reduces the Hilbert spaces of the new system blocks \( A' \) and \( B' \). Considering just the subsystem \( A' \), truncation works by selecting the \( \tilde{\chi}^A \leq \chi^A \) largest eigenvalues of the exact diagonalisation of \( \hat{\rho}_{A'} \) with corresponding eigenvectors \( |\tilde{a}\rangle_A \) and discarding the rest. If the total sum of discarded eigenvalues is small (e.g. \( 10^{-10} \)) the state remains a faithful representation to one with a complete set of eigenvectors.

Once the reduced density matrix has been truncated a transform matrix \( T_{A \rightarrow A'} \), with column vectors \( A \langle a\sigma_1 | \tilde{a} \rangle_A \) as elements, transforms the block Hamiltonian and local operators into the new reduced basis, for example the block Hamiltonian \( H^A \) transforms into \( H^{A'} = T_{A \rightarrow A'}^\dagger H^A T_{A \rightarrow A'} \). An identical process is performed on \( B' \).

The process is then repeated, enlarging the system by two-sites until the ground state properties converge at a desired chain length. The whole procedure is only possible if the reduced state dimension remains computationally manageable e.g. \( \chi \approx 100 \).

The differences between infinite and finite system algorithms is shown in Fig. 3.1. The infinite algorithm is traditionally used as a start-up procedure used to build the state to some predefined size \( N \), represented by the number of bold points inside the blocks in Fig. 3.1 (a). The decision to halt the growth of the chain and hold the system size constant leads to the application of finite DMRG. The renormalisation is applied as before, but now only on one block which grows at the expense of the other. Sites are exchanged between blocks until the edge site is reached upon which the sweep reverses, large opposing arrows in Fig. 3.1 (b). The process continue back and forth until convergence.
CHAPTER 3. NUMERICAL TECHNIQUE

The infinite chain is determined from a more complicated extrapolations. Finite size scaling is possible to find properties in the thermodynamic limit neglecting boundary effects. As it will be later revealed in the iTEBD algorithm, the two sites for large $N$ can be translationally invariant. The sites then represent a repeating two-unit cell containing all the information necessary for the infinite chain.

Figure 3.1: Redesigned from [1]. Left: Infinite DMRG. The system is split into blocks A (blue) and B (red). Two sites are added and the blocks renormalised into subsystems A and B (the superblock). The decision can be made to continue this process iteratively until a desired size is reached (1), an extrapolation technique may be used to form the chain for $N \to \infty$, or the finite algorithm commences (2). Right: From this point we can take the block to be a finite chain of length $N$. Instead of adding sites, the current ones are extracted from the blocks in pairs and refined in sweeps.

3.2 Matrix Product States

3.2.1 Schmidt decomposition

The most general bipartite pure state from (3.1) is written with two indices denoting all possible orthonormal parts in a superposition. A more convenient representation is the Schmidt decomposition. The singular value decomposition (SVD) is utilised. A type of matrix factorisation technique known from
linear algebra. Considering a general rectangular $N_A \times N_B$ matrix $M$, its SVD is $M = U\lambda V^\dagger$, where $U$ is a matrix with orthonormal column vectors, $V^\dagger$ has orthonormal row vectors and $\lambda$ is a diagonal matrix containing positive singular values. $U$ and $V^\dagger$ have dimensions $N_A \times \min\{N_A, N_B\}$ and $\min\{N_A, N_B\} \times N_B$. Using this tool a new bipartite state can be derived, essentially removing an index from (3.1) forming a more compact representation (3.4). The coefficients $c_{ij}$ are manipulated as matrix $c$ which the SVD can be applied resulting in

$$|\psi\rangle = \sum_{a=1}^{\min\{N_A, N_B\}} \left( \sum_i U_{i,a} |i\rangle_A \right) \lambda_a \left( \sum_j V_{j,a} |j\rangle_B \right)$$

(3.3)

since $U$ and $V^\dagger$ are orthonormal and from the previous assumption of the bases also being orthonormal the new bipartite bases $\{|\Phi_a\rangle\}$ also share this property. The state is now

$$|\Psi\rangle = \sum_a \lambda_a |\Phi_a\rangle_A |\Phi_a\rangle_B$$

(3.4)

the Schmidt decomposition. The Schmidt rank is the number of non-zero values $\lambda_a$, bounded by $\chi \leq \min\{N_A, N_B\}$. When $\chi = 1$ the state is unentangled i.e. a product state, and for $\chi > 1$ the state is entangled. This is the defining nature of separability in the system. At the two extremes of completely separable to maximally entangled. A partially separable state will have some middle ground between the two, limiting entanglement to a maximum of $m$-separable subsystems.

The reduction to only one index is advantageous in describing the state. The Schmidt coefficients $\lambda$ are extremely useful as the reduced density matrix has the eigenvalues $\lambda^2$. The reduced density matrices are now stated as

$$\rho_A = \sum_{a=1}^\chi \lambda_a^2 |\Phi_a\rangle_A \langle \Phi_a|_A \quad \rho_B = \sum_{a=1}^\chi \lambda_a^2 |\Phi_a\rangle_B \langle \Phi_a|_B.$$ 

(3.5)

Evidently the eigenvalues are shared between both halves of the bipartition A and B, with eigenvectors being the left and right singular vectors after performing the SVD, which can be substituted into (2.8) to find the entanglement.
CHAPTER 3. NUMERICAL TECHNIQUE

entropy. These eigenvalues redefine the von Neumann entropy (2.8) as

\[ S_{EE} = -\sum_a \lambda_a^2 \ln \lambda_a^2. \]  

(3.6)

3.2.2 Decomposition into a Matrix Product State

Consider a chain with \( N \) sites in the \( d \)-state local basis \( |\sigma_i\rangle \in \{ |0\rangle, |1\rangle, \cdots, |d\rangle \} \)

\[ |\Psi\rangle = \sum_{\sigma_1,\ldots,\sigma_N} c_{\sigma_1,\ldots,\sigma_N} |\sigma_1\rangle \otimes \cdots \otimes |\sigma_N\rangle. \]  

(3.7)

The number of coefficients \( d^N \) becomes unmanageable even for modest sized systems. Fortunately a more efficient representation exists. The vector \( c_{\sigma_1,\ldots,\sigma_N} \) is reshaped into the matrix \( \Psi \) upon which the SVD can be performed. Starting from the left the decomposition returns the three matrices as

\[
c_{\sigma_1,\ldots,\sigma_N} = \Psi_{\sigma_1,\ldots,\sigma_N}
\]

\[
= \sum_{a_1} U_{\sigma_1,a_1} \lambda_{a_1,a_1}^{(1)} (V^\dagger)_{a_1,\sigma_2,\ldots,\sigma_N}
\]

(3.8)

\[
= \sum_{a_1} A_{a_1,\sigma_2,\sigma_3,\ldots,\sigma_N}^{\sigma_1}
\]

(3.9)

\[
= \sum_{a_1} A_{a_1,\sigma_2,\ldots,\sigma_N}^{\sigma_1} \Psi_{a_1,\sigma_2,\ldots,\sigma_N}
\]

(3.10)

The left-most matrix \( U \) is reformulated into \( A_{a_1}^{\sigma_1} \), which denotes \( \chi_1 \) row vectors. A matrix multiplication of \( \lambda \) and \( V^\dagger \) returns \( c_{a_1,\sigma_2,\ldots,\sigma_N} \). This can be reshaped into a new \( \Psi_{a_1,\sigma_2,\ldots,\sigma_N} \) matrix and the SVD procedure applied recursively.

The second application of the SVD is slightly different. The resultant \( A \) matrix is now a set of matrices instead of vectors. The process is started from
As (3.10) follows

\[ C_{\sigma_1...\sigma_N} = \sum_{a_1} A_{a_1}^{\sigma_1} \Psi(a_1\sigma_2),(...\sigma_N) \] (3.11)

\[ = \sum_{a_1} A_{a_1}^{\sigma_1} \sum_{a_2} U(a_1\sigma_1,a_2) \left( \lambda_{a_2}^{[2]} (V^\dagger)_{a_2}(\sigma_3...\sigma_N) \right) \] (3.12)

\[ = \sum_{a_1,a_2} A_{a_1}^{\sigma_1} A_{a_1,a_2}^{\sigma_2} \Psi(a_2\sigma_3),(...\sigma_N) \] (3.13)

This time \( U \) retains two indices \( a_1 \) and \( a_2 \). The rest of the information is reformed into \( \Psi \) and the process applied recursively stopping at site \( n \)

\[ C_{\sigma_1...\sigma_N} = \sum_{a_1...a_n} A_{a_1}^{\sigma_1} A_{a_1,a_2}^{\sigma_2} \ldots A_{a_{n-1},a_n}^{\sigma_n} \lambda_{a_n,a_n}^{[n]} \left( (V^\dagger)_{a_n,\lambda_{n+1...\sigma_N}} \right) \] (3.14)

The set of \( A \)-matrices are subject to the left-normalisation condition, \( \sum_{\sigma_i} (A^{\sigma_i})^\dagger A^{\sigma_i} = I \). The remainder \( V^\dagger \) is acted on from the right

\[ (V^\dagger)_{a_n,\lambda_{n+1...\sigma_N}} = \Psi(a_n\sigma_{n+1...\sigma_N-1},\sigma_N) \] (3.15)

\[ = \sum_{a_{N-1}} U(a_n\sigma_{n+1...\sigma_N-1},a_{N-1}) \lambda_{a_{N-1},a_{N-1}}^{[N-1]} B_{a_{N-1}}^{\sigma_N} \] (3.16)

\[ = \sum_{a_{N-1}} \Psi(a_n\sigma_{n+1...\sigma_N-1},\sigma_{N-1}) B_{a_{N-1}}^{\sigma_N} \] (3.17)

\[ = \sum_{a_{N-2},a_{N-1}} U(a_n\sigma_{n+1...\sigma_N-2},a_{N-2}) \lambda_{a_{N-2},a_{N-2}}^{[N-2]} B_{a_{N-2},a_{N-1}}^{\sigma_{N-1}} B_{a_{N-1}}^{\sigma_N} \] (3.18)

\[ = \sum_{a_{N-2},a_{N-1}} \Psi(a_n\sigma_{n+1...\sigma_N-2},\sigma_{N-2}) B_{a_{N-2},a_{N-1}}^{\sigma_{N-1}} B_{a_{N-1}}^{\sigma_N} \] (3.19)

\[ = \sum_{a_{n+1},a_{N-1}} U(a_n\sigma_{n+1},a_{n+1}) \lambda_{a_{n+1},a_{n+1}}^{[n+1]} B_{a_{n+1},a_{n+2},...a_{N-1}}^{\sigma_{n+1}} B_{a_{N-2},a_{N-1}}^{\sigma_{N-1}} B_{a_{N-1}}^{\sigma_N} \] (3.20)

This successively generates a set of right-normalised matrices \( B_{a_{n+1},a_{n+2},...a_{N-1}}^{\sigma_{n+1}} \), with the condition \( \sum_{\sigma_i} (B^{\sigma_i})^\dagger = I \), until the two halves of the chain are accounted for having separate normalisation conditions. In MPS language the coefficients
are joined as
\[ c_{\sigma_1...\sigma_N} = \sum_{a_1...a_{N-1}} A_{a_1}^{\sigma_1} A_{a_1 a_2}^{\sigma_2} ... A_{a_{n-1} a_n}^{\sigma_n} \lambda_{a_n a_n}^{[n]} B_{a_n a_{n+1}}^{\sigma_{n+1}} B_{a_{n+1} a_{n+2}}^{\sigma_{n+2}} ... B_{a_{N-2} a_{N-1}}^{\sigma_{N-1}} B_{a_{N-1}}^{\sigma_N} \]  
(3.21)

The summations above are identical to matrix multiplications
\[ c_{\sigma_1...\sigma_N} = A_{\sigma_1}^{\sigma_2} ... A_{\sigma_{n-1}}^{\sigma_n} \lambda_{a_n}^{[n]} B_{\sigma_{n+1}}^{\sigma_{n+2}} ... B_{\sigma_N}^{\sigma_{N-1}} \]  
(3.22)

The two blocks, left (A matrices) and right (B matrices), and their respective normalisation conditions, conveniently allows for the Schmidt decomposition to be recovered at any bond \( n \)

\[ \langle \Psi | = \sum_{a_n} \left[ \left( \sum_{\sigma_1...\sigma_n} \left( A_{\sigma_1}^{\sigma_2} ... A_{\sigma_n}^{\sigma_n} \right)_{a_n} | \sigma_1; ..., \sigma_n \rangle \right) \times \lambda_{a_n}^{[n]} \left( \sum_{\sigma_{n+1}...\sigma_N} \left( B_{\sigma_{n+1}}^{\sigma_{n+2}} ... B_{\sigma_N}^{\sigma_N} \right)_{a_n} | \sigma_{n+1}; ..., \sigma_N \rangle \right) \right] \]  
(3.23)

\[ = \sum_{a_n} \lambda_{a_n}^{[n]} \langle \Phi_{a_n}^{1[...n]} | A | \Phi_{a_n}^{n+1[...N]} \rangle_B \]  
(3.24)

In the infinite case, as is vital for understanding in the next section, a spin-1/2 chain with identical Schmidt rank on all bond indices \( \chi_1 = \chi_2 = ... = \chi_N = \chi \) takes the form

\[ \langle \Psi | = \sum_{a=1}^{\chi} \lambda_{a}^{[n]} \langle \Phi_{a}^{[-\infty...n]} | A | \Phi_{a}^{n+1[...\infty]} \rangle_B \]  
(3.25)

### 3.3 Infinite Time Evolving Block Decimation

#### 3.3.1 Vidal’s decomposition

G. Vidal [46] proposed a new form of MPS where information about the local nature of sites and bonds is retained. Instead of absorbing \( \lambda \) into the A and B matrices, their coefficients are reformed into tensors

\[ c_{i_1...i_N} = \sum_{a_1,...,a_{N-1}} \Gamma_{a_1}^{[1]} \lambda_{a_1}^{[1]} \Gamma_{a_1 a_2}^{[2]} \lambda_{a_2}^{[2]} \Gamma_{a_2 a_3}^{[3]} ... \Gamma_{a_{n-1} a_n}^{[n]} \lambda_{a_n}^{[n]} \Gamma_{a_{n-1} a_{n+1}}^{[n+1]} ... \Gamma_{a_{N-2} a_{N-1}}^{[N-1]} \lambda_{a_{N-1} a_N}^{[N]} \]  
(3.26)
For each site \( n \) there is an assigned tensor with three indices \( a_n, a_{n+1} \) (omitting one index at the edges) and \( i_n \). The bond index \( a_n \) runs from 1 to \( \chi_n \) and \( i_n \) has \( d_n \) states depending on the local basis. The vectors have one index \( a_n \) and contain the information of splitting at \( n : n + 1 \). The \( d^N \) coefficients have been reduced to \( N - 1 \) vectors \( \lambda^{[n]} \) and \( N \) tensors \( \Gamma^{[n]} \). The total number of parameters is now \( (N - 1)\chi \) from the vectors and \( d [N\chi^2 - 2(\chi^2 - \chi)] \) from the tensors (the end sites are vectors and have one less index reducing the number of entries in the tensor).

