Quantum Phase Transition and Quantum Entanglement in the Generalized Cluster-XY Model

A Thesis presented

by

Aydin Deger

to

The Graduate School

in Partial Fulfillment of the

Requirements

for the Degree of

Master of Arts

in

Physics

Stony Brook University

May 2016

(include this copyright page only if you are selecting copyright through ProQuest, which is optional)

Stony Brook University

The Graduate School

Aydin Deger

We, the thesis committe for the above candidate for the

Master of Arts degree, hereby recommend

acceptance of this thesis

Dr. Tzu-Chieh Wei – Thesis Advisor
Assistant Professor, C.N. Yang Institute for Theoretical Physics

Dr. Martin Rocek – Second Reader
Professor, C.N. Yang Institute for Theoretical Physics

Dr. Matthew Dawber – Third Reader
Associate Professor, Department of Physics and Astronomy

This thesis is accepted by the Graduate School

Charles Taber
Dean of the Graduate School

Abstract of the Thesis

Quantum Phase Transition and Quantum Entanglement in the Generalized Cluster-XY Model

by

Aydin Deger

Master of Arts

in

Physics

Stony Brook University

2016

In this work, we give a detailed analytic treatment of one-dimensional anisotropic XY model in the transverse field. We present a multipartite geometric measure of entanglement per site and per block and use it for quantifying global entanglement in many-body systems. We also investigate spontaneous symmetry breaking and Quantum Phase Transition (QPT) in the model. Further, we extend the solution of the XY model to the n-site interaction and diagonalize the Hamiltonian and obtain energy levels and eigenvalues. We also examine Quantum Entanglement and QPT for next-nearest neighbor interaction and halfway interaction. At last, we introduce a Generalized Cluster-XY Hamiltonian with n-site interaction. Through this, one can diagonalize many suitable bilinear Hamiltonians by defining parameters that characterize the model. By using the model, we investigate QPT between Ferromagnetic-Paramagnetic state, GHZ-Cluster state and symmetry protected topological order and an antiferromagnetic state.

Contents

List of Figures

Acknowledgements

There are many people whom I would like to thank for their contribution in various ways, both directly and indirectly, to this thesis. First of all, special thanks to the Turkish Fulbright Commission for giving me an incredible opportunity to pursue my graduate study in the United States, and a chance to experience a different life and culture.

Further, I would like to thank the Department of Physics at Stony Brook University for giving me an opportunity to earn my master's degree at CN Yang Institute for Theoretical Physics. It was a wonderful feeling to study in the place where whole faculty is valuable and was a great pleasure to follow their courses that allowed me to gain solid knowledge in physics. It was challenging, productive, and exciting time to achieve knowledge, conduct research and enhance my passion for physics.

I would like to thank my advisor, Dr. Tzu-Chieh Wei, who introduced me a topic that turned out to be an inspiring and enjoyable journey for me. Thanks to his help, I delved into this thrilling field in which I was able to develop my skills and creativity further.

I want to acknowledge also my family for their support and belief in me. Besides, thanks to everyone who made my stay in US enjoyable and unforgettable.

1 Introduction

Integrable quantum spin chains have a significant importance for statistical physics, quantum many-body physics and quantum information theory. There are many challenges in this field. To name a few, one can study magnetism, superconductivity, quantum computing, new states of matter, and strange quantum phenomena such as quantum entanglement or quantum phase transition. Antiferromagnetic Heisenberg chain was one of the first introduced models and solved by Bethe in 1931 [1]. Over the years, many spin-1/2 and spin-1 models have been introduced in one and two dimensions. For example, these include Ising Model [2] which is a mathematical model for ferromagnetism, AKLT [3] for spin-1 systems for understanding valence-bond solids and Hubbard model [4] for investigating conducting and insulating systems.

The Ising Model was firstly introduced by Lenz [5] and studied by Ising [2] through his Ph.D. research. In 1941, Kramers and Wannier [6] studied high and low-temperature expansion of the two-dimensional Ising model and after three years, the model was exactly solved by Onsager [7] for the first time. Later, Lee and Yang investigated the partition function and its roots on complex field plane [8]. In 1964, Schultz, Mattis and Lieb [9] solved the problem using fermions. Later, all aspects of the problem and thermodynamic properties have been discussed in great detail by McCoy and Wu [10].

Lieb, Schultz, Mattis presented two soluble spin chain, including the quantum XY Model [11]. Many other authors studied all statistical properties, correlation, quantum entanglement and quantum phase transition in this model [12] [13] [14] [15] [16] [17] [18]. Three-spin interactions and triangular configuration has been also solved [19] [20] [21] [22] [23]. Many experimental realization of the model has been studied such as Ion-traps [24], Quantum dot spins and cavity [25] and Josephson junctions [26]. The bilinear form of the Hamiltonian which consists two creation and annihilation operators emerges in many models such as BCS and superfluids. To diagonalize the hamiltonian one shall use Jordan Wigner Transformation [27] [28] and Bogoliubov transformation which can be seen in the solution of the theory of BCS Superconductivity [29].

