# Quantum Phase Transitions in an Integrable One-Dimensional Spin Model

*Master of Science Thesis*

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**Abstract**

A one-dimensional spin model, recently introduced and solved exactly, is studied. The solution, showing the appearance of a first-order quantum phase transition, is explicitly carried out and verified. Moreover, new results are found by generalizing the model to include anisotropy, thereby giving additional phases with both first-order and continuous quantum phase transitions. These transitions are shown to coincide at the critical point of the original model, thus explaining its behaviour. The one-dimensional quantum compass model is shown to be a special case of this generalized model, and is described by a spin liquid with a quantum Ising type of behaviour. The entanglement present in the generalized model is also calculated, showing the absence of concurrence, but large localizable entanglement, for spins that are not nearest neighbours. The block entropy is shown to be fully equivalent to that of the corresponding quantum Ising model.

# Contents

# Chapter 1

# Introduction

This thesis will focus on a one-dimensional spin model recently introduced by Brzezicki, Dziarmaga and Oleś [1], with emphasis on the quantum phase transition it exhibits. The study of quantum phase transitions, where the ground state changes in some fundamental way as a parameter is varied [2], and in particular their relation to the concept of quantum entanglement, i.e. completely non-classical correlations between different parts of a system [3], have attracted much attention. New phases of matter, often with exotic behaviour, have been found in many systems, and in the search for new tools to describe the transitions between them, entanglement is seen as a promising alternative [4]. It not only captures the correlations that inherently show up near phase transitions, but is also recognized as a valuable resource that enables new technologies such as quantum computing and quantum communication [5]. In the search for systems that can serve as building blocks in possible quantum computers, recent results [6] have shown that a spin model, the two-dimensional quantum compass model, which can be realized as an array of superconducting Josephson junctions, has properties making it suitable as a noise-protected qubit. This model, which has not been solved exactly, shows a first-order quantum phase transition, with discontinuous correlation functions [7]. As the model has been suspected to exhibit effective dimensionality reduction into one-dimensional spin chains [8], it has been found necessary to better understand the nature of first-order quantum phase transitions in one-dimensional spin models. The model we shall study was designed to show how such transitions can occur.

The thesis is organized as follows. In this introductory chapter, basic theory of quantum phase transitions and entanglement is reviewed. Chap. 2 introduces the two-dimensional quantum compass model, studied in the context of protected qubits. In Chap. 3, the one-dimensional "XX-ZZ" model, introduced and solved by Brzezicki et al., is investi-

gated. The solution of the model, by mapping onto the exactly solvable quantum Ising model in different subspaces and proceeding with a series of transformations, is explicitly carried out. In Chap. 4 new results are presented by generalizing the XX-ZZ model to include different coupling constants of the spin $x$ and $z$ components, showing the emergence of new phases and phase transitions. By this generalization, the nature of the quantum phase transition in the XX-ZZ model is elucidated. Chap. 5 treats the one-dimensional quantum compass model, shown to be a special case of the generalized XX-ZZ model, and therefore its solution is easily accessible. The entanglement in the generalized XX-ZZ model is calculated in Chap. 6. Finally, the concluding remarks in Chap. 7 summarize this thesis.

## 1.1   Quantum Phase Transitions

A quantum phase transition, as opposed to a classical phase transition, takes place at the absolute zero of temperature [9],[2]. This means that the quantum ground state of the system changes in some fundamental way as we cross the phase boundary by varying not the temperature, but some parameter in the Hamiltonian. Note that classical phase transitions are driven only by thermal fluctuations, therefore they cannot occur at zero temperature since the classical system then freezes into a fluctuationless ground state. Quantum systems however do have fluctuations due to the Heisenberg uncertainty principle even in the ground state. These purely quantum fluctuations can then drive phase transitions at zero temperature. Quantum phase transitions, QPTs, are therefore qualitatively different, and their critical behaviour must be treated quantum mechanically.

As an example, let us consider a lattice Hamiltonian $H(g)$ that depends on a dimensionless coupling constant $g$, and where $g$ only couples to a conserved quantity. This means that the Hamiltonian can be written as $H(g) = H_0 + gH_1$, where $H_0$ and $H_1$ commute, and therefore $H_0$ and $H_1$ can be simultaneously diagonalized so that the eigenfunctions will be independent of $g$ although the eigenvalues will depend on $g$. We can then have a level crossing at a point $g = g_c$ where an excited level becomes the ground state, and this will create a non-analyticity of the ground state energy as a function of $g$. We may also have an avoided level crossing, where the levels do not actually cross in a finite lattice but where the ground state energy at this point becomes non-analytic in the infinite lattice limit, called the thermodynamic limit. For a general Hamiltonian, a quantum phase transition can be identified as a point of non-analyticity in the ground state energy of the infinite lattice system. In analogy with classical phase transitions we may define a quantum

phase transition having a discontinuous first derivative of the ground state energy as being "first-order". If the first derivative of the ground state energy is continuous but higher order derivatives are discontinuous, the QPT is called "continuous".

In contrast to the quantum phase transitions at zero temperature, all non-zero temperature continuous phase transitions are to be considered as classical. At a continuous phase transition the correlation time diverges, meaning that the coherent fluctuations in the order parameter become increasingly slower. Therefore the frequency associated with the critical fluctuations vanishes at the transition. Since a quantum system behaves classically if the temperature is much larger than all frequencies of the the system, we conclude that at non-zero temperatures the critical fluctuations will behave classically. This is true even in such highly quantum mechanical systems as superconductors and superfluid helium, because it is only the mere existence of the order parameter that is due to quantum mechanics. At long wavelengths the order parameter is governed by classical thermal fluctuations, which therefore govern the critical behaviour, for example by doing classical statistical mechanics with the Ginzburg-Landau free energy functional.

To see what happens when the temperature $T$ goes to zero, we focus our attention on the partition function $Z$

$$Z(\beta) = \operatorname{tr} e^{-\beta H}, \tag{1.1}$$

where $H$ is the Hamiltonian of the system, and $\beta \equiv 1/k_B T$. All other thermodynamic quantities can be obtained from $Z$. We now notice that the operator $e^{-\beta H}$ is equivalent to the time evolution operator $e^{-iHt/\hbar}$, if we identify the time interval $t$ with the imaginary value $t = -i\hbar\beta$. So when we write the partition function as

$$Z(\beta) = \sum_n \langle n|e^{-\beta H}|n\rangle, \tag{1.2}$$

where $n$ runs over a complete set of states, we see that $Z$ is the sum of imaginary-time transition amplitudes for the system to return to the same state after imaginary time $t = -i\hbar\beta$. So calculating the thermodynamics of a quantum system is the same as calculating the dynamics in imaginary time. This is very different from the case in classical statistical mechanics, where the dynamics and thermodynamics of a system always can be treated separately, i.e. where the position and momentum sums in the partition function are totally independent. In the quantum case position and momentum do not commute, and therefore we will not be able to separate dynamics and thermodynamics, making the situation more elaborate.

Taking things one step further, we may write

$$e^{-\beta H} = \left(e^{-\delta\tau H/\hbar}\right)^N, \tag{1.3}$$

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where $\delta\tau$ is an imaginary time interval that is small on the relevant time scales, and $N$ is a large integer such that $N\delta\tau = \hbar\beta$. Then we can insert a complete set of states between every factor in the expression for $Z$ in Eq. (1.2), which gives

$$Z(\beta) = \sum_n \sum_{m_1, m_2, \ldots, m_N} \langle n|e^{-\delta\tau H/\hbar}|m_1\rangle \times$$

$$\times \langle m_1|e^{-\delta\tau H/\hbar}|m_2\rangle \langle m_2| \cdots |m_N\rangle \langle m_N|e^{-\delta\tau H/\hbar}|n\rangle . \tag{1.4}$$

This expression for the quantum partition function has the same form as a classical partition function expressed in terms of a transfer matrix $\mathbf{T}$, if we identify $\mathbf{T}$ with $e^{-\delta\tau H/\hbar}$. The imaginary time dimension of the quantum system may therefore be treated as an additional spacial dimension of a classical system. So if we have a $d$-dimensional quantum system, it will have a partition function that looks like a classical partition function for a classical system in $d+1$ dimensions. This extra spacial dimension will however be finite in extent, its size limited to $\hbar\beta$ in units of time. But when $T \to 0$ the size of the additional spacial dimension diverges and the dual classical system gets fully $d+1$-dimensional. We may thus conclude that a quantum system in $d$ dimensions at zero temperature is closely connected to a classical system in $d+1$ dimensions (note however that this does not imply that the quantum system behaves classically, since one of the $d+1$ spacial dimensions corresponds to time in the quantum system). We may therefore expect to be able to describe quantum phase transitions using the same tools as for classical phase transitions. In particular, since diverging correlation lengths are a generic feature of classical continuous phase transitions, this implies diverging correlation length $\xi$ and correlation time $\xi_\tau$ at the continuous QPT, since both are effective correlation lengths in a dual classical system. We also expect that as the system approaches the quantum critical point by letting the parameter $g$ move towards $g_c$, they will diverge according to some critical exponents

$$\xi \sim |g - g_c|^{-\nu} , \tag{1.5}$$

$$\xi_\tau \sim \xi^z , \tag{1.6}$$

where $\nu$ is the correlation length exponent and $z$ is the dynamical-scaling exponent. The characteristic energy scale $\Delta$, given by the energy gap to the lowest excitation above the ground state, then vanishes as

$$\Delta \sim \xi_\tau^{-1} \sim |g - g_c|^{z\nu} \tag{1.7}$$

when $g \to g_c$.

We now shortly remark on the effect of a non-zero temperature. After all, this is always the case when doing a physical experiment. Since

the size $L_\tau$ of the extra spacial dimension is given by $\hbar\beta$, this means that as the temperature is increased, $L_\tau$ decreases. As long as $g$ is far enough away from the critical point $g_c$ for the correlation time $\xi_\tau$ to be smaller than $L_\tau$, the non-zero temperature does not affect the behaviour of the system. That is, the system is quantum mechanical since the characteristic fluctuations obey $\hbar\omega \gg k_B T$ at low temperatures. But when $g \to g_c$ we will eventually have $\xi_\tau > \hbar\beta$, and the system will then effectively be a $d$-dimensional classical system rather than a $d+1$-dimensional system, and the transition may therefore be of a different universality class than at $T = 0$. The formal theory of the effect of reduced dimensionality near critical points is known as "finite-size scaling". Close to the quantum critical point $g = g_c$ at $T = 0$, the transition from the $T = 0$ behaviour to the $T \neq 0$ behaviour is controlled by the physics at the quantum critical point [2]. That is, when the temperature is larger than the energy gap, $T > \Delta$, the system will be excited, and the physics is governed by the thermal excitations of the quantum critical point. Quantum and thermal effects will here play an equal role, so that the system will not be classical, but described by a continuum quantum field theory. This region above the quantum critical point is known as "quantum critical", cf. Fig. (1.1), and has many unusual features that are accessible to experiments.
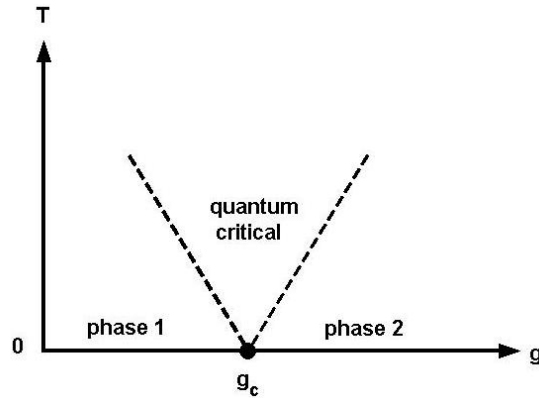


Figure 1.1: *Typical phase diagram of a system near a quantum critical point at $g = g_c$ and $T = 0$. The quantum critical region is bounded below by the energy gap $\Delta$, Eq. (1.7), and its properties are universal. There is also another class of systems where the quantum critical point at the same time is the end point of a classical phase boundary.*

Let us conclude by giving some examples of systems exhibiting quantum phase transitions. The insulators $CsCoBr_3$ and $CsCoCl_3$ behave as one-dimensional Ising magnets, and when placed in a magnetic field they are described by the one-dimensional quantum Ising model. This

model (which we will come across later on) has a continuos QPT at a critical value of the magnetic field strength. The heavy fermion material $CeCu_{6-x}Au_x$ shows a continuous QPT at a critical value of the doping $x$, where the material goes from being magnetically ordered to magnetically disordered. Quantum Hall systems, i.e. two-dimensional electron systems in transverse magnetic fields, show a rich phase diagram with a number of QPTs. First-order QPTs are found in the itinerant-electron magnets MnSi and $UGe_2$ at a critical pressure, where the exponent describing the temperature dependence of the electrical resistivity, and the magnetization, respectively, are discontinuous [10].

## 1.2 Entanglement

As we have seen, both classical and quantum continuous phase transitions show diverging correlation lengths. However, quantum systems have additional correlations that have no classical analogues, namely the correlations between presently noninteracting particles that have interacted in the past, as appearing in the famous EPR effect. These correlations come from the phenomenon of entanglement, a very counter-intuitive part of quantum mechanics that contradicts locality, one of the cornerstones of classical physics [3],[11],[12],[13]. It is now recognized that these non-local correlations, shown to be a physical reality, are a precious resource, enabling quantum computing and quantum communication [5]. Entanglement also seems to be a fundamental feature of quantum phase transitions in many-body systems [14], which have given rise to intense research on the borderline between condensed matter physics and quantum information during the last years. Since the ground state of a many-body system typically consists of a superposition of a huge number of product states, understanding this structure is equivalent to understanding how different subsystems are interrelated, i.e. entangled [15]. The long-range correlations that appear near a continuous QPT must be due to long-range entanglement in the ground state of the system, since an unentangled state always has vanishing correlation functions [16]. We may therefore expect entanglement to characterize the QPT. Actually, it has been shown that quantum phase transitions in a wide class of systems are signaled by the behaviour of the entanglement near the critical point [17]. There has even been hopes that entanglement may provide a unified framework for the understanding of complex quantum systems, since a large number of seemingly different quantum states turn out to be equivalent regarding their entanglement content [4]. Then one could possibly develop universal principles governing the behaviour of entangled states, just as the laws of thermodynamics govern the behaviour of the energy, independent of

the particular physical representation.

In order to quantify the entanglement of a system, let us start with the basic building block in quantum information, the qubit, being a state vector in a two-dimensional Hilbert space. Letting $|0\rangle$ and $|1\rangle$ be the orthogonal basis of this Hilbert space, the qubit can be in any complex linear combination of these two basis states,

$$|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle, \tag{1.8}$$

where $|\alpha|^2 + |\beta|^2 = 1$. By writing $\alpha \equiv \cos(\theta/2)$ and $\beta \equiv e^{i\phi}\sin(\theta/2)$, where $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$, we see that the single qubit can be represented as a vector on a sphere, called the "Bloch sphere". One of the most obvious ways to physically realize a qubit is as the spin of a spin-1/2 particle, and this is indeed what we will do in subsequent chapters. However, as we also shall see, an entire many-body system may also serve as a qubit.

Now, let us consider composite systems, i.e. systems made up of many components, e.g. several qubits. A general composite system is said to be in an entangled state if it cannot be written as a tensor product of states of its components. That is, it cannot be written as $|\Psi\rangle = |\phi_1\rangle|\phi_2\rangle \cdots |\phi_N\rangle$, where $|\phi_i\rangle$ is the single-component state of part $i$ (we will use the notation $|\phi_i\rangle|\phi_j\rangle \equiv |\phi_i\rangle \otimes |\phi_j\rangle$). There will then be correlations between the subsystems, since a measurement on one subsystem will affect measurements on the others, and these correlations are seen to be purely quantum mechanical.

The state $|\Psi\rangle = (1/\sqrt{2})(|0\rangle|0\rangle + |1\rangle|1\rangle)$ is an example of an entangled state, since it cannot be written as a tensor product of single-qubit states. In fact, it is maximally entangled, since the outcome of a measurement on one of the qubits completely determines the outcome of a subsequent measurement on the other. The state is one of the four maximally entangled two-qubit states, the "Bell states"

$$
\begin{aligned}
|\Psi_1\rangle &= (1/\sqrt{2})(|00\rangle + |11\rangle), \\
|\Psi_2\rangle &= (1/\sqrt{2})(|01\rangle + |10\rangle), \\
|\Psi_3\rangle &= (1/\sqrt{2})(|00\rangle - |11\rangle), \\
|\Psi_4\rangle &= (1/\sqrt{2})(|01\rangle - |10\rangle),
\end{aligned} \tag{1.9}
$$

where we use the notation $|11\rangle \equiv |1\rangle|1\rangle$. When we quantify the amount of entanglement in a general system the minimum value will correspond to an unentangled state, and the maximum value to some (generalized) Bell state.

The amount of entanglement is generally difficult to define, but in the case of a bipartite system, i.e. a system consisting of only two components, it turns out to be fairly easy. Consider first a pure bipartite

state $|\Psi\rangle$, i.e. the density operator is given by $\rho_{ij} = |\Psi\rangle\langle\Psi|$. The reduced density operators of the subsystems $i$ and $j$ are given by $\rho_i = \mathrm{tr}_j(\rho_{ij})$ and $\rho_j = \mathrm{tr}_i(\rho_{ij})$ respectively, where $\mathrm{tr}_\alpha$ is the partial trace over subsystem $\alpha = i, j$ [5]. For a pure bipartite state $|\Psi\rangle$ it turns out that there is only one unique entanglement measure, namely the **von Neumann entropy**, S, given by [11]

$$S(\Psi) = -\mathrm{tr}(\rho_\alpha \log_2 \rho_\alpha) = -\sum_n \lambda_n \log_2 \lambda_n \,, \qquad (1.10)$$

where $\alpha$ is either $i$ or $j$, $\rho_\alpha$ is the reduced density matrix of subsystem $\alpha$, and $\lambda_n$ is the $n$th eigenvalue of $\rho_\alpha$. We see that the amount of entanglement in the system is completely determined by the eigenvalues of any of the two subsystems.

Next we consider mixed bipartite states. As subsystems of a many-body system generally are in a mixed state, these are of particular importance. Things are now a bit more complicated though, as there is no unique entanglement measure for mixed states. We will consider some of the more common ones. The first one is the **entanglement of formation**. A pair of quantum systems in a mixed state will have a density matrix $\rho_{ij}$ that can be decomposed in an infinite number of ways into ensembles of pure states $|\Psi_n\rangle$ with probabilities $p_n$, so that

$$\rho_{ij} = \sum_n p_n |\Psi_n\rangle\langle\Psi_n| \,. \qquad (1.11)$$

The entanglement of formation $E_F(\rho_{ij})$ of the mixed state $\rho_{ij}$ is then defined as the average entanglement of the pure states of its decompostion, minimized over all possible decompositions [11],[13]

$$E_F(\rho_{ij}) = \min \sum_n p_n S(\Psi_n) \,, \qquad (1.12)$$

where $S(\Psi_n)$ is the von Neumann entropy of the pure state $|\Psi_n\rangle$. The physical idea behind this entanglement measure is that it quantifies the amount of entanglement needed to create the mixed state $\rho_{ij}$, without transferring quantum states [13].

For a system $\rho_{ij}$ of two qubits the entanglement of formation can be expressed as a function of a quantity called the **concurrence**, $C(\rho_{ij})$, according to [18]

$$E_F(\rho_{ij}) = h\left(\frac{1 + \sqrt{1 - C^2(\rho_{ij})}}{2}\right) \,, \qquad (1.13)$$

where the function $h$, called the "binary entropy function" is given by

$$h(x) = -x \log_2 x - (1 - x) \log_2(1 - x) \,. \qquad (1.14)$$

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As $E_F(C(\rho_{ij}))$ is monotonically increasing from 0 to 1 as $C(\rho_{ij})$ goes from 0 to 1, we may just as well use the concurrence as entanglement measure. For a *pure* state $|\Psi\rangle$ of two qubits, the concurrence is defined as [19]

$$C(\Psi) = |\langle\Psi|\tilde{\Psi}\rangle|, \qquad (1.15)$$

where the tilde denotes the flipped state $|\tilde{\Psi}\rangle = (\sigma^y \otimes \sigma^y)|\Psi^*\rangle$, where $|\Psi^*\rangle$ is the complex conjugate of $|\Psi\rangle$ when expressed in a given basis. $\sigma$ denotes the Pauli matrices. In a spin system the flipped state of course corresponds to the time-reversed state. So we see that for a pure state the concurrence measures the overlap between the states before and after the qubits have been flipped. For a product state there is of course no overlap, so the concurrence will be 0, and for the Bell states in Eq. (1.9) there is total overlap, so the concurrence will be 1. For a general state of two qubits we have to consider the density matrix $\rho_{ij}$ and the flipped density matrix

$$\tilde{\rho}_{ij} = (\sigma^y \otimes \sigma^y)\,\rho_{ij}^*\,(\sigma^y \otimes \sigma^y), \qquad (1.16)$$

where $\rho_{ij}^*$ is the complex conjugate of $\rho_{ij}$ in a given basis. The concurrence $C(\rho_{ij})$ is then given by [11],[18]

$$C(\rho_{ij}) = \max\left\{0,\, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\right\}, \qquad (1.17)$$

where $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ are the non-negative real eigenvalues of the Hermitian matrix

$$R \equiv \sqrt{\sqrt{\rho_{ij}}\tilde{\rho}_{ij}\sqrt{\rho_{ij}}}. \qquad (1.18)$$

Equivalently, the $\lambda_i$s are the square roots of the eigenvalues of the non-Hermitian matrix $\rho_{ij}\tilde{\rho}_{ij}$.

It has been shown for a quite general class of systems that the concurrence, and therefore also the entanglement of formation, has a strong connection to quantum phase transitions [17]. For these systems, a discontinuity in the concurrence is both necessary and sufficient to signal a first-order QPT. Similarly, a discontinuity or divergence in the first derivative of the concurrence is both necessary and sufficient to signal a continuous QPT.

Another set of entanglement measures arises when quantifying the amount of entanglement that can be localized to a pair of qubits by doing measurements on the rest of the system. The **localizable entanglement**, $E_L(\rho_{ij})$, is defined as the maximal amount of entanglement that can be localized in this pair by doing *local* measurements, where the measurement basis only consists of single site states, on the rest of the system [20]. In contrast, the **entanglement of assistance**, $A(\rho_{ij})$, is similarly defined except that we now allow *global* measurements, where the measurement basis may also consist of states composed of many single site states, on the rest of the system [20]. Therefore the

entanglement of assistance provides an upper bound for the localizable entanglement. Both can formally be written as [20],[21]

$$E(\rho_{ij}) = \max_{\Omega} \sum_n p_n S(\Psi_n) \,, \qquad (1.19)$$

where $\Omega = \{p_n, |\Psi_n\rangle\}$ are the pure state ensembles of the pair specified by each measurement basis, and $p_n$ denotes the probability that the pair will be in state $|\Psi_n\rangle$ after performing measurements on the rest of the system. In analogy with Eq. (1.19) the **concurrence of assistance** is defined as [22]

$$C_A(\rho_{ij}) = \max_{\Omega} \sum_n p_n C(\Psi_n) \,, \qquad (1.20)$$

where $C(\Psi_n)$ is given by Eq. (1.15). Given the square root $X$ of the reduced density matrix $\rho_{ij}$, such that $\rho_{ij} = XX^\dagger$, the concurrence of assistance is equal to [20]

$$C_A(\rho_{ij}) = \mathrm{tr}(\,|\,X^T(\sigma^y \otimes \sigma^y)X\,|\,)\,. \qquad (1.21)$$

Since for a pure state all entanglement measures are essentially equivalent, we may as well measure the localizable entanglement by the concurrence according to Eq. (1.20), and then it will be easy to at least give lower and upper bounds to the localizable entanglement. There exists a theorem stating that it always exists measurements of the other qubits such that the classical correlations $Q_{ij}^{\alpha,\beta} \equiv \langle \sigma_i^\alpha \sigma_j^\beta \rangle - \langle \sigma_i^\alpha \rangle \langle \sigma_j^\beta \rangle$, where $\alpha, \beta = x, y, z$, do not decrease on average [20]. Then it follows that a lower bound to the localizable entanglement is provided by the maximal correlation function, and an upper bound is given by the entanglement of assistance [20]

$$\max_{\alpha\,\beta}(|Q_{ij}^{\alpha,\beta}|) \leq E_L(\rho_{ij}) \leq C_A(\rho_{ij})\,, \qquad (1.22)$$

provided that $E_L(\rho_{ij})$ is measured in concurrence in the same way as the concurrence of assistance in Eq. (1.20).

We finally consider the entanglement between an entire block of qubits and the rest of the system. Let us restrict ourselves to a one-dimensional system. When the entire system is in its ground state $|\Psi_g\rangle$, the block and the rest of the system constitute a pure bipartite system. Therefore we measure the entanglement between the two subsystems as the von Neumann entropy, which we now call the **block entropy**, $S_L$, being a function of the number of qubits in the block, $L$. The interesting thing is that the block entropy as a function of $L$ obeys a universal scaling law close to a continuous quantum phase transition. More precisely, at criticality $S_L$ diverges as [15],[23]

$$S_L = \frac{c}{3} \log_2 L + A \qquad \text{when} \qquad L \to \infty\,, \qquad (1.23)$$

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where $c$ is the "central charge" of the underlying conformal field theory that describes the universal properties of the continuous QPT, and $A$ is a non-universal constant. For the universality class of the Ising model we have that $c = 1/2$, whereas for the universality class of the Heisenberg model $c = 1$. Away from the critical point $S_L$ will saturate to a finite value as $L \to \infty$.

# Chapter 2

# The Two-Dimensional Quantum Compass Model

The two-dimensional spin-1/2 quantum compass model, defined on a square $n \times n$ lattice, is given by the Hamiltonian

$$H = -J_x \sum_{i,j} \sigma_{i,j}^x \sigma_{i,j+1}^x - J_z \sum_{i,j} \sigma_{i,j}^z \sigma_{i+1,j}^z \,, \qquad (2.1)$$

with periodic boundary conditions. We see that the first term couples the $x$ components of adjacent spins in the same row of the lattice, while the second term couples the $z$ components of adjacent spins in the same column.

This spin model has not been solved exactly, and its properties still remain mostly unclear. It was introduced in 1982 by Kugel and Khomskii [24] as a simple model of orbital interactions in Mott insulating transition metal compounds. When modelling these types of systems the spin operators $\sigma$ in Eq. (2.1) are actually pseudospin operators $T$, describing orbital occupation so that e.g. the $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals corresponds to states where the eigenvalues of $T^z$ are 1/2 and -1/2, respectively [25].

The two-dimensional quantum compass model can also be physically implemented by a superconducting Josephson junction array [6]. For a Josephson junction array implementation of a spin-1/2 system the basic building block that is to operate as the "spin" at each lattice point can be realized as a loop of Josephson junctions, i.e. junctions that the Cooper pairs can only tunnel through, where the loop is penetrated by a magnetic flux $\Phi_0/2$. If the loop consists of, say, four junctions, the phase differences between the superconducting condensates must be an odd multiple of $\pm\pi/4$ across each junction in the loop, for the gauge invariant phase difference (i.e. including a phase difference $\pi$ coming from the magnetic flux) across the entire loop to be an integer multiple of $2\pi$.