### 3.3.2 Graphical representation

The mathematical notation of an MPS can be transferred into a graphical representation, shown in Fig.3.2. The state is built from two building blocks. Circles represent \( \Gamma \) tensors and diamonds \( \lambda \) tensors. The number of legs extending from these two elements carry the tensor indices. Matching leg index permits the interconnection of elements. Enclosed legs depict the summation, or matrix multiplication, of that index. This is useful in rapidly identifying correct summation conventions whilst performing index contractions, moving away from obscure mathematics and into something more intuitive.

![Diagram](image.png)

Figure 3.2: (a) Tensors \( \Gamma \) are represented by a circle with three legs for each index with conjugate inversed. (b) Bonds \( \lambda \) have one index joining the chain together. (c) Two-site MPS formed from the combination of (a) and (b) parts.
3.3.3 Time evolution and the Suzuki-Trotter expansion

Time evolution of the quantum state is performed in imaginary time from an initial state, \(|\Psi_0\rangle\), to another at later time \(|\Psi_\tau\rangle\), by application of the time evolution operator, \(\hat{U}_\tau\), containing a nearest-neighbour Hamiltonian \(H_{i,i+1}\),

\[
|\Psi_\tau\rangle = \hat{U}_\tau |\Psi_0\rangle = \exp(-\tau \hat{H}) |\Psi_0\rangle = \exp\left(-\sum_{i=1}^{N-1} \tau H_{i,i+1}\right) |\Psi_0\rangle \tag{3.27}
\]

The ground state, \(|\Psi_{gr}\rangle\), is reached after ‘long’ times \([47]\]

\[
|\Psi_{gr}\rangle = \lim_{\tau \to \infty} \exp(-\tau \hat{H}) |\Psi_0\rangle \tag{3.28}
\]

which is easily seen by expanding the wavefunction into a superposition of orthonormal eigenstates

\[
|\Psi_\tau\rangle = \sum_m c_m(\tau) \exp\left(-E_m \tau\right) |\phi_m\rangle \tag{3.29}
\]

where the energy operator \(\hat{H}\) is Hermitian acting on the basis states with real eigenvalues \(E_0 \leq E_1 \leq \ldots \leq E_m\) ordered from lowest to highest energy. Projecting onto the eigenstate \(|\phi_m\rangle\), the leading coefficient is

\[
\langle \phi_m | \Psi_\tau \rangle = \sum_m c_m'(0) \exp\left(-E_m \tau\right) \langle \phi_m | \phi_m' \rangle
\]

\[
= c_m'(0) \exp\left(-E_m \tau\right) \tag{3.30}
\]

and the lowest eigenstate coefficient

\[
\langle \phi_0 | \Psi_\tau \rangle = \sum_m c_m(0) \exp\left(-E_m \tau\right) \langle \phi_0 | \phi_m \rangle
\]

\[
= c_0(0) \exp\left(-E_0 \tau\right) \tag{3.31}
\]

The decay of the eigenstates with eigenvalues greater than the ground state is understood from the ratio of the two

\[
\frac{\langle \phi_m | \Psi_\tau \rangle}{\langle \phi_0 | \Psi_\tau \rangle} = \frac{c_m(0)}{c_0(0)} \exp\left(-(E_m - E_0) \tau\right) \tag{3.32}
\]
and an energy gap $E_0 < E_1$ has coefficients decaying quicker for larger separation. As the chain becomes more critical, the gap closes and considerably more time is required to converge to the ground state. The near critical properties can be still be studied to locate the critical point as the situation is improved with large $\chi$. In any case the ground state is asymptotically approached as $\tau \to \infty$.

In general, the terms in $\hat{H}$ do not commute. This causes trouble when decomposing the exponential sum into a product of exponentials, $\exp(A + B + C...) \neq \exp(A) \exp(B) \exp(C)...$ The decomposition is an essential part of the update. It allows for individual nearest-neighbour updates. The Hamiltonian is separated into $F$ and $G$

$$\hat{H} = \sum_{\text{even } i} F_{i,i+1} + \sum_{\text{odd } i} G_{i,i+1}$$  \hspace{1cm} (3.33)

where $F$ and $G$ are the local Hamiltonians on even and odd bonds respectively and $[F, G] \neq 0, [F', F''] = 0, [G', G''] = 0$.

$$F \equiv \sum_{\text{even } i} F_{i,i+1}$$  \hspace{1cm} (3.34)

$$G \equiv \sum_{\text{odd } i} G_{i,i+1}$$  \hspace{1cm} (3.35)

The time evolution operator is approximated by the Suzuki-Trotter expansion (for small positive $\delta$) of order $p$ [48]

$$e^{-(F+G)\tau} = [e^{-i(F+G)\delta}]^{\tau/\delta} \approx \left[f_p(U_{F\delta}, U_{G\delta})\right]^{\tau/\delta}$$  \hspace{1cm} (3.36)

with commuting products of odd and even operators

$$U_{F\delta} \equiv e^{-iF\delta} = \prod_{\text{even } i} e^{-F_{i,i+1}\delta}$$  \hspace{1cm} (3.37)

$$U_{G\delta} \equiv e^{-iG\delta} = \prod_{\text{odd } i} e^{-G_{i,i+1}\delta}$$  \hspace{1cm} (3.38)

to the first order ($p = 1$), the function $f_1(x, y) = xy$ is the expansion

$$f_1(U_{F\delta}, U_{G\delta}) = U_{F\delta}U_{G\delta} + O(\delta^2)$$  \hspace{1cm} (3.39)
CHAPTER 3. NUMERICAL TECHNIQUE

The application of $f_1$ to the chain is shown in Fig.3.3. The product of all operators in $U_F$ are applied in parallel (green) since they independently commute updating half the chain, followed by all operators in $U_G$ (red). The translational invariance is broken as odd and even parts of the decomposition are updated separately, enforcing two-site invariance on the state. The correction term is negligible as $\delta \to 0$.

![Figure 3.3: Non-commuting parts of a general Hamiltonian applied to an MPS in Vidal form.](image)

Taking $N \to \infty$ moves the free ends of the chain infinitely far from the bulk, eliminating boundary effects. This is advantageous because normally a total update on all sites in the chain would require a computational time of $O(N d\chi^3)$. But the tensors describing the state are reduced to repeating blocks of two sites $\Gamma^{[1]}$, $\Gamma^{[2]}$ and their bonds $\lambda^{[1]}$, $\lambda^{[2]}$.

It is important to note that even though the operators are Hermitian they are not necessarily unitary. Non-unitary gates affect the reliability of the Schmidt decomposition. However for $\delta \ll 1$ this problem is overcome since the operators are close to identity and approximate to unitary operators [49].

3.3.4 One- and Two-site updates

The technical details of applying the update in Fig.3.3 are presented here. This section deals with two types of update, those on one-site and those over two. Operators of this form used in the construction of nearest-neighbour Hamiltonians.
Figure 3.4: Update procedure of an MPS in iTEBD with unitary two-site operator.

The first process involves applying a one-site update. This is relatively straightforward. The matrix element $U_{i_1}^{i_1'}$ has two indices the same size as the local state space $d$. For example, the operator could be one of the Pauli matrices and its corresponding matrix elements. As it only acts on a single site just one tensor $\Gamma$ is involved in the update. The summation over the index gives

$$
\tilde{\Gamma}_{a_1,a_2}^{i_1} = \sum_{i_1'} U_{i_1}^{i_1'} \Gamma_{a_1,a_2}^{i_1'}.
$$

The second update is over two-sites. Using the infinite-MPS (3.25) and the decomposition (3.26), two neighbouring sites are extracted in the local basis with the remainder of the chain, $|\Phi_{a_1}^{[-\infty,0]}\rangle$ infinitely to the left and $|\Phi_{a_3}^{[3,\infty]}\rangle$ infinitely to the right,

$$
|\Psi\rangle = \sum_{a_1,a_2,a_3} \sum_{i_1,i_2} \lambda_{a_1}^{[1]} \Gamma_{a_1,a_2}^{[1]} \lambda_{a_2}^{[2]} \Gamma_{a_2,a_3}^{[2]} \lambda_{a_3}^{[3]} |\Phi_{a_1}^{[-\infty,0]}\rangle_{i_1} |i_2\rangle |\Phi_{a_3}^{[3,\infty]}\rangle.
$$

(3.41)
The inclusion of two-site translational invariance forms infinitely many repeating blocks $\Theta$. This is the contraction of two neighbouring tensors (3.41), noting that $\lambda_{a_3}^{[3]} = \lambda_{a_3}^{[1]}$,

$$|\Psi\rangle = \sum_{a_1,a_2,a_3} \sum_{i_1,i_2} \lambda_{a_1}^{[1]} \Gamma_{a_1,a_2}^{[1]} \lambda_{a_2}^{[2]} \Gamma_{a_2,a_3}^{[2]} \lambda_{a_3}^{[1]} |\Phi_{a_1}^{[-\infty\ldots0]}\rangle |i_1\rangle |i_2\rangle |\Phi_{a_3}^{[3\ldots\infty]}\rangle$$  (3.42)

$$= \sum_{a_1,a_3} \sum_{i_1,i_2} \Theta_{a_1,a_3}^{[1]} |\Phi_{a_1}^{[-\infty\ldots0]}\rangle |i_1\rangle |i_2\rangle |\Phi_{a_3}^{[3\ldots\infty]}\rangle$$  (3.43)

Application of the two-site operator $U_{i_1,i_2}^{r_1,r_2}$ is similar as seen previously, but now two indices are summed:

$$\tilde{\Theta}_{a_1,a_3}^{i_1,i_2} = \sum_{i_1',i_2'} U^{r_1,r_2}_{i_1,i_2} \Theta_{a_1,a_3}^{i_1',i_2'}$$  (3.44)

The graphical representation elucidates the two-site update, shown in Fig.3.4. A summary of the procedure is given (i) construct the state and operator, (ii) contract all legs of the state into $\Theta$, (iii) apply the update $U$, (iv) recover the tensors with an SVD and (v) reintroduce the bonds at the ends, finally (v) shape $X$ and $Z$ into transformed $\Gamma$ tensors. Importantly, only the $\Gamma^{[1]}$, $\Gamma^{[2]}$ and the bond $\lambda^{[2]}$ are modified ignoring the remaining left and right parts. The other bond $\lambda^{[1]}$ is modified repeating this process with an exchange of $\Gamma^{[1]}$ and $\Gamma^{[2]}$.

Computational cost of the update only grows as $O(d\chi^3)$. This is an excellent outcome since measurements can be made between any two-sites on the chain independent of the system size [46].

### 3.3.5 Physical Operators in Infinite Time Evolving Block Decimation

#### 3.3.5.1 Site operators

To perform a physical measurement an operator acting on a single site is a $d \times d$ matrix. This has the expectation value, Fig.3.5 (a)

$$\langle \Psi | U^{[1]} | \Psi \rangle = \sum_{i_1,a_1,a_2} (\lambda_{a_1}^{i_1} \Gamma_{a_1,a_2}^{i_1})^* \lambda_{a_2}^{i_2} \sum_{i_1'} U^{(1)}_{i_1,i_1'} \Gamma_{a_1,a_2}^{i_1'}$$  (3.45)
The mean of (3.44) for all sites with $U^r \in \{\sigma_r^x, \sigma_r^y, \sigma_r^z\}$ one of the Pauli matrices is the calculated magnetisation in each respective direction.

### 3.3.5.2 Bond operators

In the local tensor product space $|i_1\rangle|i_2\rangle$, the operator $U_{i_1,i_2}^{i_1',i_2'}$ is a reshaping of the matrix acting on the two-spin basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$. The expectation value is, Fig. 3.5 (b)

$$\langle \Psi | U_{1,2} | \Psi \rangle = \sum_{i_1,i_2,a_1,a_3} (\Theta_{a_1,a_3}^{i_1,i_2})^* \sum_{i_1',i_2'} U_{i_1,i_2}^{i_1',i_2'} \Theta_{a_1,a_3}^{i_1',i_2'} \tag{3.46}$$

For example, energy is measured by application of the Hamiltonian. The matrix form of the Ising model is a Kronecker product of two Pauli matrices, $J \sigma_z \otimes \sigma_z$

$$\begin{pmatrix} J/4 & 0 & 0 & 0 \\ 0 & -J/4 & 0 & 0 \\ 0 & 0 & -J/4 & 0 \\ 0 & 0 & 0 & J/4 \end{pmatrix} \tag{3.47}$$

Figure 3.5: Expectation values $\langle \Psi | U | \Psi \rangle$ of (a) site operators and (b) bond operators of an MPS at site $r$.

### 3.3.5.3 Time-evolution operator

The propagation of time requires exponentiation of the Hamiltonian. If a matrix is diagonalisable, $A = VDV^\dagger$ ($D$ a diagonal matrix of eigenvalues, $V$
CHAPTER 3. NUMERICAL TECHNIQUE

being formed of the eigenvectors of $A$ in rows, and $V^\dagger$, the conjugate transpose column form), it is simple to exponentiate. By performing the transformation and taking the exponential of all entries in $D$, the time evolution operator is represented as

$$e^A = V \begin{pmatrix} e^{-w_1\delta} & 0 \\ e^{-w_2\delta} & e^{-w_3\delta} \\ & \ddots \\ 0 & \cdots & e^{-w_n\delta} \end{pmatrix} V^T$$ (3.48)

Reshaping into $U_{i_1,i_2}^{r_1,r_2}$, the summation procedure updates the state as per Fig.3.4.