The structure of this thesis as follows. In the first section, we give an introduction to the Quantum Entanglement and Quantum Phase Transition. In the second section, we will be mostly focusing on one-dimensional generalized spin-1/2 XY model. We begin with a quick derivation of one-dimensional quantum Ising model and two-dimensional square lattice Ising model. Later we shall show an alternative solution for the spin-1 Ising model in one dimension. In the next part, we present detailed solution of the anisotropic XY model in the transverse field. We pay attention to the *cyclic chain* problem and introduce a gauge term to specify periodic/antiperiodic boundary conditions. Competition between vacuum states is also examined. Afterward we introduce Fourier transformation in many-site interaction and give a detailed treatment to Bogoliubov transformation.

Subsequently, we introduce the derivation of geometric entanglement per site and block and using global entanglement in the geometric picture we examine emergence of quantum phase transition for the model. In the next section, we solve three-site interaction of the XY model. This model also shows the quantum phase transition at the same critical point. Nevertheless, in this model disorder line $r^2 + h^2 = 1$ vanishes, which exists in the XY model.

Next we shall derive generalized Hamiltonian for n-site interaction and investigate halfway interaction ($n = N/2 - 1$) properties in the context of Quantum Phase Transition. It turns out that QPT does not occur when we consider halfway interaction. Quantum-Classical duality is also examined for this model, and we present the proper constants for mapping 1D Quantum XY model to 2D Square-lattice Ising model.

In the last section, we introduce a generalized Cluster-XY Hamiltonian and show diagonalization of the model. A similar model has been studied by

Suzuki in 1971 [30]. We define the Hamiltonian in more convenient way that one can solve many suitable bilinear Hamiltonians by defining parameters that characterize the model. We give an example of several Hamiltonians and examine Global Entanglement and Quantum Phase Transition between Ferromagnetic-Paramagnetic state, GHZ-Cluster and Symmetry protected topological order and an Antiferromagnetic state.

1.1 Quantum Entanglement

Quantum entanglement is one of the most intriguing consequence of the quantum mechanics. The term was introduced by Schrodinger as a "Verschrankung" for the first time in 1935 [31]. It was discussed and objected in the famous EPR paper [32] and defined by Einstein as a "spooky action at a distance." This spooky non-local correlation had been a very counter-intuitive subject until Bell introduced a series of inequalities [33]. Bell's theorem says that "No physical theory of local hidden variables can ever reproduce all of the predictions of quantum mechanics." The existence of entangled states was tested by many experiments over the years [34] [35]. Assume that Alice and Bob are sharing the entangled state.

$$|\psi\rangle = (|\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B) \tag{1}$$

It does not matter how far Alice and Bob are apart from each other, their state would stay entangled [36]. Now, let's assume Alice decided to make a *measurement* and find out her state. Bob's state function also collapsed *instantaneously* when Alice makes a measurement in her own state. Unfortunately, Bob still needs to know which direction he needs to measure to verify to collapse and it has to be done in the classical channels. Unfortunately, therefore quantum entanglement can not be used for transferring useful information faster than the speed of light.

Quantum entanglement has gained more attention with the emergence of Quantum Information Science [37] and has played a major role in the very different areas such as the theory of black holes, quantum many-body physics, and quantum computation. Most of the subareas of quantum information science are based on quantum entanglement. To list a few, entanglement is needed for Quantum teleportation [38]; Quantum search and factoring algorithms [39] [40] require entangling gates; Quantum Communication and Quantum Cryptography [41] can be achieved with the use of entanglement;

Quantum Error Correction [42] uses entangled states. As an unexpected application, Quantum entanglement exhibits dramatic change and divergence in the quantum critical point. Thus, it is very useful for detecting Quantum Phase Transition at strongly correlated many body systems.

There has been much work done in detecting and quantifying entanglement in bipartite and multipartite quantum systems the over years [43] [44]. Many different methods have been introduced for measuring entanglement [45]. At this point, we shall start by defining some basic concepts. The bipartite system can be described as the composition of two Hilbert Space $H = H_A \otimes H_B$. Bipartite pure state $|\psi\rangle = |\psi_A\rangle \otimes |\psi_B\rangle$ is separable —unentangled—if it can be written in the following form by using Schmidt Decomposition.