This will then give two (nearly) degenerate ground states of this loop, where the phase difference between two opposite sides of the loop is either $\pi/2$ or $-\pi/2$, that are the representations of "spin up" and "spin down". For an isolated loop these states will only be close to degenerate due to transitions between them that lift the degeneracy.

Recently the two-dimensional quantum compass model has been proposed as a realistic model to create protected qubits, i.e. qubits protected from external noise [6]. In order to protect a qubit from outside noise the two lowest states $|0\rangle$ and $|1\rangle$ need to be separated from the higher states by an energy gap, but they also must be degenerate. If there were an energy difference between $|0\rangle$ and $|1\rangle$ it would clearly be affected by fluctuations in the physical quantity that determines the energy scale. Stable degeneracies are mostly due to some symmetries of the system. So when using a lattice system to implement a qubit, it is necessary that these symmetries remain even if some parts of the system are perturbed by noise.

In general, states are degenerate if there are symmetry operators that commute with the Hamiltonian but not with each other. To see this, suppose that we have two symmetry operators $A$ and $B$, and that the state $|0\rangle$ is a simultaneous eigenstate of $A$ and the Hamiltonian $H$, with $A|0\rangle = a|0\rangle$. Then the state $|1\rangle \equiv B|0\rangle$ will be degenerate with $|0\rangle$, since $H|1\rangle = HB|0\rangle = BH|0\rangle$. We also get

$$[A, B]|0\rangle = AB|0\rangle - BA|0\rangle = AB|0\rangle - aB|0\rangle = (A - a)|1\rangle . \qquad (2.2)$$

This applies to all eigenstates of $A$. Thus if $[A, B] \neq 0$, the states $|0\rangle$ and $|1\rangle$ are not equivalent, i.e. we cannot write $|1\rangle \propto |0\rangle$, and therefore each eigenstate of $H$ is degenerate.

Local noise introduces terms in the Hamiltonian that might not commute with some symmetry operators. So in order to preserve the degeneracy we need two non-commuting sets, $\{P_i\}$ and $\{Q_i\}$, of symmetry operators, so that if the noise fields only affect one $P_i$ and one $Q_i$ each, the degeneracy will only be broken if all noise fields act simultaneously. Also, the symmetry operators should of course not result in higher than twofold degeneracy for the system to be a qubit. It turns out that the two-dimensional quantum compass model has these properties, as shown by Douçot et al. [6].

The Hamiltonian in Eq. (2.1) has two sets, $\{P_i\}$ and $\{Q_i\}$, of symmetry operators, where

$$P_i = \prod_j \sigma_{i,j}^z , \qquad (2.3)$$

$$Q_j = \prod_i \sigma_{i,j}^x . \qquad (2.4)$$

We see that $P_i$ flips all $x$ spin components in the $i$th row, and that $Q_j$ flips all $z$ spin components in the $j$th column. These Hermitian operators are clearly seen to commute with the Hamiltonian, $[P_i, H] = 0$ and $[Q_i, H] = 0$ for all $i$. We also have that

$$[P_i, P_j] = 0 \qquad \forall\, i, j\,, \tag{2.5}$$

$$[Q_i, Q_j] = 0 \qquad \forall\, i, j\,, \tag{2.6}$$

$$\{P_i, Q_j\} = 0 \qquad \forall\, i, j\,. \tag{2.7}$$

Note that $P_i$ and $Q_j$ *anti*commute with each other. These conditions are sufficient for each state to be doubly, and only doubly, degenerate (with the exception of possible accidental degeneracies, of course). We now prove this claim. Noting that $[Q_i, P_m P_n] = 0$, $\forall\, i, m, n$, we see that the operators $H$, $\{Q_i\}$, $\{Q_i Q_j\}$ and $\{P_i P_j\}$ can all be diagonalized simultaneously. Thus if we start with an eigenstate $|0\rangle$ of the Hamiltonian that is a simultaneous eigenstate of all these operators, we have that $Q_i|0\rangle \propto |0\rangle$, $Q_i Q_j|0\rangle \propto |0\rangle$ and $P_i P_j|0\rangle \propto |0\rangle$, $\forall\, i, j$. But $P_i|0\rangle$ will be linearly independent of $|0\rangle$ since $[P_i, Q_j] \neq 0$. Let us define $P_1|0\rangle \equiv |1\rangle$. Since $[P_1, H] = 0$, $|0\rangle$ and $|1\rangle$ will be degenerate. We have that $P_1|1\rangle = P_1 P_1|0\rangle \propto |0\rangle$, since $|0\rangle$ is an eigenstate of $\{P_i P_j\}$. Therefore $P_i P_1|1\rangle = P_i P_1 P_1|0\rangle = P_1(P_i P_1)|0\rangle \propto P_1|0\rangle \equiv |1\rangle$. Then $|1\rangle \propto P_i P_1|1\rangle = P_i P_1 P_1|0\rangle \propto P_i|0\rangle$, $\forall\, i$. Thus $P_i|0\rangle \propto |1\rangle$ for all $i$, and not just for $i = 1$. So, no matter which symmetry operator that acts on $|0\rangle$, we only get back the states $|0\rangle$ or $|1\rangle$. Furhermore, $Q_i|1\rangle = Q_i P_1|0\rangle = -P_1 Q_i|0\rangle \propto -P_1|0\rangle \propto |1\rangle$, $\forall\, i$, and since $|0\rangle$ is an eigenstate of $\{P_i P_j\}$ we have that $P_i|1\rangle = P_i P_1|0\rangle \propto |0\rangle$, $\forall\, i$. Thus, no matter which symmetry operator that acts on $|1\rangle$, we only get back the states $|0\rangle$ or $|1\rangle$. Therefore, when acting with the symmetry operators on the states $|0\rangle$ and $|1\rangle$, we never leave the subspace spanned by these two states. A completely similar argument can be given if we instead start with an eigenstate of the operators $H$, $\{P_i\}$, $\{Q_i Q_j\}$ and $\{P_i P_j\}$ (since $[P_i, Q_m Q_n] = 0$, $\forall\, i, m, n$). The conclusion is therefore that, apart from accidental degeneracies, every state will be doubly, and only doubly, degenerate.

The total Hilbert space of the system can be divided into symmetry sectors, i.e. subspaces that are not mixed with each other by the Hamiltonian, which are characterized by the eigenvalues of the $P_i$ (or $Q_i$) operators that clearly are integrals of motion. Numerical diagonalization of finite systems have shown that in each symmetry sector of the Hamiltonian (2.1), there exists a finite energy gap between the ground states and the lowest excited states. However, this gap closes exponentially fast as the size $n$ of the system grows. It was first thought that this gap would remain finite even in the thermodynamic limit close to the isotropic point $J_x = J_z$, but later calculations have shown that the

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gap vanishes exponentially up to the isotropic point [7]. But for medium size systems (4×4 or 5×5 lattice points) the results indicate that these systems would provide a good protection from outside noise, suppressing its effect by many orders of magnitude [6].

The properties of the quantum compass model, Eq. (2.1), are particularly interesting near the isotropic point $J_x = J_z$. At this point the system becomes intrinsically frustrated, leading to enhanced fluctuations, that possibly might destroy long-range order altogether leading to a "spin liquid" state, and an increased ground state degeneracy in the thermodynamic limit. In fact, numerical results indicate that there is a first-order quantum phase transition at $J_x = J_z$, with diverging spin fluctuations and discontinuous correlation functions [7]. The system goes from spin ordering in the $z$ direction for $J_z > J_x$ to spin ordering in the $x$ direction for $J_x > J_z$. These indications have been further strengthened by recent analytical results using both a mean-field approximation and perturbation theory [8].

The symmetries of the model may actually suggest a one-dimensional type of behaviour of the system [8],[26]. This is clearly seen if we consider the limits $J_x = 0$ and $J_z = 0$. In these limits we simply get $n$ decoupled one-dimensional Ising chains. When the other coupling constant is slightly increased we can treat these transverse couplings as small perturbations, leading to separate excitations in the chains [6]. In the two-dimensional *classical* compass model, it has been shown both numerically and in the spin-wave approximation that the system shows spontaneous dimensionality reduction by essentially decoupling into one-dimensional chains in either the $x$ or the $z$ directions at low non-zero temperatures [27].

Altogether, these developments provide us with a clear motivation for a better understanding of possible mechanisms behind first-order quantum phase transitions in one-dimensional spin systems.

# Chapter 3

# The One-Dimensional XX-ZZ Model

## 3.1 The Hamiltonian and its Symmetries

We now consider the one-dimensional spin-1/2 model recently introduced by Brzezicki, Dziarmaga and Oleś [1]. Following these authors we will refer to the model as "the XX-ZZ model". It was designed to show, by exact solution, a mechanism behind a first-order QPT in a one-dimensional spin model, and to clarify the properties of the ground state of the one-dimensional quantum compass model.

The XX-ZZ model for a chain of $N$ spins, and with a parameter $\alpha \in [0, 2]$, is defined by the Hamiltonian

$$H(\alpha) = J \sum_{i=1}^{N'} \left[ (1 - \alpha)\, \sigma_{2i-1}^z \sigma_{2i}^z + \alpha\, \sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z \right] \qquad (3.1)$$

for $0 \leq \alpha \leq 1$, and

$$H(\alpha) = J \sum_{i=1}^{N'} \left[ \sigma_{2i-1}^x \sigma_{2i}^x + (2 - \alpha)\, \sigma_{2i}^z \sigma_{2i+1}^z + (\alpha - 1)\, \sigma_{2i}^x \sigma_{2i+1}^x \right] \qquad (3.2)$$

for $1 \leq \alpha \leq 2$, where $N' \equiv N/2$. It is assumed that the number $N'$ is even, and that the boundary conditions are periodic, $\sigma_{N+1} = \sigma_1$. We also assume that $J$ is positive. Note that the spin-1/2 operators $\sigma$ have a mixed fermionic and bosonic character,

$$\{ \sigma_i^\alpha, \sigma_i^\beta \} = 2\delta_{\alpha,\beta}, \qquad (3.3)$$

$$[ \sigma_i^\alpha, \sigma_j^\beta ] = 0 \qquad i \neq j. \qquad (3.4)$$

Thus $\sigma$ operators on the same lattice site obey fermionic anticommutation relations, and $\sigma$ operators on different lattice sites obey bosonic

commutation relations.

The model interpolates between the Z Ising model at $\alpha = 0$,

$$H(0) = J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z \,, \tag{3.5}$$

and the X Ising model at $\alpha = 2$,

$$H(2) = J \sum_{i=1}^{N} \sigma_i^x \sigma_{i+1}^x \,. \tag{3.6}$$

In the middle, at $\alpha = 1$, we have the one-dimensional quantum compass model

$$H(1) = J \sum_{i=1}^{N} \left[ \sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z \right] \,, \tag{3.7}$$

which is intrinsically frustrated. Calling the $\{2i, 2i+1\}$ pair an even bond, and the $\{2i-1, 2i\}$ pair an odd bond, we see that the 1D quantum compass model favours antiferromagnetic ordering on the $x$ spin component on odd bonds, and of the $z$ spin component on even bonds. These two orderings are clearly incompatible, and give rise to a very interesting behaviour at this point. Since the XX-ZZ model makes antiferromagnetic order on the $z$ spin component more favourable when $\alpha < 1$, and on the $x$ spin component more favourable when $\alpha > 1$, we might suspect that there will be a QPT at $\alpha = 1$, and as we shall see this is indeed the case. Note that the model we consider in this chapter has the same coupling constant $J$ for both the $x$ and $z$ spin components. In later chapters the model will be generalized to include different coupling constants for the two components.

First of all, we note that the Hamiltonian (3.1) for $0 \leq \alpha \leq 1$, and the Hamiltonian (3.2) for $1 \leq \alpha \leq 2$, actually are mapped onto each other by the simultaneous symmetry operation

$$\sigma_i^x \leftrightarrow \sigma_i^z \quad \forall\, i \,, \qquad 2i \leftrightarrow 2i - 1 \quad \forall\, i \,, \qquad (1 - \alpha) \leftrightarrow (\alpha - 1) \,. \tag{3.8}$$

So we only need to solve the model for $0 \leq \alpha \leq 1$, Eq. (3.1). Then the solution for $1 \leq \alpha \leq 2$ is simply given by applying the symmetry operation of Eq. (3.8).

Before we solve the model, Eq. (3.1), let us take a look at the symmetries of this Hamiltonian. We readily identify the Hermitian symmetry operators

$$P_i \;\; \equiv \;\; \sigma_{2i-1}^z \sigma_{2i}^z \,, \tag{3.9}$$

$$Q \;\; \equiv \;\; \prod_{i=1}^{N} \sigma_i^x \,, \tag{3.10}$$

since $P_i H P_i = H$ due to that $\sigma_i^z \sigma_i^x \sigma_i^z = -\sigma_i^x$ and similarly $QHQ = H$ because $\sigma_i^x \sigma_i^z \sigma_i^x = -\sigma_i^z$. By applying these basic symmetry operators one after another we can create composite symmetry operators, like e.g.

$$P \equiv \prod_i P_i = \prod_j \sigma_j^z \qquad \text{and} \qquad PQ = \prod_j \sigma_j^y. \qquad (3.11)$$

Clearly, since the Pauli matrices form a group under multiplication, so do the total number of symmetry operators. Now, the $P_i$ operators commute with each other, and also with $Q$, since

$$\sigma_{2i-1}^z \sigma_{2i}^z \sigma_{2i-1}^x \sigma_{2i}^x \sigma_{2i-1}^z \sigma_{2i}^z = \sigma_{2i-1}^x \sigma_{2i}^x. \qquad (3.12)$$

Thus the symmetry operators form an Abelian group. This has the implication that every eigenstate of the Hamiltonian of the XX-ZZ model in general is non-degenerate, apart from possible accidental degeneracies, cf. Eq. (2.2). However, at the special points $\alpha = 0$ and $\alpha = 1$, where the Hamiltonian is given by Eq. (3.5) and Eq. (3.7), respectively, the symmetry group gets larger. Here there will be non-commuting symmetry operators, resulting in degeneracies at these points.

When we now solve the model for $\alpha \in [0, 1]$, it is most convenient to do so in the eigenbasis of the Z Ising model at $\alpha = 0$, Eq (3.5). That is, we will work in the basis $\{|\uparrow\rangle, |\downarrow\rangle\}$ of eigenstates of the $\sigma_i^z$ operators.

The fact that the Hamiltonian (3.1) has the symmetry operators $P_i$, Eq (3.9), is crucial in our solution of the model. It clearly implies that the eigenvalues of $P_i$, $\forall\, i$, are constants of motion. Or to put it more explicitly, the Hamiltonian does only flip the spins in odd bond pairs. The only terms in the Hamiltonian that alter the spins are those who contain $\sigma^x$ operators, and these terms all have the form $\sigma_{2i-1}^x \sigma_{2i}^x$, so that the only transitions that can occur flip spins on $\{2i - 1, 2i\}$ bonds, i.e. odd bonds, simultaneously. A state where a particular odd bond is parallel, $|\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$, will not be mixed with a state were that bond is antiparallel, $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$. This means that the Hilbert space of the spin chain can be divided into subspaces that are not mixed by the Hamiltonian. Each subspace can be labelled by a vector $\vec{s} = (s_1, s_2, \ldots, s_{N'})$, where the element $s_i = 1$ when the odd bond $\{2i - 1, 2i\}$ is parallel and $s_i = 0$ when it is antiparallel. The Hamiltonian can then be diagonalized in each subspace $\vec{s}$ independently.

## 3.2   Mapping onto the Quantum Ising Model

In each subspace $\vec{s}$, the contribution to the energy from the terms involving $\sigma_{2i-1}^z \sigma_{2i}^z$ in the Hamiltonian (3.1), will be a constant. Since every antiparallel odd bond is contributing $-J(1 - \alpha)$, and every parallel odd

bond is contributing $J(1 - \alpha)$, to the energy, this constant is given by

$$C_s(\alpha) \equiv J(1 - \alpha) \sum_{i=1}^{N'} \sigma_{2i-1}^z \sigma_{2i}^z = -J(1 - \alpha)(N' - 2s), \qquad (3.13)$$

where $s \equiv \sum_{i=1}^{N'} s_i$ is the number of parallel odd bonds in the subspace $\vec{s}$. The Hamiltonian (3.1) may then be written as

$$H_{\vec{s}}(\alpha) = J \sum_{i=1}^{N'} \left[ \alpha\, \sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z \right] + C_s(\alpha). \qquad (3.14)$$

Since, in each subspace $\vec{s}$, the Hilbert space of each odd bond in effect is only two-dimensional ($\{|\uparrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ for $s_i = 1$ and $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ for $s_i = 0$), each odd bond actually can be seen as a spin-1/2 entity itself, being the eigenstate of a $\tau_i^z$ operator and being flipped by a $\tau_i^x$ operator. We define

$$
\begin{aligned}
\tau_i^x &\equiv -\left( |\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow| \right), \\
\tau_i^y &\equiv -(-1)^{\sum_{j=1}^{i-1} s_j} \left( i\, |\uparrow\downarrow\rangle\langle\downarrow\uparrow| - i\, |\downarrow\uparrow\rangle\langle\uparrow\downarrow| \right), \\
\tau_i^z &\equiv -(-1)^{\sum_{j=1}^{i-1} s_j} \left( |\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow| \right),
\end{aligned} \qquad (3.15)
$$

for the antiparallel ($s_i = 0$) odd bond $\{2i - 1, 2i\}$, and

$$
\begin{aligned}
\tau_i^x &\equiv -\left( |\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow| \right), \\
\tau_i^y &\equiv -(-1)^{\sum_{j=1}^{i-1} s_j} \left( i\, |\uparrow\uparrow\rangle\langle\downarrow\downarrow| - i\, |\downarrow\downarrow\rangle\langle\uparrow\uparrow| \right), \\
\tau_i^z &\equiv -(-1)^{\sum_{j=1}^{i-1} s_j} \left( |\uparrow\uparrow\rangle\langle\uparrow\uparrow| - |\downarrow\downarrow\rangle\langle\downarrow\downarrow| \right),
\end{aligned} \qquad (3.16)
$$

for the parallel ($s_i = 1$) odd bond $\{2i - 1, 2i\}$. It is seen that the $\tau$ operators are completely analogous to the $\sigma$ operators, in that

$$
\begin{aligned}
\{ \tau_i^\alpha, \tau_i^\beta \} &= 2\delta_{\alpha,\beta}, & (3.17) \\
[ \tau_i^\alpha, \tau_j^\beta ] &= 0 \qquad i \neq j. & (3.18)
\end{aligned}
$$

With this choice of nonlocal $\tau$ operators, the Hamiltonian (3.14) can be reduced to a quantum Ising model. To see this, let us consider the different terms in the Hamiltonian. For the first term, we have that

$$\sigma_{2i-1}^x \sigma_{2i}^x = -\tau_i^x, \qquad (3.19)$$

since $\sigma_{2i-1}^x \sigma_{2i}^x$ merely consists of simultaneously flipping the two spins on the odd bond $\{2i - 1, 2i\}$. For the second term, which includes two adjacent odd bonds, we must be more careful. When all odd bonds are antiparallel, i.e. in the $s{=}0$ subspace, we have that $\sigma_{2i-1}^z = -\tau_i^z$ and

$\sigma_{2i}^z = \tau_i^z$, giving $\sigma_{2i}^z \sigma_{2i+1}^z = -\tau_i^z \tau_{i+1}^z$. When $s \neq 0$, there are odd bonds that are not antiparallel. Every time a parallel odd bond appears, say at lattice index $j$, all subsequent operators $\tau_i^z$, $\forall i > j$, acquire an additional minus sign due to the factor $(-1)^{\sum_{j=1}^{i-1} s_i}$ in Eqs. (3.15)-(3.16). This additional minus sign takes care of the effect of the bond being parallel. Therefore the construction of the $\tau_i^z$ operators leads to that $\sigma_{2i}^z \sigma_{2i+1}^z = -\tau_i^z \tau_{i+1}^z$ for all $s$ and for all $i$, except at the boundary. For the boundary term, $\sigma_{2N'}^z \sigma_1^z$, we must compensate for that $\sigma_1^z$ does not contain the factor $(-1)^{\sum_{j=1}^{N'} s_i}$, by inserting a factor $(-1)^s$. So the Hamiltonian (3.14) is reduced to

$$H_{\vec{s}}(\alpha) = -J \sum_{i=1}^{N'-1} \left[ \alpha \, \tau_i^x + \tau_i^z \tau_{i+1}^z \right] - J[\alpha \tau_{N'}^x + (-1)^s \tau_{N'}^z \tau_1^z] + C_s(\alpha) \,. \quad (3.20)$$

This is recognized as the Hamiltonian for the ferromagnetic quantum Ising model, with periodic boundary conditions when $s$ is even and antiperiodic boundary conditions when $s$ is odd.

## 3.3 Exact Solution

The solution to the quantum Ising model is very well known, and the fact that this relatively simple model may be solved exactly makes it somewhat of a prototype system in the study of QPTs. Its exact solution was found in 1961 by Lieb, Schultz and Mattis [28] in the context of the XY model, and by Katsura [29] in 1962 who generalized their solution to include the transverse term that couples to the parameter $\alpha$.

### 3.3.1 Jordan-Wigner Transformation

The Hamiltonian (3.20) is solved by first making the Jordan-Wigner transformation of the $\tau$ operators:

$$\tau_i^x = 1 - 2c_i^\dagger c_i \,, \quad (3.21)$$

$$\tau_i^y = i \left( c_i - c_i^\dagger \right) \prod_{j < i} (1 - 2c_j^\dagger c_j) \,, \quad (3.22)$$

$$\tau_i^z = -(c_i + c_i^\dagger) \prod_{j < i} (1 - 2c_j^\dagger c_j) \,, \quad (3.23)$$

where $c_i^\dagger$ and $c_i$ are fully fermionic creation and annihilation operators at lattice site $i$, obeying

$$\begin{aligned}
\{c_i, c_j^\dagger\} &= \delta_{i,j} \,, \\
\{c_i, c_j\} &= 0 \,, \\
\{c_i^\dagger, c_j^\dagger\} &= 0 \,.
\end{aligned} \quad (3.24)$$

The meaning of the $c$ operators is easier to appreciate when instead looking at the raising and lowering operators in the $x$ spin direction, $\tau_i^+ \equiv -(\tau_i^z - i\,\tau_i^y)/2$ and $\tau_i^- \equiv -(\tau_i^z + i\,\tau_i^y)/2$ (rotation $x \to -z$ and $z \to x$ of spin $z$ raising and lowering operators). Then $\tau_i^+$ and $\tau_i^-$ are given by

$$\tau_i^+ = c_i^\dagger \prod_{j<i}(1 - 2c_j^\dagger c_j)\,, \tag{3.25}$$

$$\tau_i^- = c_i \prod_{j<i}(1 - 2c_j^\dagger c_j)\,. \tag{3.26}$$

Therefore the $c$ operators are acting like raising and lowering operators in the $x$ spin direction. The crucial feature of the Jordan-Wigner transformation is that it will transform the Hamiltonian (3.20), expressed in $\tau$ operators with mixed fermionic and bosonic properties, into a Hamiltonian that is expressed in fully fermionic $c$ operators.

It is readily checked that the fermionic anticommutation relations, Eq. (3.24), for the $c$ operators implies that the Jordan-Wigner transformation, Eqs. (3.21)-(3.23), preserves the commutation and anticommutation relations, Eqs. (3.17)-(3.18), for the $\tau$ operators. We get

$$\begin{aligned}
\{\tau_i^x, \tau_i^x\} &= 2\,(1 - 2c_i^\dagger c_i)(1 - 2c_i^\dagger c_i) \\
&= 2(1 - 4c_i^\dagger c_i + 4c_i^\dagger c_i c_i^\dagger c_i) \\
&= 2(1 - 4c_i^\dagger c_i + 4c_i^\dagger c_i - 4c_i^\dagger c_i^\dagger c_i c_i) = 2\,,
\end{aligned} \tag{3.27}$$

where the anticommutation relations, Eq. (3.24), for the $c$ operators were used. Note that these relations lead to $c_i^\dagger c_i^\dagger = 0$ and $c_i c_i = 0$, always. Further,

$$\begin{aligned}
\tau_i^z \tau_i^x &= -(c_i + c_i^\dagger) \prod_{j<i}(1 - 2c_j^\dagger c_j)(1 - 2c_i^\dagger c_i) \\
&= -(c_i + c_i^\dagger)(1 - 2c_i^\dagger c_i) \prod_{j<i}(1 - 2c_j^\dagger c_j) \\
&= (1 - 2c_i^\dagger c_i)(c_i + c_i^\dagger) \prod_{j<i}(1 - 2c_j^\dagger c_j) = -\tau_i^x \tau_i^z
\end{aligned}$$

$$\Rightarrow \qquad \{\tau_i^x, \tau_i^z\} = 0\,, \tag{3.28}$$

where we used that

$$\begin{aligned}
(c_i + c_i^\dagger)(1 - 2c_i^\dagger c_i) &= c_i + c_i^\dagger - 2c_i c_i^\dagger c_i - 2c_i^\dagger c_i^\dagger c_i \\
&= c_i + c_i^\dagger - 2c_i + 2c_i^\dagger c_i c_i - 2c_i^\dagger + 2c_i^\dagger c_i c_i^\dagger \\
&= -(1 - 2c_i^\dagger c_i)(c_i + c_i^\dagger)\,. \tag{3.29}
\end{aligned}$$

For $\{\tau_i^z, \tau_i^z\}$, we get

$$
\begin{aligned}
\{\tau_i^z, \tau_i^z\} &= 2(c_i + c_i^\dagger) \prod_{j<i}(1 - 2c_j^\dagger c_j)(c_i + c_i^\dagger) \prod_{j'<i}(1 - 2c_{j'}^\dagger c_{j'}) \\
&= 2 \prod_{j<i}(1 - 2c_j^\dagger c_j) \prod_{j'<i}(1 - 2c_{j'}^\dagger c_{j'})(c_i + c_i^\dagger)(c_i + c_i^\dagger) \\
&= 2 \prod_{j<i}(1 - 2c_j^\dagger c_j)(1 - 2c_j^\dagger c_j)(c_i c_i + c_i^\dagger c_i + c_i c_i^\dagger + c_i^\dagger c_i^\dagger) \\
&= 2,
\end{aligned}
\tag{3.30}
$$

since

$$
\begin{aligned}
(c_i + c_i^\dagger)(c_i + c_i^\dagger) &= c_i c_i + c_i^\dagger c_i + c_i c_i^\dagger + c_i^\dagger c_i^\dagger \\
&= c_i^\dagger c_i + c_i c_i^\dagger = 1,
\end{aligned}
\tag{3.31}
$$

and

$$
\begin{aligned}
(1 - 2c_i^\dagger c_i)(1 - 2c_i^\dagger c_i) &= 1 - 2c_i^\dagger c_i - 2c_i^\dagger c_i + 4c_i^\dagger c_i c_i^\dagger c_i \\
&= 1 - 4c_i^\dagger c_i + 4c_i^\dagger c_i = 1.
\end{aligned}
\tag{3.32}
$$

Also, for different sites, $i \neq j$, we get (assuming here that $i > j$)

$$
\begin{aligned}
\tau_j^z \tau_i^z &= (c_j + c_j^\dagger) \prod_{m<j}(1 - 2c_m^\dagger c_m)(c_i + c_i^\dagger) \prod_{n<i}(1 - 2c_n^\dagger c_n) \\
&= (c_j + c_j^\dagger)(c_i + c_i^\dagger) \prod_{n<i}(1 - 2c_n^\dagger c_n) \prod_{m<j}(1 - 2c_m^\dagger c_m) \\
&= -(c_i + c_i^\dagger)(c_j + c_j^\dagger) \prod_{n<i}(1 - 2c_n^\dagger c_n) \prod_{m<j}(1 - 2c_m^\dagger c_m) \\
&= -(c_i + c_i^\dagger) \prod_{\substack{n<i \\ n\neq j}}(1 - 2c_n^\dagger c_n)(c_j + c_j^\dagger)(1 - 2c_j^\dagger c_j) \prod_{m<j}(1 - 2c_m^\dagger c_m) \\
&= (c_i + c_i^\dagger) \prod_{n<i}(1 - 2c_n^\dagger c_n)(c_j + c_j^\dagger) \prod_{m<j}(1 - 2c_m^\dagger c_m) = \tau_i^z \tau_j^z \\
\Rightarrow \quad & [\tau_i^z, \tau_j^z] = 0 \qquad \forall\, i \neq j,
\end{aligned}
\tag{3.33}
$$

where again we used Eq. (3.29). Similar calculations for the other commutation and anticommutation relations show that the Jordan-Wigner transformation with fully fermionic $c$ operators indeed preserves the anticommutation, Eq. (3.17), and commutation, Eq. (3.18), relations of the $\tau$ operators.