3.3.5.4 Correlation function

Correlation between sites 1 and $r$ takes advantage of translational invariance. As the full description of the state is only stored in the two-site invariant tensors the chain is built iteratively from these. Firstly, the self-correlation (normalised) is calculated $\langle O_1 \cdot O_r = 1 \rangle$ using (3.44). Next, units of the grey cell in Fig.3.6 build the state from the previously stored odd and even tensors by inserting them with correct parity. Omitting the grey cell is similar to a double version of (3.44) and calculates the nearest-neighbour correlation. The equation (3.48) for calculating the correlation over any distance $r$ is represented in Fig.3.6.

$$\langle U_1 U_r \rangle = \sum_{i_1 \cdots i_r} \sum_{a_1 \cdots a_r} \sum_{a'_1 \cdots a'_r} \lambda_{a_1}^2 \left( \Gamma^{[1]}_{a_1,a'_2} \right)^* \left( \sum_{i'_1} \Gamma^{[1]}_{a'_1,i'_1} \Gamma^{[1]}_{a_1,a'_2} \right) \times \left( \prod_{j=2}^{r-1} \left( \lambda_{a_j} \Gamma_{a_j,a_{j+1}}^{i_j} \right)^* \lambda_{a_j} \Gamma_{a_j,a_{j+1}}^{i_j} \right) \times \left( \Gamma^{[r]}_{a_r,a'_1} \right)^* \left( \sum_{i'_r} \Gamma^{[r]}_{a_r,i'_r} \Gamma^{[r]}_{a_r,a'_1} \right) \lambda_{a_1}^2$$ (3.49)
Sections of (3.49) are conveniently identified as the Quantum Transfer Matrix (shaded cell in Fig. 3.6) useful in the calculation of the correlation length as follows

\[ T_{a_j a'_{j+1}} = \sum_{i_j} (\lambda^{ij}_{a_j a'_{j+1}})^* \lambda^{ij}_{a_j a'_{j+1}} \]  

(3.50)

Figure 3.6: MPS with one-site operators \( O_1 \) at site 1 and \( O_r \) at site \( r \). The quantum transfer matrix (shaded) inserted \( r - 1 \) times is used to build the central part of the chain. This generates distance between correlations.

3.4 Finite entanglement scaling

As the state in iTEBD is infinite the length \( L \) is no longer a limiting factor. The finite size scaling is transformed into a finite entanglement scaling by the new resource \( \chi \) which now limits the representation of the state. The universal formula for the entanglement entropy is transformed into [50]

\[ S \sim \frac{c}{6} \log \left( \frac{\xi}{a} \right) \]  

(3.51)

and depends on the correlation length \( \xi \) calculated from the dominant eigenvalues of the quantum transfer matrix (3.49)

\[ \xi = 1/\ln(\lambda_1/|\lambda_2|) = -1/ \ln |\lambda_2| \]  

(3.52)
As the MPS has been built in canonical form with orthonormal left and right
eigenvectors, the first eigenvalue in the transfer matrix is 1 leaving importance
on the second eigenvalue. The correlation length scales inversely with energy
gap until it diverges at the critical point when the gap vanishes. The constant
a is not important as the gradient of the equation is the only value of concern
used to find the central charge.

The entanglement entropy is calculated from the Schmidt decompositions
singular values using the von Neumann entropy (3.6)

\[ S = -\sum_{a_n} (\lambda_{a_n}^{[0]})^2 \ln (\lambda_{a_n}^{[0]})^2 = -\sum_{a_n} (\lambda_{a_n}^{[1]})^2 \ln (\lambda_{a_n}^{[1]})^2 \]  

(3.53)

The values are identical for either half of the chain (odd or even bond) and
the bipartite splitting of the MPS has entropy that is maximally entangled
at \( \log \chi \). This is clearly at odds with the diverging nature of the correlation
length in (3.50).

The critical properties of the system can be revealed with finite entangle-
ment scaling. In a critical chain the scaling equation

\[ \xi \propto \chi^\kappa \]  

(3.54)

holds, with \( \chi \) the number of states kept and \( \kappa \) a constant dependent only on
the central charge of the model [50]. This relation matters when considering
the diverging nature of \( \xi \). A perfect representation of the state at a critical
point requires \( \chi \) to also diverge to infinity. Limits from the finite nature of \( \chi \)
lead to an effective finite correlation length \( \xi_\chi \) at the critical point. The phase
transition is seen at the peak in a curve as the control parameter \( g \) passes
through the critical point. Depending on the number of states retained the
peak can be broad for low values of \( \chi \) and give an inaccurate representation of
the exact critical point. For larger values of \( \chi \) the peak becomes sharper and
more reliable. This will be seen later in Fig.4.5. The near critical properties
are seen as a mixture with competition between saturation and scaling.
4.1 Background

4.1.1 Origins in ferroelectricity

The Transverse Field Ising model was originally introduced in its recognisable form using a pseudo-spin formulation. It was used by [51] to describe the collective motion of protons in the ferroelectric KH$_2$PO$_4$, then extended by [52] as a possible microscopic theory of ferroelectricity. DeGennes stated the model as

$$\begin{align*}
H &= -\sum_{i=1}^{N} J_{ij} S_i^z S_j^z + 2\Omega_T \sum_{i=1}^{N} S_i^x.
\end{align*}$$

(4.1)

$S_i^z, S_i^x$ operators measure the $z$ and $x$ component of spin at site $i$, $\Omega_T$ is the tunnelling integral and fights for collective motion and $J_{ij}$ is a constant interaction strength between sites $i$ and $j$ working to isolate protons.

Using a classical spin approximation the ground state is solved exactly. Interestingly, $\Omega_T < J/2$ presents a partially polarised state and $\Omega_T > J/2$ is completely unpolarised. This is an important result and will look remarkably familiar later when considering the ferromagnetic model where the notation changes from $\Omega_T$ to $h$ which denotes the magnetic field strength.
4.1.2 Adoption in ferromagnetism

In ferromagnetism, the pseudo-spin representation (4.1) is reformulated into a
spin-1/2 chain of particles with nearest neighbour interactions. The spins are
now described as quantum mechanical entities. This is the natural extension to
the famous Ising model and can be introduced down this route by considering
Heisenberg and Ising’s work in the 1920’s and simply applying a magnetic field
transversely. Comparing to (4.1), the form of the equation has two analogous
parts

\[ H = -\sum_{i=1}^{N} J_{ij} S^x_i S^x_j - h \sum_{i=1}^{N} S^z_i \]  

(4.2)

where a canonical transformation has been imposed, \( S^x \rightarrow S^z, S^z \rightarrow -S^x \) [53]
for ease of diagonalisation later. The ordering term is analogous to the collec-
tive motion of hydrogen bonds previously mentioned restricted to two vibra-
tional states assigned spin-up and -down. In quantum mechanics the wave-
function describing fermions is antisymmetric with respect to spatial and spin
exchange. The nature of exchange symmetry determines the exchange integral
which includes all inter-particle repulsions and attractions between electrons
and protons. This in turn determines the strength and sign of \( J_{ij} \). Simplifying
for two nearest-neighbour spins the ordering strength is short ranged aligning
parallel \( J > 0 \) and anti-parallel \( J < 0 \). The transverse field strength param-
eter \( h \) acts to cause disorder by flipping spins. This model, though simple, has
a vast range of applications. A good review of successes applied to various
materials can be found in [54].

4.2 Numerical benchmark

4.2.1 Exact Diagonalisation

The exact diagonalisation for the eigenvalue spectrum is performed in section
(4.3.3) in the thermodynamic limit with periodic boundary conditions. To
save repetition the full calculation is left until later following a nearly identical
diagonalisation process with a slight addition to the characteristic form. In its
diagonal form the Hamiltonian (4.2) becomes

$$H = \sum_k \epsilon_k (\gamma_k^\dagger \gamma_k - 1/2)$$ (4.3)

$$|\epsilon_k| = \sqrt{J^2 + h^2 + 2Jh \cos k}$$ (4.4)

with Bogoliubov fermion operators $\gamma$. The ground state energy is

$$E_0 = -\frac{1}{2} \sum_k |\epsilon_k|$$ (4.5)

and solving in the thermodynamic limit

$$E_0 = -\frac{1}{\pi} \int_0^\pi |\epsilon_k| \, dk$$ (4.6)

We calculate also the ground state energy numerically by applying as a bond
operator the Hamiltonian and extract the result. There are no finite-size effects
as the MPS representation is infinite and the algorithm minimises to the ground
state for each magnetic field point. At the critical point the simulation is
slower taking more steps increasing the error generated by the Suzuki-Trotter
expansion. Despite this the energy still minimizes in an efficient time scale.

The exact energy result $E_0$ from Eq.(4.6) is compared to the numerical re-
sult $E_{num}$, Fig. 4.1. The relative error, $|E_0 - E_{num}|/E_0$, between the two mea-
surements demonstrates the accuracy of iTEBD. This is a preliminary result to
determine the success of the method as a benchmark for further computations.
The worst performance occurs under critical conditions at $h/J = 1.0$. There
is a distinct peak as the error sharply increases. The entanglement spectrum
reveals the limitation at the critical point as seen later in, Fig. 4.4. The spec-
trum decays slower and more states need to be incorporated in the simulation.
Even so the energy is minimises to an acceptable order of $10^{-7}$.
Figure 4.1: (a) Exact ground state energy for TFIM compared to numerical iTEBD. (b) Relative error: $|E_0 - E_{\text{num}}|/E_0$. 
4.2.2 Order parameter

Identification and computation of the order parameter which accounts for broken rotational symmetry, is very essential. The collective order of spins in the system determines the ferromagnetic or paramagnetic nature of the model. If the local magnetic moment for all sites is measured in direction $a$, their thermodynamic average is the magnetization $M_a = \langle s_i^a \rangle$ of the system. In the TFIM there is the region of finite magnetisation (ordered) and the one with zero magnetization (disordered region). In particular $M_z$ is the choice of order parameter because in the paramagnetic region it is zero, and as the rotational symmetry is broken, it becomes finite in the ferromagnetic region.

For $h < 1$ the analytical behaviour [53] of $M_z$ is

$$M_z = \frac{1}{2} \left(1 - (2h/J)^2\right)^{1/8} \quad (4.7)$$

otherwise $M_z = 0$, and $M_x$ takes the form of two elliptic integrals

$$M_x = \frac{1}{\pi} \left[ \int_0^\pi dk \, \epsilon_k^{-1} + \frac{J}{2h} \int_0^\pi dk \, \epsilon_k^{-1} \cos k \right] \quad (4.8)$$

Fig.4.2 shows a plot of the results gathered using iTEBD compared to the exact result for the magnetizations $M_z$ in (a) and $M_x$ in (b). The numerical results faithfully match the calculated lines (4.7) and (4.8). The phase transition is clearly present in (a) as the spontaneous magnetization of $M_z$ is reduced with increasing magnetic field strength. The suitability of selection of $M_z$ as an order parameter is evident in the figure. Its holds a zero value at and beyond the critical value of $h/J = 1.0$. Both results for $M_z$ and $M_x$ saturate to 1.0 at $h = 0$ and $h \to \infty$ respectively.
4.2.3 Spin-spin correlation function

To understand the effect of spin interactions on sites beyond nearest-neighbours, we need to compute the spin-spin correlations. We choose a particular site and measure the product of the value of the spin at that site with the spin at a certain distance along the chain, we average over the initial choice for the same distance. In more detail, the form of the correlation function is

\[ \rho_{ab}(R) = \langle 0 | S_i^a S_j^b | 0 \rangle \quad a, b \in x, y, z. \quad (4.9) \]

The separation between spins is given by the difference in site indices \( R = |i - j| \). The first point \( i \) measures the spin in a direction \( a \) and then correlates this with the second point \( j \) in direction \( b \) in one of three perpendicular directions.
CHAPTER 4. TRANSVERSE FIELD ISING MODEL

\( x, y, z \). Triangular brackets \( \langle \cdot \rangle \) denote the thermodynamic average for the system in equilibrium.

Correlation effects occur over small distances even in disordered states. Since the TFIM model is restricted to interactions in the \( z \) or \( x \) directions. It would be convenient to observe how the main correlating \( zz \) interaction is affected by the disordered \( x \) field. Typically disordered effects, like thermal or magnetic, destroy the correlations and the general function has an exponentially decaying form

\[
\rho_{zz}(R) \propto \frac{1}{R^{d-2\eta}} \exp \left( \frac{-R}{\xi} \right) \tag{4.10}
\]

It is important to recognise the correlation exponents as those previously mentioned in Chapter 2. The dimension of the system \( d \) and correlation scaling exponent \( \eta \). Also note the correlation length \( \xi \) which determines the nature of the exponential decay.

In critical systems \( \xi \) diverges and the exponential part of (4.10) is changed to a power law contribution. Moving through the transition point into the ordered state the system has an infinite correlation length. All two-point correlations in the ordering direction \( z \) returns \( \rho_{zz} \) with a constant value. There is complete coherence across the chain and all spins are uniformly ordered in the same direction, even if they are separated by a great distance. The nature of this interaction is long-range and is given the name long-range order.

Fig. 4.3 is the numerical result obtained by measuring the correlations (a) \( \rho_{zz} \) and (b) \( \rho_{xx} \) in the transverse field Ising model. At low field \( \rho_{zz} \) is a constant function with strong correlation between spins until the critical field is reached. Power law decay is observed at the critical point. Beyond this varying degrees of exponential decay can be seen as the model becomes disordered. The other correlation \( \rho_{xx} \) transitions in a similar way generating correlations as the magnetic field is increased. Correlations only hold if the magnetic field is present as expected in a paramagnetic state.
Figure 4.3: Ising model spin-spin correlation functions (a) $\rho_{zz}(R)$ and (b) $\rho_{xx}(R)$ with site distance $R = |i - j|$ over magnetic field $h$ from 0 to 1.9.
4.2.4 Entanglement properties

4.2.4.1 Singular values

A slightly entangled system is defined as a quantum state displaying limited half-chain entanglement. The notion of slight in this sense means the singular values of the Schmidt decomposition (3.24) decay rapidly with bond index $\alpha$.

The singular values of the TFIM are presented for a bipartition at bond $\lambda_1$ with $\chi_1 = 30$, Fig. 4.4. The selection of $\chi_1$ is sufficient to observe decay in the magnitudes of the singular values, which should diminish quickly. The singular values are extracted from $\lambda_{\alpha}^{[1]}$ after initialising in a product state and performing the simulation procedure in Fig.3.4.

![Figure 4.4: iTEBD: singular values for $\lambda_1$ decay rapidly as a function of alpha (log-linear).](image)

The spectrum of $\lambda_{\alpha}^{[1]}$ for the transverse field Ising model is plotted in Fig.4.4. The saturation is due to a minimum threshold of $10^{-20}$ set in the numerics. A
clear picture of rapidly decreasing singular values demonstrates the locality of entanglement in the system. The number of states contributing includes only those in close proximity of the bipartition and is small compared to $\chi_1$, even at the critical point where decay is reduced as entanglement grows.