$$|\psi\rangle = \sum_{i,j} c_{i,j} \left|e_i\right\rangle_A \otimes \left|e_j\right\rangle_B \tag{2}$$

where $|e_i\rangle$ and $|e_j\rangle$ are the basis of H

One can easily check the separability by using Schmidt Decomposition

$$|\psi\rangle = \sum_{k=1}^{n} \lambda_k \left|u_k\right\rangle_A \otimes \left|v_k\right\rangle_B \tag{3}$$

where $\sum \lambda_k^2 \geq 0$ and $n = min\Big[dim\left(H_A\right), dim\left(H_B\right)\Big]$. Schmidt coefficient λ is useful for testing entanglement. If there is only one non-zero Schmidt coefficient, then $|\psi\rangle$ is separable otherwise it is entangled [36] [46]. For deciding separability in mixed states, one shall look at the density matrices of the system. Mixed state is separable if and only if it is written in the following form

$$\rho = \sum_{i} p_i \left|e_i\right\rangle_A \left\langle e_i\right|_A \otimes \left|e_i\right\rangle_B \left\langle e_i\right|_B \tag{4}$$

If there is more than two Hilbert spaces, $H = H_A \otimes H_B \otimes H_C \otimes H_D \ldots$ it is called multipartite system [47]. We shall consider the following multi state

$$|\Psi\rangle = |\psi_1\rangle_{E,F} \otimes |\psi_2\rangle_{B,C,D} \otimes |\psi_3\rangle_A \tag{5}$$

As one can see in the first state, it can not be written as a product state of E and F. In the same way, B, C, D are entangled with each other. One need to consider all entanglement between partitions. Because of this reason, quantifying entanglement in the multipartite system is a less simple problem. GHZ and W state can be an example for multipartite states [48] which we discuss below. For an N-qubit, GHZ and W can be defined as following

$$|GHZ\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle^{\otimes\ N} + |1\rangle^{\otimes\ N} \right) \tag{6}$$

$$|W\rangle = \frac{1}{\sqrt{N}} \Big(|100\ldots00\rangle + |010\ldots00\rangle + |000\ldots01\rangle \Big) \tag{7}$$

For N=3 qubit example, one expects to see bipartite entanglement even one of the particle lost. On the other hand, GHZ would lose quantum correlation and become a separable mixed state.

There are many methods for measuring entanglement in bipartite systems. To name a few, Von Neumann Entanglement Entropy, Concurrence, Entanglement of Formation [49] [50], distillable entanglement, relative entropy of entanglement. Introducing all of the entanglement methods is beyond the scope of this paper. Thus, we will only present first two of the list.

Entanglement of Entropy—Von Neumann Entropy—is one of the simplest technique for measuring entanglement. It is very helpful for solving problem from Condensed Matter Theory to String Theory. By using density matrix

$$\rho = \sum_i \lambda_i \, |e_i\rangle \, \langle e_i| \tag{8}$$

Von Neumann Entropy can be define as following

$$S(\rho) = -Tr\,(\rho\ log_2\rho) \tag{9}$$

One can measure the Entanglement of entropy by taking partial trace $\rho_A = Tr_B(\rho)$ of one of the states.

$$E(\psi) = S(\rho_A) = S(\rho_B) \tag{10}$$

For pure p_A or p_B, entanglement will give 0. On the other hand, for any *Bell States*, entanglement would give 1 which is maximally entangled. One can also use entanglement of formation [49] for pure and mixed states.

$$E(\rho) = min \sum_i p_i E(\psi_i) \tag{11}$$

It is average of entanglement over minimum of all decompositions of ρ. This function can be derived for the standard basis. Wootters [49] derived the formula for the entanglement of formation of two qubits.

$$E(\psi) = \mathcal{E}\,(C) = h\left(\frac{1+\sqrt{1-C^2}}{2}\right) \tag{12}$$

where h is Shannon Entropy

$$h(x) = -x\ log_2 x - (1-x)\ log_2(1-x) \tag{13}$$

C is defined as *concurrence*. Let us define the state

$$|\Psi\rangle = \alpha\,|00\rangle + \beta\,|01\rangle + \gamma\,|10\rangle + \delta\,|11\rangle \tag{14}$$

and concurrence is

$$C(\Psi) = |\langle\Psi|\tilde{\Psi}\rangle\,| \tag{15}$$

$$|\tilde{\Psi}\rangle = (\sigma_y \otimes \sigma_y)\,|\Psi^*\rangle \tag{16}$$

The entanglement is a monotonic function of concurrence. The range of concurrence change between 0 to 1. Thus, it can be an another way to quantify entanglement. For mixed states,

$$C(p) = max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \tag{17}$$

where λ are the eigenvalues of the R matrix in descending order

$$R = \sqrt{\sqrt{p}\tilde{p}\sqrt{p}} \tag{18}$$

$$\tilde{p} = (\sigma_y \otimes \sigma_y)\ p^*\ (\sigma_y \otimes \sigma_y) \tag{19}$$

Quantifying entanglement is a broad research area. There are many successful techniques for a bipartite system. On the other hand quantifying entanglement in a multipartite system is more challenging. Geometric measure of entanglement is one of the promising methods for quantifying multipartite system. It was first time introduced by Shimony [51] for the bipartite systems and generalized to multipartite systems by Barnum and Linden [52]. Then, Wei and Goldbart [53] developed it further and applied it to the XY model [54]. It has also been studied in two-dimensional systems [55].