Applying the Jordan-Wigner transformation, Eqs. (3.21)-(3.23), to

the Hamiltonian (3.20), gives

$$H_{\vec{s}}(\alpha) \quad - \quad C_s(\alpha) \;=\; -J \sum_{i=1}^{N'-1} [\alpha\,\tau_i^x + \tau_i^z\tau_{i+1}^z] - J[\alpha\tau_{N'}^x + (-1)^s\tau_{N'}^z\tau_1^z]$$

$$= \quad -J \sum_{i=1}^{N'-1} [\,\alpha(1 - 2c_i^\dagger c_i) + (c_i + c_i^\dagger)\prod_{j<i}(1 - 2c_j^\dagger c_j)$$

$$\times (c_{i+1} + c_{i+1}^\dagger)\prod_{m<i+1}(1 - 2c_m^\dagger c_m)\,]$$

$$-J\,[\,\alpha(1 - 2c_{N'}^\dagger c_{N'}) + (-1)^s(c_{N'} + c_{N'}^\dagger)$$

$$\times \prod_{n<N'}(1 - 2c_n^\dagger c_n)(c_1 + c_1^\dagger)\,]$$

$$= \quad -J\alpha N' - J\sum_{i=1}^{N'-1}[\,-2\alpha c_i^\dagger c_i + (c_i + c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger)$$

$$\times (1 - 2c_i^\dagger c_i)\prod_{j<i}\underbrace{(1 - 2c_j^\dagger c_j)(1 - 2c_j^\dagger c_j)}_{1}\,]$$

$$-J\,[\,-2\alpha c_{N'}^\dagger c_{N'} - (-1)^s(c_{N'} + c_{N'}^\dagger)(c_1 + c_1^\dagger)$$

$$\times \prod_{n<N'}(1 - 2c_n^\dagger c_n)\,]$$

$$= \quad -J\alpha N' + J\sum_{i=1}^{N'-1}[\,2\alpha c_i^\dagger c_i - (c_i + c_i^\dagger)(1 - 2c_i^\dagger c_i)(c_{i+1} + c_{i+1}^\dagger)\,]$$

$$+J\,[\,2\alpha c_{N'}^\dagger c_{N'} + (-1)^s(c_{N'} + c_{N'}^\dagger)(c_1 + c_1^\dagger)\prod_{n<N'}(1 - 2c_n^\dagger c_n)\,]$$

$$= \quad -J\alpha N' + J\sum_{i=1}^{N'-1}[\,2\alpha c_i^\dagger c_i + (c_i - c_i^\dagger)(c_{i+1} + c_{i+1}^\dagger)\,]$$

$$+J\,[\,2\alpha c_{N'}^\dagger c_{N'} - (-1)^s(c_{N'} + c_{N'}^\dagger)$$

$$\times \prod_{n<N'}(1 - 2c_n^\dagger c_n)(c_1 + c_1^\dagger)\,]$$

$$= \quad -J\alpha N' + J\sum_{i=1}^{N'-1}[\,2\alpha c_i^\dagger c_i - c_i^\dagger c_{i+1} - c_i^\dagger c_{i+1}^\dagger + c_i c_{i+1} + c_i c_{i+1}^\dagger\,]$$

$$+J\,[\,2\alpha c_{N'}^\dagger c_{N'} + (-1)^s(c_{N'}^\dagger - c_{N'})(c_1 + c_1^\dagger)\underbrace{\prod_{n\le N'}(1 - 2c_n^\dagger c_n)}_{(-1)^{\Sigma_{j=1}^{N'} c_j^\dagger c_j}}\,]$$

$$= \quad -J\alpha N' + J\sum_{i=1}^{N'-1}[\,2\alpha c_i^\dagger c_i - c_i^\dagger c_{i+1} - c_i^\dagger c_{i+1}^\dagger$$

$$-c_{i+1}c_i - c_{i+1}^\dagger c_i\,] +$$

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$$+J\left[2\alpha c_{N'}^\dagger c_{N'} + (c_{N'}^\dagger c_1 + c_{N'}^\dagger c_1^\dagger - c_{N'}c_1 - c_{N'}c_1^\dagger)\right.$$
$$\left.\times(-1)^s(-1)^{\sum_{j=1}^{N'} c_j^\dagger c_j}\right]$$
$$= -J\alpha N' + J\sum_{i=1}^{N'-1}\left[2\alpha c_i^\dagger c_i - c_i^\dagger c_{i+1} - c_{i+1}c_i - c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1}^\dagger\right]$$
$$+J\left[2\alpha c_{N'}^\dagger c_{N'} + (-c_{N'}^\dagger c_1 - c_1 c_{N'} - c_1^\dagger c_{N'} - c_{N'}^\dagger c_1^\dagger)(-1)^{1+s+\sum_{j=1}^{N'} c_j^\dagger c_j}\right],$$
$$(3.34)$$

where the relations

$$(1 - 2c_i^\dagger c_i)(c_i + c_i^\dagger) = -(c_i + c_i^\dagger)(1 - 2c_i^\dagger c_i), \qquad (3.35)$$
$$(c_{N'} + c_{N'}^\dagger) = (c_{N'}^\dagger - c_{N'})(1 - 2c_{N'}^\dagger c_{N'}) \qquad (3.36)$$

were used. Thus the result of the Jordan-Wigner transformation of the Hamiltonian (3.20) is

$$H_{\vec{s}}(\alpha) = J\sum_{i=1}^{N'-1}\left[2\alpha c_i^\dagger c_i - c_i^\dagger c_{i+1} - c_{i+1}c_i - c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1}^\dagger\right]$$
$$+J\left[2\alpha c_{N'}^\dagger c_{N'} + (-c_{N'}^\dagger c_1 - c_1 c_{N'} - c_1^\dagger c_{N'} - c_{N'}^\dagger c_1^\dagger)\right.$$
$$\left.\times(-1)^{1+s+\sum_{j=1}^{N'} c_j^\dagger c_j}\right] - J\alpha N' + C_s(\alpha).$$
$$(3.37)$$

Note the appearance of the factor $(-1)^{1+s+\sum_{j=1}^{N'} c_j^\dagger c_j}$ in the Hamiltonian (3.37). This is an integral of motion, since it only depends on whether the number of $c$ particles, $\sum_{j=1}^{N'} c_j^\dagger c_j$, is odd or even, and as seen in the Hamiltonian (3.37) the $c$ particles can only be created or destroyed in pairs.

In order to simplify the Hamiltonian (3.37), projection operators $P^\pm$ are introduced, given by

$$P^\pm = \frac{1}{2}\left[1 \pm \prod_{i=1}^{N'}(1 - 2c_i^\dagger c_i)\right], \qquad (3.38)$$

thereby projecting states onto the subspaces with even $(+)$ and odd $(-)$ number of $c$ particles, thus splitting the Hamiltonian into

$$H_{\vec{s}}(\alpha) = P^+ H_{\vec{s}}^+(\alpha)P^+ + P^- H_{\vec{s}}^-(\alpha)P^-. \qquad (3.39)$$

Then the Hamiltonian (3.37), given by $H_{\vec{s}}^+(\alpha)$ and $H_{\vec{s}}^-(\alpha)$ in the $+$ and $-$ subspace, respectively, can be written as

$$H_{\vec{s}}^\pm(\alpha) = J\sum_{i=1}^{N'}\left[2\alpha c_i^\dagger c_i - c_i^\dagger c_{i+1} - c_{i+1}c_i - c_{i+1}^\dagger c_i - c_i^\dagger c_{i+1}^\dagger\right]$$
$$-J\alpha N' + C_s(\alpha). \qquad (3.40)$$

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The boundary terms have here been included in the general sum, and therefore the boundary conditions must be specified for the different subspaces. In the Hamiltonian (3.37), we see that the boundary conditions are determined by the factor $(-1)^{1+s+\sum_{j=1}^{N'} c_j^\dagger c_j}$. Thus it is clear that when $s + \sum_{j=1}^{N'} \langle c_j^\dagger c_j \rangle$ is even, the boundary conditions are antiperiodic ($c_{N'+1}^\dagger \equiv -c_1^\dagger$), and when it is odd, the boundary conditions are periodic ($c_{N'+1}^\dagger \equiv c_1^\dagger$).

### 3.3.2 Fourier Transformation

The next step in the solution is to make a Fourier transformation of the $c$ operators, defined by

$$c_j \equiv \frac{1}{\sqrt{N'}} \sum_k c_k e^{ikj} \,, \tag{3.41}$$

giving for $c_j^\dagger$, the Hermitian adjoint of $c_j$,

$$c_j^\dagger \equiv \frac{1}{\sqrt{N'}} \sum_k c_k^\dagger e^{-ikj} \,, \tag{3.42}$$

where $c_k$ are $c$ operators in $k$ space, obeying fermionic anticommutation relations. The quantized $k$ values depend on the boundary conditions. By

$$c_{N'+1} = \frac{1}{\sqrt{N'}} \sum_k c_k e^{ik(N'+1)} = \frac{1}{\sqrt{N'}} \sum_k c_k e^{ik} e^{ikN'} \tag{3.43}$$

it follows that, since we have assumed that $N'$ is even, $k$ takes the values

$$k = 0, \, \pm \frac{2\pi}{N'}, \, \pm 2 \frac{2\pi}{N'}, \dots, \pi \tag{3.44}$$

for periodic boundary conditions, and

$$k = \pm \frac{1}{2} \frac{2\pi}{N'}, \, \pm \frac{3}{2} \frac{2\pi}{N'}, \dots, \frac{1}{2}(N'-1) \frac{2\pi}{N'} \tag{3.45}$$

for antiperiodic boundary conditions. Clearly, the Fourier transformation preserves the fermionic anticommutation relations of the $c_j$ operators, since

$$\{c_m^\dagger, c_n\} = \frac{1}{N'} \sum_{k\,k'} \underbrace{\{c_k^\dagger, c_{k'}\}}_{\delta_{k,k'}} e^{-ikm} e^{ik'n} = \frac{1}{N'} \sum_k e^{ik(n-m)} = \delta_{m,n} \,,$$

$$\tag{3.46}$$

and similar calculations show that $\{c_m, c_n\} = 0$ and $\{c_m^\dagger, c_n^\dagger\} = 0$ with fermionic $c_k$ operators.

The sums that appear in the Hamiltonian (3.37) now become

$$
\begin{aligned}
\sum_{i=1}^{N'} c_i^\dagger c_{i+1} &= \sum_{j=1}^{N'} \left[ \left( \frac{1}{\sqrt{N'}} \sum_k c_k^\dagger e^{-ikj} \right) \left( \frac{1}{\sqrt{N'}} \sum_{k'} c_{k'} e^{ik'(j+1)} \right) \right] \\
&= \sum_{k,\,k'} c_k^\dagger c_{k'} e^{ik'} \underbrace{\frac{1}{N'} \sum_{j=1}^{N'} e^{ij(k'-k)}}_{\delta_{k,k'}} = \sum_k c_k^\dagger c_k e^{ik} ,
\end{aligned}
$$

$$(3.47)$$

$$
\begin{aligned}
\sum_{i=1}^{N'} c_{i+1} c_i &= \sum_{j=1}^{N'} \left[ \left( \frac{1}{\sqrt{N'}} \sum_k c_k e^{ik(j+1)} \right) \left( \frac{1}{\sqrt{N'}} \sum_{k'} c_{k'} e^{ik'j} \right) \right] \\
&= \sum_{k,\,k'} c_k c_{k'} e^{ik} \underbrace{\frac{1}{N'} \sum_{j=1}^{N'} e^{ij(k+k')}}_{\delta_{k,-k'}} \\
&= \frac{1}{2} \left[ \sum_k c_k c_{-k} e^{ik} + \sum_{k'} c_{-k'} c_{k'} e^{-ik'} \right] \\
&= -\frac{1}{2} \sum_k \left[ c_{-k} c_k \left( e^{ik} - e^{-ik} \right) \right] \\
&= -\sum_k \left[ (i \sin k) c_{-k} c_k \right] ,
\end{aligned}
$$

$$(3.48)$$

$$
\begin{aligned}
\sum_{i=1}^{N'} c_i^\dagger c_i &= \sum_{j=1}^{N'} \left[ \left( \frac{1}{\sqrt{N'}} \sum_k c_k^\dagger e^{-ikj} \right) \left( \frac{1}{\sqrt{N'}} \sum_{k'} c_{k'} e^{ik'j} \right) \right] \\
&= \sum_{k,\,k'} c_k^\dagger c_{k'} \underbrace{\frac{1}{N'} \sum_{j=1}^{N'} e^{ij(k'-k)}}_{\delta_{k,k'}} = \sum_k c_k^\dagger c_k .
\end{aligned}
$$

$$(3.49)$$

The remaining two sums are given by the Hermitian adjoints of already calculated sums:

$$
\sum_{i=1}^{N'} c_{i+1}^\dagger c_i = \left( \sum_{i=1}^{N'} c_i^\dagger c_{i+1} \right)^\dagger = \sum_k c_k^\dagger c_k e^{-ik} ,
$$

$$(3.50)$$

$$
\sum_{i=1}^{N'} c_i^\dagger c_{i+1}^\dagger = \left( \sum_{i=1}^{N'} c_{i+1} c_i \right)^\dagger = -\sum_k \left[ (i \sin k) c_{-k}^\dagger c_k^\dagger \right] .
$$

$$(3.51)$$

Summing the terms in the Hamiltonian (3.40) then gives

$$
\begin{aligned}
H_{\vec{s}}^{\pm}(\alpha) \;=\;& J\sum_k \big[\, 2\alpha c_k^\dagger c_k - e^{ik} c_k^\dagger c_k + i\sin k\, c_{-k} c_k \\
& -e^{-ik} c_k^\dagger c_k + i\sin k\, c_{-k}^\dagger c_k^\dagger \,\big] - J\alpha N' + C_s(\alpha)\,, \quad (3.52)
\end{aligned}
$$

which can be simplified as

$$
\begin{aligned}
H_{\vec{s}}^{\pm}(\alpha) \;=\;& J\sum_k \big[\, 2(\alpha - \cos k) c_k^\dagger c_k + i\sin k\,(c_{-k}^\dagger c_k^\dagger + c_{-k} c_k)\,\big] \\
& -J\alpha N' + C_s(\alpha)\,. \quad (3.53)
\end{aligned}
$$

### 3.3.3  Bogoliubov Transformation

The Hamiltonian (3.53) has the same form as the model Hamiltonian appearing in the BCS theory of superconductivity, and it can therefore be diagonalized using the procedure of Bogoliubov transformation. It consists of transforming the $c_k$ operators according to

$$
c_k = u_k \gamma_k - i v_{-k} \gamma_{-k}^\dagger\,, \qquad (3.54)
$$

where the $\gamma$ operators are fully fermionic

$$
\begin{aligned}
\{\gamma_k^\dagger, \gamma_{k'}\} &= \delta_{k,k'}\,, \\
\{\gamma_k, \gamma_{k'}\} &= 0\,, \\
\{\gamma_k^\dagger, \gamma_{k'}^\dagger\} &= 0\,,
\end{aligned} \qquad (3.55)
$$

and where the real constants $u_k$ and $v_k$ obey

$$
\begin{aligned}
u_{-k} &= u_k\,, & (3.56) \\
v_{-k} &= -v_k\,, & (3.57) \\
u_k^2 + v_k^2 &= 1\,. & (3.58)
\end{aligned}
$$

These relations give the transformations of all the different types of $c_k$ operators as

$$
\begin{aligned}
c_k &= u_k \gamma_k - i v_{-k} \gamma_{-k}^\dagger\,, & \\
c_k^\dagger &= u_k \gamma_k^\dagger + i v_{-k} \gamma_{-k}\,, & (3.59) \\
c_{-k} &= u_k \gamma_{-k} - i v_k \gamma_k^\dagger\,, & (3.60) \\
c_{-k}^\dagger &= u_k \gamma_{-k}^\dagger + i v_k \gamma_k\,. & (3.61)
\end{aligned}
$$

It is now easily seen that the inverse of the Bogoliubov transformation (3.54) is given by

$$
\gamma_k = u_k c_k - i v_k c_{-k}^\dagger\,. \qquad (3.62)
$$

The Bogoliubov transformation preserves the fermionic anticommutation relations for $c_k^\dagger$ and $c_k$, as is readily verified:

$$
\begin{aligned}
\{c_k^\dagger, c_{k'}\} &= \{u_k\gamma_k^\dagger + iv_{-k}\gamma_{-k}\,,\; u_{k'}\gamma_{k'} - iv_{-k'}\gamma_{-k'}^\dagger\} \\
&= u_k u_{k'}\underbrace{\{\gamma_k^\dagger, \gamma_{k'}\}}_{\delta_{k,k'}} - iu_k v_{-k'}\underbrace{\{\gamma_k^\dagger, \gamma_{-k'}^\dagger\}}_{0} + iv_{-k}u_{k'}\underbrace{\{\gamma_{-k}, \gamma_{k'}\}}_{0} \\
&\quad + v_{-k}v_{-k'}\underbrace{\{\gamma_{-k}, \gamma_{-k'}^\dagger\}}_{\delta_{k,k'}} \\
&= (u_k^2 + v_k^2)\,\delta_{k,k'} = \delta_{k,k'}\,.
\end{aligned}
\tag{3.63}
$$

Similar manipulations show that $\{c_k, c_{k'}\} = 0$ and $\{c_k^\dagger, c_{k'}^\dagger\} = 0$ also still hold.

Applying the Bogoliubov transformation to the $c_k$ operators in the Hamiltonian (3.53) gives

$$
\begin{aligned}
H_{\vec{s}}^{\pm}(\alpha) &= J\sum_k\big[\,2(\alpha - \cos k)(u_k\gamma_k^\dagger + iv_{-k}\gamma_{-k})(u_k\gamma_k - iv_{-k}\gamma_{-k}^\dagger) \\
&\quad +i\sin k\,(\,(u_k\gamma_{-k}^\dagger + iv_k\gamma_k)(u_k\gamma_k^\dagger + iv_{-k}\gamma_{-k}) \\
&\quad\quad +(u_k\gamma_{-k} - iv_k\gamma_k^\dagger)(u_k\gamma_k - iv_{-k}\gamma_{-k}^\dagger)\,)\,\big] - J\alpha N' + C_s(\alpha) \\
&= J\sum_k\big[\,2(\alpha - \cos k)(u_k^2\gamma_k^\dagger\gamma_k + iu_k v_k\gamma_k^\dagger\gamma_{-k}^\dagger - iu_k v_k\gamma_{-k}\gamma_k \\
&\quad +v_k^2\gamma_{-k}\gamma_{-k}^\dagger) + i\sin k\,(u_k^2\gamma_{-k}^\dagger\gamma_k^\dagger - iu_k v_k\gamma_{-k}^\dagger\gamma_{-k} + iu_k v_k\gamma_k\gamma_k^\dagger \\
&\quad +v_k^2\gamma_k\gamma_{-k} + u_k^2\gamma_{-k}\gamma_k + iu_k v_k\gamma_{-k}\gamma_{-k}^\dagger - iu_k v_k\gamma_k^\dagger\gamma_k \\
&\quad +v_k^2\gamma_k^\dagger\gamma_{-k}^\dagger) - \alpha\,\big] + C_s(\alpha) \\
&= J\sum_k\big[\,2(\alpha - \cos k)(u_k^2\gamma_k^\dagger\gamma_k + v_k^2\,\underbrace{\gamma_{-k}\gamma_{-k}^\dagger}_{1-\gamma_{-k}^\dagger\gamma_{-k}}) \\
&\quad +i\sin k(-iu_k v_k\gamma_{-k}^\dagger\gamma_{-k} + iu_k v_k\,\underbrace{\gamma_k\gamma_k^\dagger}_{1-\gamma_k^\dagger\gamma_k} \\
&\quad +iu_k v_k\,\underbrace{\gamma_{-k}\gamma_{-k}^\dagger}_{1-\gamma_{-k}^\dagger\gamma_{-k}} - iu_k v_k\gamma_k^\dagger\gamma_k) - \alpha\,\big] \\
&\quad +J\sum_k\big[\,2(\alpha - \cos k)(iu_k v_k\gamma_k^\dagger\gamma_{-k}^\dagger - iu_k v_k\gamma_{-k}\gamma_k) \\
&\quad +i\sin k\,(u_k^2\,\underbrace{\gamma_{-k}^\dagger\gamma_k^\dagger}_{-\gamma_k^\dagger\gamma_{-k}^\dagger} + v_k^2\,\underbrace{\gamma_k\gamma_{-k}}_{-\gamma_{-k}\gamma_k} \\
&\quad +u_k^2\gamma_{-k}\gamma_k + v_k^2\gamma_k^\dagger\gamma_{-k}^\dagger)\,\big] + C_s(\alpha)
\end{aligned}
$$

$$
\begin{aligned}
= \quad & J \sum_k \left[ \left( 2(\alpha - \cos k)(u_k^2 - v_k^2) + 4\sin k\,(u_k v_k) \right) \gamma_k^\dagger \gamma_k \right. \\
& \left. + \left( 2(\alpha - \cos k)v_k^2 - 2\sin k\,(u_k v_k) - \alpha \right) \right] \\
& + J \sum_k \left[ \left( 2i(\alpha - \cos k)u_k v_k - i\sin k\,(u_k^2 - v_k^2) \right) \gamma_k^\dagger \gamma_{-k}^\dagger \right. \\
& \left. \left( -2i(\alpha - \cos k)u_k v_k + i\sin k\,(u_k^2 - v_k^2) \right) \gamma_{-k}\gamma_k \right] + C_s(\alpha) \\
= \quad & J \sum_k \left[ \left( 2(\alpha - \cos k)(u_k^2 - v_k^2) + 4\sin k\,(u_k v_k) \right) \gamma_k^\dagger \gamma_k \right. \\
& \left. + \left( \underbrace{2(\alpha - \cos k)v_k^2 - \alpha}_{-(\alpha-\cos k)(u_k^2 - v_k^2) - \cos k} - 2\sin k\,(u_k v_k) \right) \right] \\
& + J \sum_k \left[ \left( 2i(\alpha - \cos k)u_k v_k - i\sin k\,(u_k^2 - v_k^2) \right) \gamma_k^\dagger \gamma_{-k}^\dagger \right. \\
& \left. \left( -2i(\alpha - \cos k)u_k v_k + i\sin k\,(u_k^2 - v_k^2) \right) \gamma_{-k}\gamma_k \right] + C_s(\alpha) \\
= \quad & J \sum_k \left[ \left( 2(\alpha - \cos k)(u_k^2 - v_k^2) + 4\sin k\,(u_k v_k) \right) \left( \gamma_k^\dagger \gamma_k - \frac{1}{2} \right) \right] \\
& + C_s(\alpha) - J \underbrace{\sum_k \cos k}_{0} \\
& + J \sum_k \left[ \left( 2i(\alpha - \cos k)u_k v_k - i\sin k\,(u_k^2 - v_k^2) \right) \left( \gamma_k^\dagger \gamma_{-k}^\dagger - \gamma_{-k}\gamma_k \right) \right].
\end{aligned}
$$
$$(3.64)$$

Thus the Bogoliubov transformation, Eq. (3.54), diagonalizes the Hamiltonian (3.53) if the coefficients of the nondiagonal terms vanish, i.e. if

$$
2i(\alpha - \cos k)u_k v_k - i\sin k\,(u_k^2 - v_k^2) = 0\,,
$$

which leads to the condition

$$
\frac{2\,u_k v_k}{u_k^2 - v_k^2} = \frac{\sin k}{\alpha - \cos k} \tag{3.65}
$$

on $u_k$ and $v_k$, for the Hamiltonian to be diagonalized. Then the Hamiltonian (3.53) becomes

$$
H_{\vec{s}}^{\pm}(\alpha) = \sum_k \epsilon_k \left( \gamma_k^\dagger \gamma_k - \frac{1}{2} \right) + C_s(\alpha)\,, \tag{3.66}
$$

with

$$
\epsilon_k = 2J(\alpha - \cos k)(u_k^2 - v_k^2) + 4J\sin k\,(u_k v_k)\,. \tag{3.67}
$$

The eigenenergies $\epsilon_k$ and the constants $u_k$ and $v_k$ are then fixed by Eqs. (3.58), (3.65) and (3.67). However, Eqs. (3.65) and (3.67) can be replaced

by two simpler equations, known as the Bogoliubov-de Gennes equations. These two coupled equations for $\epsilon_k$, $u_k$ and $v_k$ are general for any Hamiltonian of the form of (3.53), but we will derive them for the special case of our model. For the Hamiltonian (3.53), we get

$$
\begin{aligned}
[\,c_k, H_{\vec{s}}^{\pm}(\alpha)\,] &= J\sum_{k'}\big(\,2(\alpha - \cos k')[c_k, c_{k'}^{\dagger} c_{k'}]\\
&\qquad + i\sin k'\,(\,[c_k, c_{-k'}^{\dagger} c_{k'}^{\dagger}] + [c_k, c_{-k'} c_{k'}]\,)\,\big)\\
&= J\sum_{k'}\big(\,2(\alpha - \cos k')(c_k c_{k'}^{\dagger} c_{k'} - c_{k'}^{\dagger} c_{k'} c_k)\\
&\qquad + i\sin k'\,(\,c_k c_{-k'}^{\dagger} c_{k'}^{\dagger} - c_{-k'}^{\dagger} c_{k'}^{\dagger} c_k\\
&\qquad\qquad + c_k c_{-k'} c_{k'} - c_{-k'} c_{k'} c_k\,)\,\big)\\
&= J\sum_{k'}\big(\,2(\alpha - \cos k')(c_{k'}\delta_{k,k'} - \underbrace{c_{k'}^{\dagger} c_k c_{k'} - c_{k'}^{\dagger} c_{k'} c_k}_{0})\\
&\qquad + i\sin k'\,(\,c_{k'}^{\dagger}\delta_{k,-k'}\underbrace{-c_{-k'}^{\dagger} c_k c_{k'}^{\dagger} - c_{-k'}^{\dagger} c_{k'}^{\dagger} c_k}_{-c_{-k'}^{\dagger}\delta_{k,k'}}\\
&\qquad\qquad \underbrace{-c_{-k'} c_k c_{k'} - c_{-k'} c_{k'} c_k}_{0}\,)\,\big)\\
&= J\,(\,2(\alpha - \cos k)\,c_k - 2i\sin k\,c_{-k}^{\dagger}\,)\,. \quad (3.68)
\end{aligned}
$$