Negligible contributions to the state are discarded by truncating at the appropriate index $\chi_{\text{max}} \leq \chi_1$ according to the percentage of the state retained

$$\eta = \frac{\sum_{i=1}^{\chi_{\text{max}}} \lambda_i^{[1]} / \sum_{\alpha} \lambda_{\alpha}^{[1]} > 0.999}{}$$ (4.11)

Although some of the information about the state is lost, this is not important as the neglected weight contributes a minimal percentage (0.001%) to the total. Consequently large bond dimensions $\chi_1$ can potentially be greatly reduced if $\chi_{\text{max}}$ is small, simplifying the complexity of the problem.

4.2.4.2 Scaling at the critical point

As detailed in Chapter 3.4, a critical and non-critical spin chain exhibit different scaling behaviours. The non-critical chain has a finite correlation length $\xi$ whilst a complete description of the state at a critical point exhibits diverging entanglement and thereby $\xi$ also diverges. However solving for the two largest eigenvalues of the (finite) quantum transfer matrix presents a finite correlation length $\xi_\chi$ over the entire region. The system wants to diverge to $\xi \to \infty$ as $\chi \to \infty$ meaning some effective correlation length $\chi_c$ is inflicted on the system. The comparative lack of states in the finite MPS to a description that takes into account infinite entanglement gives rise to this cost.

Fig.4.5 shows the TFIM in the vicinity of the critical point $h=1$ using iTEBD. The effective correlation length grows and a broad peak sharply narrows to a point as $\chi$ is increased. Keeping at least $\chi=30$ states gives an accurate representation of the ground state. Interestingly at the critical point retaining more states i.e. larger $\chi$, not only increases the correlation length but also improves the algorithms ability to determine the true transition point $h_c$. The relation $|h_\chi - h_c|/h_c \sim \chi^{-\kappa/\nu}$ is derived from (2.1) and (2.3) and has
Figure 4.5: Effective correlation length $\xi_\chi$ in the TFIM near the quantum critical point at $h=1$.

been previously investigated [55]. The universal exponent $\nu$ for the TFIM has a known value of 1 [56] and $\kappa$ is extracted from the polynomial fit in Fig.4.6 as 1.99(4) in agreement with the accepted value $\approx 2$ [50,55].

The central charge $c$ is to equal to 1/2 at the quantum critical point $h =1$ and $c=0$ away from criticality. Fig.4.7 is plotted with a line of best fit following (3.51). This example of scaling will continue to appear throughout this work as the central charge is extracted from the gradient $\sim c/6$. 
CHAPTER 4. TRANSVERSE FIELD ISING MODEL

Figure 4.6: The scaling behaviour of the effective correlation length $\xi_\chi$ with $\chi$ using iTEBD in the TFIM.

Figure 4.7: Half-chain entanglement properties for the TFIM at the critical point $h=1.0$. The entropy scales with correlation length with a gradient of $1/12$ equivalent to a central charge $c = 1/2$. 
4.3 Non-equilibrium steady-state

The previous discussion sets up the foundation for moving into a more complex situation. Here we discuss the effect of driving the system out of equilibrium. Non-equilibrium thermodynamics has become an increasingly popular field of study with recent advances in controllable quantum simulators [57]. A review outlining the triple approach of numerical, analytical and experimental physics is found here [58]. Focus in these studies is on the dynamics of the system which become increasingly important along with transport properties and dissipation. Power-law decay is expected to be a general feature of the long-time, two-point spin correlation function. Observations have been made in lattice gases and spin-glasses [59,60].

The establishment of a non-equilibrium steady-state (NESS) in the realm of a Matrix Product State representation has been achieved using one and two spin baths coupled to the ends of a spin chain [61]. Further work is needed to extend the ‘openness’ of the system to a coupled bath with effective classical size. Ideally the bath should exchange particles and energy on a macroscopic scale. An alternative route to a NESS is in closed systems. The Hamiltonian drives the system with terms that influences spin or energy currents. This is easy to implement numerically with the time evolution operator in iTEBD.

The path set out for non-equilibrium quantum spin chains involves the consideration of integrability and how that relates to conserved quantities. The integrability of the model depends on its solubility within the framework of the algebraic Bethe ansatz. If the Yang-Baxter equation [62] is solved by the construction of $R$ matrices for a spin model, a sequence of conserved charges $Q_n$ are obtained. This has important implications later and a longer exposition is given in Chapter 5 where integrability becomes the main focus.

The nearest neighbour Hamiltonian is in general a sum of two-site interactions. It is defined as $H = Q_2$ and commutes with all $Q_n$, the operator with interactions over $n$-points. It is conjectured that the existence of $Q_3$ is a necessary and sometimes sufficient condition for integrability [63]. $Q_3$ is a sign
that the $R$ matrices generate an infinite family of conserved charges necessary for integrability. This is an important quantity since $Q_3$ has physical significance. The conserved flow of $Q_3$ through the system depends on the local energy operator. The flow of energy (energy current), is derived from the time derivative of the local Hamiltonian in Appendix B.

### 4.3.1 Energy current derivation

Using the calculation method presented in Appendix B, the local Hamiltonian of the TFIM, where $H = \sum_i h_{i,i+1}$, is used to derive the energy current

$$j^E_i = -i[h_{i-1,i}, h_{i,i+1}]$$

$$= -i[J\sigma^z_{i-1}\sigma^z_i + h(\sigma^z_{i-1} + \sigma^z_i), J\sigma^z_i\sigma^z_{i+1} + h(\sigma^z_i + \sigma^z_{i+1})]$$

$$= -i(J^2[\sigma^z_{i-1}\sigma^z_i, \sigma^z_i\sigma^z_{i+1}] + Jh[\sigma^z_{i-1}\sigma^z_i, (\sigma^z_i + \sigma^z_{i+1})])$$

$$+ Jh[(\sigma^z_{i-1} + \sigma^z_i), \sigma^z_i\sigma^z_{i+1}] + h^2[(\sigma^z_{i-1} + \sigma^z_i), (\sigma^z_i + \sigma^z_{i+1})])$$

$$= -i(Jh(\sigma^z_{i-1}[\sigma^z_i, \sigma^z_i] + [\sigma^z_i, \sigma^z_i]\sigma^z_{i+1}))$$

$$= Jh(\sigma^z_{i-1}\sigma^y_i - \sigma^y_i\sigma^z_{i+1}) \quad (4.12)$$

Physically, this is the Dzyaloshinskii-Moriya (DM) interaction $\vec{D} \cdot (\vec{S}_i \times \vec{S}_j)$ with the chiral order alignment vector $\vec{D}$ pointing in the $x$-direction. Phenomenologically introduced by Dzyaloshinskii using symmetry considerations [64], then later derived by Moriya using spin-orbit coupling as a mechanism for an anisotropic superexchange interaction [65]. The theory was used to describe weak ferromagnetism in low symmetry antiferromagnetic systems. Provided the strength of the DM interaction has a magnitude comparable to the exchange interaction; spins rotate with a tendency to align in the $Y \cdot Z$ plane, illustrated in. The interaction is asymmetric meaning spins tilt in a favourable direction lowering the energy state, but cost energy in the opposite direction.

A wealth of applications of this model have found use in condensed matter systems. Thin films have a tendency to have broken inversion symmetry on their surfaces where spin-orbit coupling is strengthened. In bilayer Fe the DM
interaction is strong and can describe the orientation of magnetic domains [66]. Weak ferromagnetism has been investigated in the cuprates, typically used in the study of superconductivity [67]. The existence of multiferroic effects, i.e. the interplay of ferroelectricity and magnetism, in the perovskites is explained within this mechanism of superexchange [68].

4.3.2 Exact calculation of energy spectrum with energy current

The Hamiltonian for the Transverse Field Ising model is modified in the presence of energy current reading:

\[
H' (J, h, \lambda) = - \sum_{n=1}^{N} (J \sigma_n^z \sigma_{n+1}^z + h \sigma_n^x) + \lambda j_n^E
\]  

(4.13)
where the Lagrange multiplier $\lambda$ subjects the system to the current term

$$H_{\text{current}} = \lambda \left( \frac{J}{2} \right) h \sum_n (\sigma^z_n \sigma^y_{n+1} - \sigma^y_n \sigma^z_{n+1})$$  \hspace{1cm} (4.14)

$$L = \lambda J h \hspace{1cm} (4.15)$$

The exact solution for the eigenvalues of this model can be found by transforming the spin operators to proper fermionic creation and annihilation operators. A Jordan-Wigner transformation correctly accounts for the anti-commutation between spins on different sites by introducing a non-local factor. The Fourier transform collects all terms in momentum space $k$. Appendix A gives a detailed mathematical solution to this model. Halting at the step (A.17), a simple way to diagonalize the Hamiltonian is to reform and identify the central matrix of the transformation

$$H = \sum_{k>0} \left( \begin{array}{cc} c^+_k & c_{-k} \\ c_k & c^+_{-k} \end{array} \right) \left( \begin{array}{cc} \frac{J}{2} \cos k + h & -i \frac{J}{2} \sin k \\ i \frac{J}{2} \sin k & \frac{J}{2} \cos k - h \end{array} \right) \left( \begin{array}{c} c_k \\ c^+_{-k} \end{array} \right)$$

as $C$ for the bare TFIM. Neglecting any immediate details about Bogoliubov fermions, the solution can be calculated by simply taking the determinant of this matrix $C$, and the $\gamma$-operators follow naturally from this.

Applying the steps in Appendix A, the energy current can be independently diagonalised. A quick description of the calculation is given as follows.

(1) Second quantisation

$$H_{\text{current}} = \frac{L}{4} \sum_n [i (a_n^+ a_n)(a_{n+1}^+ - a_{n+1}) - i (a_n^+ - a_n)(a_{n+1}^+ + a_{n+1})] \hspace{1cm} (4.16)$$

$$= \frac{Li}{4} \sum_n [2 a_n a_{n+1}^+ - 2 a_n^+ a_{n+1}] \hspace{1cm} (4.17)$$

(2) Jordan-Wigner transformation

$$c_n = \exp (\pi i \sum_{j=1}^{n-1} a_j^+ a_j) a_n \hspace{1cm} (4.18)$$

$$c_n^+ = a_n^+ \exp (-\pi i \sum_{j=1}^{n-1} a_j^+ a_j) \hspace{1cm} (4.19)$$
\[ H_{\text{current}} = \frac{Li}{2} \sum_n [c_n c_{n+1} \exp (\pi i c_j^\dagger c_j) - \exp (-\pi i c_j^\dagger c_j)] c_n^\dagger c_{n+1} \] (4.20)

\[ = \frac{Li}{2} \sum_n [-(1 - 2c_n^\dagger c_n)c_n^\dagger c_{n+1}^\dagger - c_n^\dagger(1 - 2c_n^\dagger c_n)c_{n+1}] \] (4.21)

\[ = -\frac{Li}{2} \sum_n [c_n c_{n+1}^\dagger + c_n^\dagger c_{n+1}] \] (4.22)

(3) Fourier transformation

\[ c_k = \frac{1}{\sqrt{N}} \sum_j c_j \exp (ikj) \] (4.23)

\[ c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j c_j^\dagger \exp (-ikj) \] (4.24)

\[ H_{\text{current}} = -\frac{Li}{2} \sum_k c_k c_k^\dagger \exp (-ik) + c_k^\dagger c_k \exp (ik) \] (4.25)

\[ = L \sum_k c_k^\dagger c_k \frac{(\exp (ik) - \exp (-ik))}{2i} \] (4.26)

\[ = L \sum_{k>0} [c_k^\dagger c_k \sin k - c_{-k}^\dagger c_{-k} \sin k] \] (4.27)

(4) Calculate determinant: Matrix \( C \) is modified by the addition of current terms included from (4.27) by matching the correct \( c \)-operators. These happen to appear only along to diagonal making their inclusion easier, forming a new matrix \( C' \)

\[ H' = \sum_{k>0} \begin{pmatrix} c_k^\dagger & c_{-k} \end{pmatrix} \begin{pmatrix} \frac{i}{2} \cos k + h + L \sin k & -i \frac{L}{2} \sin k \\ i \frac{L}{2} \sin k & -\frac{i}{2} \cos k - h + L \sin k \end{pmatrix} \begin{pmatrix} c_k \\ c_{-k} \end{pmatrix} \]

The eigenvalues of the problem are found from the characteristic equation

\[ \det[C' - \mathbf{I} \epsilon_k^r] = \det \begin{pmatrix} \frac{i}{2} \cos k + h + L \sin k & -i \frac{L}{2} \sin k \\ i \frac{L}{2} \sin k & -\frac{i}{2} \cos k - h + L \sin k \end{pmatrix} \]
Rearranging for $\epsilon'_k$ gives the energy spectrum as

$$\epsilon'_k = L \sin k \pm \sqrt{\left(\frac{J}{2} \cos k + h\right)^2 + \left(\frac{J}{2}\right)^2 \sin^2 k}$$  \hspace{1cm} (4.28)$$

$$= L \sin k \pm \sqrt{\left(\frac{J}{2}\right)^2 + h^2 + Jh \cos k}$$ \hspace{1cm} (4.29)$$

This diagonalisation procedure obscures details of the transformation on the $c$-operators. The diagonal form of $C'$ is expressed as $D = P^{-1}C'P$. Eigen-vectors of $C'$ are arranged as column vectors in the matrix $P$. Subsequent application of $P$ transforms the $c$-operators into a new linear combination of terms. The outcome then, is identical to a Bogoliubov transformation. The linear combination defines new $\gamma$ fermions and the Hamiltonian is written as

$$H' = \sum_k \epsilon'_k (\gamma_k^\dagger \gamma_k - 1/2).$$ \hspace{1cm} (4.30)$$

Figure 4.9: Energy dispersion relation for the TFIM with energy current. Values of energy current $L = 0 - 2$ and magnetic field $h = 0 - 2$. 

51
In Fig. 4.9 the newly calculated energy dispersion relation $\epsilon'_k$ is plotted displaying instances of gapless excitations at $\epsilon'_k(h_c, L_c) = 0$. This suggests the presence of distinct phases under a combination of critical field $h_c$ and current $L_c$ conditions. A more explicit definition of the phase boundaries is derived by solving (4.29) when the gap closes. The two conditions $\epsilon'_k = 0$ and $\frac{\partial \epsilon'_k}{\partial k} = 0$ are solved and define two new phase lines separating the ferromagnetic (FM) and paramagnetic (PM) states from a new current-carrying region (CC), Fig. 4.10.

Figure 4.10: Schematic diagram of the Transverse Field Ising model with energy current. A new current-carrying (CC) phase exists as the energy current flows beyond a critical value.