To introduce this measure, let us define n-partite, normalized state

$$|\Psi\rangle = \sum_{p_1 \cdots p_n} \Psi_{p_1 p_2 \cdots p_n} |e_{p_1}^{(1)} e_{p_2}^{(2)} \dots e_{p_n}^{(n)}\rangle \tag{20}$$

The main idea of analyzing entanglement is finding a distance between entangled state and separable state. If we define general product state as follows

$$|\Phi\rangle \equiv \otimes_{i=1}^{n} |\phi^{(i)}\rangle \tag{21}$$

The proximity can be calculated by taking overlap of entangled and separable state

$$\Lambda_{max}(\Psi) \equiv \max_{\Phi} \langle \Phi | \Psi \rangle \tag{22}$$

where Λ_{max} is inversely proportional to entanglement of $|\Psi\rangle$. Normalizing entanglement for Bell States and giving 0 for separable states

$$E_{log_2}(\Psi) \equiv -log_2 \; \Lambda^2_{max}(\Psi) \tag{23}$$

entanglement density can be defined as following for N-particle

$$\mathcal{E} \equiv \frac{E_{log_2}(\Psi)}{N} \tag{24}$$

detailed treatment for Geometric entanglement per site and Geometric Entanglement per block will be given in the *Section 2.2.5*

1.2 Quantum Phase Transition

Phase transition in a classical manner can be defined as the transformation between states of the matters due to fluctuations in the temperature or other system parameters. Boiling of water or water freezing to ice are common phase transition that we experience in our daily life. The phase transition is studied very well and can be shown in a phase diagram. On the other hand, there is also phase transition which is happening in the quantum system. Quantum Phase Transition (QPT) [56] is driven by quantum fluctuations due to Heisenberg's uncertainty principle. It happened at zero temperature and induced by the change in physical parameters such as magnetic field or chemical potential. QPT is a change in the ground state of the many body systems between low-lying energy levels. It is known that there is an abrupt change in the entanglement near the critical point due to divergence in long-range correlation. Thus, Quantum Phase Transition can be characterized by entanglement near the critical points. It has been widely studied by many authors [57] [58].

Let us consider a Hamiltonian in the finite lattice $H = H_0 + g\ H_1$ where $[H_0, H_1] = 0$. Thus, there will be a critical point in g_c where the ground state meets with the first excited state. Correlation in the energy gap Δ can be shown

$$\Delta \sim J\ |g - g_c|^{zv} \sim \xi^{-z} \tag{25}$$

zv is a critical exponent and ξ is correlation length. If the transition occurs at a non-zero temperature T_c, correlation time is [59]

$$\tau \sim \xi^z \sim |t|^{-zv} \tag{26}$$

where

$$t = \frac{|T - T_c|}{T_c} \tag{27}$$

Main differences between quantum phase transition and classical phase transition are the energy scales and temperature. Typical energy scale in the quantum systems is $\hbar w_c$ while thermal energy is $k_B T$. As long as $\hbar w_c \ll k_B T$ classical phase transition can be considered since quantum effects would be overshadowed by the thermal fluctuations. Nevertheless, if there is no thermal fluctuations but only non-thermal variables change, transition in the critical point can be defined as Quantum Phase Transition.

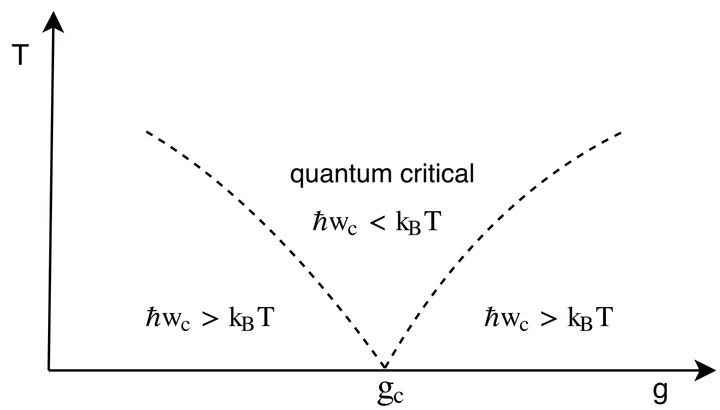

Figure 1: Quantum phase transition lies in quantum critical area

Symmetry breaking is an important phenomenon for the quantum phase transition. Symmetry breaking is defined as the systems has lower symmetry than the initial. In terms of group theory, broken symmetry is invariance on the transformation of one of the subgroups of the initial system [60] [61]. Explicit symmetry breaking occurs when one or more terms of the perturbation does not obey the symmetry of the unperturbed. Hydrogen atom in a magnetic field can be an example for this type of symmetry breaking

$$H = H_0 + H_1 \tag{28}$$

where $H_1 = -\vec{\mu}\,\vec{B}$ is a small perturbation due to magnetic field $\vec{B}$ and

$$H_0 = \frac{\vec{p}^2}{2m_e} - \frac{e^2}{4\pi e_0 r} \tag{29}$$

H_0 is invariant under rotational symmetry, on the other hand, H_1 is not in the same symmetry group. Thus, symmetry is broken, and degeneracy is lifted. On the other hand, spontaneous symmetry breaking occurs when the Hamiltonian has an overall symmetry while ground states break the symmetry and exhibit degeneracy. It is one of the most crucial concepts in theoretical physics. It is also associated with Phase Transition. Ferromagnets, Bose–Einstein condensate and standard model can be given an example of this phenomena. The order parameter is a physical property of the system that quantifies the strength of symmetry whereas it changes between disorder—high symmetry and order—low symmetry.