Inserting $c_k = u_k\gamma_k - iv_{-k}\gamma_{-k}^{\dagger}$ and $c_{-k}^{\dagger} = u_k\gamma_{-k}^{\dagger} + iv_k\gamma_k$, this becomes

$$
\begin{aligned}
[\,c_k, H_{\vec{s}}^{\pm}(\alpha)\,] &= J\,(\,2(\alpha - \cos k)\,c_k - 2i\sin k\,c_{-k}^{\dagger}\,)\\
&= [\,2J(\alpha - \cos k)\,u_k + 2J\sin k\,v_k\,]\,\gamma_k\\
&\quad + [\,2iJ(\alpha - \cos k)\,v_k - 2iJ\sin k\,u_k\,]\,\gamma_{-k}^{\dagger}\,. \quad (3.69)
\end{aligned}
$$

But at the same time, as the $\gamma$ particles diagonalize the Hamiltonian, with eigenenergies $\epsilon_k$, cf. Eq. (3.66), we get

$$
\begin{aligned}
[\,c_k, H_{\vec{s}}^{\pm}(\alpha)\,] &= [\,u_k\gamma_k - iv_{-k}\gamma_{-k}^{\dagger}, H_{\vec{s}}^{\pm}(\alpha)\,]\\
&= u_k\underbrace{[\gamma_k, H_{\vec{s}}(\alpha)]}_{\epsilon_k\gamma_k} - iv_{-k}\underbrace{[\gamma_{-k}^{\dagger}, H_{\vec{s}}(\alpha)]}_{-\epsilon_{-k}\gamma_{-k}^{\dagger}}\\
&= u_k\epsilon_k\gamma_k - iv_k\epsilon_{-k}\gamma_{-k}^{\dagger}\,. \quad (3.70)
\end{aligned}
$$

Equating the coefficients of $\gamma_k$ and $\gamma_{-k}^{\dagger}$ in Eqs. (3.69) and (3.70), gives

$$
\begin{aligned}
u_k\epsilon_k &= 2J(\alpha - \cos k)\,u_k + 2J\sin k\,v_k\,, \quad (3.71)\\
-iv_k\epsilon_{-k} &= 2iJ(\alpha - \cos k)\,v_k - 2iJ\sin k\,u_k\,. \quad (3.72)
\end{aligned}
$$

Letting $k \to -k$ in Eq. (3.72) and simplifying, gives us the **Bogoliubov-de Gennes equations**

$$\epsilon_k u_k = 2J(\alpha - \cos k)\, u_k + 2J \sin k\, v_k\,, \qquad (3.73)$$

$$\epsilon_k v_k = 2J \sin k\, u_k - 2J(\alpha - \cos k)\, v_k\,. \qquad (3.74)$$

These two coupled linear equations, together with Eq. (3.58), completely determine $\epsilon_k$, $u_k$ and $v_k$. We now readily see from Eqs. (3.73) and (3.74) that Eq. (3.58) gives

$$
\begin{aligned}
\epsilon_k &= \sqrt{(\epsilon_k u_k)^2 + (\epsilon_k v_k)^2} \\
&= 2J\sqrt{((\alpha - \cos k)\, u_k + \sin k\, v_k)^2 + ((\alpha - \cos k)\, v_k - \sin k\, u_k)^2} \\
&= 2J\sqrt{(\alpha - \cos k)^2 + \sin^2 k} \;=\; 2J\sqrt{1 + \alpha^2 - 2\alpha \cos k}\,, \qquad (3.75)
\end{aligned}
$$

and, when $k \neq 0$ and $k \neq \pi$, that

$$v_k = \left( \frac{\epsilon_k - 2J(\alpha - \cos k)}{2J \sin k} \right) u_k\,. \qquad (3.76)$$

Eqs. (3.58) and (3.76) now give us $u_k$ as

$$u_k = \frac{\sqrt{2}\, J \sin k}{\sqrt{\epsilon_k(\epsilon_k - 2J(\alpha - \cos k))}}\,. \qquad (3.77)$$

For future reference, these relations imply that

$$
\begin{aligned}
v_k^2 &= \left( \frac{\epsilon_k - 2J(\alpha - \cos k)}{2J \sin k} \right)^2 \left( \frac{2J^2 \sin^2 k}{\epsilon_k(\epsilon_k - 2J(\alpha - \cos k))} \right) \\
&= \frac{1}{2}\left( 1 - \frac{(\alpha - \cos k)}{\sqrt{(\alpha - \cos k)^2 + \sin^2 k}} \right)\,, \qquad (3.78)
\end{aligned}
$$

and

$$
\begin{aligned}
u_k v_k &= \left( \frac{\epsilon_k - 2J(\alpha - \cos k)}{2J \sin k} \right) \left( \frac{2J^2 \sin^2 k}{\epsilon_k(\epsilon_k - 2J(\alpha - \cos k))} \right) \\
&= \frac{\sin k}{2\sqrt{(\alpha - \cos k)^2 + \sin^2 k}}\,. \qquad (3.79)
\end{aligned}
$$

The special cases $k = 0$ and $k = \pi$ must be treated separately. For $k = 0$, the Bogoliubov-de Gennes equations become

$$(1 - \alpha)u_0 = -(1 - \alpha)u_0\,,$$

$$(1 - \alpha)v_0 = (1 - \alpha)v_0\,,$$

which gives

$$u_0 \quad = \quad 0 \,, \tag{3.80}$$
$$|v_0| \quad = \quad 1 \,. \tag{3.81}$$

Similarly, for $k = \pi$ the Bogoliubov-de Gennes equations become

$$(1 + \alpha)u_\pi \quad = \quad (1 + \alpha)u_\pi \,,$$
$$(1 + \alpha)v_\pi \quad = \quad -(1 + \alpha)v_\pi \,,$$

which gives

$$|u_\pi| \quad = \quad 1 \,, \tag{3.82}$$
$$v_\pi \quad = \quad 0 \,. \tag{3.83}$$

To summarize, the Bogoliubov transformation has diagonalized the Hamiltonian (3.53), bringing it on the form

$$H_{\bar{s}}^{\pm}(\alpha) = \sum_k \epsilon_k \left( \gamma_k^\dagger \gamma_k - \frac{1}{2} \right) + C_s(\alpha) \,, \tag{3.84}$$

with the eigenenergies $\epsilon_k$ given by

$$\epsilon_k = 2J\sqrt{1 + \alpha^2 - 2\alpha \cos k} \,. \tag{3.85}$$

### 3.3.4   The Physical Spectrum

The ground state of the Hamiltonian (3.84) will be the state that is annihilated by $\gamma_k$, $\forall\, k$, called the "Bogoliubov vacuum" $|\Psi_0\rangle$.

For antiperiodic boundary conditions (where $\sin k \neq 0$ for all allowed $k$ values) the Bogoliubov vacuum is given by

$$|\Psi_0^{(ap)}\rangle \equiv \prod_{k>0} (u_k + iv_k c_k^\dagger c_{-k}^\dagger) |0\rangle \,, \tag{3.86}$$

where $|0\rangle$ is the $c$ vacuum, i.e. the state that is annihilated by $c_k$, $\forall\, k$. This is shown by calculating

$$
\begin{aligned}
\gamma_k |\Psi_0^{(ap)}\rangle &= (u_k c_k - iv_k c_{-k}^\dagger) \prod_{k'>0} (u_{k'} + iv_{k'} c_{k'}^\dagger c_{-k'}^\dagger) |0\rangle \\
&= \prod_{\substack{k'>0 \\ k' \neq \pm k}} (u_{k'} + iv_{k'} c_{k'}^\dagger c_{-k'}^\dagger)(u_k c_k - iv_k c_{-k}^\dagger)(u_k + iv_k c_k^\dagger c_{-k}^\dagger) |0\rangle \\
&= \prod_{\substack{k'>0 \\ k' \neq \pm k}} (u_{k'} + iv_{k'} c_{k'}^\dagger c_{-k'}^\dagger)(u_k^2 c_k + iu_k v_k \underbrace{c_k c_k^\dagger}_{1 - c_k^\dagger c_k} c_{-k}^\dagger \\
&\qquad\qquad - iu_k v_k c_{-k}^\dagger + v_k^2 c_{-k}^\dagger \underbrace{c_k^\dagger c_{-k}^\dagger}_{-c_{-k}^\dagger c_k^\dagger}) |0\rangle \\
&= 0 \,. \tag{3.87}
\end{aligned}
$$

Note that $|\Psi_0^{(ap)}\rangle$ contains an even number of $c$ particles, since they always are created in pairs $c_k^\dagger c_{-k}^\dagger$, cf. Eq. (3.86). Thus antiperiodic boundary conditions imply an even number of $c$ particles in the Bogoliubov vacuum.

For periodic boundary conditions, we must take extra care of the $c_0$ and $c_\pi$ particles. Note that the Hamiltonian (3.53) can be written as

$$H_{\vec{s}}^\pm(\alpha) = J\left[\, 2(\alpha-1)c_0^\dagger c_0 + 2(\alpha+1)c_\pi^\dagger c_\pi + \sum_{\substack{k\neq 0 \\ k\neq \pi}} (\ldots)\,\right]. \tag{3.88}$$

Thus, since for $0 \leq \alpha < 1$ we get $(\alpha-1) < 0$ and $(\alpha+1) > 0$, the ground state will contain the $c_0$, but not the $c_\pi$, particle, as this will lower the energy. Therefore the Bogoliubov vacuum for periodic boundary conditions is given by

$$|\Psi_0^{(p)}\rangle \equiv c_0^\dagger \prod_{\substack{k>0 \\ k\neq \pi}} (u_k + iv_k c_k^\dagger c_{-k}^\dagger)\,|0\rangle\,. \tag{3.89}$$

Since Eqs. (3.62) and (3.80)-(3.83) give $\gamma_0 = -iv_0 c_0^\dagger$ and $\gamma_\pi = u_\pi c_\pi$, we easily prove that $|\Psi_0^{(p)}\rangle$ is the Bogoliubov vacuum by calculating

$$\gamma_0|\Psi_0^{(p)}\rangle = -iv_0 \underbrace{c_0^\dagger c_0^\dagger}_{0} \prod_{\substack{k>0 \\ k\neq\pi}} (u_k + iv_k c_k^\dagger c_{-k}^\dagger)\,|0\rangle = 0\,, \tag{3.90}$$

$$\gamma_\pi|\Psi_0^{(p)}\rangle = u_\pi c_\pi c_0^\dagger \prod_{\substack{k>0 \\ k\neq\pi}} (u_k + iv_k c_k^\dagger c_{-k}^\dagger)\,|0\rangle = 0\,, \tag{3.91}$$

and by observing that for all other $k$ values, $\gamma_k|\Psi_0^{(p)}\rangle = 0$ follows from Eq. (3.87). We now note that $|\Psi_0^{(p)}\rangle$ contains an odd number of $c$ particles, since the $c_0$ particle has been added to the state of even numbers of $c$ particles. Thus periodic boundary conditions imply an odd number of $c$ particles in the Bogoliubov vacuum.

The solution on the form of the Hamiltonian (3.84), $H_{\vec{s}}^\pm(\alpha)$, is for each $+$ and $-$ subspace, i.e. the subspaces with even and odd number of $c$ particles, separately. Since $\gamma_k^\dagger = u_k c_k^\dagger + iv_k c_{-k}$, the addition of a $\gamma$ particle would make the system leave the subspace of even or odd number of $c$ particles it belonged to. But due to the projection operators, $P^+$ and $P^-$, in the decomposition of $H_{\vec{s}}(\alpha)$ in Eq. (3.39), the physical Hamiltonian $H_{\vec{s}}(\alpha)$, will only let $H_{\vec{s}}^+(\alpha)$ and $H_{\vec{s}}^-(\alpha)$ act on states with either even or odd number of $c$ particles. Thus the physical spectrum of $H_{\vec{s}}^\pm(\alpha)$ will only contain states with the same parity (i.e. odd or even) on the number of $\gamma$ particles. In fact, when $s$ is even, the spectrum of $H_{\vec{s}}(\alpha)$

will only consist of states with an even number of $\gamma$ particles, and when $s$ is odd the spectrum will only consist of an odd number of $\gamma$ particles. To see this, note that:

- When $s$ is even and the number of $c$ particles is even, the boundary conditions are antiperiodic. This means that the Bogoliubov vacuum contains an even number of $c$ particles. In order to stay in the $+$ subspace of even parity on the number of $c$ particles, we can only add an even number of $\gamma$ particles to the vacuum.

- When $s$ is even and the number of $c$ particles is odd, the boundary conditions are periodic. This means that the Bogoliubov vacuum contains an odd number of $c$ particles. In order to stay in the $-$ subspace, we can only add an even number of $\gamma$ particles to the vacuum.

- When $s$ is odd and the number of $c$ particles is even, the boundary conditions are periodic. This means that the Bogoliubov vacuum contains an odd number of $c$ particles. In order to be in the $+$ subspace, we can only have an odd number of $\gamma$ particles.

- When $s$ is odd and the number of $c$ particles is odd, the boundary conditions are antiperiodic. This means that the Bogoliubov vacuum contains an even number of $c$ particles. In order to be in the $-$ subspace, we can only have an odd number of $\gamma$ particles.

This proves the assertion. Note that when $s$ is odd, the ground state is not the Bogoliubov vacuum, but a state with one $\gamma$ particle with minimal energy $\epsilon_k$. As seen in Eq. (3.85), $\epsilon_k$ is minimized by $k = 0$ in a $+$ subspace ($s$ odd and $+$ subspace give periodic boundary conditions, cf. page 25), and by $k = \pm\pi/N'$ in a $-$ subspace.

Thus, the energy levels of the Hamiltonian $H_{\vec{s}}(\alpha)$, given by

$$H_{\vec{s}}^{\pm}(\alpha) = \sum_k \epsilon_k \left(\gamma_k^{\dagger}\gamma_k - \frac{1}{2}\right) - (1-\alpha)J(N' - 2s)\,, \qquad (3.92)$$

where the $k$ values depend on whether the boundary conditions are periodic or antiperiodic, and $0 \leq \alpha \leq 1$, are given by, for each $s = 0, 1, 2, \ldots, N'$ and for periodic and antiperiodic boundary conditions, having even numbers of $\gamma$ particles for even $s$, and odd numbers of $\gamma$ particles for odd $s$. The energy levels for $1 \leq \alpha \leq 2$ are, by the symmetry of the model, Eq. (3.8), given by letting $\alpha \to (2 - \alpha)$.

Let us take a finite system as an example. When $N = 8$, i.e. $N' = 4$, we get for even values of $s$, $s = 0, 2, 4$, that the number of possible excitations is 8 (the number of ways of picking an even number of $k$ values

among a total number of 4 values of $k$) per $s$ value, and since we also have the two possible boundary conditions, this gives $3 \times 8 \times 2 = 48$ number of energy levels. For odd $s$, i.e. $s = 1, 3$, we get 8 possible excitations, together with two possible boundary conditions, giving $2 \times 8 \times 2 = 32$ number of energy levels. In total we therefore get 80 (degenerate) energy levels for $N = 8$. Plotting these energy levels gives the energy diagram of Fig. (3.1). Note that each $s$ value is $(N'!/((N' - s)!s!))$-fold degenerate, giving $(1 + 6 + 1) \times 8 \times 2 = 128$ states with even $s$, and $(4 + 4) \times 8 \times 2 = 128$ states with odd $s$, i.e. in total 256 states, in agreement with the size of the total Hilbert space of the system ($2^8 = 256$).
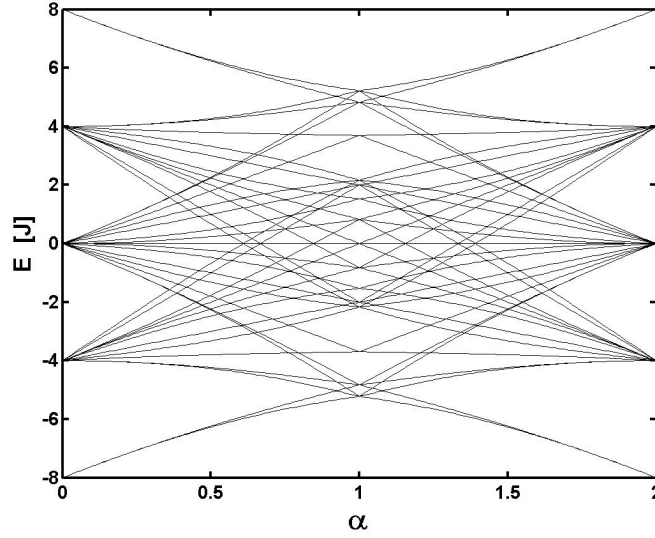


Figure 3.1: *Eigenspectrum of the XX-ZZ model, for a chain of N=8 spins.*

In general, at $\alpha = 0$, where $\epsilon_k = 2J$, the Hamiltonian (3.92) becomes

$$H_{\vec{s}}^{\pm}(0) = 2J \sum_k \gamma_k^{\dagger} \gamma_k + 2Js - 2JN', \qquad (3.93)$$

so the spectrum will at this point go from the lowest lying energy level ($s = 0$, $\langle \gamma_k^{\dagger} \gamma_k \rangle = 0$, $\pm$ subspace, i.e. twofold degeneracy) at $E = -2JN' = -JN$, in discrete steps of $\Delta E = 4J$ to the highest energy level at $E = 2JN' = JN$. By the symmetry (3.8) of the model, this result also applies to the point $\alpha = 2$.

At the other special point, $\alpha = 1$, where $\epsilon_k = 2J\sqrt{2}\sqrt{1 - \cos k}$, the Hamiltonian (3.92) becomes

$$H_{\vec{s}}^{\pm}(1) = 2J\sqrt{2} \sum_k [(\sqrt{1 - \cos k})(\gamma_k^{\dagger} \gamma_k - \frac{1}{2})], \qquad (3.94)$$

so at this point the spectrum will go from the lowest energy level at $E = -J\sqrt{2}\sum_k \sqrt{1 - \cos k}$ , to the highest level at $E = J\sqrt{2}\sum_k \sqrt{1 - \cos k}$ . In the thermodynamic limit, $N \to \infty$, we get

$$\sum_k \sqrt{1 - \cos k} \;\to\; \frac{N'}{2\pi} \int_{-\pi}^{\pi} \sqrt{1 - \cos k}\, dk \;=\; \frac{N'}{2\pi} 4\sqrt{2}\,, \qquad (3.95)$$

so then the spectrum at $\alpha = 1$ will be quasicontinuous, going from $E = -2JN/\pi$ to $E = 2JN/\pi$, with the separation between the levels going to zero as

$$\begin{aligned} \Delta E \;&\sim\; 2J\sqrt{2}\sqrt{1 - \cos \frac{\pi}{N'}} \;\sim\; 2J\sqrt{2}\sqrt{\frac{1}{2}\left(\frac{\pi}{N'}\right)^2} \\ &=\; 2J\pi \frac{1}{N'} \;\sim\; \frac{1}{N} \end{aligned} \qquad (3.96)$$

when $N \to \infty$.

## 3.4  The Quantum Phase Transition

The ground state of the Hamiltonian (3.92) is, for $0 < \alpha < 1$, readily seen to be in the $s{=}0$ subspace and with no $\gamma$ particles ($\langle \gamma_k^\dagger \gamma_k \rangle = 0$), whence the ground state energy is given by

$$E_0 = -\frac{1}{2}\sum_k \epsilon_k - (1 - \alpha)JN'\,. \qquad (3.97)$$

It is easily checked numerically that, for finite $N$, the term $-(1/2)\sum_k \epsilon_k$ is minimized for antiperiodic boundary conditions. Thus, for $N < \infty$, the ground state will be in the $\{s = 0, +\}$ subspace. Therefore the ground state is non-degenerate for finite $N$. In the thermodynamic limit however, where the summation over $k$ can be replaced by an integral, the lowest energy eigenstates in the $\{s = 0, +\}$ and $\{s = 0, -\}$ subspaces become degenerate, resulting in double degeneracy of the ground state. The ground state energy for $\alpha \in [0, 1]$ is then

$$E_0 = -JN\frac{1}{2\pi}\int_0^{\pi} \sqrt{1 + \alpha^2 - 2\alpha \cos k}\, dk - \frac{1}{2}(1 - \alpha)JN \qquad (3.98)$$

when $N \to \infty$. For $\alpha \in [1, 2]$ we simply do the symmetry transformation $\alpha \to (2 - \alpha)$, cf. Eq. (3.8). When plotting this ground state energy for $\alpha \in [0, 2]$, together with its derivative $\partial E_0/\partial \alpha$, we clearly see that the ground state energy has a discontinuous first derivative at $\alpha = 1$, cf. Fig. (4.2). Thus the XX-ZZ model has a first-order quantum phase transition at $\alpha = 1$.
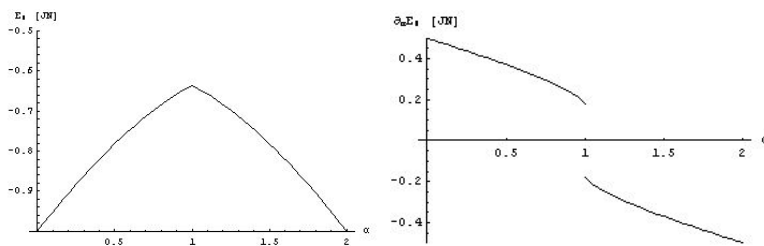
Figure 3.2: *Left: The ground state energy $E_0(\alpha)$ of the XX-ZZ model in the thermodynamic limit ($N \to \infty$). Right: The first derivative $\partial E_0/\partial \alpha$ of the ground state energy with respect to the parameter $\alpha$. The discontinuity in $\partial E_0/\partial \alpha$ at $\alpha = 1$ shows that there is a first-order QPT at this point.*

As previously noted, the ground state is twofold degenerate at $\alpha = 0$ and $\alpha = 2$, and non-degenerate for $0 < \alpha < 1$ and $1 < \alpha < 2$, when $N < \infty$. In the thermodynamic limit the ground state degeneracy is twofold for $0 \leq \alpha < 1$ and $1 < \alpha \leq 2$. At the QPT at $\alpha = 1$, however, there is large degeneracy. Eq. (3.94) shows that the energy eigenvalues are independent of $s$ at $\alpha = 1$, and therefore all subspaces $\vec{s}$ will contribute to the ground state degeneracy. For even values of $s$, all states with no $\gamma$ particles and, for $N \to \infty$, both the $+$ and $-$ subspaces, will contribute. For odd values of $s$, every state will contain at least one $\gamma$ particle, cf. page 34. In the $+$ subspaces, where the boundary conditions then are periodic, the eigenenergy of the $\gamma_0$ particle will be $\epsilon_{k=0} = 2J\sqrt{1 + 1 - 2} = 0$, thus the states with $\langle \gamma_0^\dagger \gamma_0 \rangle = 1$ will nevertheless be ground states. In the $-$ subspaces, the minimal eigenenergy will be $\min \epsilon_k = 2J\sqrt{2 - 2\cos(2\pi/N)}$ which goes to zero as $1/N$ when $N \to \infty$, cf. Eq. (3.96), so that these states with $\gamma$ particles of momentum $k = \pm\pi/N'$ also are ground states. Therefore, in the thermodynamic limit each subspace $\vec{s}$ with $s$ even contributes two states to the ground state degeneracy (the states $\{\langle \gamma_k \gamma_k \rangle = 0, \pm\}$), and each subspace $\vec{s}$ with $s$ odd contributes three states (the states $\{\langle \gamma_0^\dagger \gamma_0 \rangle = 1, +\}$ and $\{\langle \gamma_{\pm\pi/N'}^\dagger \gamma_{\pm\pi/N'} \rangle = 1, -\}$). Therefore the ground state degeneracy $d$ will be on the order of the total number of $\vec{s}$ subspaces, i.e. $d \sim 2^{N'} = 2^{N/2}$.

The state with the second lowest energy, i.e. the first excited state, will for $\alpha \in [0, 1]$ be given by $\{s = 2, \langle \gamma_k^\dagger \gamma_k \rangle = 0 \,\forall\, k\}$, and also by the $\{s = 1, \langle \gamma_0^\dagger \gamma_0 \rangle = 1\}$ state, with eigenenergy $E_1$. The energy gap $\Delta$ that separates these lowest excited states from the ground state is (cf. Eq. (3.92))

$$\Delta = E_1 - E_0 = E_0 + (1 - \alpha)2J \times 2 - E_0 = 4J(1 - \alpha) \qquad (3.99)$$

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when $0 \leq \alpha < 1$. For $1 < \alpha \leq 2$, the symmetry (3.8) of the model then implies that we simply need to let $(1 - \alpha) \rightarrow (\alpha - 1)$, so that the gap is then given by

$$\Delta = 4J(\alpha - 1) \tag{3.100}$$

when $1 < \alpha \leq 2$. This enables us to write

$$\Delta = 4J|\alpha - 1| \qquad \alpha \in [0, 2] , \tag{3.101}$$

which obviously is on the form $\Delta \sim |\alpha - \alpha_c|^{z\nu}$, cf. Eq. (1.7), with $z\nu = 1$. The first-order QPT of the XX-ZZ model therefore has an energy gap that goes to zero as in a continuous QPT in the universality class of the quantum Ising model.

## 3.5 Correlation Functions

To understand the nature of the QPT in the XX-ZZ model, we must quantify how the ground state changes as $\alpha$ is varied. For $0 \leq \alpha < 1$, the ground state $|\Psi_0\rangle$ is given by the Bogoliubov vacuum in the $s{=}0$ subspace, i.e. by $|\Psi_0^{(ap)}\rangle$ (Eq. (3.86)) in the $+$ subspace and by $|\Psi_0^{(p)}\rangle$ (Eq. (3.89)) in the $-$ subspace.