For $h < 1$ and $L < 1$ the ground state is separated from excited states marking one phase boundary between magnetic order and disorder. The gap closes at the critical value $h_c = 1$ and grows again beyond this point. Interestingly there is another region for the conditions $L \geq h_c$ and $L > h_{PM}$. The
notation PM denotes a second paramagnetic boundary for the line \( L = h > 1 \). The current forces asymmetry in the spectrum as the gap disappears in the negative half of the momentum space. The excitations once again become gapless as energy is favourably minimised by current flow in one direction.

4.3.3 Correlations

4.3.3.1 Spin-spin correlations

The behaviour of the spin-spin correlation function \( \langle \sigma_z^1 \sigma_z^{1+R} \rangle \) reveals distinct properties within the current region (\( L > 1 \) in Fig.4.11). We confirm the oscillatory behavior accompanied by a power-law decay (as \( R^{-\omega} \)), where \( \omega = 1/2 \) and \( R \) is the distance between the two correlated spins, as obtained in [69]. The specific power-law is considered to govern the critical region of non-equilibrium steady-state models in general [70]. The power \( \omega \) is a nonequilibrium dynamic exponent and in an arbitrary dimension \( d \) satisfies the relation \( \omega \geq d/2 \). This result demonstrates the success of the iTEBD method in the critical regime.

Table 4.1: Numerical data showing how the wavelength \( R \) and wavenumber \( k \) vary with current \( L \)

<table>
<thead>
<tr>
<th>( L )</th>
<th>( \mathcal{R} )</th>
<th>( k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.2</td>
<td>10.3103448276</td>
<td>0.609405932803</td>
</tr>
<tr>
<td>1.4</td>
<td>7.66666666667</td>
<td>0.819545909632</td>
</tr>
<tr>
<td>1.6</td>
<td>7.29268292683</td>
<td>0.861573904998</td>
</tr>
<tr>
<td>1.8</td>
<td>6.10204081633</td>
<td>1.02968588646</td>
</tr>
<tr>
<td>2.0</td>
<td>5.98</td>
<td>1.05069988414</td>
</tr>
</tbody>
</table>

Using least squares fitting, an approximate expression for the damped sinusoidal correlation function is found

\[
\langle \sigma_z^n \sigma_z^{n+R} \rangle \sim \frac{Q(h, L)}{\sqrt{R}} \cos (kR)
\]  

(4.31)
Figure 4.11: TFIM with energy current $L$ in range $\{0, 0.2, \ldots, 1.8, 2.0\}$ and magnetic field $h = 0.5$ below the critical value $h_c = 1$. The oscillatory behaviour of the $\sigma_z^z$-correlation function is shown above critical value of the energy current $L_c = 1$. In the region $L \leq 1$ normal FM correlations are observed. Inset: A Fast Fourier transform (FFT) is used to calculate the period as it shifts with $L$. 
The amplitude decreases strongly as the phase boundary is approached \( h \to 2 \), more details on the analysis of \( Q(h, L) \) can be found in [69].

The wavelength of the correlations has been also investigated in [69] and found to be independent of \( h \). The formula discovered is given as a function of wavenumber \( k \) and depends only on \( L \) as

\[
k = \arccos(1/L). \tag{4.32}
\]

Using a Fast Fourier Transform (FFT), the peak of the oscillations in space determines the wavelength \( R = 2\pi/k \). Table 4.1 lists results for current, wavelength and wavenumber. A least squares fit of this data remains reliably close to (4.32) with

\[
k = (1.01 \pm 0.06) \arccos[(0.99 \pm 0.05)/L]. \tag{4.33}
\]

The fitted values are calculated with errors extracted from the covariance matrix. Error sources are mainly from the numerical method and difficulty maximising the resolution of the FFT peak.

### 4.3.3.2 Chiral order

The transition into the current carrying region can be described more clearly by defining a chiral order parameter. It characterises asymmetry between spins generated from the strength current in the system. It takes of the form of the average energy current over all bonds

\[
C_{zy} = \sum_n (\sigma_n^z \sigma_{n+1}^y - \sigma_n^y \sigma_{n+1}^z). \tag{4.34}
\]

Chiral order is zero in non-current carrying regions and at the transition point the Dzyaloshinskii-Moriya term gains significance as \( C_{zy} \) continuously grows with current strength \( L \). The physics is generated from inversion symmetry breaking. A magnetic spiral state emerges under these conditions and chiral order grows. Both FM and AFM orders demonstrate identical growth in \( C_{zy} \) i.e. \( L > |J| \).
Figure 4.12: Chiral order parameter of the TFIM at $h = 0.5$.

Figure 4.13: The behaviour of a chiral order parameter $C_{zy}$ as a function of magnetic field in the TFIM with energy current $L = 2.0$.

Fig. 4.12 is a numerical non-linear curved fit of the chiral order. Two coefficients are used in the fit and extracted leaving the current $L$ as a free
CHAPTER 4. TRANSVERSE FIELD ISING MODEL

parameter. It is zero for $L \leq 1$ and increases with the fitting function as shown.

Regarding the dependence of the chiral order on the magnetic field strength, the current flow is suppressed as the system moves into the paramagnetic state under a strong magnetic field $h_{PM} > L/|J|$. Fig.4.13 shows $C_{zy}$ for constant current $L = 2$ as the PM boundary is approached. The trend of the data is identified and plotted with a rearrangement of variables into a linear form. The relationship extracted in the figure agrees with [69] as

$$C_{zy} \propto |h_{PM}^2 - h^2|^{1/2}.$$  \hfill (4.35)

4.3.4 Entanglement properties

The entanglement properties differ as the current is able to flow through the TFIM. We focus on the boundary moving between the current-carrying phase into the paramagnetic state. The main result of this section reveals the nature of the central charge in the current-carrying region where a sudden change in $c$ is expected to occur crossing the boundary.

As the system is forced into a non-equilibrium steady-state the model becomes critical. The entanglement entropy scales as $S = \frac{c}{6} \log(\xi)$. For example, Fig.4.14 demonstrates one set of critical parameters. Fixing the current at $L = 1.2$ with a (non-critical) transverse field $h = 0.5$ the system sits in the current region. Extracting the precise value for $c$ from Fig.4.14 determines the severity of the scaling, expressed as the gradient $\approx 1/6$.

The scaling is investigated with dependence on $h$, Fig.4.15. A series of points either side of and the point on the boundary are analysed. The central charge is extracted from the two inset figures from the linear relationship $S = \frac{c}{6} \log(\xi)$. In low field, to the left of the graph, the system remains in the current-carrying region and shows a central charge falling along the $c = 1$ dotted line. The left inset shows the scaling behaviour. Further increase of the field strength into the non-critical PM region hits the boundary at $h = L$ identifying the critical transition parameter $L_c = 1.2$. A sharp drop to $c = 0$ is
observed. These points have non-critical scaling as $S$ is either zero or constant and logarithmic scaling no longer applies.

Figure 4.14: Central charge $c = 1$ in the current-carrying TFIM ($h = 0.5$ and $L = 1.2$). $S = \frac{c}{6} \log(\xi)$. 
Figure 4.15: The central charge as a function of the transverse field $h$ in the current-carrying TFIM at $L = 1.2$. Left inset: Central charge $c = 1$ is determined in the current-carrying region from the calculation of $S = \xi \log(\xi)$. Right inset: The scaling disappears crossing into the paramagnetic phase and $S$ is constant or zero.
Chapter 5

Transverse Field Ising model with integrability breaking perturbations

Integrability is defined with connection to exact solubility. The eigenfunctions and eigenvalues can be obtained exactly. These solutions are calculated with analytical methods which exclude limiting approximations. That is, any non-perturbative mathematical technique [11, 71]. This is a useful but ill-defined way to characterise integrability. It is based on the vague notion of solubility. A more concrete definition of integrability is needed. In the study of integrable lattice models some known processes are used. For example the Bethe ansatz has found success in a limited class of local one-dimensional models. The origin of integrability can be traced to classical mechanics [63]. A system with $N$ degrees of freedom is integrable if it has $N$ constants of motion. The Poisson bracket has state variables which are reinterpreted in quantum mechanics as commutation relations and operators respectively with $N$ Liouville-von Neumann equations

$$i\hbar \frac{d}{dt} \hat{Q}_i = [\hat{Q}_i, \hat{H}] = 0 \quad (5.1)$$
For the system to be completely integrable this equation states that all the operators $\hat{Q}_i$ must commute with the Hamiltonian and be independent of time. The measured quantity $Q$ is one of the $N$ conserved constants of motion. For a quantum spin chain in the thermodynamic limit, the system has an infinite number of spin degrees of freedom. Therefore quantum integrability in this sense has an infinite number of conservation laws. In contrast, non-integrable models only have one conserved quantity which is the energy [72].

In addition to analytical calculations, computational methods are highly effective in a wide variety of cases, and can additionally probe situations in the absence of integrability especially since alternative analytical methods like a perturbative expansion can diverge with strong interactions.

## 5.1 Non-integrability as a function of $D$

Integrability breaking can be achieved by introducing certain perturbation terms in the TFIM. One way in particular is to include the interaction $D\sigma_i^x\sigma_{i+1}^x$ longitudinal to the magnetic field direction $x$ and transverse to the original spin ordering interaction $z$. The system is perturbed into an integrability breaking regime and non-integrability is controlled by the parameter $D$. The inclusion of this interaction is a largely unexplored method to break integrability. The Hamiltonian reads

$$H_{\text{non}} = -\sum_{i=1}^{N} J\sigma_i^z\sigma_{i+1}^z + h\sigma_i^x + D\sigma_i^x\sigma_{i+1}^x \quad (5.2)$$

The model approaches the TFIM as $D \to 0$. It is expected that creating a small perturbation by gradually increasing $D$ will move the system out of integrability and into an area of new physics.

Before an attempt at a numerical simulation, some discussion of known solutions to the model is informative. If the spin couplings have equivalent interaction strength $D/J=1$ the Hamiltonian is recognised as the isotropic XY model in an integrability breaking magnetic field. Additionally, in the absence
of magnetic field $h=0$, if the interaction strength $D$ is no longer constrained to equal $J$, i.e. it holds any value $|D| \geq J$, the XY model with anisotropy emerges. This has a known exact solution calculated (using Appendix.A) with energy dispersion relation

$$
\epsilon_k^{h=0} = \left( 1 - \left[ 1 - \left( \frac{1 + D/J}{1 - D/J} \right)^2 \right] \sin^2(k) \right)^{1/2}
$$

As a consequence it is expected that upon arrival to the separate limits for the TFIM and XY model, the system regains integrability with known entanglement properties.

![Figure 5.1: Correlations of the non-integrable TFIM at $h=0.5$ with integrability breaking parameter $D$. Triangles (blue) denote long-range order, stars (colourless) critical correlations and circles (red) exponential decay.](image-url)
5.1.1 Spin-spin correlations

The system passes through a critical point as $D$ increases. To show this the $zz$-correlations are presented in Fig. 5.1. At low values of $D$ there is long-range order until the critical point is reached at $D_c$ and correlations with power law decay emerge. The non-integrable term acts similarly to a transverse field, and at $D_c$, the system experiences a phase transition from a $Z_2$ symmetry breaking FM to PM phase.

The correlation length $\xi$ is a factor in the exponential part of the general correlation function $(4.10) \sim \exp\left(-R/\xi\right)$, and at the critical point $\xi$ is infinite sending the exponential to 1. The remainder of the function governing the decay is a power law. The specific power of this is obtained by linearising the critical line in Fig. 5.1 with a log-log transformation. Using the $(4.10)$ the critical correlation exponent is calculated to be $\eta = 0.48 \pm 0.05$.

5.1.2 Entanglement properties

There are two known critical points for the model Hamiltonian (5.2). One at $h = J, D = 0$ and $h = 0, D = J$; the isotropic XY and TFIM limits, with central charges 0.5 and 1, respectively [41]. A critical line with nonzero central charge is expected to connect these two points. This is evident from the fact that a phase transition is unavoidable as the parameters are physically unable to be tuned around the critical points. Therefore a symmetry breaking transition must occur.

The critical line that connects the two known critical points is located by observing a peak in the effective correlation length $\xi_\chi$ as it increases with $\chi$. Fig. 5.2 shows an example point, when $D/J = -0.25$ the field causing the transition is found to be $h/J = 0.607$. The location of the exact critical field requires a discrete number of points to trace the curve. Numerical inaccuracies arise when using relatively few points to find the peak in the effective correlation length, as this reduces the number of significant figures available by the re-
finement. Also, $\chi$ has a direct relation to the sharpness of the peak and using limited $\chi$ presents a broad peak.

![Graph](image)

Figure 5.2: Effective correlation length at $D = 0.25$, critical $h \approx 0.607$.

The exact nature of the entanglement scaling is used to map this critical line by repeating the process in the previous paragraph at selection of points. The points are chosen to include the scaling behaviour at the furthest extents of the line i.e. the XY and TFIM limits, and a few example points falling in between these are all shown in Fig. 5.3. The graph shows the central charge is $c=0.5$ at all points except at the XY point, where $c=1$. This is convincing evidence of the critical line and more points are measured until a sufficient number map the full phase diagram, as presented in Fig. 5.4. The critical line separates a FM from a PM region.
Figure 5.3: Entanglement entropy scaling of the non-integrable critical line. The XY point is shown on the left with central charge $c \approx 1.0$. The remaining lines starting with the TFIM on the right have central charges $c \approx 0.5$ with the rest lines falling in between these two points.
Figure 5.4: Phase diagram of the TFIM with integrability breaking term $D/J$ as function of the transverse field $h/J$. 