Ising Ferromagnet may be given an example of spontaneous symmetry breaking [2].

$$H = -J \sum \sigma_i \sigma_j \tag{30}$$

where J is the coupling constant. There is nearest neighbor interaction in the system which leads unpaired couples to be aligned. In the case $J > 0$ system is ferromagnetic and spin point $\uparrow$ (up) direction. Hamiltonian enjoys the Ising symmetry that is invariant under the change of $\sigma_i \to -\sigma_i$. The energy of the system remains unchanged under this transformation. On the other hand, the ground state may choose a specific orientation depending on the temperature.

Ferromagnet is a material which shows spontaneous symmetry breaking at the *Curie temperature*. Magnetization is the differences between spin up and spin down states. Below the Curie temperature, magnetization gives a non-zero value and choose a particular direction that breaks the symmetry of the system. Quantum phase transition occurs from ferromagnetic to paramagnetic phase at the critical temperature.

In statistical physics and Condensed Matter Physics one can examine the relation between d dimensional quantum and (d+1) dimensional classical systems. One can reach the classical partition function by mapping temperature into imaginary time in the quantum partition function. Thus, imaginary time acts as an additional dimension at zero temperature.

In classical partition function kinetic and potential part of Hamiltonian commutes.

$$Z = Tr\left(e^{-H/k_bT}\right) \tag{31}$$

where $H = H_{kin} + H_{pot}$ Thus partition function $Z = Z_{kin}Z_{pot}$ can be factorizable which means dynamics and static parts are decoupled. On the other hand in quantum mechanics, kinetic and potential terms do not commute $[T, V] \neq 0$ which indicates static and dynamics are coupled. Density operator in the partition function looks very similar to time evolution operator. By choosing imaginary time τ

$$\tau = \frac{1}{k_bT} = \frac{-it}{\hbar} \tag{32}$$

where t is real time, one can show at zero temperature (T) imaginary time can be considered as an extra dimension [59].

2 Integrable Quantum Spin Chains

Most of the physical phenomena can be expressed in spin, fermionic or bosonic language. One's main aim is solving—diagonolizing—Hamiltonian and finding partition functions so that statistical mechanics of the system can be easily derived. For instance, one can study Heisenberg spin model for studying magnetism.

$$H = -\frac{1}{2}\sum_{j=1}^{N}\left(J_x\sigma_j^x\sigma_{j+1}^x + J_y\sigma_j^y\sigma_{j+1}^y + J_z\sigma_j^z\sigma_{j+1}^z + h\sigma_j^z\right) \tag{33}$$

where J are coupling constants. For the spin 1/2 systems σ_i are Pauli spin matrices.

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{34a}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{34b}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{34c}$$

In the case $J > 0$ ground state is ferromagnet otherwise antiferromagnet. In the limit of $J = J_x = J_y \neq J_z$ called Heisenberg XXZ model [62] [63].

There are several methods solving for the spin chain problems. One approach is using certain similarities between spin operators (σ_i) and fermionic (c_i) or bosonic (b_i) operators. For instance, Holstein-Primakoff transformation [64] is useful for mapping spin operators to bosonic annihilation and creation operators. While bosonic canonical commutation relations (CCR)

$$[b_i, b_j^\dagger] = \delta_{i,j} \tag{35}$$

we define transformation where $S_i = \dfrac{\sigma_i}{2}$ and spin s

$$S_i^+ = S_{ix} + i\ S_{iy} = \sqrt{2s}\ \sqrt{1 - \frac{b_i^\dagger b_i}{2s}}\ b_i \tag{36a}$$

$$S_i^- = S_{ix} - i\ S_{iy} = \sqrt{2s}\ b_i^\dagger\ \sqrt{1 - \frac{b_i^\dagger b_i}{2s}} \tag{36b}$$

$$S_z = s - b_i^\dagger b_i \tag{36c}$$

using this transformation one can work with bosons and expand the square root for further analysis. One must note that total boson number can not exceed twice spin number since square root must be a real number $b_i^\dagger b_i \leq 2s$