Since the ground state is in the $s{=}0$ subspace, this means that there will be no magnetization of the system in any spin direction for any $\alpha$, because all spins are paired with another antiparallel spin. Furthermore, the expectation values of the spin components on each lattice site are all zero, i.e. for all $i$,

$$\langle \Psi_0 | \sigma_i^x | \Psi_0 \rangle = 0 , \tag{3.102}$$
$$\langle \Psi_0 | \sigma_i^y | \Psi_0 \rangle = 0 , \tag{3.103}$$
$$\langle \Psi_0 | \sigma_i^z | \Psi_0 \rangle = 0 . \tag{3.104}$$

For $\sigma_i^x$ and $\sigma_i^y$, this is easily recognized since these operators flip a single spin, thereby making the odd bond of the site $i$ parallel, thus $\sigma_i^x | \Psi_0 \rangle$ and $\sigma_i^y | \Psi_0 \rangle$ will not belong to the $s{=}0$ subspace, making these states orthogonal to $|\Psi_0\rangle$. For $\sigma_i^z$, we have that $\sigma_{2i}^z \propto \tau_i^z = -(c_i + c_i^\dagger) \prod_{j<i} (1 - 2c_j^\dagger c_j)$, containing an odd number of $c$ operators, therefore $\sigma_{2i}^z$, as well as $\sigma_{2i-1}^z \propto \sigma_{2i}^z$, changes the parity of the number of $c$ particles, and takes states out of the $\pm$ subspace they were in. However, we know that at the point $\alpha = 0$, the two ground states are eigenstates of the $\sigma_i^z$ operators. This simply means that at this point it is possible to make linear combinations of the two degenerate ground states $|\Psi_0^{(ap)}\rangle$ and $|\Psi_0^{(p)}\rangle$, that are eigenstates of both the Hamiltonian and the $\sigma_i^z$ operators. So, we do not get any information about the changes in the ground states by looking at simple expectation values. Instead we must look at the correlation

functions $\langle\Psi_0|\sigma_i^\alpha\sigma_j^\beta|\Psi_0\rangle - \langle\Psi_0|\sigma_i^\alpha|\Psi_0\rangle\langle\Psi_0|\sigma_j^\beta|\Psi_0\rangle = \langle\Psi_0|\sigma_i^\alpha\sigma_j^\beta|\Psi_0\rangle$.

In the $s=0$ subspace, it is trivial that $\langle\Psi_0|\sigma_{2i-1}^z\sigma_{2i}^z|\Psi_0\rangle = -1$, since in this subspace all odd bonds are antiparallel. The correlation function $\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle$ is, by Eq (3.15), given by $-\langle\Psi_0|\tau_i^x|\Psi_0\rangle$, thus

$$
\begin{aligned}
\langle\Psi_0|\sigma_{2j-1}^x\sigma_{2j}^x|\Psi_0\rangle &= -\langle\Psi_0|\tau_j^x|\Psi_0\rangle = -\langle\Psi_0|(1-2c_j^\dagger c_j)|\Psi_0\rangle \\
&= -1 + 2\langle\Psi_0|(\frac{1}{\sqrt{N'}}\sum_k c_k^\dagger e^{-ijk})(\frac{1}{\sqrt{N'}}\sum_{k'} c_{k'}e^{ijk'})|\Psi_0\rangle \\
&= -1 + \frac{2}{N'}\sum_{k,k'}[e^{i(k'-k)j}\langle\Psi_0|c_k^\dagger c_{k'}|\Psi_0\rangle] \\
&= -1 + \frac{2}{N'}\sum_{k,k'}[e^{i(k'-k)j}\langle\Psi_0|(u_k\gamma_k^\dagger - iv_k\gamma_{-k}) \\
&\qquad\qquad\qquad \times(u_{k'}\gamma_{k'} + iv_{k'}\gamma_{-k'}^\dagger)|\Psi_0\rangle] \\
&= -1 + \frac{2}{N'}\sum_{k,k'}[e^{i(k'-k)j}v_kv_{k'}\underbrace{\langle\Psi_0|\gamma_{-k}\gamma_{-k'}^\dagger|\Psi_0\rangle}_{\delta_{k,k'}}] \\
&= -1 + \frac{2}{N'}\sum_k v_k^2. \qquad\qquad\qquad\qquad\text{(3.105)}
\end{aligned}
$$

For spin pairs $\{i,j\}$ on different odd bonds, one gets $\langle\Psi_0|\sigma_i^x\sigma_j^x|\Psi_0\rangle = 0$, since $\sigma_i^x\sigma_j^x$ then flips two spins on two different antiparallel odd bonds, making these two bonds parallel, thus taking the state out of the $s=0$ subspace, and therefore $\sigma_i^x\sigma_j^x|\Psi_0\rangle$ will be orthogonal to $|\Psi_0\rangle$. We write this as $\langle\Psi_0|\sigma_{2i-m}^x\sigma_{2j-n}^x|\Psi_0\rangle = 0$, where $i \neq j$ and $m,n = 0,1$. The remaining type of correlation functions, namely between the $z$ spin components of spins on different odd bonds, is more involved. By Eq. (3.15), $\langle\Psi_0|\sigma_{2i-m}^z\sigma_{2j-n}^z|\Psi_0\rangle = (-1)^{m+n}\langle\Psi_0|\tau_i^z\tau_j^z|\Psi_0\rangle$, when $i \neq j$ and $m,n = 0,1$. Writing $j = i + r$, this becomes

$$
\begin{aligned}
\langle\Psi_0|\tau_i^z\tau_{i+r}^z|\Psi_0\rangle &= \langle\Psi_0|(c_i^\dagger + c_i)\prod_{j<i}(1-2c_j^\dagger c_j) \\
&\qquad\qquad \times \prod_{j'<i+r}(1-2c_{j'}^\dagger c_{j'})(c_{i+r}^\dagger + c_{i+r})|\Psi_0\rangle \\
&= \langle\Psi_0|(c_i^\dagger + c_i)\prod_{i\leq j<i+r}(1-2c_j^\dagger c_j)(c_{i+r}^\dagger + c_{i+r})|\Psi_0\rangle \\
&= \langle\Psi_0|(c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1})(c_{i+1}^\dagger - c_{i+1})\ldots \\
&\qquad \times\ldots(c_{i+r-1}^\dagger + c_{i+r-1})(c_{i+r-1}^\dagger - c_{i+r-1})(c_{i+r}^\dagger + c_{i+r})|\Psi_0\rangle \\
&= \langle\Psi_0|B_iA_{i+1}B_{i+1}A_{i+2}B_{i+2}\ldots A_{i+r-1}B_{i+r-1}A_{i+r}|\Psi_0\rangle,
\end{aligned}
$$
$$\text{(3.106)}$$

where

$$A_j \equiv c_j^\dagger + c_j, \tag{3.107}$$

$$B_j \equiv c_j^\dagger - c_j. \tag{3.108}$$

Since the $A_i$ and $B_i$ operators obey fermionic anticommutation relations,

$$\{A_i, A_j\} = 0 \qquad i \neq j, \tag{3.109}$$

$$\{B_i, B_j\} = 0 \qquad i \neq j, \tag{3.110}$$

$$\{A_i, B_j\} = 0 \qquad \forall\, i, j, \tag{3.111}$$

we can use Wick's theorem to calculate the expectation value (3.106) as the sum of all possible products of contractions of pairs of the operators:

$$\langle \Psi_0 | B_i \dots A_{i+r} | \Psi_0 \rangle = \sum_{\substack{all\ possible \\ pairings}} \left[ (-1)^p \prod_{all\ pairs} (contractions\ of\ pairs) \right].$$

There are three types of contractions that need to be calculated, $A_i^{\cdot} A_j^{\cdot}$, $B_i^{\cdot} B_j^{\cdot}$ and $B_i^{\cdot} A_j^{\cdot}$, where the contraction is defined as

$$X^{\cdot} Y^{\cdot} \equiv XY - N[XY], \tag{3.112}$$

where $N[\ ]$ is the normal ordering operator; here the normal ordering is with respect to the $\gamma$ operators, since they can annihilate $|\Psi_0\rangle$. Now, since

$$\begin{aligned}
B_n A_m &= (c_n^\dagger - c_n)(c_m^\dagger + c_m) = c_n^\dagger c_m^\dagger + c_n^\dagger c_m - c_n c_m^\dagger - c_n c_m \\
&= c_n^\dagger c_m^\dagger + c_n^\dagger c_m + c_m^\dagger c_n + c_m c_n - \delta_{m,n} \\
&= c_n^\dagger c_m^\dagger + c_n^\dagger c_m + (c_n^\dagger c_m)^\dagger + (c_n^\dagger c_m^\dagger)^\dagger - \delta_{m,n}, \tag{3.113}
\end{aligned}$$

we need to calculate the contractions of the first two terms.

$$\begin{aligned}
c_n^\dagger c_m^\dagger &= \frac{1}{N'} \sum_{k,k'} [\,(u_k \gamma_k^\dagger - i v_k \gamma_{-k}) e^{-ikn} (u_{k'} \gamma_{k'}^\dagger - i v_{k'} \gamma_{-k'}) e^{-ik'm}\,] \\
&= \frac{1}{N'} \sum_{k,k'} [\,(u_k u_{k'} \gamma_k^\dagger \gamma_{k'}^\dagger - i u_k v_{k'} \gamma_k^\dagger \gamma_{-k'} - i u_{k'} v_k \underbrace{\gamma_{-k} \gamma_{k'}^\dagger}_{\substack{\delta_{-k,k'} - \\ -\gamma_{k'}^\dagger \gamma_{-k}}} \\
&\qquad - v_k v_{-k'} \gamma_{-k} \gamma_{-k'}) e^{-ikn} e^{-ik'm}] \\
&= N[c_n^\dagger c_m^\dagger] - i\frac{1}{N'} \sum_{k,k'} [\,u_{k'} v_k \delta_{-k,k'} e^{-ikn} e^{-ik'm}\,] \\
&= N[c_n^\dagger c_m^\dagger] + i\frac{1}{N'} \sum_{k} u_k v_k e^{ik(n-m)}, \tag{3.114}
\end{aligned}$$

and

$$c_n^\dagger c_m = \frac{1}{N'} \sum_{k,k'} [\, (u_k \gamma_k^\dagger - iv_k \gamma_{-k}) e^{-ikn} (u_{k'} \gamma_{k'} + iv_{k'} \gamma_{-k'}^\dagger) e^{ik'm} \,]$$

$$= \frac{1}{N'} \sum_{k,k'} [\, (u_k u_{k'} \gamma_k^\dagger \gamma_{k'} + iu_k v_{k'} \gamma_k^\dagger \gamma_{-k'}^\dagger - iu_{k'} v_k \gamma_{-k} \gamma_{k'}$$

$$+ v_k v_{k'} \gamma_{-k} \gamma_{-k'}^\dagger ) e^{-ikn} e^{ik'm} ]$$

$$= N[c_n^\dagger c_m] + \frac{1}{N'} \sum_{k,k'} [\, v_k v_{k'} \delta_{-k,-k'} e^{-ikn} e^{ik'm} \,]$$

$$= N[c_n^\dagger c_m] + \frac{1}{N'} \sum_k v_k^2 e^{-ik(n-m)} , \qquad (3.115)$$

gives for Eq. (3.113)

$$B_n A_m = N[B_n A_m] + \frac{1}{N'} \sum_k v_k^2 e^{ik(n-m)} + \frac{1}{N'} \sum_k v_k^2 e^{-ik(n-m)}$$

$$+ i \frac{1}{N'} \sum_k u_k v_k e^{ik(n-m)} - i \frac{1}{N'} \sum_k u_k v_k e^{-ik(n-m)} - \delta_{m,n}$$

$$= N[B_n A_m] + \frac{2}{N'} \sum_k v_k^2 \cos(k(n-m))$$

$$- \frac{2}{N'} \sum_k u_k v_k \sin(k(n-m)) \, - \, \delta_{m,n} . \qquad (3.116)$$

Thus the contraction becomes

$$B_n^{\cdot} A_m^{\cdot} = -\delta_{m,n} + \frac{2}{N'} \sum_k v_k^2 \cos(k(n-m)) - \frac{2}{N'} \sum_k u_k v_k \sin(k(n-m)) ,$$
$$(3.117)$$

which can be written as

$$B_i^{\cdot} A_{i+r'}^{\cdot} = -\delta_{r',0} + \frac{2}{N'} \sum_k v_k^2 \cos(kr') + \frac{2}{N'} \sum_k u_k v_k \sin(kr') . \quad (3.118)$$

Similar calculations show that

$$A_n^{\cdot} A_m^{\cdot} = \delta_{m,n} , \qquad (3.119)$$
$$B_n^{\cdot} B_m^{\cdot} = -\delta_{m,n} . \qquad (3.120)$$

Since we do not have any two $A_i$s or $B_i$s with the same $i$ in the expression for $\tau_i^z \tau_{i+r}^z$, Eq. (3.106), all contractions of two $A_i$s or $B_i$s will give zero, due to Eqs. (3.119) and (3.120). Thus only the terms where only

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$A_i$s are contracted with $B_i$s, and vice versa, will contribute to the sum. Since the operators must stand next to each other to be contracted, and since all operators anticommute, every time we interchange two operators the term acquires a minus sign. We get all the different terms by holding the $B_i$s fixed, and permuting the $A_i$s amongst each other, and then contracting the nearest neighbours. The sign of a particular term is then decided by how many times we have permuted the $A_i$s amongst themselves. This procedure is what makes a determinant. Further, in every term, the sum of the index differences $r'$ must always add up to $r$. The result (which was outlined in Ref. [28]) is that the correlation function $\langle \Psi_0 | \tau_i^z \tau_{i+r}^z | \Psi_0 \rangle$ is given by the Toeplitz determinant

$$\langle \Psi_0 | \tau_i^z \tau_{i+r}^z | \Psi_0 \rangle = \begin{vmatrix} f_1 & f_2 & f_3 & \cdots & f_r \\ f_0 & f_1 & f_2 & & \\ f_{-1} & f_0 & f_1 & & \\ \vdots & & & \ddots & \\ f_{-r+2} & \cdots & & & f_1 \end{vmatrix}, \qquad (3.121)$$

where $f_{r'} \equiv B_i^{\cdot} A_{i+r'}^{\cdot}$.

For nearest neighbour spins on two different odd bonds, the above results for $0 \leq \alpha < 1$ give that

$$\langle \Psi_0 | \sigma_{2i}^x \sigma_{2i+1}^x | \Psi_0 \rangle = 0 \,, \qquad (3.122)$$

and

$$\begin{aligned} \langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle &= -\langle \Psi_0 | \tau_i^z \tau_{i+1}^z | \Psi_0 \rangle = -f_1 \\ &= -\frac{2}{N'} \sum_k v_k^2 \cos k - \frac{2}{N'} \sum_k u_k v_k \sin k \,. \end{aligned}$$
$$(3.123)$$

In summary, the nearest neighbour spin correlation functions for $0 \leq \alpha < 1$ are given by

$$\langle \Psi_0 | \sigma_{2i-1}^z \sigma_{2i}^z | \Psi_0 \rangle = -1 \,, \qquad (3.124)$$

$$\langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle = -1 + \frac{2}{N'} \sum_k v_k^2 \,, \qquad (3.125)$$

$$\langle \Psi_0 | \sigma_{2i}^x \sigma_{2i+1}^x | \Psi_0 \rangle = 0 \,, \qquad (3.126)$$

$$\langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle = -\frac{2}{N'} \sum_k v_k^2 \cos k - \frac{2}{N'} \sum_k u_k v_k \sin k \,. \qquad (3.127)$$

When calculating $\langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle$ and $\langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle$, the expressions for $v_k^2$ and $u_k v_k$ are given by Eqs. (3.78) and (3.79). For $1 < \alpha \leq 2$, the
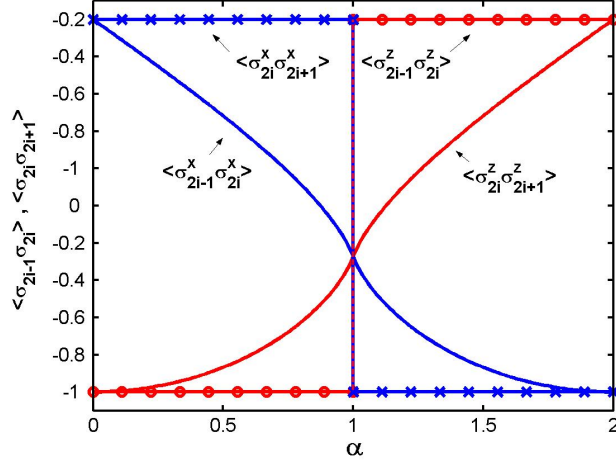
Figure 3.3: *Correlation functions in the ground state of the XX-ZZ model, calculated in the thermodynamic limit ($N \to \infty$). Note the discontinuities in $\langle\Psi_0|\sigma_{2i}^x\sigma_{2i+1}^x|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i-1}^z\sigma_{2i}^z|\Psi_0\rangle$ at the QCP at $\alpha = 1$.*

symmetry (3.8) relates the correlation functions to those already calculated. Plotting the correlation functions for nearest neighbour spins, Eqs. (3.124)-(3.127), gives the curves shown in Fig. (3.3). The correlation functions $\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle$ are continuous at the QCP ($\alpha = 1$), as is seen by applying Eqs. (3.78) and (3.79) to Eqs. (3.125) and (3.127):

$$\lim_{\alpha \to 1^-} \langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle = -\frac{\sqrt{2}}{4\pi}\int_{-\pi}^{\pi}\sqrt{1-\cos k}\,dk = -\frac{2}{\pi}, \quad (3.128)$$

$$\lim_{\alpha \to 1^-} \langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^x|\Psi_0\rangle = -\frac{\sqrt{2}}{4\pi}\int_{-\pi}^{\pi}\sqrt{1-\cos k}\,dk = -\frac{2}{\pi}, \quad (3.129)$$

so that, by the symmetry (3.8), $\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle$ are continuous at $\alpha = 1$. In contrast, $\langle\Psi_0|\sigma_{2i-1}^z\sigma_{2i}^z|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i}^x\sigma_{2i+1}^x|\Psi_0\rangle$ are obviously discontinuous at the QCP. Thus the QPT is due to a level crossing at $\alpha = 1$ where the ground state abruptly changes from ordering in the $z$ spin direction on odd bonds to ordering of the $x$ spin component on even bonds.

As previously noted, the only long-range correlations for $\alpha \in [0, 1)$ are between the $z$ spin components. Since $\langle\Psi_0|\sigma_{2i-m}^z\sigma_{2j-n}^z|\Psi_0\rangle = (-1)^{m+n}$ $\times\langle\Psi_0|\tau_i^z\tau_j^z|\Psi_0\rangle$, where $i \neq j$ and $m, n = 0, 1$, this correlation function behaves as in the quantum Ising model, where it is well known that the correlation length $\xi$ of the $\tau_i^z\tau_j^z$ correlations diverges as $\xi \sim |1 - \alpha|^{-1}$ as $\alpha \to 1$. Thus the $z$ spin components have a correlation length which diverges in the Ising universality class as $\alpha \to 1^-$, but due to the sym-

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metry (3.8) their correlation length vanishes for $\alpha \in (1, 2]$. Instead the correlation length of the spin $x$ components diverges when $\alpha \to 1^+$.

The conclusion is thus that the first-order QPT at $\alpha = 1$ is characterized by a number of discontinuous correlation functions, together with a vanishing excitation gap and diverging correlation length, both in the Ising universality class.

When the temperature $T$ is larger than the excitation energy gap $\Delta$, the system will be excited. Since the lowest excitation is given by $\gamma_0^\dagger \propto c_0 \propto \sum_j c_j$, and by Eq. (3.26) the $c_j$ operators act as lowering operators on the $\tau$ spins, it is seen that these excitations will destroy the $z$ spin correlations for $\sigma$ spins on different odd bonds. This is consistent with the general fact that quantum critical regions are described by the physics of the quantum critical point (cf. page 5), since the long-range correlations are undefined at the QCP. Further, excitations to degenerate states in different $\vec{s}$ subspaces will lead to non-trivial correlations between spins on the same odd bonds for energies larger than the gap $\Delta$. Therefore, combining the expression for the excitation gap, Eq. (3.101), with the results for the correlation functions, the phase diagram of the XX-ZZ model may be constructed, and is shown in Fig. (3.4).

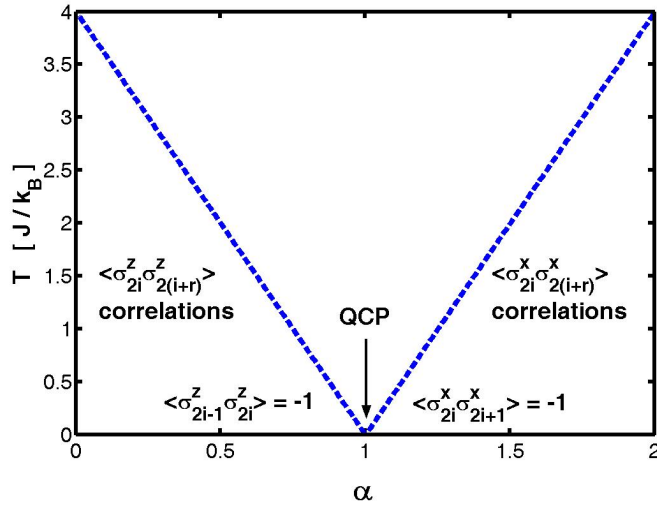This concludes the derivation of the results in Ref. [1].



Figure 3.4: *Phase diagram of the XX-ZZ model. The dashed line is the excitation energy gap $\Delta = 4J|\alpha - 1|$, separating the phases where the system is in its quantum ground state from the quantum critical phase, where the system is excited. $\Delta$ vanishes at the QCP at $\alpha = 1$, marking the phase boundary between ordering of $z$ spin components on odd bonds and ordering of $x$ spin components on even bonds.*

# Chapter 4

# Generalization of the One-Dimensional XX-ZZ Model

## 4.1 Introducing Different Coupling Constants

The one-dimensional XX-ZZ model, as defined by Eqs. (3.1) and (3.2), can be generalized by introducing different coupling constants $J_x$ and $J_z$ for the interactions in the $x$ and $z$ spin directions, respectively. The generalized model, which we then can refer to as "the anisotropic XX-ZZ model", will be given by the Hamiltonian

$$H(\alpha) = \sum_{i=1}^{N'} \left[ J_z \left( 1 - \alpha \right) \sigma_{2i-1}^z \sigma_{2i}^z + J_x \alpha \, \sigma_{2i-1}^x \sigma_{2i}^x + J_z \sigma_{2i}^z \sigma_{2i+1}^z \right] \qquad (4.1)$$

for $0 \leq \alpha \leq 1$, and

$$H(\alpha) = \sum_{i=1}^{N'} \left[ J_x \sigma_{2i-1}^x \sigma_{2i}^x + J_z \left( 2 - \alpha \right) \sigma_{2i}^z \sigma_{2i+1}^z + J_x \left( \alpha - 1 \right) \sigma_{2i}^x \sigma_{2i+1}^x \right] \quad (4.2)$$

for $1 \leq \alpha \leq 2$, where as before $N' \equiv N/2$. The symmetry, Eq. (3.8), relating the Hamiltonians for $0 \leq \alpha \leq 1$ and $1 \leq \alpha \leq 2$, is now modified to include the exchange of the coupling constants. Thus the symmetry transformation relating the Hamiltonians (4.1) and (4.2) is

$$\sigma_i^x \leftrightarrow \sigma_i^z \;\; \forall\, i\,, \quad 2i \leftrightarrow 2i - 1 \;\; \forall\, i\,, \quad \left( 1 - \alpha \right) \leftrightarrow \left( \alpha - 1 \right), \quad J_x \leftrightarrow J_z\,. \quad (4.3)$$

Thus, once again only the Hamiltonian for $0 \leq \alpha \leq 1$ needs to be solved. In every subspace $\vec{s}$, of the Hamiltonian (4.1), the terms involving $\sigma_{2i-1}^z \sigma_{2i}^z$ will only give a constant contribution $C_s(\alpha)$, now given

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by (cf. Eq. (3.13))

$$C_s(\alpha) = J_z(1 - \alpha) \sum_{i=1}^{N'} \sigma_{2i-1}^z \sigma_{2i}^z = -J_z(1 - \alpha)(N' - 2s) \, . \qquad (4.4)$$

The Hamiltonian (4.1) then becomes

$$
\begin{aligned}
H_{\vec{s}}(\alpha) &= \sum_{i=1}^{N'} \left[ J_x \alpha \, \sigma_{2i-1}^x \sigma_{2i}^x + J_z \sigma_{2i}^z \sigma_{2i+1}^z \right] + C_s(\alpha) \\
&= J_z \sum_{i=1}^{N'} \left[ \frac{J_x}{J_z} \alpha \, \sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z \right] - J_z(1 - \alpha)(N' - 2s) \, .
\end{aligned}
$$
$$(4.5)$$

Comparing Eq. (4.5) with Eq. (3.14), given by

$$H_{\vec{s}}(\alpha) = J \sum_{i=1}^{N'} \left[ \alpha \, \sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z \right] - J(1 - \alpha)(N' - 2s) \, , \qquad (4.6)$$

it is readily seen that the anisotropic model simply corresponds to making the transformation

$$\alpha \to \frac{J_x}{J_z} \alpha \, , \qquad J \to J_z \qquad (4.7)$$

everywhere in the Hamiltonian, except in the constant term $C_s(\alpha)$, where only the transformation $J \to J_z$ is made. Since the term $C_s(\alpha)$ is only a constant, this difference will only add an $\alpha$-dependent shift to the energy spectrum, without influencing any correlation functions or any other properties of the ground state. Thus the fact that this constant obeys another transformation is of no importance. The solution to the anisotropic model is hence given by simply applying the transformation (4.7) to the solution, Eq. (3.84), of the isotropic model, giving

$$
\begin{aligned}
H_{\vec{s}}^{\pm}(\alpha) &= \sum_k \epsilon_k \, (\gamma_k^\dagger \gamma_k - \frac{1}{2}) + C_s(\alpha) \\
&= 2J_z \sum_k \left[ \sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k} \, (\gamma_k^\dagger \gamma_k - \frac{1}{2}) \right] \\
&\qquad\qquad - J_z(1 - \alpha)(N' - 2s) \, .
\end{aligned}
$$
$$(4.8)$$

This solution readily gives the energy spectrum. In order to determine whether to have an odd or even number of $\gamma$ particles, we express the Hamiltonian in $c$ operators, by applying the transformation (4.7) to the

Hamiltonian (3.53), giving

$$H_{\vec{s}}^{\pm}(\alpha) = J_z \sum_k \left[ 2(\frac{J_x}{J_z}\alpha - \cos k)c_k^{\dagger}c_k + i \sin k \, (c_{-k}^{\dagger}c_k^{\dagger} + c_{-k}c_k) \right]$$
$$-J_x\alpha N' + C_s(\alpha) \,. \tag{4.9}$$

Recognizing that the ground state still will be in the $s$=0 subspace for $\alpha \in [0, 1)$, we see that antiperiodic boundary conditions (where $k \neq 0$, $\pi$) implies an even number of $c$ particles in the Bogoliubov vacuum (cf. page 33). For periodic boundary conditions, the terms in the Hamiltonian involving the $c_0$ and $c_{\pi}$ particles become

$$J_z \left[ 2(\frac{J_x}{J_z}\alpha - 1)c_0^{\dagger}c_0 + 2(\frac{J_x}{J_z}\alpha + 1)c_{\pi}^{\dagger}c_{\pi} \right].$$

Thus in the ground state $\langle c_{\pi}^{\dagger}c_{\pi} \rangle = 0$, and

$$\langle c_0^{\dagger}c_0 \rangle = 1 \quad \text{when} \quad \frac{J_x}{J_z}\alpha \leq 1 \,, \tag{4.10}$$

$$\langle c_0^{\dagger}c_0 \rangle = 0 \quad \text{when} \quad \frac{J_x}{J_z}\alpha \geq 1 \,. \tag{4.11}$$

Then we get

- $s$ even and BCs antiperiodic $\Rightarrow$ even number of $\gamma$ particles

- $s$ even and BCs periodic and $\frac{J_x}{J_z}\alpha \leq 1 \Rightarrow$ even number of $\gamma$s

- $s$ even and BCs periodic and $\frac{J_x}{J_z}\alpha \geq 1 \Rightarrow$ odd number of $\gamma$ particles

- $s$ odd and BCs antiperiodic $\Rightarrow$ odd number of $\gamma$ particles

- $s$ odd and BCs periodic and $\frac{J_x}{J_z}\alpha \leq 1 \Rightarrow$ odd number of $\gamma$ particles

- $s$ odd and BCs periodic and $\frac{J_x}{J_z}\alpha \geq 1 \Rightarrow$ even number of $\gamma$ particles

Thus, in the thermodynamic limit, for $(J_x/J_z)\alpha < 1$ both $\{\langle \gamma_k^{\dagger}\gamma_k \rangle = 0, s = 0, +\}$ and $\{\langle \gamma_k^{\dagger}\gamma_k \rangle = 0, s = 0, -\}$ will be ground states, i.e. double degeneracy. For $(J_x/J_z)\alpha > 1$, only $\{\langle \gamma_k^{\dagger}\gamma_k \rangle = 0, s = 0, +\}$ will be a ground state, i.e. no degeneracy.