.png
5.2 Integrability breaking in the presence of energy current

The energy current is once again calculated from (B.9). The local Hamiltonian

\[ h_{i,i+1} = J \sigma_i^z \sigma_{i+1}^z + D \sigma_i^x \sigma_{i+1}^x + h (\sigma_i^z + \sigma_{i+1}^x) \]  

(5.4)

is substituted into the commutation relation (B.9) as

\[ J_{i,i+1}^{\text{non}} = -i \left[ J \sigma_{i-1}^z \sigma_i^z + D \sigma_{i-1}^x \sigma_i^x + h (\sigma_{i-1}^z + \sigma_i^x), \right. \\
J \sigma_i^z \sigma_{i+1}^z + D \sigma_i^x \sigma_{i+1}^x + h (\sigma_i^z + \sigma_{i+1}^x) \right] \\
= -i \left( J^2 [\sigma_{i-1}^z \sigma_i^z, \sigma_i^z \sigma_{i+1}^z] + JD [\sigma_{i-1}^z \sigma_i^z, \sigma_i^z \sigma_{i+1}^z] \\
+ Jh [\sigma_{i-1}^z \sigma_i^z, (\sigma_i^z + \sigma_{i+1}^x)] + JD [\sigma_{i-1}^z \sigma_i^z, \sigma_i^z \sigma_{i+1}^z] \\
+ D^2 [\sigma_{i-1}^z \sigma_i^z, \sigma_i^z \sigma_{i+1}^z] + Dh [\sigma_{i-1}^z \sigma_i^z, (\sigma_i^z + \sigma_{i+1}^x)] \\
+ Jh [(\sigma_{i-1}^z + \sigma_i^z), \sigma_i^z \sigma_{i+1}^z] + Dh [(\sigma_{i-1}^z + \sigma_i^z), \sigma_i^z \sigma_{i+1}^z] \\
+ h^2 [1] \right) \\
= J \left( D (\sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z + \sigma_{i-1}^z [\sigma_i^z, \sigma_i^z] \sigma_{i+1}^z) \\
+ Jh (\sigma_{i-1}^z [\sigma_i^z, \sigma_i^z] + [\sigma_i^z, \sigma_i^z] \sigma_{i+1}^z) \right) \\
= JD (\sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z - \sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z) + Jh (\sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z - \sigma_{i-1}^z \sigma_i^z \sigma_{i+1}^z) \]  

(5.5)

Interestingly, the energy current contains two parts. The second term has been seen before and is simply the TFIM energy current. The first term is dependent on \( D \) and contains a two terms which are cyclic permutation of their spin-directions

\[ J_{\text{non}}^{E} = \sum_i (JD (\sigma_{i-1}^z \sigma_i^y \sigma_{i+1}^x - \sigma_{i-1}^z \sigma_i^y \sigma_{i+1}^x) + Jh (\sigma_{i-1}^z \sigma_i^y \sigma_{i+1}^z - \sigma_{i-1}^z \sigma_i^y \sigma_{i+1}^z)) \]  

(5.6)

This is an expected result considering the Heisenberg model has an energy current with three conflicting spin directions resulting in all 3! = 6 non-commuting relations [73]. The non-integrable model has only two spin directions with only 2! = 2 non-commutators.
A collection of the parameters $L_1=JD\lambda$ and $L_2=Jh\lambda$ gives the equation for two controlled currents as the Lagrange multiplier is applied

$$J_{non}^E = \sum_i \left( L_1(\sigma_{i-1}^x\sigma_i^y\sigma_{i+1}^z - \sigma_{i-1}^x\sigma_i^y\sigma_{i+1}^z) + L_2(\sigma_i^z\sigma_{i+1}^y - \sigma_i^z\sigma_{i+1}^z) \right)$$

(5.7)

The new Hamiltonian is

$$H = \sum_i J\sigma_i^z\sigma_{i+1}^z + D\sigma_i^x\sigma_{i+1}^x + h(\sigma_i^x + \sigma_{i+1}^x) + L_1(\sigma_{i-1}^x\sigma_i^y\sigma_{i+1}^z - \sigma_{i-1}^x\sigma_i^y\sigma_{i+1}^z) + L_2(\sigma_i^z\sigma_{i+1}^y - \sigma_i^z\sigma_{i+1}^z)$$

(5.8)

Non-integrable current gives a situation which is plagued by numerical convergence problems. The number of parameters available presents an issue with selecting a set which will exhibit interesting entanglement scaling properties. To simplify the situation, it is found that after testing for convergence, the selection of the current strengths set to equal $L=L_1=L_2$ mitigates numerical obstacles. As the calculations are quite extensive only one large value for the current is chosen. Now only $D$ and $h$ are free as $L$ takes a constant value.

Fig.5.5 shows the situation on a colour map. The current is taken as $L=2$, from previous experience with the TFIM this was a sufficient to force the system into a non-equilibrium steady state. In Fig.5.4 there is only line of entanglement scaling, whereas the current in this situation facilitates scaling behaviour in the region. The remnants of no scaling are seen on the left hand side of the diagram. The XY critical point is still distinct in the top left corner.
Figure 5.5: The central charge of the TFIM with a non-integrability breaking term and energy current, $L=2$. 
Chapter 6

Transverse Field Ising Model with periodically weakened bond

We consider an extension of the Ising model when interactions on different sites are not equal i.e. $J_i \neq J_j$ with $i \neq j$. It is natural to assume that sites may not have equivalent bond strengths or spin magnetic moments since lattices are not always monatomic or fully occupied. These types of models have been useful in describing magnetic systems, in particular those with non-magnetic or diatomic lattice constituents, for example Fe-Mn alloys [74]. This is another way to introduce disorder into the system since mixed-bonds dilute the magnetic effects of the representation. These concepts provide a useful framework for studying ferrimagnetism [75]. This chapter deals with a particular bond dilution in the form of an alternating weakened bond. This is one of the simplest models with mixed-bond interactions and considers alternating bond strengths. In the main section one bond of strength $J$ has two neighbouring bonds of strength $J'$, which in turn have neighbouring bonds of strength $J$; therefore the sequence of bonds is repeated with period 2. This model is a reduced version of the more general extended quantum compass model [76],
which has been used in the description of the degeneracy of orbitals [77]. There is a second-order Ising-like phase transition in this system and we examine the critical entanglement scaling properties as a result. Subsequently, the more general case is studied taking a block of \( n - 1 \) spins identically interacting with strength \( J \), having a bond impurity of strength \( J' \) at every \( n \)th bond. We again look for phase transitions and entanglement scaling properties.

\section*{6.1 Results}

\subsection*{6.1.1 Exact diagonalisation for alternate weak bond}

This problem considers the weak bond Hamiltonian

\[ H_{wb} = -\sum_{i=1}^{N/2} J \sigma_{2i-1}^z \sigma_{2i}^z + J' \sigma_{2i}^z \sigma_{2i+1}^z + h (\sigma_{2i-1}^x + \sigma_{2i}^x) \]  

and is formed from the summation of odd \((2i-1)\) and even \((2i)\) spin operators over \(N/2\). This consideration splits the chain into two halves; even bonds with exchange strength \( J \) and odd bonds with exchange strength \( J' \) with the transverse magnetic field acting on all sites equally. Using the Jordan-Wigner transformation, defined in Appendix.A, the spins transform into fermion operators

\[ H_{wb} = -\sum_{i=1}^{N/2} \{J(c_{2i-1}^\dagger c_{2i-1}) (c_{2i}^\dagger + c_{2i}) + J' (c_{2i}^\dagger - c_{2i}) (c_{2i+1}^\dagger + c_{2i+1}) \} + 2h (c_{2i}^\dagger c_{2i-1} + c_{2i}^\dagger c_{2i}) \]  

Two independent Majorana fermions populations can be identified at site \( i \) if the lattice is re-framed with two sites per cell [76]. The two independent fermions operators are denoted with an additional subscript \( q \) and \( p \) and the lattice cells are rescaled \( 2i - 1 \rightarrow i \) and \( 2i \rightarrow i \). After a Fourier transformation

\begin{align*}
\end{align*}
the Hamiltonian can be written as

$$H_{wb} = -\sum_k [B_k c_q^\dagger c_p^\dagger + A_k c_q^\dagger c_p^\dagger + A_k^* c_q c_p^\dagger + B_k c_p c_q^\dagger + 2h(c_q^\dagger c_p + c_p^\dagger c_q) - Nh]$$

(6.3)

where $A_k = J + J' \exp(ik)$ and $B_k = J - J' \exp(ik)$.

Instead of the two-dimensional Bogoliubov process presented in Appendix A, a four-dimensional Bogoliubov transformation, using the associated Bogoliubov-de Gennes equations $[c_q^\dagger, H]$ and $[c_p^\dagger, H]$, is used to link linear expressions of the $c$ operators to $\gamma$ operators. The diagonal form of the Hamiltonian is found after a lengthy process and two independent Majorana fermion populations are found as

$$H_{wb} = -\sum_k \left( \epsilon_q^k \left( \gamma_q^k \gamma_q^k - \frac{1}{2} \right) + \epsilon_p^k \left( \gamma_p^k \gamma_p^k - \frac{1}{2} \right) \right)$$

(6.4)

where the dispersion relations $\epsilon_q^k = \sqrt{a + 2\sqrt{b}}$ and $\epsilon_p^k = \sqrt{a - 2\sqrt{b}}$, such that $a = 2J^2 + 2J'^2 + 4h^2$ and $b = (J^2 - J'^2)^2 + 4h^4(J^2 + J'^2) + 8JJ'h^2 \cos ka$. The ground state is found from (6.4) as

$$E_0 = -\frac{1}{2} \sum_k (\epsilon_q^k + \epsilon_p^k).$$

(6.5)

### 6.1.2 Order parameter

Integrating (6.5) over $k$ for $N \to \infty$, the exact ground state energy $E_0$ is calculated. The second derivative of $E_0$ with respect to $J'$ shows susceptibility to bond weakening $E''_0 = d^2E_0/dJ'^2$, analogous to magnetic susceptibility with magnetic field, and diverges at sufficiently weak $J'$. Fig.6.1 presents the exact analytical solution against one obtained using iTEBD. The peaks in the Figure indicate critical bond strengths $J'_c$ for multiple lines at different field strengths $h$. A linearised plot of $\log(J'_c/J)$ against $\log(h/J)$ is shown later in Fig.6.6 and includes this case with period $n=2$ where $J'_c/J = (h/J)^2$.

A second-order phase transition occurs passing through the critical points. This is seen in Fig.6.2 with a numerical solution for magnetisations $M_z$ and
CHAPTER 6. TRANSVERSE FIELD ISING MODEL WITH
PERIODICALLY WEAKENED BOND

\( M_x \) using iTEBD at \( h=0.5J \). The order parameter \( M_x \) changes continuously to zero upon reduction of \( J' \) to the critical bond strength. The model moves from a saturated FM state to one where the order parameter is zero in the PM state. The nature of \( M_x \) demonstrates typical magnetization behaviour for a PM phase, as seen previously in Fig. 4.2. This transition is equivalent to passing through the critical magnetic field in the TFIM and studies of the universal behaviour at the quantum critical points shows identical scaling exponents. For example, the relation near the transition \( E_0'' \propto |J' - J|^{-\nu} \) holds where \( \nu=1 \).

![Graph showing susceptibility to bond weakening](image)

Figure 6.1: The susceptibility to bond weakening, \( d^2E_0/dJ'^2 \), describes the response of the weak bond transverse field Ising model to reducing \( J' \). The divergence of the lines, \( d^2E_0/dJ'^2 \to \infty \), indicates quantum critical points. The numerical iTEBD solutions are pictured as vertical dashed lines at the peaks. The critical points are \( J'/J = (h/J)^2 \). The peaks are normalised for clarity since their magnitudes decay with increasing field
CHAPTER 6. TRANSVERSE FIELD ISING MODEL WITH PERIODICALLY WEAKENED BOND

6.1.3 Spin-spin correlations

Fig.6.3 shows the correlations as every even bond is weakened through the transition point at $J'_c = 0.25J$ when $h = 0.5J$. This coincides with the peak in Fig.6.1. Long-range order is maintained until $J'$ is tuned to $J_c$ and power-law decay appears. On the other side of the transition $J_c < 0.25J$ the region experiences exponential decay. When the bond strength is completely diminished
CHAPTER 6. TRANSVERSE FIELD ISING MODEL WITH PERIODICALLY WEAKENED BOND

$J' = 0$ and the chain is isolated into pairs, the correlations are instantaneously cut-off and the chain ceases to correlate beyond the first neighbour.

Short-range interactions are modified from the usual equivalent bond strength TFIM. The odd bond preserves a modulated pairing between spins experiencing the full strength $J$. Correlations show an almost sawtooth decay instead of a smooth curve.

Figure 6.3: Correlations for the TFIM with weakened bond at $h=0.5$.

6.1.4 Entanglement scaling and central charge

The entanglement scaling properties are investigated at the divergent points in Fig. 6.1. The critical nature at $(J_c/J) = (h/J)^2$ shares universal properties
with the TFIM. As it falls in the same universality class, the entanglement scaling exhibits similar behavior with the same central charge.

This is indeed what we find as presented in Fig. 6.4 which is the plot of the central charge at the critical points; the central charge is identical to the TFIM. Otherwise, when $J'/J \neq (h/J)^2$ the system is tuned away from criticality, the scaling disappears and the central charge is zero.

Figure 6.4: Central charge as a function of $(h/J)^2$ in the weakened bond transverse field Ising model at critical $J'$. Inset is the entanglement scaling where the central charge of $c=0.5$ is extracted from.
6.1.5 In the presence of energy current

In the situation where an energy current is introduced in the system, in a similar to the homogeneous TFIM, then it can be proved that there is no energy current conservation; the system then is not in a steady state. To show this we shall take the energy current over two consecutive bonds, as schematically seen in Fig.6.5 and find its time derivative. The energy current density over two sites \(2n, 2n+1\) that involves three bonds as indicated in Fig.6.5 reads

\[
j_{2n} + j_{2n+1} = J'h\sigma_{2n-1}^z\sigma_{2n}^y - Jh\sigma_{2n}^y\sigma_{2n+1}^z + Jh\sigma_{2n}^z\sigma_{2n+1}^y - J'h\sigma_{2n+1}^y\sigma_{2n+2}^z. \quad (6.6)
\]

The continuity equation then takes the form

\[
\partial_t(j_{2n} + j_{2n+1}) = -i[H,j_{2n} + j_{2n+1}] = 2h(J'^2 - J^2)(\sigma_{2n}^x - \sigma_{2n+1}^x) + 2J'h^2 \left[ (\sigma_{2n-1}^y\sigma_{2n}^y - \sigma_{2n-1}^z\sigma_{2n}^z) - (\sigma_{2n}^y\sigma_{2n+1}^y - \sigma_{2n+1}^z\sigma_{2n+2}^z) \right]. \quad (6.7)
\]

![Figure 6.5: Illustration of the sites, the corresponding interactions, the energy currents and the bonds that are involved. Due to the symmetry of the problem, the energy current \(j_{2n}\) and \(j_{2n+1}\) need to be considered in the continuity equation.](image)

The form of equation (6.7) indicates that upon summation over all sites, the last term on the right hand side, proportional to \(J'h^2\), will vanish except from the boundaries, but the first term on the right hand side will only vanish if \(J' = J\). Thus, there is no energy current conservation in the system, contrary to the homogeneous case.
6.1.6 Generalisation to \( n \)-sites

The previous discussion considered the weakening of every second bond. The generalisation to a periodically weakened bond of a period \( n \)-sites reveals a relationship for the critical \( J' \) that scales with the transverse field as \( J'_c/J = (h/J)^n \). Fig.6.6 shows the critical lines for \( n \) from 2 to 6.