On the other hand, as we consider fermionic picture, Jordan-Wigner transformation [65] is very useful tool for diagonalizing spin chain problems. This time we are mapping spin Hilbert space to the fermionic Fock space whereas fermionic CCR [66]

$$\{c_i, c_j^\dagger\} = \delta_{i,j} \tag{37a}$$

$$\{c_i, c_j\} = 0 \tag{37b}$$

One can easily see the problem here. Fermionic CCR obeys the anticommutation relation. Therefore, we can not naively map spin operators into fermionic operators since spin operators do not hold anticommutation relations for multi-site problems

$$\{S_i^+, S_j^+\} \neq 0 \tag{38}$$

Thus one need an extra phase to solve correct anticommutation-commutation problem. We define the Jordan-Wigner transformation

$$S_i^+ = c_i^\dagger \; e^{i\pi \sum_{j=1}^{i-1} c_j^\dagger c_j} \tag{39a}$$

$$S_i^- = e^{-i\pi \sum_{j=1}^{i-1} c_j^\dagger c_j} \; c_i \tag{39b}$$

$$S_z = c_i^\dagger c_i - 1/2 \tag{39c}$$

where $n_i = c_i^\dagger c_i$ is the number of the fermion at a site. Thus desired commutation $[S_i^+, S_j^+] = 0$ can be derived easily

$$S_i^+ S_j^+ = S_j^+ S_i^+ \tag{40}$$

Now, one can safely use the transformation for mapping spin operators to fermionic operators. This transformation has been examined in detailed in the section 2.2.1

2.1 Ising Model in a Transverse Field

Ising model is the simplest model for explaining ferromagnetism. As we consider N atoms and their magnetic moments represented by opposite direction of $\uparrow$ and $\downarrow$ spins in each site on the lattice. It can be represented in various lattice and dimensions despite the fact that 3D dimensional classical Ising model has not been solved properly. We shall give a quick derivation of one and two dimensional Ising model since we will be referring this section later for quantum-classical duality of XY-Ising Model.

2.1.1 One and Two Dimensional Square-lattice Ising Model

We begin with defining the two dimensional Hamiltonian for the model [9]

$$H(\sigma_{11},\dots\sigma_{NM}) = -h\sum\sigma_{nm} - J_1\sum\sigma_{nm}\sigma_{n+1,m} - J_2\sum\sigma_{nm}\sigma_{n,m+1} \quad (41)$$

J_1 and J_2 is the bond strengths in the n-th row and m-th column. σ_{nm} can take ±1 values. We assumed that it has periodic boundry conditions $\sigma_{n,M+1} = \sigma_{n1}$ and $\sigma_{N+1,m} = \sigma_{1m}$. Then partition function can be defined

$$Z \equiv \sum_{\sigma_{11}=\pm1}\dots\sum_{\sigma_{NM}=\pm1} e^{-\beta H(\sigma_{11},\dots\sigma_{NM})} \quad (42)$$

Solving one-dimensional problem and generalizing to 2D is the most practical way to derive. Then we define 1D cyclic lattice where $K_1 = \beta J_1$ and $H = \beta h$

$$Z = \sum_{\sigma_1\dots\sigma_N} e^{K_1\sum\sigma_n\sigma_{n+1}}e^{H\sum\sigma_n} \quad (43)$$

Expanding Z terms

$$Z = \sum_{\sigma_{1'}\sigma_1\dots\sigma_N\sigma_{N'}} e^{K_1\sigma_{1'}\sigma_2}e^{H\sigma_2\delta_{\sigma_2\sigma_{2'}}}\dots e^{K_1\sigma_{N'}\sigma_1}e^{H\sigma_1\delta_{\sigma_1\sigma_{1'}}} \quad (44)$$

defining matrix for each exponential term $(V_1)_{\sigma_i \sigma_j} = e^{K_1 \sigma_i \sigma_j}$

$$V_1 = \begin{pmatrix} e^{K_1} & e^{-K_1} \\ e^{-K_1} & e^{K_1} \end{pmatrix} \tag{45}$$

and $(V_2)_{\sigma_i \sigma_j} = e^{H \sigma_i} \delta_{\sigma_i \sigma_j}$

$$V_2 = \begin{pmatrix} e^{H} & 0 \\ 0 & e^{-H} \end{pmatrix} \tag{46}$$

then Z can be written as the trace of a matrix product under the cyclic permutations of factors

$$Z = trV_1V_2 \ldots V_1V_2 = tr(V_1V_2)^N = tr(V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}})^N = trV^N \tag{47}$$

V is called the transfer Matrix. Then largest eigenvalue of this matrix is the solution of Hamiltonian.