In Fig. (4.1) the energy spectrum at $J_x/J_z = 2$ for a finite system of $N = 8$ spins is plotted, and when comparing with the spectrum for $J_x/J_z = 1$ in Fig. (3.1), we clearly see how the level crossing at $\alpha = 1$ persists for $J_x/J_z \neq 1$, whereas no level crossing is present at $(J_x/J_z)\alpha = 1$, for $\alpha < 1$, in this finite system (as we shall see, there is an avoided level crossing at this point).
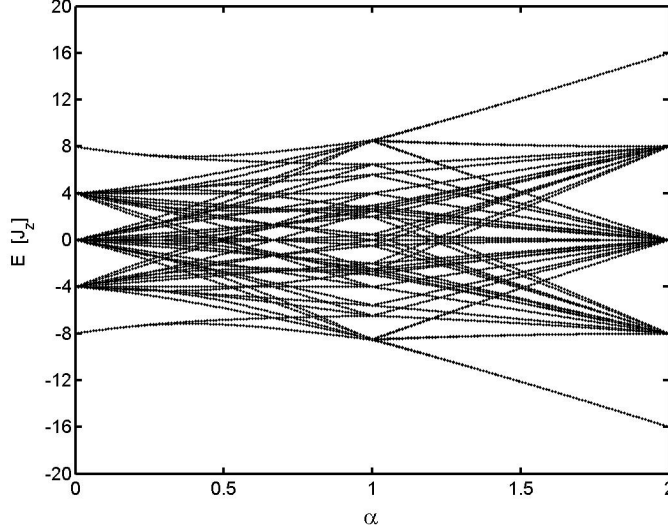
Figure 4.1: *Energy spectrum of the generalized XX-ZZ model at $J_x/J_z = 2$, for a chain of N=8 spins.*

## 4.2 The Quantum Phase Transitions

The ground state energy for $0 \leq \alpha < 1$ is, in the thermodynamic limit where the summation over $k$ in Eq. (4.8) is replaced by an integral, given by

$$E_0(\alpha, \frac{J_x}{J_z}) = -J_z \frac{N'}{2\pi} \int_{-\pi}^{\pi} \sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k} \, dk$$
$$- J_z(1 - \alpha)N'. \tag{4.12}$$

The integral appearing in Eq. (4.12) is the same as the one appearing in the ground state energy of the quantum Ising model (QIM), with parameter $(J_x/J_z)\alpha$. Thus we immediately see that the generalized XX-ZZ model will exhibit a continuous QPT at $(J_x/J_z)\alpha = 1$ when $\alpha \in [0, 1)$, and, by the symmetry (4.3), at $(J_z/J_x)(2 - \alpha) = 1$ when $\alpha \in (1, 2]$. The ground state energy $E_0$ and its first derivative $\partial E_0/\partial \alpha$ with respect to $\alpha$ are plotted in Fig. (4.2). The discontinuous first derivative indicating a first-order QPT is seen to be present at $\alpha = 1$ for all values of $J_x/J_z$. In Fig. (4.3) we see a divergence in the second derivative $\partial^2 E_0/\partial \alpha^2$, and a discontinuity in the third derivative $\partial^3 E_0/\partial \alpha^3$, at $(J_x/J_z)\alpha = 1$ when $\alpha \in [0, 1)$, and at $(J_z/J_x)(2 - \alpha) = 1$ when $\alpha \in (1, 2]$, confirming the presence of a continuous QPT at these points (cf. the definition on page 3). The behaviour of the ground state energy at these points of continuous

QPTs is completely determined by the integral

$$I \equiv \int_0^\pi \sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k} \, dk \,, \qquad (4.13)$$

which is also found in the quantum Ising model, and is plotted in Fig (4.4). Here the divergence in the second derivative, and the discontinuity in the third derivative, at $(J_x/J_z)\alpha = 1$ is clearly visible.
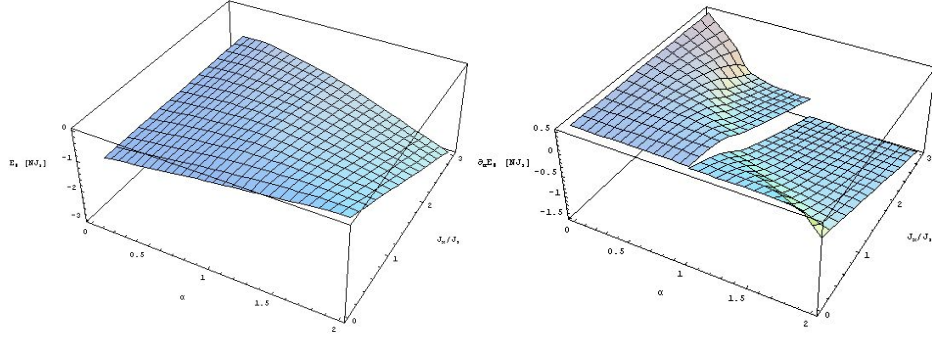


Figure 4.2: *Left: Ground state energy $E_0$ of the generalized XX-ZZ model, as a function of $\alpha$ and $J_x/J_z$. Right: The derivative $\partial E_0/\partial \alpha$ of the ground state energy with respect to $\alpha$. Note the discontinuity in $\partial E_0/\partial \alpha$ at $\alpha = 1$ for all values of $J_x/J_z$, showing the presence of a first-order QPT at these points.*
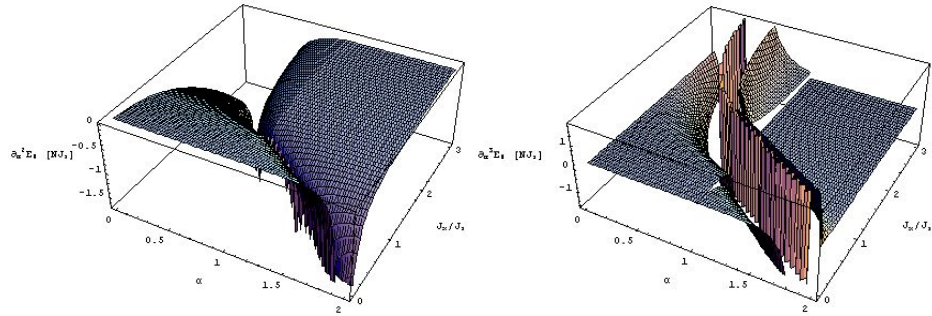


Figure 4.3: *Left: The second derivative $\partial^2 E_0/\partial \alpha^2$ of the ground state energy with respect to $\alpha$. Right: The third derivative $\partial^3 E_0/\partial \alpha^3$ of the ground state energy with respect to $\alpha$. Note the divergence of $\partial^2 E_0/\partial \alpha^2$, and the discontinuity in $\partial^3 E_0/\partial \alpha^3$, at $(J_x/J_z)\alpha = 1$ when $\alpha \in [0,1)$, and at $(J_z/J_x)(2 - \alpha) = 1$ when $\alpha \in (1,2]$, showing the presence of a continuous QPT at these points.*
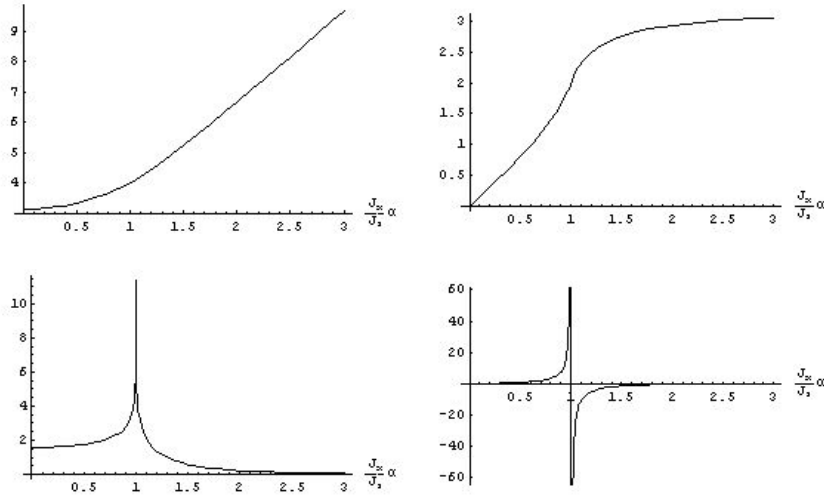
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Figure 4.4: *Upper left: The integral $I(x)$, defined in Eq. (4.13), which determines the ground state energy, plotted as a function of $x \equiv (J_x/J_z)\alpha$. Upper right: $\partial I / \partial x$. Lower left: $\partial^2 I / \partial x^2$. Lower right: $\partial^3 I / \partial x^3$.*

## 4.3 Energy Gap and Correlation Functions

Calculating the gaps between the ground state and the low lying excited states in the thermodynamic limit, using Eq. (4.8) and the following discussion, gives

$$\{\langle \gamma_0^\dagger \gamma_0 \rangle = 1, \langle \gamma_{\pm 2\pi/N'}^\dagger \gamma_{\pm 2\pi/N'} \rangle = 1, s = 0\} :$$

$$\Delta_1 = \begin{cases} 4J_z(1 - \frac{J_x}{J_z}\alpha) & \text{when } \frac{J_x}{J_z}\alpha < 1 \\ 2J_z(1 - \alpha) & \text{when } \frac{J_x}{J_z}\alpha > 1 \end{cases}$$

$$\{\langle \gamma_k^\dagger \gamma_k \rangle = 0 \ \forall k, s = 2\} : \qquad \Delta_2 = 4J_z(1 - \alpha)$$

$$\{\langle \gamma_0^\dagger \gamma_0 \rangle = 1, s = 0\} : \qquad \Delta_3 = 2J_z(\frac{J_x}{J_z}\alpha - 1) \qquad \text{when } \frac{J_x}{J_z}\alpha > 1 .$$

$$(4.14)$$

Note that the state $\{\langle \gamma_0^\dagger \gamma_0 \rangle = 1, s = 0\}$ can only exist for $(J_x/J_z)\alpha > 1$. For all $\alpha \in [0, 1)$, the energy gap $\Delta = \min_i \Delta_i$, is thus given by

$$\Delta = \begin{cases} 4J_z(1 - \alpha) & \text{when } \frac{J_x}{J_z} < 1 \\ 4J_z(1 - \frac{J_x}{J_z}\alpha) & \text{when } \frac{J_x}{J_z} > 1 \text{ and } \frac{J_x}{J_z}\alpha < 1 \\ 2J_z(\frac{J_x}{J_z}\alpha - 1) & \text{when } \frac{J_x}{J_z} > 1 \text{ and } \frac{J_x}{J_z}\alpha > 1 \text{ and } \alpha < \frac{2}{\frac{J_x}{J_z}+1} \\ 2J_z(1 - \alpha) & \text{when } \frac{J_x}{J_z} > 1 \text{ and } \frac{J_x}{J_z}\alpha > 1 \text{ and } \alpha > \frac{2}{\frac{J_x}{J_z}+1} . \end{cases}$$

$$(4.15)$$

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This gives the gap as a function of the parameters $\alpha$ and $J_x/J_z$, and is plotted in Fig. (4.5). Gapless states occur not only for all $\alpha = 1$, but also for $(J_x/J_z)\alpha = 1$ when $(J_x/J_z) > 1$ and $\alpha \in [0,1)$, and, by the symmetry (4.3), for $(J_z/J_x)(2 - \alpha) = 1$ when $(J_x/J_z) < 1$ and $\alpha \in (1,2]$. Thus both the first-order and continuous QPTs are associated with vanishing excitation energy gaps.

The correlation functions of the isotropic XX-ZZ model, Eqs. (3.124)-(3.127), are easily generalized to the anisotropic model by the transformation (4.7). They then, for $0 \leq \alpha < 1$, become

$$\langle \Psi_0 | \sigma_{2i-1}^z \sigma_{2i}^z | \Psi_0 \rangle = -1 \,, \tag{4.16}$$

$$\langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle = -1 + \frac{2}{N'} \sum_k v_k^2$$

$$= -\frac{1}{N'} \sum_k \left[ \frac{(J_x/J_z)\alpha - \cos k}{\sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k}} \right] ,$$
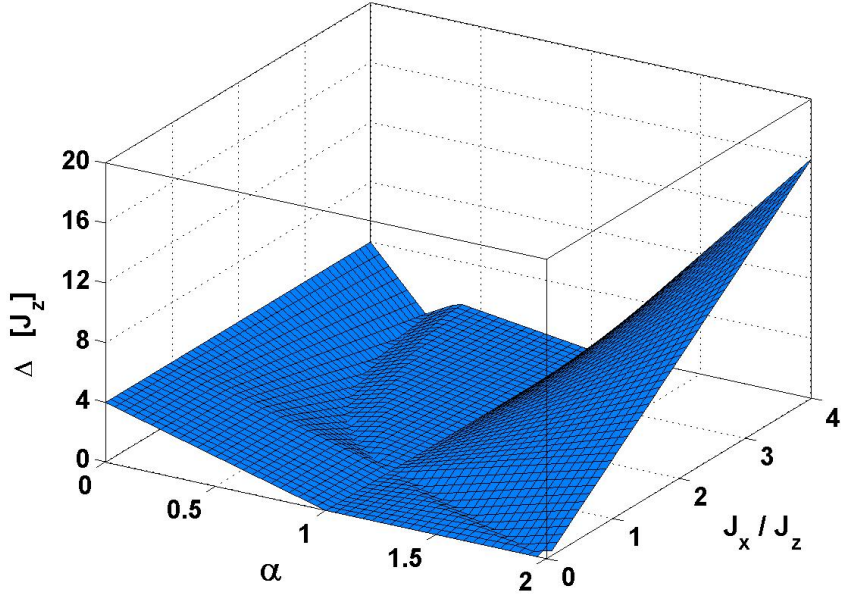
$$\tag{4.17}$$



Figure 4.5: *Energy gap $\Delta$ (Eq. (4.15)) in the generalized XX-ZZ model as a function of the parameters $\alpha$ and $J_x/J_z$, when $N \to \infty$. Note how the gap not only vanishes for all $\alpha = 1$, but also for $(J_x/J_z)\alpha = 1$ when $(J_x/J_z) > 1$ and $\alpha \in [0,1)$, and for $(J_z/J_x)(2 - \alpha) = 1$ when $(J_x/J_z) < 1$ and $\alpha \in (1,2]$.*

$$\langle\Psi_0|\sigma_{2i}^x\sigma_{2i+1}^x|\Psi_0\rangle \;=\; 0\,, \tag{4.18}$$

$$\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle \;=\; -\frac{2}{N'}\sum_k v_k^2\cos k - \frac{2}{N'}\sum_k u_k v_k\sin k$$

$$=\; -\frac{1}{N'}\sum_k\Big[\,\frac{1-(J_x/J_z)\alpha\cos k}{\sqrt{1+((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha\cos k}}\,\Big]\,,$$

$$\tag{4.19}$$

which are related to the correlation functions for $1 < \alpha \le 2$ by the symmetry transformation, Eq. (4.3). These nearest neighbour correlation functions are shown in Fig. (4.6), for a representative number of values of the anisotropy parameter $Q \equiv J_x/J_z$. $\langle\Psi_0|\sigma_{2i-1}^z\sigma_{2i}^z|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i}^x\sigma_{2i+1}^x|\Psi_0\rangle$ are unaffected by the anisotropy, whereas the correlations $|\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle|$ increase, and the correlations $|\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle|$ decrease, for larger values of $J_x/J_z$. We note that both of the correlation functions $\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle$ and $\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle$ are continuous at $\alpha = 1$, since
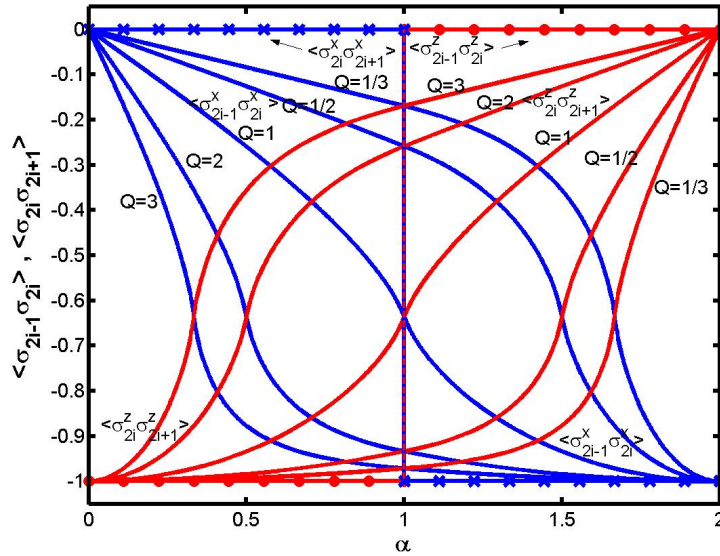


Figure 4.6: *Correlation functions between nearest neighbour spins in the ground state of the generalized XX-ZZ model for some different values of the anisotropy parameter $Q \equiv J_x/J_z$. Note how increasing coupling $J_x$ relative to the coupling $J_z$ leads to increased correlations between $\sigma^x$s on odd bonds and decreasing correlations between $\sigma^z$s on even bonds, while the correlations between $\sigma^z$s on odd bonds and $\sigma^x$s on even bonds remain unaffected by variations in $J_x/J_z$*

$$\lim_{\alpha \to 1^-} \langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle = -\frac{1}{N'} \sum_k \left[ \frac{(J_x/J_z) - \cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}} \right],$$

$$\lim_{\alpha \to 1^-} \langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle = -\frac{1}{N'} \sum_k \left[ \frac{1 - (J_x/J_z)\cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}} \right],$$

$$\lim_{\alpha \to 1^+} \langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle = -\frac{1}{N'} \sum_k \left[ \frac{1 - (J_z/J_x)\cos k}{\sqrt{1 + (J_z/J_x)^2 - 2(J_z/J_x)\cos k}} \right]$$

$$= -\frac{1}{N'} \sum_k \left[ \frac{(J_x/J_z) - \cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}} \right],$$

$$\lim_{\alpha \to 1^+} \langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle = -\frac{1}{N'} \sum_k \left[ \frac{(J_z/J_x) - \cos k}{\sqrt{1 + (J_z/J_x)^2 - 2(J_z/J_x)\cos k}} \right]$$

$$= -\frac{1}{N'} \sum_k \left[ \frac{1 - (J_x/J_z)\cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}} \right].$$

## 4.4 Emergence of a New Phase

The correlation functions, as shown in Fig. (4.6), reveal the nature of the first-order and continuous QPTs in the generalized XX-ZZ model. It is clearly seen that the continuous QPT at $(J_x/J_z)\alpha = 1$ when $(J_x/J_z) > 1$ and $\alpha < 1$, is due to a continuous transition from dominating antiparallel ordering of spin $z$ components on even bonds for $(J_x/J_z)\alpha < 1$, to dominating antiparallel ordering of spin $x$ components on odd bonds for $(J_x/J_z)\alpha > 1$, while maintaining the perfect antiparallel ordering of spin $z$ components on odd bonds and total non-ordering of spin $x$ components on even bonds. This new type of ordering did not occur in the isotropic model, since the constraint $J_x/J_z = 1$ makes the condition $(J_x/J_z)\alpha = 1$ impossible to fulfill for $\alpha < 1$. Note that this new phase of the system is equivalent to the magnetically ordered phase in the QIM for the $\tau$ spins, cf. Eq. (3.20), since $\sigma_{2i-1}^x \sigma_{2i}^x = -\tau_i^x$ and $\sigma_{2i}^z \sigma_{2i+1}^z = -\tau_i^z \tau_{i+1}^z$ in the ground state.

It has now been shown that the generalized XX-ZZ model possesses four distinct phases, apart from the frustrated "spin liquid" phase at $\alpha = 1$. The two phases for $\alpha < 1$ were considered above. For $1 < \alpha \le 2$ the phases are given by the symmetry of the model, Eq. (4.3). Thus, here there will, for $J_x/J_z < 1$, be a separation between a phase with dominating ordering of spin $z$ components on even bonds for $(J_z/J_x)(2 - \alpha) > 1$, and a phase of dominating ordering of spin $x$ components on odd bonds for $(J_z/J_x)(2 - \alpha) < 1$, both with perfect antiparallel ordering of spin $x$

components on even bonds and total non-ordering of spin $z$ components on odd bonds. As pointed out on page 47, for $\alpha \in [0, 1)$, the "magnetically disordered" phase for $(J_x/J_z)\alpha < 1$ has a doubly degenerate ground state, while the "magnetically ordered" state for $(J_x/J_z)\alpha > 1$ has a non-degenerate ground state. At $\alpha = 1$ the ground state degeneracy $d$ will be on the order of $d \sim 2^{N/2}$, since the Hamiltonian (4.8) becomes independent of $s$. The characteristics of the different phases and phase transitions of the generalized XX-ZZ model are graphically summarized in Fig. (4.7), for three representative values of $J_x/J_z$.

By considering the $\tau$ spins, it is clearly seen that at the continuous QPT (where $(J_x/J_z)\alpha = 1$ for $\alpha \in [0, 1)$) the effective quantum Ising model (Eq. (3.20) with $\alpha \rightarrow (J_x/J_z)\alpha$) for the $\tau$ spins is critical, meaning that $\langle\Psi_0|\tau_i^z\tau_{i+r}^z|\Psi_0\rangle$, and therefore also $\langle\Psi_0|\sigma_{2i}^z\sigma_{2(i+r)}^z|\Psi_0\rangle$, show diverging correlation length. On the other hand, at the first-order QPT at $\alpha = 1$ there will be no diverging correlation length since the $\tau$ spins are then controlled by a non-critical QIM.

We may now also gain further insight into the nature of the QPT at
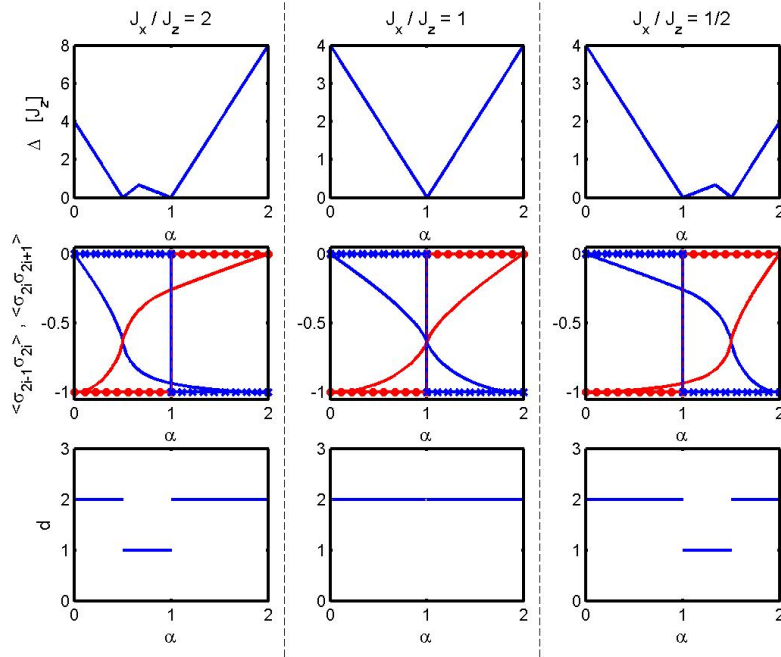


Figure 4.7: *Summary of the properties of the generalized XX-ZZ model in the thermodynamic limit. Left column: $J_x/J_z = 2$. Middle column: $J_x/J_z = 1$. Right column: $J_x/J_z = 1/2$. Upper row: Energy gap $\Delta$. Middle row: Correlation functions in the ground state (cf. Fig. (4.6) for clarification). Lower row: Ground state degeneracy $d$.*

$\alpha = 1$ and $J_x/J_z = 1$, which is the one that was studied in Chap. 3, by observing the behaviour around this point in the $\alpha$-$(J_x/J_z)$-plane of the generalized model. It is clearly seen, cf. Fig. (4.8), that $\alpha = J_x/J_z = 1$ is the special point where the phase boundaries of the first-order and continuous QPTs coincide, thus explaining the mixed first-order and continuous behaviour at this point. The discontinuities of certain correlation functions are obviously attributed to the $\alpha = 1$ first-order QPT, whereas the diverging correlation length is due to the "simultaneous" $(J_x/J_z)\alpha = 1$ continuous QPT. The vanishing excitation energy gap comes with both transitions.
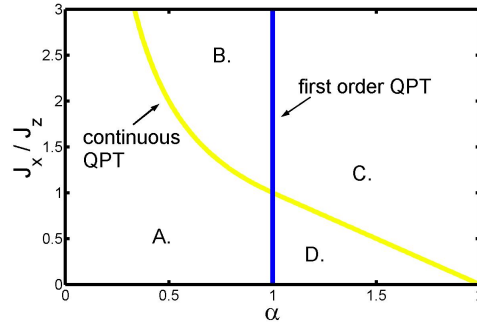


Figure 4.8: *Phase diagram at zero temperature of the generalized XX-ZZ model. The first-order and continuous QPTs are shown, marking the boundaries between the four phases. (A.) and (B.):* $\langle \sigma^z_{2i-1}\sigma^z_{2i} \rangle = -1$. *(C.) and (D.):* $\langle \sigma^x_{2i}\sigma^x_{2i+1} \rangle = -1$. *(A.) and (D.):* $|\langle \sigma^z_{2i}\sigma^z_{2i+1} \rangle| > |\langle \sigma^x_{2i-1}\sigma^x_{2i} \rangle|$. *(B.) and (C.):* $|\langle \sigma^z_{2i}\sigma^z_{2i+1} \rangle| < |\langle \sigma^x_{2i-1}\sigma^x_{2i} \rangle|$.

## 4.5  The Signs of the Coupling Constants

So far we have only considered the case when both coupling constants $J_x$ and $J_z$ are positive, $J_x > 0$ and $J_z > 0$. It will now be shown that this actually was no loss of generality.