![Figure 6.6: Critical boundary for transverse Ising model with weakened bond over \( n \)-sites, \( (J'_c/J) = (h/J)^n \). Second-order phase transition occurs crossing the line from above (ordered to disordered).](image-url)
CHAPTER 6. TRANSVERSE FIELD ISING MODEL WITH
PERIODICALLY WEAKENED BOND

The physics behind the above result is that as the distance between the weakened bonds becomes larger, lower values of $J'$ are required to produce the same effect. In the limit of very large $n$ then $J'_c$ approaches 0, which indicates that it effectively requires cutting the chain in order to produce the same result. The analytical treatment and proof of this relation is beyond the scope of the present work and will be presented elsewhere as it involves the non-trivial diagonalisation of a chain of $n$ spins with periodically modulated couplings and periodic boundary conditions [78]. The case of a single site with transverse field in an $n$-periodic chain has been investigated analytically, e.g. in Ref. [79]; the treatment there is simplified by the fact that the defect is site rather than bond.
Chapter 7

Heisenberg model with anisotropic term

This chapter outlines a brief exposition into spin chains with integer spin values. We motivate further work and present some preliminary findings on questions related to the physics of the Haldane phase [80], especially out of equilibrium.

7.1 Topological order and symmetry

The starting point in understanding order in condensed matter physics is the study of symmetries. A phase transition between one state of matter to another necessitates a difference in symmetry between the two. A high-symmetry state, which is usually high temperature in thermal phase transitions, experiences a reduction in symmetry as a phase transition occurs to a more ordered state. Landau theory provides a phenomenological framework to describe symmetry-breaking phase transitions, away from the microscopic interactions of the model, and the key strength is the generality in which it can be applied. As symmetry is the focus of the theory, very different systems microscopically, with similar symmetries, can have identical universal properties. Topological
order is a type of order which is beyond symmetry-breaking, Ref [81] gives a precise definition of a topological phase if, “at low temperatures and energies, and long wavelengths... all observable properties are independent of the choice of spacetime coordinates”; the physical state of the system can change, but cannot be described by a conventional local order parameter as local correlations vanish. Instead the wave function contains non-local correlations or entanglement [82]. A global topological invariant, such as the entanglement entropy, has to be considered. Ground state degeneracy can also partially characterise topological order and it is required that the ground states have a finite energy gap for excitations.

There are two types of topological order, intrinsic and symmetry-protected [83]. These are respectively, models without any symmetries to break and ones actively protected by one. The latter is the class important in the Haldane phase.

7.2 Haldane phase

The Haldane phase is an example of topological order. Haldane’s conjecture introduced a new way of thinking about the physics of integer and half-integer spins chains. It states that a finite energy gap with exponentially decaying correlations is present in integer chains. On the other hand half-integer chains have no gap and power law decay in correlations [80]. The body of evidence convincingly supports Haldane’s conjecture [84].

Formally the resilience of the Haldane phase is determined by an adiabatic connection from the topological phase to the topologically trivial state with degenerate and non-degenerate eigenvalues respectively. In other words, for the Haldane phase to be stable a phase transition is expected to occur when going from the integer spin Haldane phase to the trivial state. The stability of this in a spin-1 Heisenberg chain has been investigated under symmetry breaking conditions [85]. The three symmetries which protect topological order are $\pi$ rotations about two orthogonal axis i.e. the dihedral group $D_2$. 

81
time-reversal symmetry and spatial inversion. The usefulness and limitations of the symmetries follow a hierarchy in characterising the Haldane phase. Although, provided only the inversion symmetry holds, double degeneracy in the entanglement spectrum exists as a method to detect the Haldane phase.

7.3 The $S = 1$ Heisenberg model

To study the related physics, we use the Heisenberg model with on-site anisotropy that reads:

$$H_{\text{Heis}} = -\sum_{i=1}^{N} J\vec{S}_{i}\vec{S}_{i+1} + D(S_{z}^{i})^{2}$$  \hfill (7.1)

This is the simplest model with a tunable parameter $D$ which enables investigation into the Haldane phase [85]. Experimental evidence for the Haldane phase in this model has been achieved using neutron scattering and has shown a gapped excitation spectrum in the quasi-1D material CsNiCl$_3$ [86]. The ions of which are spin-1 with AFM couplings and is well-modelled by (7.1).

The control of parameter $D$ allows a phase transition of the system between one of the following phases. In the limit of large-$D$ the state is topologically trivial i.e. a simple product state. In the large negative $D$ case an AFM state presides. In between these two states exists the Haldane phase which persists from $D \approx -0.2$ to $D \approx 1$ [87]. Within this region one of the three symmetries listed previously protects the degeneracy of the entanglement spectrum.

Fig.7.1 presents a numerical result using iTEBD to confirm the double degeneracy of the first two Schmidt coefficients of the entanglement spectrum. The state is evolved in time with $D(t)=1.5J - 2t/40$ in small time steps $t = 0, 1, 2, ..., 40J$. The system is evolved slowly keeping the evolution adiabatic. The Haldane phase is present in the centre of the figure when $\lambda_{1} - \lambda_{2} = 0$, connecting the large-$D$ and AFM phases. A natural question in extension to this adiabatic nature is: 'Will the Haldane phase remain after a quantum quench?'. The procedure requires evolving from an initial Hamiltonian with $D(0)$ supporting topological order, then suddenly evolving with a
new Hamiltonian with a sudden jump to $D(t)$ that might not support topological order. Little is known about the fate of the 1D Haldane phase in non-equilibrium conditions, but previous efforts using the Toric Code Model indicate the possibility of quenches which can either preserve or destroy topological order [88]. Subjecting models like these to adverse conditions, such as noise or thermal mixing, will play a part in realising new quantum technologies based on topological order. It is also a non-trivial question with potential application in the area of topological quantum computations, apart from being a fundamental one.
Chapter 8

Discussion and Conclusion

The aim of this thesis has been to study the physics of one-dimensional quantum spin chains. In principle, low-dimensional systems exhibit phenomena absent in higher dimensions. The confinement of electron wavefunctions in 1D leads to intriguing physics relating to strongly correlated systems, of which magnetism is the main topic in this thesis. Nevertheless, we can draw conclusions for electron systems as well because, it is well known that, we can map the interacting spins in certain models in 1D to free or interacting fermions. Furthermore, increasing our understanding of the fundamental properties of magnetic systems has the potential to guide development of new technologies. In particular, the existence of magnetic phase transitions or the presence of entangled states has important implications in quantum information science. These can be used as a resource for communication or computation tasks. Although many studies have been performed, there is still a lot unknown about out-of-equilibrium systems and their properties. As this is a ubiquitous consequence of the world, generated from noise or heat baths, the fate of these systems under these conditions is of fundamental importance in all experimental realisations.

In Chapter 1, an introduction to the theoretical and experimental background of strongly correlated electron systems is given. A discussion on the origin of magnetism is presented along with historical context of previous work.
CHAPTER 8. DISCUSSION AND CONCLUSION

in the field. The Hubbard and Heisenberg models are introduced as a general way to describe magnetism, with a list of known analytical and numerical approaches used to solve problems in 1D. The transverse field Ising model can be thought of as a limit of the Heisenberg model and it was discussed in the context of quantum information theory.

In Chapter 2, the theory of quantum phase transitions is outlined. A general classification scheme of phase transitions as first and second or higher order is given. We have focused on zero temperature quantum phase transitions and quantum criticality. This set the main background as critical entanglement properties and the extraction of the central charge have been investigated in the following chapters.

In Chapter 3, the main numerical technique is outlined. The algorithm called infinite-time evolving block decimation (iTEBD) has been used to study strongly correlated systems. Taking advantage of a matrix product state (MPS) representation for the quantum state, imaginary time evolution can be simulated until ground state convergence is reached. This works extremely well when the system is gapped and 1D. In gapless systems convergence times are longer but still possible with careful selection of parameters and increasing the available bond size \( \chi \). The success of this method relies on the Schmidt decomposition. Corresponding Schmidt coefficients for a bipartite split are used to define two-halves of the chains entanglement entropy. When they decay at a sufficient rate the system is considered to be slightly entangled and the MPS is truncated. The reduction in matrix dimensions simplifies the complexity of the problem only discarding a minute weight of the original state. This is possible as only a small amount of information is lost about the state. The two-site state invariance imposed by the time evolution operator allows for a parallelised update of the chain. These conditions enable an effective infinite chain to be simulated. This reduces the complexity of the problem further by specifying a limited number of tensors in the description of the state. Errors in the method result from the truncation of Hilbert space and the Suzuki-Trotter expansion of the time evolution operator. As long as the discarded weight is
small the truncation procedure should lead to an approximate quantum state with fidelity an arbitrary distance from the true state. The order-$p$ of the Suzuki-Trotter expansion and small size of $\delta$ should ensure the evolution error is minimised.

In Chapter 4, the transverse field Ising model (TFIM) is used as a simple preliminary model to test the numerical method. The Hamiltonian consists of two competing terms. A spin ordering term in form of an exchange interaction $J$ for the $z-$component of the spins and a term that induces quantum dynamics in the form of a magnetic field $h$ in a transverse direction. The combined nature of these exhibits quantum behaviour in a well-known manner. We started by confirming the known quantum critical point at the critical magnetic field $h/J = 1$. The magnetisation in $z$-direction is used as an order parameter and the spin-spin correlation function demonstrates the ferromagnetic to paramagnetic transition. The entanglement properties were then investigated. We confirmed also the value of the central charge $c = 0.5$. This value is important within conformal field theory (CFT) and $c$ has its origins in the two-point correlation function of the stress-energy tensor from quantum theory. Observables and critical properties are directly related to operators in a particular CFT describing the spin chain.

The next part of the chapter involved inducing a non-equilibrium steady-state in the TFIM. An energy current was injected through the bonds and the effect on the correlations and entanglement properties was studied. The form of the current coincidently takes the form of the Dzyaloshinskii-Moriya interaction used to describe weak ferromagnetism. Establishing the existence of the current-carrying phase was the first step, where oscillatory correlations are already known to exist. Novel results were found in the entanglement properties within the current-carrying phase. We have clearly observed doubling of the central charge which is now $c = 1.0$.

In Chapter 5, a model that breaks the integrability of the TFIM is investigated. The question regarding how an integrability breaking perturbation affects the physical properties of the model was studied. The correlation func-
tion was numerically calculated to identify a change from long-range order to power-law decay at a critical parameter $D_c$. This change is attributed to the perturbation effectively acting as a transverse magnetic field. Critical entanglement properties are used to map the phase diagram of the system, which has been originally calculated, with particular interest in the central charge along the critical line. One limit of the model is the anisotropic XY model and the majority of work in the literature considers the exactly solvable case with a transverse field. The study here presented a new result with a longitudinal magnetic field. This is not exactly solvable and a numerical method was required.

In Chapter 6, the TFIM is analysed when subjected to a periodic alternate weakening of the interaction strength. The model is based on previous work with the extended quantum compass model. An order parameter is calculated from the second derivative of the free energy and a phase transition was seen. The key result of the chapter is the relation of the critical weak bond $J'_c$ to its spatial period $n$ (in units of lattice spacing) within the chain and magnetic field strength $h$, given by $J'_c/J = (h/J)^n$. The behaviour is due to the strength of $J'$ required to effectively cut the chain at a bond. The bond energy required is weaker the longer the period in order to observe the transition.

In Chapter 7, we have presented a brief look at the Haldane phase in the spin-1 Heisenberg model with on-site anisotropy. The question as to how a quench could induce a non-equilibrium state was presented and left for future work to determine whether the stability of the Haldane phase is retained.

There were several questions left open in relation to the topological phases as well as the possibility to include a form of noise (such as $1/f$) in the system. This will also be important for real applications in quantum computing. In principle, the numerical calculations could accommodate such problems and could be performed with increasing $\chi$ which would lead to more intensive computations.
References


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Appendix A

Eigenvalue spectrum

Method example: Transverse Field Ising model

A.1 Second quantisation

The Transverse Field Ising model in 1D is exactly diagonalised. First calculated by [53], the procedure followed is: Jordan-Wigner transformation $\rightarrow$ Fourier transform $\rightarrow$ Bogoliubov transformation.

The first step rewrites the Hamiltonian in second quantisation language as creation and annihilation operators

\[
a_i^\dagger \equiv S_i^x + iS_i^y, \quad a_i \equiv S_i^x - iS_i^y
\]  

spin operator terms are derived and combined to form the Hamiltonian.

The transverse field from the product of (A.1) and (A.2)

\[
a_i^\dagger a_i = (S_i^x + iS_i^y)(S_i^x - iS_i^y) = S_i^z - (S_i^x)^2 + i[S_i^x, S_i^y]
\]  

\[
= s(s + 1) - (m_s)^2 + S_i^z
\]  

where $s = \frac{1}{2}$, $\hbar = 1$ (dimensionless) and $m_s = \pm \frac{1}{2}$, therefore,

\[
S_i^z = a_i^\dagger a_i - \frac{1}{2}
\]  

97
and the quadratic term can be found from the product of the following two terms,

\[ a_i^\dagger + a_i = 2S_x^i \]  
\[ a_{i+1}^\dagger + a_{i+1} = 2S_x^{i+1} \]  

The Hamiltonian 4.2 becomes,

\[ H = -\sum_i \left[ \frac{J}{4} \left( a_i^\dagger + a_i \right) \left( a_{i+1}^\dagger + a_{i+1} \right) + h \left( a_i^\dagger a_i - \frac{1}{2} \right) \right] \]  

\[ (A.8) \]

A.2 Jordan-Wigner transformation

The creation and annihilation operators must satisfy fermionic commutation relations \( \{ a_i^\dagger, a_j \} = \delta_{i,j}, \{ a_i^\dagger, a_j^\dagger \} = 0 \) and \( \{ a_i, a_j \} = 0 \). But presently, \( [a_i^\dagger, a_j] = 0 \) for \( i \neq j \). They commute like bosons between sites, which is a problem for modelling a chain of fermions. Independent non-interacting fermions need to anti-commute to obey the Pauli exclusion principle. Using the Jordan-Wigner transformation \[89\] a string function introduces a phase factor to the operators, defining new ‘\( c \)’-operators

\[ a_i^\dagger \equiv c_i^\dagger \exp \left[ \pi i \sum_{j=1}^{i-1} a_j^\dagger a_j \right] \quad a_i \equiv \exp \left[ -\pi i \sum_{j=1}^{i-1} a_j^\dagger a_j \right] c_i \]  
\[ (A.9) \]

the second being the conjugate of the first. This saves the representation by recovering the appropriate anti-commutation relations \( \{ c_i^\dagger, c_j \} = \delta_{i,j}, \{ c_i^\dagger, c_j^\dagger \} = 0 \) and \( \{ c_i, c_j \} = 0 \). Applying this

\[ H = -\sum_i \left[ h \left( c_i^\dagger c_i - \frac{1}{2} \right) + \frac{J}{4} \left( c_i^\dagger - c_i \right) \left( c_{i+1}^\dagger + c_{i+1} \right) \right] \]

\[ + \frac{J}{4} \left( c_N^\dagger - c_N \right) \left( c_1^\dagger + c_1 \right) \left( \exp[i\pi \sum_{j=1}^{N} c_j^\dagger c_j] + 1 \right) \]  
\[ (A.10) \]

at the boundary the correction term (second line of \( (A.10) \)) at \( i = N \) is negligible for large systems.
A.3 Fourier transformation