$$Z = \Lambda_1^N + \Lambda_2^N = \Lambda_1^N [1 + (\frac{\Lambda_1}{\Lambda_2})^N] \tag{48}$$

when $N \to \infty$ only largest eigenvalue will contribute. Next step is writing the matrices in terms of Pauli spins (τ^x, τ^y, τ^z)

$$V_1 = e^{K_1} \mathbb{1} + e^{-K_1} \tau^x = e^{K_1} (\mathbb{1} + e^{-2K_1} \tau^x) \tag{49}$$

$$V_2 = \mathbb{1} \cosh H + \tau^z \sinh H \tag{50}$$

Using the followings property

$$e^{a\tau^i} = \mathbb{1} \cosh a + \tau^i \sinh a = \cosh a \ (\mathbb{1} + \tau^i \ \tanh a) \tag{51}$$

and defining and using simple identities

$$\tanh K_1' \equiv e^{-2K_1} \tag{52}$$

$$\tanh K_1 \equiv e^{-2K_1'} \tag{53}$$

$$\sinh 2K_1 \sinh 2K_1' \equiv 1 \tag{54}$$

we have reached

$$V_1 = (2\sinh\ 2K_1)^{\frac{1}{2}}\ e^{-2K_1'\ \tau^x} \tag{55}$$

$$V_2 = e^{H\tau^z} \tag{56}$$

Generalization of 2D Ising model is following. In every row, we are taking 2^M configuration.

$$\tau_m^z = \mathbb{1} \ldots \tau^z \ldots \mathbb{1} \tag{57}$$

$$\tau_m^x = \mathbb{1} \ldots \tau^x \ldots \mathbb{1} \tag{58}$$

we have reached the two-dimensional solution

$$V_1 = (2\sinh 2K_1)^{M/2}\ \ e^{-2K_1'\ \tau^x} \tag{59}$$

$$V_2 = e^{K_2 \sum \tau_m^z \tau_{m+1}^z + H \sum \tau_m^z} \tag{60}$$

$$Z = tr\left(V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}}\right)^N = trV^N \tag{61}$$

Ising model with a transverse field in one-dimension will be introduced in the next section.

2.1.2 Spin-1 Ising model in a transverse crystal field

In this part, we shall consider spin-1 Ising Model with a transverse single-ion crystal-field term. Pfeuty has given the exact solution of this model [67]. Later, Oitmaa and Brasch [68] have shown that spin-1 Hamiltonian can be solved by mapping to traditional spin-1/2 transverse Ising Model. Here we show the quick derivation of the exact location of critical point in one dimension by this transformation. Hamiltonian of a spin-1 Ising model is the following:

$$H = -J \sum_{<i,j>} S_i^z S_j^z - \Delta \sum_i (S_i^x)^2 \tag{62}$$

This Hamiltonian shows similarity with spin-1/2 Ising model under the right transformation when one is only concerned with the ground state:

$$H_{TIM} = -J \sum_{<i,j>} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x \tag{63}$$

If N is the number of sites,

$$N_0 = N - \sum_i (S_i^z)^2 \tag{64}$$

N_0 indicates the number of sites in the ground states which commutes with H since $[(S_i^z)^2, (S_i^x)^2] = 0$ To see the eigenvalues we expand S_i^x term.

$$(S_i^x)^2 = \left(\frac{S_i^+ + S_i^-}{2}\right)^2 = \frac{1}{4} \sum_i \left(S_i^+ S_i^+ + S_i^+ S_i^- + S_i^- S_i^+ + S_i^- S_i^-\right) \tag{65}$$

It appears that there are no sites in the zero state and ($m_i = 0$) [68]. Thus, there are two states per site ($m = \pm 1$). Defining transformation

$$S_i^z \longrightarrow \sigma_i^z \tag{66a}$$
$$S_i^+ S_i^+ \longrightarrow 2\sigma_i^+ \tag{66b}$$
$$S_i^- S_i^- \longrightarrow 2\sigma_i^- \tag{66c}$$
$$S_i^+ S_i^- \longrightarrow 1 + \sigma_i^z \tag{66d}$$
$$S_i^- S_i^+ \longrightarrow 1 - \sigma_i^z \tag{66e}$$

using Equation (66), one can map each spin-1 operator to a σ operator

$$(S_i^x)^2 = \frac{1}{4}\sum_i 2\sigma_i^+ + 2\sigma_i^- + 1 + \sigma_i^z + 1 - \sigma_i^z \tag{67a}$$
$$= \frac{1}{2}\sum_i \left(\sigma_i^+ + \sigma_i^- + 1\right) \tag{67b}$$
$$= \frac{1}{2}\sum_i (\sigma_x + 1) \tag{67c}$$

By doing this conversion, we can calculate crystal field term (V) in terms of σ and later H_{eff}. This is the same result with H_{TIM} with a constant $-\frac{1}{2}N\Delta$

$$V = -\frac{1}{4}\Delta \sum_i (S_i^\dagger S_i^\dagger + S_i^\dagger S_i + S_i S_i^\dagger + S_i S_i) \tag{68}$$

$$H \longrightarrow H_{eff} = -\frac{1}{2}N\Delta - J \sum_{<i,j>} \sigma_i^z \sigma_j^z - \frac{1}{2}\Delta \sum_i \sigma_i^x \tag{69}$$