Consider first the case when $J_x > 0$ and $J_z < 0$, i.e. antiferromagnetic coupling of the $x$ spin components and ferromagnetic coupling of the $z$ spin components. Then the Hamiltonian (4.1) for $0 \le \alpha \le 1$ can be written as (cf. Eq. (4.5))

$$
\begin{aligned}
H_{\vec{s}}(\alpha) &= J_z \sum_{i=1}^{N'} \left[ \frac{J_x}{J_z}\alpha\, \sigma^x_{2i-1}\sigma^x_{2i} + \sigma^z_{2i}\sigma^z_{2i+1} \right] - J_z(1-\alpha)(N'-2s) \\
&= -|J_z| \sum_{i=1}^{N'} \left[ -\frac{J_x}{|J_z|}\alpha\, \sigma^x_{2i-1}\sigma^x_{2i} + \sigma^z_{2i}\sigma^z_{2i+1} \right] + |J_z|(1-\alpha)(N'-2s).
\end{aligned}
$$

Thus the ground state will now be in the $s = N'$ subspace. Redefining the $\tau$ operators of Eqs. (3.15) and (3.16) as

$$\tau_j^x \equiv -(|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|)\,, \tag{4.20}$$

$$\tau_j^z \equiv -(-1)^j(-1)^{\sum_{j'=1}^{j-1} s_{j'}}(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow|) \tag{4.21}$$

for the antiparallel ($s_j = 0$) odd bond $\{2j - 1, 2j\}$, and

$$\tau_j^x \equiv -(|\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow|)\,, \tag{4.22}$$

$$\tau_j^z \equiv -(-1)^j(-1)^{\sum_{j'=1}^{j-1} s_{j'}}(|\uparrow\uparrow\rangle\langle\uparrow\uparrow| - |\downarrow\downarrow\rangle\langle\downarrow\downarrow|) \tag{4.23}$$

for the parallel ($s_j = 1$) odd bond $\{2j - 1, 2j\}$, by putting a minus sign on $\tau_j^z$ for every second pair, gives

$$\sigma_{2i-1}^x \sigma_{2i}^x = -\tau_i^x\,, \tag{4.24}$$

$$\sigma_{2i}^z \sigma_{2i+1}^z = \tau_i^z \tau_{i+1}^z\,. \tag{4.25}$$

Then the Hamiltonian becomes

$$H_{\vec{s}}(\alpha) = -|J_z| \sum_{i=1}^{N'-1} \left[\frac{J_x}{|J_z|}\alpha\,\tau_i^x + \tau_i^z \tau_{i+1}^z\right] - |J_z|\left[\frac{J_x}{|J_z|}\alpha\tau_{N'}^x + (-1)^s \tau_{N'}^z \tau_1^z\right]$$

$$+ |J_z|(1-\alpha)(N' - 2s)\,. \tag{4.26}$$

Thus the solution will be the same as for $J_x > 0$ and $J_z = |J_z|$, but every second $\tau_i^z$ operator has acquired a minus sign relative to the $\sigma$ operators, and the energy levels are reversed with respect to $s$ ($s \leftrightarrow N' - s$). The correlation functions in the ground state are now given by

$$\langle\Psi_0|\sigma_{2i}^z \sigma_{2i+1}^z|\Psi_0\rangle = \langle\Psi_0|\tau_i^z \tau_{i+1}^z|\Psi_0\rangle\,, \tag{4.27}$$

$$\langle\Psi_0|\sigma_{2i-1}^z \sigma_{2i}^z|\Psi_0\rangle = 1\,, \tag{4.28}$$

$$\langle\Psi_0|\sigma_{2i-1}^x \sigma_{2i}^x|\Psi_0\rangle = -\langle\Psi_0|\tau_i^x|\Psi_0\rangle\,, \tag{4.29}$$

$$\langle\Psi_0|\sigma_{2i}^x \sigma_{2i+1}^x|\Psi_0\rangle = 0 \tag{4.30}$$

for $\alpha \in [0, 1)$, where the $\tau$ operators obey the same QIM Hamiltonian as for positive coupling constants. It is seen that we now get antiferromagnetic ordering of $x$ spin components, and ferromagnetic ordering of $z$ spin components, between nearest neighbour $\sigma$ spins.

The case $J_x < 0$ and $J_z > 0$ is treated similarly. The Hamiltonian is written as

$$H_{\vec{s}}(\alpha) = J_z \sum_{i=1}^{N'} \left[\frac{J_x}{J_z}\alpha\,\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z\right] - J_z(1-\alpha)(N' - 2s)$$

$$= J_z \sum_{i=1}^{N'} \left[-\frac{|J_x|}{J_z}\alpha\,\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z\right] - J_z(1-\alpha)(N' - 2s)\,.$$

Now the ground state is in the $s = 0$ subspace. The $\tau$ operators of Eqs. (3.15) and (3.16) are now redefined as

$$\tau_i^x \equiv (|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|)\,, \tag{4.31}$$

$$\tau_i^z \equiv -(-1)^{\sum_{j'=1}^{j-1} s_{j'}} (|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow|) \tag{4.32}$$

for the antiparallel ($s_i = 0$) odd bond $\{2i - 1, 2i\}$, and

$$\tau_i^x \equiv (|\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow|)\,, \tag{4.33}$$

$$\tau_i^z \equiv -(-1)^{\sum_{j=1}^{i-1} s_j} (|\uparrow\uparrow\rangle\langle\uparrow\uparrow| - |\downarrow\downarrow\rangle\langle\downarrow\downarrow|) \tag{4.34}$$

for the parallel ($s_i = 1$) odd bond $\{2i - 1, 2i\}$, giving

$$\sigma_{2i-1}^x \sigma_{2i}^x = \tau_i^x\,, \tag{4.35}$$

$$\sigma_{2i}^z \sigma_{2i+1}^z = -\tau_i^z \tau_{i+1}^z\,, \tag{4.36}$$

so that the Hamiltonian becomes

$$H_{\vec{s}}(\alpha) = -J_z \sum_{i=1}^{N'-1} \left[\frac{|J_x|}{J_z}\alpha\,\tau_i^x + \tau_i^z \tau_{i+1}^z\right] - J_z\left[\frac{|J_x|}{J_z}\alpha\tau_{N'}^x + (-1)^s \tau_{N'}^z \tau_1^z\right]$$
$$- J_z(1 - \alpha)(N' - 2s)\,. \tag{4.37}$$

Thus the solution will be the same as for $J_x = |J_x|$ and $J_z > 0$, apart from that the $\tau_i^x$ operators have acquired a minus sign relative to the $\sigma$ operators. The correlation functions for $\alpha \in [0, 1)$ are then given by

$$\langle\Psi_0|\sigma_{2i}^z \sigma_{2i+1}^z|\Psi_0\rangle = -\langle\Psi_0|\tau_i^z \tau_{i+1}^z|\Psi_0\rangle\,, \tag{4.38}$$

$$\langle\Psi_0|\sigma_{2i-1}^z \sigma_{2i}^z|\Psi_0\rangle = -1\,, \tag{4.39}$$

$$\langle\Psi_0|\sigma_{2i-1}^x \sigma_{2i}^x|\Psi_0\rangle = \langle\Psi_0|\tau_i^x|\Psi_0\rangle\,, \tag{4.40}$$

$$\langle\Psi_0|\sigma_{2i}^x \sigma_{2i+1}^x|\Psi_0\rangle = 0\,. \tag{4.41}$$

Finally, for the case $J_x < 0$ and $J_z < 0$, the Hamiltonian can be written

$$H_{\vec{s}}(\alpha) = J_z \sum_{i=1}^{N'} \left[\frac{J_x}{J_z}\alpha\,\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z\right] - J_z(1 - \alpha)(N' - 2s)$$

$$= -|J_z| \sum_{i=1}^{N'} \left[\frac{|J_x|}{|J_z|}\alpha\,\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i}^z \sigma_{2i+1}^z\right] + |J_z|(1 - \alpha)(N' - 2s)\,.$$

Thus the ground state will be in the $s = N'$ subspace. This time we redefine the $\tau$ operators as

$$\tau_j^x \equiv (|\uparrow\downarrow\rangle\langle\downarrow\uparrow| + |\downarrow\uparrow\rangle\langle\uparrow\downarrow|)\,, \tag{4.42}$$

$$\tau_j^z \equiv -(-1)^j (-1)^{\sum_{j'=1}^{j-1} s_{j'}} (|\uparrow\downarrow\rangle\langle\uparrow\downarrow| - |\downarrow\uparrow\rangle\langle\downarrow\uparrow|) \tag{4.43}$$

for the antiparallel ($s_j = 0$) odd bond $\{2j-1, 2j\}$, and

$$
\begin{align}
\tau_j^x &\equiv \left( |\uparrow\uparrow\rangle\langle\downarrow\downarrow| + |\downarrow\downarrow\rangle\langle\uparrow\uparrow| \right), \tag{4.44}\\
\tau_j^z &\equiv -(-1)^j \, (-1)^{\sum_{j'=1}^{j-1} s_{j'}} \left( |\uparrow\uparrow\rangle\langle\uparrow\uparrow| - |\downarrow\downarrow\rangle\langle\downarrow\downarrow| \right) \tag{4.45}
\end{align}
$$

for the parallel ($s_j = 1$) odd bond $\{2j-1, 2j\}$. This gives

$$
\begin{align}
\sigma_{2i-1}^x \sigma_{2i}^x &= \tau_i^x, \tag{4.46}\\
\sigma_{2i}^z \sigma_{2i+1}^z &= \tau_i^z \tau_{i+1}^z. \tag{4.47}
\end{align}
$$

The Hamiltonian becomes

$$
\begin{aligned}
H_{\vec{s}}(\alpha) &= -|J_z| \sum_{i=1}^{N'-1} \left[ \frac{|J_x|}{|J_z|}\alpha\,\tau_i^x + \tau_i^z \tau_{i+1}^z \right] - |J_z| \left[ \frac{|J_x|}{|J_z|}\alpha\tau_{N'}^x + (-1)^s \tau_{N'}^z \tau_1^z \right] \\
&\quad + |J_z|(1-\alpha)(N'-2s).
\end{aligned} \tag{4.48}
$$

Thus the solution will be the same as for $J_x = |J_x|$ and $J_z = |J_z|$, but every second $\tau_i^z$ operator, and every $\tau_i^x$ operator, have acquired a minus sign relative to the $\sigma$ operators, and the energy levels are reversed with respect to $s$ ($s \leftrightarrow N' - s$). Now the correlation functions in the ground state are, for negative values of $J_x$ and $J_z$, given by

$$
\begin{align}
\langle\Psi_0|\sigma_{2i}^z\sigma_{2i+1}^z|\Psi_0\rangle &= \langle\Psi_0|\tau_i^z\tau_{i+1}^z|\Psi_0\rangle, \tag{4.49}\\
\langle\Psi_0|\sigma_{2i-1}^z\sigma_{2i}^z|\Psi_0\rangle &= 1, \tag{4.50}\\
\langle\Psi_0|\sigma_{2i-1}^x\sigma_{2i}^x|\Psi_0\rangle &= \langle\Psi_0|\tau_i^x|\Psi_0\rangle, \tag{4.51}\\
\langle\Psi_0|\sigma_{2i}^x\sigma_{2i+1}^x|\Psi_0\rangle &= 0 \tag{4.52}
\end{align}
$$

for $\alpha \in [0, 1)$, where the $\tau$ operators obey the same QIM Hamiltonian as for positive coupling constants.

Therefore, the signs of the coupling constants $J_x$ and $J_z$ only influence the interpretation of the $\sigma$ spins as $\tau$ spins in the associated QIM, whereas this QIM for the $\tau$ spins will be the same as for only positive coupling constants. The $x$ spin components of nearest neighbour $\sigma$ spins on odd bonds will order themselves ferromagnetically for negative coupling constant $J_x$ or antiferromagnetically for positive $J_x$. Independently the $z$ spin components of nearest neighbour $\sigma$ spins will have ferromagnetic ordering for negative coupling constant $J_z$ or antiferromagnetic ordering for positive $J_z$.

# Chapter 5

# QPT in the One-Dimensional Quantum Compass Model

At $\alpha = 1$, the generalized XX-ZZ model, Eqs. (4.1) and (4.2), becomes

$$H(1) = \sum_{i=1}^{N'} \left[ J_x \sigma_{2i-1}^x \sigma_{2i}^x + J_z \sigma_{2i}^z \sigma_{2i+1}^z \right] , \qquad (5.1)$$

which is nothing but the one-dimensional quantum compass model, cf. Eq. (3.7), where the parameter is the ratio $J_x/J_z$ between the two different coupling constants $J_x$ and $J_z$. Therefore, the solution to the generalized XX-ZZ model automatically gives us the solution to the one-dimensional quantum compass model. Thus, the ground state energy will be given by the the limit when $\alpha \to 1^-$ and $\alpha \to 1^+$ of Eq. (4.12), which becomes

$$E_0(\frac{J_x}{J_z}) = -J_z \frac{N'}{2\pi} \int_{-\pi}^{\pi} \sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k} \, dk . \qquad (5.2)$$

Therefore, when we view the Hamiltonian as parameterized by $J_x/J_z$, it is immediately clear that the one-dimensional quantum compass model exhibits a continuous QPT at $J_x/J_z = 1$, since the integral appearing in Eq. (5.2) is the same as the one, Eq. (4.13), appearing in the QIM, and which was plotted in Fig. (4.4). At the point $J_x/J_z = 1$, the correlation length diverges, since it is at the continuous QPT of the generalized XX-ZZ model. At all other points, the correlation length will be finite since then the effective quantum Ising model of the $\tau$ spins will be non-critical. The solution to Eq. (5.1) is, by analogy with Eq. (4.8) in the limits $\alpha \to 1^-$ and $\alpha \to 1^+$, given by

$$H_{\vec{s}}^{\pm}(\alpha) = 2J_z \sum_k \left[ \sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k} \, (\gamma_k^\dagger \gamma_k - \frac{1}{2}) \right] . \qquad (5.3)$$

Thus the energy gap to the lowest lying excitation will be

$$\Delta = 2J_z\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)} = 2J_z\left|1 - \frac{J_x}{J_z}\right|, \qquad (5.4)$$

where we used the results on page 47 for the $\gamma$ particles in the different subspaces. The gap $\Delta$ is plotted in Fig. (5.1).
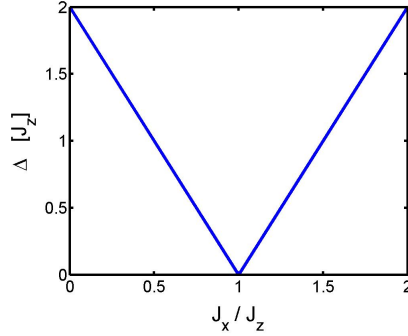


Figure 5.1: *Energy excitation gap $\Delta$ in the one-dimensional quantum compass model, in the thermodynamic limit. Vanishing excitation energy gap at $J_x/J_z = 1$ marks the continuous QPT.*

The correlation functions $\langle\Psi_0|\sigma^z_{2i-1}\sigma^z_{2i}|\Psi_0\rangle$ and $\langle\Psi_0|\sigma^x_{2i}\sigma^x_{2i+1}|\Psi_0\rangle$ are discontinuous at $\alpha = 1$ in the generalized XX-ZZ model, therefore they have no definite values in the one-dimensional quantum compass model. The two other nearest neighbour correlation functions are given by

$$
\begin{aligned}
\langle\Psi_0|\sigma^x_{2i-1}\sigma^x_{2i}|\Psi_0\rangle &= -1 + \frac{2}{N'}\sum_k v_k^2 \\
&= -\frac{1}{N'}\sum_k \left[\frac{(J_x/J_z) - \cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}}\right],
\end{aligned}
$$
$$(5.5)$$

$$
\begin{aligned}
\langle\Psi_0|\sigma^z_{2i}\sigma^z_{2i+1}|\Psi_0\rangle &= -\frac{2}{N'}\sum_k v_k^2\cos k - \frac{2}{N'}\sum_k u_k v_k \sin k \\
&= -\frac{1}{N'}\sum_k \left[\frac{1 - (J_x/J_z)\cos k}{\sqrt{1 + (J_x/J_z)^2 - 2(J_x/J_z)\cos k}}\right],
\end{aligned}
$$
$$(5.6)$$

using Eqs. (4.17) and (4.19), since these correlation functions are continuous at $\alpha = 1$. Eqs. (5.5) and (5.6) are nothing but the correlation functions $-\langle\Psi_0|\tau^x_i|\Psi_0\rangle$ and $-\langle\Psi_0|\tau^z_i\tau^z_{i+1}|\Psi_0\rangle$ of the QIM with parameter $J_x/J_z$. Therefore it is clear that the continuous QPT of the one-dimensional quantum compass model is associated with a transition

from a phase with dominating correlations between spin $z$ components on even bonds for $J_x/J_z < 1$ to a phase with dominating correlations between spin $x$ components on odd bonds for $J_x/J_z > 1$, cf. Fig. (5.2). The long-range correlations in the generalized XX-ZZ model are all discontinuous at $\alpha = 1$, and therefore undefined in the one-dimensional quantum compass model, so that this system will be in a spin liquid state, i.e. a state where there are only short-range correlations.
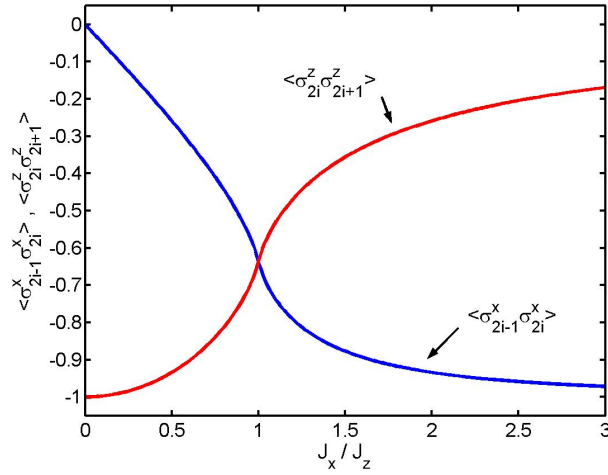


Figure 5.2: *Correlation functions $\langle \Psi_0 | \sigma_{2i-1}^x \sigma_{2i}^x | \Psi_0 \rangle$ and $\langle \Psi_0 | \sigma_{2i}^z \sigma_{2i+1}^z | \Psi_0 \rangle$ in the ground state of the one-dimensional quantum compass model, in the thermodynamic limit. The QPT at $J_x/J_z = 1$ is characterized by balance between the two correlation functions.*

It has thus been shown that the one-dimensional quantum compass model, which arises when holding $\alpha = 1$ fixed and varying $J_x/J_z$ in the generalized XX-ZZ model, does not exhibit any first-order, but well a continuous, QPT. First-order QPTs in quantum compass models therefore apparently require higher dimensionality of the system, if it at all is justified to call this one-dimensional model a quantum compass model. After all, the resemblance to different couplings along different axes is rather superficial, since there is only one axis in one dimension (cf. Eqs. (2.1) and (5.1)). But this solution also shows that merely interpolating between two spin models with incompatible types of ordering is not sufficient to create a first-order QPT in one dimension. There must clearly be additional interactions, such as in Eq. (4.1), leading to a discontinuity in the ordering.

# Chapter 6

# Entanglement in the Generalized XX-ZZ Model

With the solution to the generalized XX-ZZ model, in the form of the correlation functions, at hand, it is now rather straightforward to calculate the entanglement present in the ground state of this system.

## 6.1  Concurrence of Spin Pairs

The calculation of the concurrence, cf. page 8, between a pair of spins requires the reduced density matrix of this pair, which will be a $4{\times}4$ matrix. Since the Pauli matrices $\{\sigma^\mu\}$, where $\mu = 0, 1, 2, 3$ and $\sigma^0 \equiv \mathbf{1}$ and $\sigma^{1,2,3} \equiv \sigma^{x,y,z}$, form a basis for all $2{\times}2$ matrices, $\{\sigma^\mu \otimes \sigma^\nu\}$ will form a basis for all $4{\times}4$ matrices. Therefore the reduced density matrix $\rho_{ij}$ of the spin pair $\{i, j\}$ can be expanded as

$$\rho_{ij} = \frac{1}{4} \sum_{\mu,\nu=0}^{3} q_{\mu\nu}\, \sigma_i^\mu \sigma_j^\nu \,, \tag{6.1}$$

where $q_{\mu\nu}$ are coefficients that can be determined by using

$$
\begin{aligned}
\langle \sigma_i^\mu \sigma_j^\nu \rangle &= \operatorname{tr}(\sigma_i^\mu \sigma_j^\nu \rho_{ij}) = \frac{1}{4} \operatorname{tr}\left( \sigma_i^\mu \sigma_j^\nu \sum_{\mu',\nu'=0}^{3} q_{\mu'\nu'}\, \sigma_i^{\mu'} \sigma_j^{\nu'} \right) \\
&= \frac{1}{4} \sum_{\mu',\nu'=0}^{3} q_{\mu'\nu'}\, \operatorname{tr}\left( \sigma_i^\mu \sigma_j^\nu \sigma_i^{\mu'} \sigma_j^{\nu'} \right) \\
&= \frac{1}{4}\, q_{\mu\nu}\, \operatorname{tr} \mathbf{1} = q_{\mu\nu} \,, \tag{6.2}
\end{aligned}
$$

where in the following all expectation values are understood to be taken in the ground state $|\Psi_0\rangle$. Thus $q_{\mu\nu} = \langle \sigma_i^\mu \sigma_j^\nu \rangle$ and we get

$$\rho_{ij} = \frac{1}{4} \sum_{\mu,\,\nu\,=\,0}^{3} \langle \sigma_i^\mu \sigma_j^\nu \rangle \, \sigma_i^\mu \sigma_j^\nu \,. \tag{6.3}$$

From Eqs. (3.102)-(3.104) we have that $\langle \sigma_i^\mu \rangle = 0$ for $\mu = 1, 2, 3$. Trivially, $\langle \sigma_i^0 \rangle = 1$. $\langle \sigma_i^x \sigma_j^x \rangle$ and $\langle \sigma_i^z \sigma_j^z \rangle$ were calculated in Sec. 3.5. The correlation function $\langle \sigma_i^x \sigma_j^y \rangle$ must be zero, since the matrix $\sigma_i^x \sigma_j^y$ will be imaginary, and because $\rho_{ij}$ must be real as the Hamiltonian is real, $\langle \sigma_i^x \sigma_j^y \rangle$ must vanish (cf. the discussion in Ref. [4]). The same argument gives that $\langle \sigma_i^z \sigma_j^y \rangle$ must be zero. $\langle \sigma_i^x \sigma_j^z \rangle$ is easily seen to be zero since $\sigma_i^x$ flips only one spin on an odd bond, giving a state in a different subspace than the ground state. For the correlation function $\langle \sigma_i^y \sigma_j^y \rangle$, the matrix $\sigma_i^y \sigma_j^y$ is given by

$$\sigma_i^y \sigma_j^y = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} . \tag{6.4}$$

Therefore, in the subspace $s{=}0$, which is where the ground state is, we get $\langle \sigma_i^y \sigma_j^y \rangle = \langle \sigma_i^x \sigma_j^x \rangle$. Thus the reduced density matrix (6.3) will be given by

$$\rho_{ij} = \frac{1}{4} \big( \mathbf{1} + \langle \sigma_i^x \sigma_j^x \rangle \, (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) + \langle \sigma_i^z \sigma_j^z \rangle \, \sigma_i^z \sigma_j^z \big) \,. \tag{6.5}$$

Explicitly, this is

$$\rho_{ij} = \frac{1}{4} \begin{pmatrix} 1 + \langle \sigma_i^z \sigma_j^z \rangle & 0 & 0 & 0 \\ 0 & 1 - \langle \sigma_i^z \sigma_j^z \rangle & 2 \langle \sigma_i^x \sigma_j^x \rangle & 0 \\ 0 & 2 \langle \sigma_i^x \sigma_j^x \rangle & 1 - \langle \sigma_i^z \sigma_j^z \rangle & 0 \\ 0 & 0 & 0 & 1 + \langle \sigma_i^z \sigma_j^z \rangle \end{pmatrix} . \tag{6.6}$$

The "flipped" density matrix, Eq. (1.16), is now given by

$$\tilde{\rho}_{ij} \equiv (\sigma_i^y \sigma_j^y) \, \rho_{ij}^* \, (\sigma_i^y \sigma_j^y) = \rho_{ij} \,, \tag{6.7}$$

using Eqs. (6.4) and (6.6). Thus $\rho_{ij} \tilde{\rho}_{ij}$ is simply given by $\rho_{ij}^2$. Explicitly

$$\rho_{ij}^2 = \frac{1}{16} \begin{pmatrix} A^2 & 0 & 0 & 0 \\ 0 & B^2 + (2C)^2 & 4BC & 0 \\ 0 & 4BC & B^2 + (2C)^2 & 0 \\ 0 & 0 & 0 & A^2 \end{pmatrix} , \tag{6.8}$$

where

$$A \equiv 1 + \langle \sigma_i^z \sigma_j^z \rangle \,, \tag{6.9}$$
$$B \equiv 1 - \langle \sigma_i^z \sigma_j^z \rangle \,, \tag{6.10}$$
$$C \equiv \langle \sigma_i^x \sigma_j^x \rangle \,. \tag{6.11}$$