Transforming into Fourier space,
\[ c_k = \frac{1}{\sqrt{N}} \sum_j c_j \exp(i k a j) \]  \hspace{1cm} (A.11)

\[ c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j c_j^\dagger \exp(-i k a j) \]  \hspace{1cm} (A.12)

expand the second term in (A.10)
\[ \sum_i (c_i^\dagger - c_i) (c_{i+1}^\dagger + c_{i+1}) = \sum_i \left( c_i^\dagger c_{i+1}^\dagger - c_i c_{i+1}^\dagger + c_i^\dagger c_{i+1} - c_i c_{i+1} \right) \]  \hspace{1cm} (A.13)

where the lattice spacing \( a = 1 \), and by carefully considering summations and Dirac delta functions the transformation into momentum space reduces the problem making all terms dependent on only \( k \) as follows
\[ \sum_i c_i^\dagger c_{i+1} = \sum_{k,k'} \exp(i k') c_k^\dagger c_k^\prime \frac{1}{N} \sum_j \exp(i j (k-k')) \]
\[ = \sum_{k,k'} \exp(i k') c_k^\dagger c_k^\prime \delta(k-k') \]
\[ = \sum_k \exp(i k) c_k^\dagger c_k \]  \hspace{1cm} (A.14)

\[ \sum_i c_i c_{i+1} = \sum_{k,k'} \exp(i k') c_k c_k^\prime \frac{1}{N} \sum_j \exp(i j (k+k')) \]
\[ = \sum_{k,k'} \exp(i k') c_k c_k^\prime \delta(k+k') \]
\[ = \sum_k \exp(-i k) c_k c_{-k} \]
\[ = \frac{1}{2} \sum_k \exp(-i k) c_k c_{-k} + \exp(i k) c_{-k} c_k \]
\[ = \frac{1}{2} \sum_k c_k c_{-k} \left( \exp(-i k) - \exp(i k) \right) \]
\[ = \sum_k (-i \sin k) c_k c_{-k} \]  \hspace{1cm} (A.15)
with the preference of keeping $k$ instead of $k'$ after the sum is evaluated.

Performing the Fourier transform for all terms in (A.13) using (A.14), (A.15) and their Hermitian conjugates

$$\sum_k \left( \exp(ik)c_k^\dagger c_k + \exp(-ik)c_k^\dagger c_k - i \sin k \ c_k c_{-k} - i \sin k \ c_{-k}^\dagger c_k^\dagger \right)$$  \hspace{1cm} (A.16)

The Hamiltonian (A.10) becomes

$$-\sum_k \left( \left[ \frac{J}{2} \cos k + h \right] c_k^\dagger c_k - \frac{iJ}{4} \sin k \left[ c_{-k}^\dagger c_k^\dagger + c_{-k} c_k \right] - \frac{h}{2} \right)$$  \hspace{1cm} (A.17)

### A.4 Bogoliubov transformation

Finally the Bogoliubov transform introduces new $\gamma$-operators

$$\gamma_k = u_k c_k + iv_k c_{-k}^\dagger$$  \hspace{1cm} (A.18)

$$\gamma_{-k}^\dagger = u_k c_{-k}^\dagger + iv_k c_k$$  \hspace{1cm} (A.19)

with the inverse transformations summarised below

$$
\begin{align*}
c_k &= u_k \gamma_k + iv_k \gamma_{-k}^\dagger & u_{-k} &= u_k \\
c_k^\dagger &= u_k \gamma_k^\dagger - iv_k \gamma_{-k} & v_{-k} &= -v_k \\
c_{-k} &= u_k \gamma_{-k} - iv_k \gamma_k^\dagger & u_k^2 + v_k^2 &= 1 \\
c_{-k}^\dagger &= u_k \gamma_{-k}^\dagger + iv_k \gamma_k & c_{-k}^\dagger c_{-k} &= \frac{1}{2}
\end{align*}
$$

The right column includes restrictions on $u$ and $v$. They are real numbers with a square sum equal to one. The three operator products in (A.17) are evaluated in terms of Bogoliubov fermions. The diagonal term

$$c_k^\dagger c_k = (u_k \gamma_k^\dagger - iv_k \gamma_{-k})(u_k \gamma_k + iv_k \gamma_{-k}^\dagger)$$

$$= u_k^2 \gamma_k^\dagger \gamma_k + iv_k v_k \gamma_k^\dagger \gamma_{-k}^\dagger - iv_k u_k \gamma_{-k} \gamma_k + v_k^2 \gamma_{-k}^\dagger \gamma_{-k}$$

$$= u_k^2 \gamma_k^\dagger \gamma_k + v_k^2 (1 - \gamma_{-k}^\dagger \gamma_{-k}) + iu_k v_k \gamma_k^\dagger \gamma_{-k}^\dagger + iv_k u_k \gamma_{-k} \gamma_k$$  \hspace{1cm} (A.20)
and the two off-diagonal terms

\[
c^\dagger_{-k}c^\dagger_k = (u^\dagger_k \gamma^\dagger_{-k} + iv_k \gamma_k)(u^\dagger_k \gamma^\dagger_k - iv_k \gamma_{-k})
\]

\[
= u^2_{k\gamma^\dagger_{-k}} - u^2_{k\gamma^\dagger_k} + iv_k v_k \gamma_k \gamma_{-k} + u^2_{k\gamma^\dagger_k} - iv_k v_k \gamma_{-k}
\]

\[
= -iv_k v_k \gamma_{-k} + u^2_{k\gamma^\dagger_{-k}} - iv_k v_k (1 - \gamma^\dagger_k \gamma_k) + u^2_{k\gamma^\dagger_k} - iv_k v_k \gamma_{-k} \tag{A.21}
\]

\[
c_{-k}c_k = (u^\dagger_k \gamma_{-k} - iv_k \gamma_{-k}^\dagger)(u_k \gamma_k + iv_k \gamma_{-k}^\dagger)
\]

\[
= u^2_{k\gamma_{-k}} - u^2_{k\gamma_{-k}^\dagger} - iv_k v_k \gamma_{-k} + u^2_{k\gamma_{-k}^\dagger} - iv_k v_k \gamma_{-k}
\]

\[
= -iv_k v_k \gamma_{-k} - iv_k v_k (1 - \gamma^\dagger_k \gamma_{-k}) + u^2_{k\gamma^\dagger_{-k}} - iv_k v_k \gamma_{-k} \tag{A.22}
\]

Collecting identical fermion operators with \( A = \left[ \frac{\gamma}{2} \cos k + h \right] \) and \( B = \left[ \frac{i\gamma}{4} \sin k \right] \)

\[
H = -\sum_k A \left[ (u^2_k - v^2_k) \gamma^\dagger_{-k} + v^2_k \right] - B \left[ (-4iv_k v_k) \gamma^\dagger_k \gamma_k + 2iv_k v_k \right] - \frac{h}{2}
\]

\[
+ \left[ A (iv_k v_k) + B \left( u^2_k - v^2_k \right) \right] \gamma^\dagger_{-k} + \left[ A (iv_k v_k) + B \left( u^2_k - v^2_k \right) \right] \gamma_{-k}
\]

\[
= -\sum_k \left[ A (u^2_k - v^2_k) + 4iB(u_k v_k) \right] \gamma^\dagger_{-k} + Av^2 - 2iB(u_k v_k) - \frac{h}{2}
\]

\[
+ \left[ A (iv_k v_k) + B \left( u^2_k - v^2_k \right) \right] \left( \gamma^\dagger_{-k} + \gamma_{-k} \right) \tag{A.23}
\]

restating \( (Av^2 - \frac{h}{2}) \) by adding a sum zero term \( \left( \frac{\gamma}{4} u^2_k \cos k - \frac{\gamma}{4} v^2_k \cos k \right) \) to factorise into a more convenient form \( -\left( \frac{\gamma}{4} \cos k + \frac{\gamma}{4} \right) \left( u^2_k - v^2_k \right) \)\( + \frac{\gamma}{4} \cos k = -\frac{1}{2} \left( u^2_k - v^2_k \right) + \frac{\gamma}{4} \cos k \), a constant can be brought outside the bracket

\[
H = -\sum_k \left[ A (u^2_k - v^2_k) + 4iB(u_k v_k) \right] \left( \gamma^\dagger_{-k} - \frac{1}{2} \right)
\]

\[
+ \left[ A (iv_k v_k) + B \left( u^2_k - v^2_k \right) \right] \left( \gamma^\dagger_{-k} + \gamma_{-k} \right) \tag{A.24}
\]

where \( \sum_k \cos k = 0 \).

To eliminate the off-diagonal contribution, set to zero

\[
\left[ A (iv_k v_k) + B \left( u^2_k - v^2_k \right) \right] = 0 \tag{A.25}
\]
which rearranges to
\[ \frac{u_k v_k}{u_k^2 - v_k^2} = -\frac{B}{A_i} \] (A.26)

The Bogoliubov-de Gennes equations form linear expressions of the \( c \) operators in terms of \( u_k \) and \( v_k \)
\[ [c_k, H] = -\sum_{k'} A[c_k, c_{k'}^\dagger] - B \left( [c_k, c_{-k'}^\dagger c_{k'}] + [c_k, c_{-k'} c_{k'}^\dagger] \right) \]
\[ = -\sum_{k'} A c_{k'} \delta_{k,k'} - B \left( c_{k'}^\dagger \delta_{k,-k'} - c_{-k'}^\dagger \delta_{k,k'} \right) \]
\[ = -(A c_{-k} - 2B c_{-k}^\dagger) \]
into \( \gamma \)-operators
\[ = - \left( A (u_k \gamma_k + iv_k \gamma_{-k}^\dagger) - 2B \left( u_k \gamma_{-k}^\dagger + iv_k \gamma_k \right) \right) \]
\[ = - \left( (A u_k - 2B iv_k) \gamma_k + (Aiv_k - 2Bu_k) \gamma_{-k}^\dagger \right) \] (A.27)
alternatively we can equate this starting with \( \gamma \)-operators with commutation relation
\[ [c_k, H] = [u_k \gamma_k + iv_k \gamma_{-k}^\dagger, H] \]
\[ = u_k [\gamma_k, H] + iv_k [\gamma_{-k}^\dagger, H] \]
\[ = \sum_{k'} u_{k'} \epsilon_{k'} \gamma_{k'} \delta_{k,k'} - iv_{k'} \epsilon_{k'} \gamma_{-k}^\dagger \delta_{k,k'} \]
\[ = u_k \epsilon_k \gamma_k - iv_k \epsilon_{-k} \gamma_{-k}^\dagger \]
then just match the coefficients in the two methods
\[ u_k \epsilon_k = -Au_k + 2Biv_k \] (A.28)
\[ -iv_k \epsilon_{-k} = -Aiv_k + 2Bu_k \] (A.29)
and since \( \epsilon_k^2 = (u_k \epsilon_k)^2 + (v_k \epsilon_k)^2 \) this leads to
\[ \epsilon_k = \sqrt{\left( \frac{J}{2} \right)^2 + h^2 + Jh \cos k} \] (A.30)
The diagonalised Hamiltonian is finally written as,
\[ H = \sum_k \epsilon_k \left( \gamma_k^\dagger \gamma_k - \frac{1}{2} \right) \] (A.31)
Appendix B

Energy current calculation

By applying a form of energy flow, inducing a non-equilibrium state, the behaviour of systems under flux can be investigated. The energy current we consider creates a non-equilibrium steady-state (NESS). The importance of a steady-state is that it allows energy to move through the system at a constant rate in a continuous manner, there are no impulses causing discontinuous energy transfer. It is conserved and thus characterised by a conservation law. This is expressed in the form of the following continuity equation [73]

\[ \frac{\partial h_{i,i+1}(t)}{\partial t} + \Delta j_i = 0 \]  (B.1)

importance placed on \( \Delta j_i = j_{i+1} - j_i \) the discrete divergence of the current.

Applying a unitary transformation (Heisenberg picture)

\[ h_{i,i+1}(t) = U h_{i,i+1} U^{-1} = e^{iHt} h_{i,i+1} e^{-iHt} \]

the derivative can now be taken

\[ \frac{\partial h_{i,i+1}(t)}{\partial t} = U h_{i,i+1} \frac{\partial (U^{-1})}{\partial t} + U \frac{\partial (h_{i,i+1})}{\partial t} U^{-1} \]
\[ + \frac{\partial (U)}{\partial t} h_{i,i+1} U^{-1} \]
\[ = U h_{i,i+1} (-iH) U^{-1} + (iH) U h_{i,i+1} U^{-1} \]
\[ = i[H, h_{i,i+1}(t)] \]  (B.4)
where we have made use of \( dU/dt = iHU \) and \([H, U] = [H, U^{-1}] = 0\) to find the commutation relation in the final line.

Simplifying this commutator with \( H = h_{1.2} + \cdots + h_{i,i+1} + \cdots + h_{N,N+1} \) and \([h_{i,i+1}, h_{i-1,i}] \neq 0\)

\[
i[H, h_{i,i-1}(t)] = iH h_{i,i+1}(t) - ih_{i,i+1}(t)H
= i(h_{i-1,i} h_{i,i+1}(t) + h_{i+1,i+2} h_{i,i+1}(t))
- i(h_{i,i+1}(t) h_{i-1,i} + h_{i,i+1}(t) h_{i+1,i+2})
= i[h_{i-1,i}, h_{i,i+1}(t)] - i[h_{i,i+1}(t), h_{i+1,i+2}]\]

These two commutation relations have dependencies on the previous \( i - 1 \) and next \( i + 1 \) sites. They can be identified as the local current operators \( j_i \) and \( j_{i+1} \) respectively, and referring back to the original continuity equation (B.1)

\[
\frac{\partial h_{i,i+1}(t)}{\partial t} = j_i(t) - j_{i+1}(t)
\]

this gives an explicit calculation for the two local current operators \( \Delta j_i \) with a comparison of (B.1) to (B.8). Therefore the energy current equation is

\[
j^E_i = -i[h_{i-1,i}, h_{i,i+1}]\]