The eigenvalues $\lambda_1^2$, $\lambda_2^2$, $\lambda_3^2$ and $\lambda_4^2$ of $\rho_{ij}\tilde{\rho}_{ij}$ are then given by

$$\lambda_1^2 = \lambda_2^2 \;\; = \;\; \frac{1}{16}A^2\,, \tag{6.12}$$

$$\lambda_3^2 \;\; = \;\; \frac{1}{16}(B + 2C)^2\,, \tag{6.13}$$

$$\lambda_4^2 \;\; = \;\; \frac{1}{16}(B - 2C)^2\,. \tag{6.14}$$

Therefore the positive eigenvalues $\lambda_i$ of $R(\rho_{ij})$, Eq. (1.18), are given by

$$\lambda_1 = \lambda_2 \;\; = \;\; \frac{1}{4}\left(1 + \langle\sigma_i^z\sigma_j^z\rangle\right), \tag{6.15}$$

$$\lambda_3 \;\; = \;\; \frac{1}{4}\left|1 - \langle\sigma_i^z\sigma_j^z\rangle + 2\langle\sigma_i^x\sigma_j^x\rangle\right|, \tag{6.16}$$

$$\lambda_4 \;\; = \;\; \frac{1}{4}\left|1 - \langle\sigma_i^z\sigma_j^z\rangle - 2\langle\sigma_i^x\sigma_j^x\rangle\right| \tag{6.17}$$

for $\alpha \in [0, 1)$. The concurrence of the spins $i$ and $j$ is now given by Eq. (1.17). It is immediately clear that the concurrence of two spins that are not on the same odd bond is zero for $\alpha \in [0, 1)$, since then $\langle\sigma_i^x\sigma_j^x\rangle = 0$, making $\lambda_3 = \lambda_4$, and thus $C(\rho_{ij}) = \max(0, -2\lambda_1) = 0$. For two spins $\{i, j\} = \{2i - 1, 2i\}$ that are on the same odd bond, we have for $\alpha \in [0, 1)$ that $\langle\sigma_{2i-1}^z\sigma_{2i}^z\rangle = -1$ and $\langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle \in [-1, 0]$, giving for the eigenvalues of $R(\rho_{2i-1,2i})$, Eqs. (6.15)-(6.17),

$$\lambda_1 = \lambda_2 \;\; = \;\; 0\,, \tag{6.18}$$

$$\lambda_3 \;\; = \;\; \frac{1}{2}(1 + \langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle)\,, \tag{6.19}$$

$$\lambda_4 \;\; = \;\; \frac{1}{2}(1 - \langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle)\,, \tag{6.20}$$

making

$$\begin{aligned}
C(\rho_{2i-1,2i}) \;\; &= \;\; \max\{0\,, \lambda_4 - \lambda_3 - \lambda_2 - \lambda_1\} = \max\{0\,, \lambda_4 - \lambda_3\} \\
&= \;\; \max\{0\,, \frac{1}{2}(1 - \langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle - 1 - \langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle)\} \\
&= \;\; -\langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle \tag{6.21}
\end{aligned}$$

for all $\alpha \in [0, 1)$ and $J_x/J_z$, where $\langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle$ is given by Eq. (3.125). $C(\rho_{i,j})$ for $\alpha \in (1, 2]$ is given by the symmetry transformation (4.3). Therefore, we get that $C(\rho_{i,j})$ is zero for all spins $\{i, j\}$ that are not nearest neighbours, and for nearest neighbours, $C(\rho_{2i-1,2i}) = -\langle\sigma_{2i-1}^x\sigma_{2i}^x\rangle$ and $C(\rho_{2i,2i+1}) = 0$ for $\alpha \in [0, 1)$, and for $\alpha \in (1, 2]$ we have that $C(\rho_{2i,2i+1}) = -\langle\sigma_{2i}^z\sigma_{2i+1}^z\rangle$ and $C(\rho_{2i-1,2i}) = 0$, with $J_x \leftrightarrow J_z$. This gives us the concurrence of all nearest neighbour pairs as plotted in Fig. (6.1) for three representative values of $J_x/J_z$.
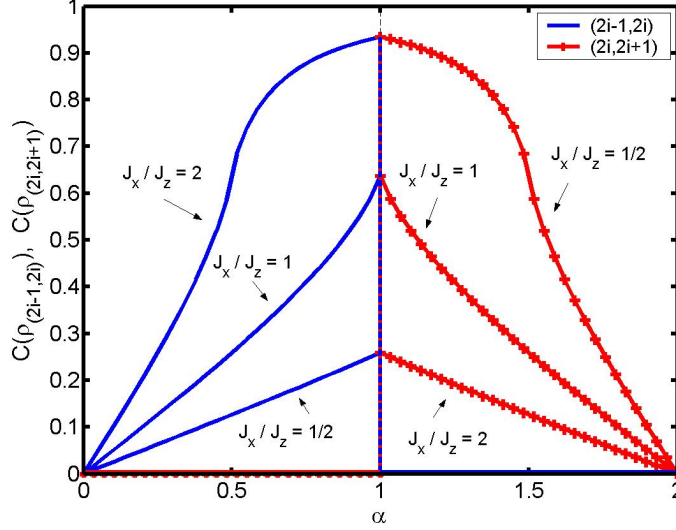
Figure 6.1: *Concurrence of nearest neighbour pairs of spins in the generalized XX-ZZ model, for three representative values of $J_x/J_z$. For spins that are not nearest neighbours, the pairwise concurrence is always zero.*

The analytic expression for the concurrence in the thermodynamic limit will, by Eqs. (3.125) and (3.78), be given by

$$
\begin{aligned}
C(\rho_{2i-1,2i}) &= -\langle \sigma_{2i-1}^x \sigma_{2i}^x \rangle = 1 - \frac{2}{N'} \sum_k v_k^2 \\
&= 1 - \frac{1}{2\pi} \int_{-\pi}^{\pi} \left( 1 - \frac{((J_x/J_z)\alpha - \cos k)}{\sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k}} \right) dk \\
&= \frac{1}{\pi} \int_0^{\pi} \frac{(J_x/J_z)\alpha - \cos k}{\sqrt{1 + ((J_x/J_z)\alpha)^2 - 2(J_x/J_z)\alpha \cos k}} \, dk \,, \qquad \textbf{(6.22)}
\end{aligned}
$$

where the integral is recognized as the derivative of the integral $I(x)$, defined in Eq. (4.13), where $x \equiv (J_x/J_z)\alpha$:

$$
C(\rho_{2i-1,2i}) = \frac{1}{\pi} \frac{\partial I(x)}{\partial x} \,. \qquad \textbf{(6.23)}
$$

This function $\partial I/\partial x$ was plotted in Fig. (4.4), where it was clearly seen that it had a diverging derivative $\partial^2 I/\partial x^2 = \pi \, \partial C/\partial x$ at $(J_x/J_z)\alpha = 1$. The concurrence $C(\rho_{2i-1,2i})$ of a spin pair on an odd bond, and its derivative $\partial C(\rho_{2i-1,2i})/\partial \alpha$, are plotted in Fig. (6.2) for $\alpha \in [0,1)$, as functions of $\alpha$ and $J_x/J_z$. Thus, for the generalized XX-ZZ model, the first-order QPTs at $\alpha = 1$ are associated with a discontinuous pairwise concurrence, and the continuous QPTs are associated with a diverging

derivative of the pairwise concurrence. These results clearly agree with the general analysis of Ref. [17], quoted on page 9.
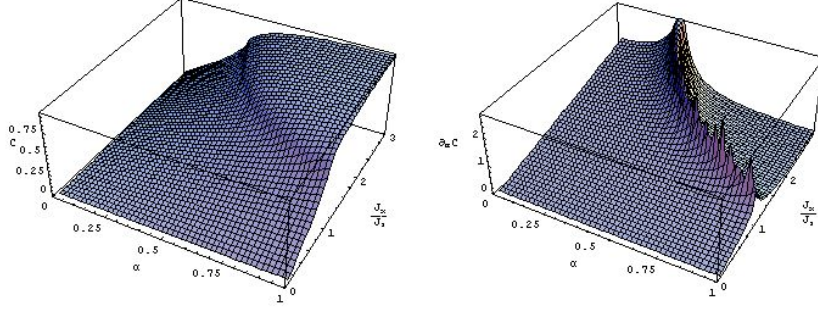


Figure 6.2: *Left: Concurrence $C(\rho_{2i-1,2i})$ of a pair of spins on the same odd bond as a function of $\alpha \in [0,1)$ and $J_x/J_z$. Right: The derivative $\partial C(\rho_{2i-1,2i})/\partial\alpha$ on the same interval. Since the concurrence $C(\rho_{2i-1,2i})$ is zero for $\alpha \in (1,2]$, it is clearly seen that the first-order QPT at $\alpha = 1$ is associated with a discontinuity in the pairwise concurrence. The second order QPT in the generalized XX-ZZ model is similarly seen to be associated with a divergence in the derivative $\partial C/\partial\alpha$ of the pairwise concurrence. Concurrence of non-nearest neighbour pairs is zero for all $\alpha \in [0,2]$.*

## 6.2 Localizable Entanglement of Spin Pairs

The concurrence of spin pairs was previously seen to be zero for all spins that are not nearest neighbours, but this does not by necessity mean that all these spins are totally unentangled, since entanglement may come in other than simple pairwise forms. We shall now investigate the localizable entanglement and the entanglement of assistance of the generalized XX-ZZ model, measuring the amount of entanglement that can be localized in a pair of spins by doing local and global measurements, respectively, on the rest of the system, cf. page 9.

The localizable entanglement of a spin pair is bounded below by the maximal absolute value of the correlation functions of this pair, cf. Eq. (1.22). For $\alpha \in [0,1)$, a pair on the same odd bond has $|\langle\sigma_{2i-1}^z\sigma_{2i}^z\rangle| = 1$, and therefore this pair has $E_L(\rho_{2i-1,2i}) = 1$. Pairs that are not on the same odd bond will have maximal correlation function

$$\max_{\alpha\beta}(|Q_{2i-m,2j-n}^{\alpha,\beta}|) = |\langle\sigma_{2i-m}^z\sigma_{2j-n}^z\rangle| = \langle\tau_i^z\tau_j^z\rangle, \qquad (6.24)$$

where $i \neq j$ and $m,n = 0,1$, and $\langle\tau_i^z\tau_j^z\rangle$ is given by Eq. (3.121). Thus

$$\langle\tau_i^z\tau_j^z\rangle \leq E_L(\rho_{2i-m,2j-n}) \qquad i \neq j \quad m,n = 0,1. \qquad (6.25)$$

The lower bounds can be written on the compact form

$$| \langle \sigma_i^z \sigma_j^z \rangle | \; \leq \; E_L(\rho_{ij}) \qquad \forall \, i,j \, . \tag{6.26}$$

The upper bounds of the localizable entanglement are given by the entanglement of assistance, given by Eq. (1.21). For pairs $\{i,j\}$ that are not on the same odd bond, the reduced density matrix $\rho_{ij}$ is, by Eq. (6.5),

$$\rho_{ij} = \frac{1}{4} \begin{pmatrix} 1+Z & 0 & 0 & 0 \\ 0 & 1-Z & 0 & 0 \\ 0 & 0 & 1-Z & 0 \\ 0 & 0 & 0 & 1+Z \end{pmatrix}, \tag{6.27}$$

where $Z \equiv \langle \sigma_i^z \sigma_j^z \rangle$. Since $1 \pm Z \geq 0$, we get

$$\sqrt{\rho_{ij}} = \frac{1}{2} \begin{pmatrix} \sqrt{1+Z} & 0 & 0 & 0 \\ 0 & \sqrt{1-Z} & 0 & 0 \\ 0 & 0 & \sqrt{1-Z} & 0 \\ 0 & 0 & 0 & \sqrt{1+Z} \end{pmatrix}. \tag{6.28}$$

Then

$$\sqrt{\rho_{ij}}^T \sigma_i^y \sigma_j^y \sqrt{\rho_{ij}} = \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & -(1+Z) \\ 0 & 0 & 1-Z & 0 \\ 0 & 1-Z & 0 & 0 \\ -(1+Z) & 0 & 0 & 0 \end{pmatrix}, \tag{6.29}$$

with eigenvalues $\lambda_{1,2} = \pm (1/4)(1+Z)$ and $\lambda_{3,4} = \pm (1/4)(1-Z)$. Therefore

$$\begin{aligned} C_A(\rho_{ij}) &= \mathrm{tr}( \, | \, \sqrt{\rho_{ij}}^T \sigma_i^y \sigma_j^y \sqrt{\rho_{ij}} \, | \, ) \\ &= \sum_i |\lambda_i| = \frac{1}{2} ( (1+Z) + (1-Z) ) = 1 \, . \end{aligned} \tag{6.30}$$

Thus the entanglement of assistance between a pair of spins will always be maximal for all $\alpha \in [0,1]$ and independent of the separation between the two spins.

The bounds on the localizable entanglement are now given by

$$| \langle \sigma_i^z \sigma_j^z \rangle | \; \leq \; E_L(\rho_{ij}) \; \leq \; 1 \qquad \forall \, i,j \tag{6.31}$$

for $\alpha \in [0,1)$. For $\alpha \in (1,2]$, the bound are given by applying the symmetry (4.3) to Eq. (6.31). The lower bounds are plotted in Fig. (6.3) for separations up to 20 bonds between spins, when $J_x/J_z = 2$. Since the upper bound of the localizable entanglement is unity, it is clear that this entanglement measure does not monotonically increase as the critical points are approached, like the concurrence does (cf. Fig. (6.1)). In fact,
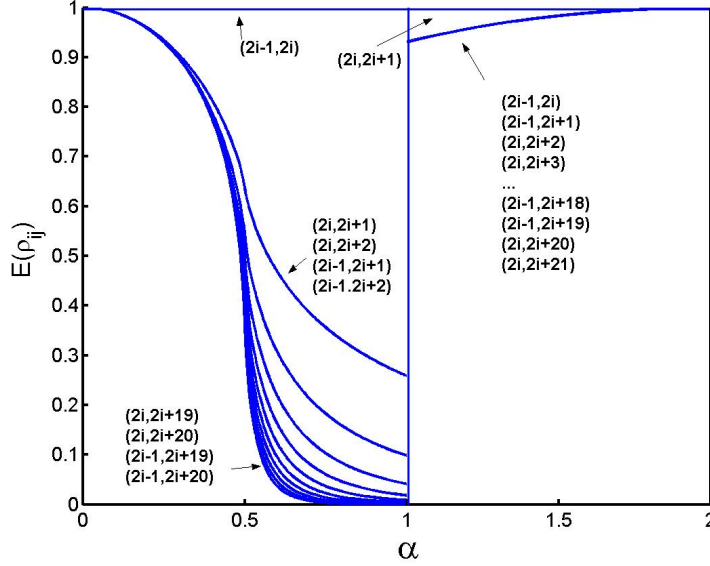
Figure 6.3: *Lower bounds on the localizable entanglement of spin pairs with separations up to 20 bonds in the generalized XX-ZZ model, given by $|\langle \sigma_i^z \sigma_j^z \rangle|$ for $\alpha \in [0,1)$. The upper bound of the localizable entanglement, given by the entanglement of assistance, is $C_A(\rho_{ij}) = 1$ for all pairs $\{i,j\}$ for all $\alpha \in [0,2]$.*

as the system approaches the continuous QPT from $\alpha = 0$, it is clear that the localizable entanglement can only be constant or decrease.

For pairs that are not nearest neighbours, we see that the entanglement of assistance is always maximal whereas the concurrence, or equivalently the entanglement of formation, is always minimal (cf. page 64). This seems to be a consequence of the duality between these two entanglement measures, where the entanglement of formation, Eq. (1.12), gives a lower bound, and the entanglement of assistance, Eq. (1.19), gives an upper bound, to the average entanglement of the pure state decompositions of the state under consideration [21]. Thus the concurrence will be minimal if the ground state $\rho_{ij}$ can be decomposed into pure states with no entanglement between the two spins, and the entanglement of assistance will be maximal if the ground state can be decomposed into pure states with maximal entanglement between the two spins. At the point $\alpha = 0$, where we know that the solution can be written as any linear combination of the two states $|\Psi_0^1\rangle \equiv |\uparrow\downarrow\uparrow\downarrow \ldots \uparrow\downarrow\rangle$ and $|\Psi_0^2\rangle \equiv |\downarrow\uparrow\downarrow\uparrow \ldots \downarrow\uparrow\rangle$, the reduced density matrix can be written as

$$\rho_{ij} = \frac{1}{2}|X\rangle\langle X| + \frac{1}{2}|Y\rangle\langle Y|. \tag{6.32}$$

We can have $|X\rangle = |A\rangle$ and $|Y\rangle = |B\rangle$, where $|A\rangle = |\uparrow\downarrow\rangle$ and $|B\rangle = |\downarrow\uparrow\rangle$, or $|A\rangle = |\uparrow\uparrow\rangle$ and $|B\rangle = |\downarrow\downarrow\rangle$, depending on the positions of the spins $\{i, j\}$. In this case the pure state decomposition has minimal entanglement, therefore the concurrence will be minimal at $\alpha = 0$. At the same time, we can have $|X\rangle = |A\rangle + |B\rangle$ and $|Y\rangle = |A\rangle - |B\rangle$, which are maximally entangled, so that the entanglement of assistance will be maximal at $\alpha = 0$. The striking difference between the concurrence and the entanglement of assistance therefore comes as a consequence of the fact that the pair will be in a mixed state, and of the different ways these two mixed-state entanglement measures are defined. That this behaviour persists for non-nearest neighbour spins for all values of $\alpha$ seems to indicate a similar structure of the ground state for other values of $\alpha$ than $\alpha = 0$.

## 6.3 Block Entropy

The block entropy measures the entanglement between an entire block of adjacent spins and the rest of the system, cf. the discussion on page 10. Since the odd bond pairs of spins can be considered as $\tau$ spins governed by a quantum Ising Hamiltonian (3.20), it is intuitively clear that a block of an even number of $\sigma$ spins that fully cover an integer number of $\tau$ spins will have an equal amount of entanglement with the rest of the system as that block would have in the QIM. This will now be formally shown.

The reduced density matrix $\rho_L$ for a block of $L$ spins $\sigma_1, \ldots, \sigma_L$, where $L$ is even and $\sigma_1$ and $\sigma_2$ are on the same odd bond, can be expanded as (cf. Eq. (6.3))

$$\rho_L = \frac{1}{2^L} \sum_{\mu_1,\ldots,\mu_L = 0,x,y,z} \langle \sigma_1^{\mu_1} \ldots \sigma_L^{\mu_L} \rangle \, \sigma_1^{\mu_1} \ldots \sigma_L^{\mu_L} \, . \tag{6.33}$$

Note that if we have one $\sigma_i^0$, then the other spin operator on the same odd bond must be either $\sigma_j^0$ or $\sigma_j^z$, for the expectation value $\langle \sigma_1^{\mu_1} \ldots \sigma_L^{\mu_L} \rangle$ not to be zero. In this way, one finds that the allowed pairs of $\sigma$ operators on every odd bond are

$$
\begin{aligned}
\sigma_{2i-1}^0 \sigma_{2i}^0 &\leftrightarrow & \tau_i^0 \\
\sigma_{2i-1}^z \sigma_{2i}^z &\leftrightarrow & -\tau_i^0 \\
\sigma_{2i-1}^z \sigma_{2i}^0 &\leftrightarrow & -\tau_i^z \\
\sigma_{2i-1}^0 \sigma_{2i}^z &\leftrightarrow & \tau_i^z \\
\sigma_{2i-1}^x \sigma_{2i}^x &\leftrightarrow & -\tau_i^x \\
\sigma_{2i-1}^y \sigma_{2i}^y &\leftrightarrow & -\tau_i^x \\
\sigma_{2i-1}^y \sigma_{2i}^x &\leftrightarrow & \tau_i^y \\
\sigma_{2i-1}^x \sigma_{2i}^y &\leftrightarrow & -\tau_i^y \, .
\end{aligned}
$$

Therefore

$$\sum_{\mu_1,\ldots,\mu_L} \langle \sigma_1^{\mu_1} \ldots \sigma_{2i-1}^{\mu_{2i-1}} \sigma_{2i}^{\mu_{2i}} \ldots \sigma_L^{\mu_L} \rangle \, \sigma_1^{\mu_1} \ldots \sigma_{2i-1}^{\mu_{2i-1}} \sigma_{2i}^{\mu_{2i}} \ldots \sigma_L^{\mu_L}$$

$$= \sum_{\mu_1,\ldots,\mu_{2i-2},\mu_{2i+1},\ldots,\mu_L} [\, \langle \ldots \tau_i^0 \ldots \rangle (\ldots (\sigma_{2i-1}^0 \sigma_{2i}^0 - \sigma_{2i-1}^z \sigma_{2i}^z) \ldots )$$

$$- \langle \ldots \tau_i^z \ldots \rangle (\ldots (\sigma_{2i-1}^z \sigma_{2i}^0 - \sigma_{2i-1}^0 \sigma_{2i}^z) \ldots )$$

$$- \langle \ldots \tau_i^x \ldots \rangle (\ldots (\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i-1}^y \sigma_{2i}^y) \ldots )$$

$$+ \langle \ldots \tau_i^y \ldots \rangle (\ldots (\sigma_{2i-1}^y \sigma_{2i}^x - \sigma_{2i-1}^x \sigma_{2i}^y) \ldots ) \,].$$

$$(6.34)$$

Since

$$\sigma_{2i-1}^0 \sigma_{2i}^0 - \sigma_{2i-1}^z \sigma_{2i}^z \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \;=\; 2\tau_i^0,$$

$$\sigma_{2i-1}^z \sigma_{2i}^0 - \sigma_{2i-1}^0 \sigma_{2i}^z \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \;=\; -2\tau_i^z,$$

$$\sigma_{2i-1}^x \sigma_{2i}^x + \sigma_{2i-1}^y \sigma_{2i}^y \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \;=\; -2\tau_i^x,$$

$$\sigma_{2i-1}^y \sigma_{2i}^x - \sigma_{2i-1}^x \sigma_{2i}^y \;=\; \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -2i & 0 \\ 0 & 2i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \;=\; 2\tau_i^y$$

in the $s{=}0$ subspace of the ground state, this becomes

$$\sum_{\mu_1,\ldots,\mu_{2i-2},\mu_{2i+1},\ldots,\mu_L} 2[\, \langle \ldots \tau_i^0 \ldots \rangle (\ldots \tau_i^0 \ldots )$$

$$+ \langle \ldots \tau_i^z \ldots \rangle (\ldots \tau_i^z \ldots )$$

$$+ \langle \ldots \tau_i^x \ldots \rangle (\ldots \tau_i^x \ldots )$$

$$+ \langle \ldots \tau_i^y \ldots \rangle (\ldots \tau_i^y \ldots ) \,]$$

$$= \sum_{\nu_1,\ldots,\nu_{L/2}} 2^{L/2} \langle \tau_1^{\nu_1} \ldots \tau_{L/2}^{\nu_{L/2}} \rangle \, \tau_1^{\nu_1} \ldots \tau_{L/2}^{\nu_{L/2}},$$

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giving

$$\rho_L = \frac{1}{2^{L/2}} \sum_{\nu_1,\dots,\nu_{L/2}=0,x,y,z} \langle \tau_1^{\nu_1} \dots \tau_{L/2}^{\nu_{L/2}} \rangle \, \tau_1^{\nu_1} \dots \tau_{L/2}^{\nu_{L/2}} , \qquad (6.35)$$

which is the reduced density matrix for $L/2$ spins $\tau_i$ governed by the quantum Ising model. Note that although the reduced density matrix, when expressed in the basis of eigenstates of the $\sigma_i^z$ operators, will contain a large number of columns and rows with only zeros, these rows and columns will only contribute eigenvalues zero, without affecting remaining eigenvalues. Since the block entropy

$$S_L = -\sum_i \lambda_i \log_2 \lambda_i \qquad (6.36)$$

is not affected by additional eigenvalues $\lambda_i$ that are zero, it is clear that the block entropy of $L$ spins in the generalized XX-ZZ model is the same as the block entropy of $L/2$ spins in the quantum Ising model, for the same value of the parameter $(J_x/J_z)\alpha$ when $\alpha \in [0,1)$. Thus the continuous QPT at $(J_x/J_z)\alpha = 1$ will correspond to a critical QIM, with diverging block entropy according to Eq. (1.23) and central charge $c = 1/2$. The first-order QPT at $\alpha = 1$ will, for $J_x/J_z \neq 1$, correspond to a non-critical QIM, with saturated block entropy. An analytic expression for the block entropy near the continuous QPTs, cited in Ref. [23], suggests that the saturation value $S_{L\to\infty}$ of the block entropy in general is discontinuous at $\alpha = 1$ when $J_x/J_z \neq 1$.

# Chapter 7

# Conclusions

The solution to the XX-ZZ model, introduced and solved by Brzezicki, Dziarmaga and Oleś [1], has been explicitly verified. This model, with parameter $\alpha \in [0, 2]$, was shown to exhibit a first-order quantum phase transition at parameter value $\alpha = 1$, with discontinuous correlation functions and a vanishing energy gap and diverging correlation length that behaved as at the QPT of the quantum Ising model.

A generalization of the XX-ZZ model was presented in Chap. 4. By introducing different coupling constants $J_x$ and $J_z$ in the $x$ and $z$ spin directions, respectively, it was shown that the mixed first-order and continuous behaviour at the QCP of the original model is due to the meeting of one first-order and one continuous QPT phase boundary at that particular point. The continuous QPT is in all respects Ising like, since the mapping of the XX-ZZ model onto QIMs in the different subspaces results in effective QIMs, with parameter $(J_x/J_z)\alpha$ when $\alpha < 1$, for spin pairs on both sides of $\alpha = 1$. This point marks a discontinuous transition between two different QIMs with incompatible ordering of the original spins. The separation of the QPT of the XX-ZZ model into one first-order and one continuous results in the emergence of a new phase between these two QPTs, that is not accessible in the original model where the parameter never exceeds the critical value of the QIM. This new phase is characterized by a non-degenerate ground state with reversed dominance of the two non-trivial pair correlation functions relative to the phase in the isotropic model, cf. Fig. (4.7).

The generalization of the XX-ZZ model also allows us to identify the one-dimensional quantum compass model as a particular cross-section $\alpha = 1$ of the parameter space of the generalized XX-ZZ model, making its solution a trivial special case. The one-dimensional quantum compass model behaves entirely similar to the QIM with parameter $J_x/J_z$. It was shown that the ground state is described by a spin liquid state where some correlation functions are undefined and the rest

are mapped onto correlation functions of the QIM with parameter $J_x/J_z$. Thus the one-dimensional quantum compass model exhibits a continuous QPT at the critical point $J_x/J_z = 1$, with energy gap vanishing as $\Delta \sim |(J_x/J_z) - 1|$ but with undefined correlation length.

The pairwise entanglement, as measured by the concurrence, in the ground state of the generalized XX-ZZ model, was shown to be nonzero only for spins on the same odd bond when $\alpha \in [0, 1)$ and spins on the same even bond when $\alpha \in (1, 2]$. This pairwise concurrence is discontinuous at the first-order QPT, and has a diverging first derivative $\partial C/\partial \alpha$ at the continuous QPT, in accordance with the general analysis of Ref. [17]. Therefore, the concurrence appears to be the appropriate measure of the critical entanglement content in the generalized XX-ZZ model, as it signals the orders of the QPTs. The absence of any concurrence at $\alpha = 0$ and $\alpha = 2$ is expected, since at these points we know that the ground states can be written as unentangled product states. However, the absence of any concurrence for all values of $\alpha$ between spins not on the same odd bond, clearly a consequence of the absence of any correlations between the $x$ spin components for these spins, is rather peculiar since the spins do possess long-range correlations between their $z$ spin components that must be due to entanglement in the ground state. In fact, the entanglement of assistance between any two spins, no matter how far apart, was shown to be maximal for all values of $\alpha \in [0, 2]$, clearly showing the presence of long-range entanglement in this model. For the localizable entanglement, the bounds calculated are only able to show that this entanglement measure is close to maximal for all spin pairs in the neighbourhood of the points $\alpha = 0$ and $\alpha = 2$. This total difference between the concurrence and the entanglement of assistance comes as a consequence of the different ways they measure the entanglement content of the mixed-state subsystem. The result that the concurrence vanishes for non-nearest neighbour spins for all values of $\alpha$ is however somewhat surprising as the spins of the effective QIM show non-vanishing long-range concurrence near its continuous QPT [4]. The inability of any of the calculated pairwise measures of entanglement to both indicate the different orders of the QPTs in the model as well as any long-range entanglement close to the continuous transitions, clearly points out the imperfectness of our present entanglement measures. For the block entropy, when the block covers an integer number of odd bonds, it was shown that the entanglement between this block and the rest of the system is the same as for the equivalent QIM block of half the number of spins. This shows that the continuous QPTs in the generalized XX-ZZ model are in the universality class of the QIM. The first-order QPTs probably show up as discontinuities in the saturation values $S_{L\to\infty}$ of the block entropy at $\alpha = 1$.

The XX-ZZ model apparently shows how one-dimensional spin mod-

els with first-order QPTs can be constructed by letting the model continuously interpolate between two models with incompatible types of ordering in such a way as to make some correlations discontinuous at the critical point. By also introducing a second parameter describing anisotropy, it has now been shown in this thesis how one can tune the location of the continuous QPT that also arises in this model. It can either be separated from the first-order one, giving rise to a new phase between the two QPTs, or to coincide with the one of first-order, giving rise to a first-order QPT with the same type of critical long-range correlations as in a continuous phase transition when the critical point is approached from either direction.

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