If we consider more general Hamiltonian by adding a $(S_i^y)^2$ term

$$H = -J \sum_{<i,j>} S_i^z S_j^z - \Delta_x \sum_i (S_i^x)^2 - \Delta_y \sum_i (S_i^y)^2 \tag{70}$$

and using same conversation and keeping in mind that ground state lies in the $N_0 = 0$ we will get the following

$$H \longrightarrow H_{eff} = -\frac{1}{2}N(\Delta_x + \Delta_y) - J\sum_{<i,j>}\sigma_i^z\sigma_j^z - \frac{1}{2}(\Delta_x - \Delta_y)\sum_i \sigma_i^x \quad (71)$$

In order to have Blume-Capel model [69], one can choose $\Delta_x = \Delta_y = \Delta$ and equation (70) become

$$H = -J\sum_{<i,j>} S_i^z S_j^z - \Delta\sum_i((S_i^x)^2 + (S_i^y)^2) \quad (72)$$

where we use $(S_i^x)^2 + (S_i^y)^2 = (S_i)^2 - (S_i^z)^2$

$$H = -J\sum_{<i,j>} S_i^z S_j^z + \Delta\sum_i (S_i^z)^2 - 2N\Delta \quad (73)$$

2.2 The Anisotropic XY Model in One Dimension

Quantum entanglement and Quantum Phase transition in XY Model is a broad topic. There are several methods to diagonalize the Hamiltonian. Firstly, we shall define Hamiltonian of the anisotropic XY model [11].

$$H_{XY} = -\sum_{j=1}^{N}(\frac{1+r}{2})\sigma_j^x\sigma_{j+1}^x + (\frac{1-r}{2})\sigma_j^y\sigma_{j+1}^y + h\sigma_j^z \tag{74}$$

where N is the number of the site, and r indicate the anisotropy between σ_x and σ_y terms. $r = 0$ is isotropic XY limit and $r = 1$ Ising limit in the transverse field (h)

Diagonalization of this Hamiltonian can be done by mapping spin operators into the fermionic picture and define boundary conditions. In this paper, we are going to use only cyclic chain which is $\sigma_{N+1}^x = \sigma_1^x$ and $\sigma_{N+1}^y = \sigma_1^y$. Later we will perform Fourier Transformation and Bogoliubov transformation to cancel out non-diagonal terms.

2.2.1 Jordan-Wigner Transformation

Let us begin with defining Jordan-Wigner Transformation for this problem.

$$\sigma_i^x = \prod_{j=1}^{i-1}\left(1 - 2c_j^\dagger c_j\right)\left(c_i + c_i^\dagger\right) \tag{75a}$$

$$\sigma_i^y = -i\prod_{j=1}^{i-1}\left(1 - 2c_j^\dagger c_j\right)\left(c_i - c_i^\dagger\right) \tag{75b}$$

$$\sigma_i^z = 1 - 2c_i^\dagger c_i \tag{75c}$$

bearing in mind that $j \leq i - 1$. In order to determine correct boundary conditions we check the last term of the chain [54]

$$\sigma_N^x\sigma_{N+1}^x = \sigma_N^x\sigma_1^x \tag{76}$$

$$\left(c_N + c_N^\dagger\right)\left(c_{N+1} + c_{N+1}^\dagger\right) = \sigma_1^x = -\prod_{j=1}^{N}\left(1 - 2c_j^\dagger c_j\right)\left(c_N + c_N^\dagger\right)\left(c_1 + c_1^\dagger\right) \tag{77}$$

One can easily notice that there is two possibility to hold the above equation. First is the periodic boundary condition occurs where total number of site N is odd

$$\prod_{j=1}^{N}\left(1 - 2c_j^\dagger c_j\right) = -1 \tag{78}$$

$$c_{N+1} = c_1 \tag{79}$$

and other is the antiperiodic boundary condition where the total number of site N is even

$$\prod_{j=1}^{N}\left(1 - 2c_j^\dagger c_j\right) = 1 \tag{80}$$

$$c_{N+1} = -c_1 \tag{81}$$

With the help of Jordan-Wigner transformation (75) in the Hamiltonian (74) one can reach the fermionic Hamiltonian

$$\begin{aligned} -H_{XY} = \sum_{j=1}^{N}(\frac{1+r}{2})\prod_{i=1}^{j-1}(1-2c_i^\dagger c_i)(c_j + c_j^\dagger)\prod_{i=1}^{j}(1-2c_i^\dagger c_i)(c_{j+1} + c_{j+1}^\dagger) \\ + (-i)^2(\frac{1-r}{2})\prod_{i=1}^{j-1}(1-2c_i^\dagger c_i)(c_j - c_j^\dagger)\prod_{i=1}^{j}(1-2c_i^\dagger c_i)(c_{j+1} - c_{j+1}^\dagger) \\ + h(1-2c_j^\dagger c_j) \end{aligned} \tag{82}$$

After canceling terms and simplifying, we have

$$-H_{XY} = \sum_{j=1}^{N} (\frac{1+r}{2})(c_j + c_j^\dagger)(1 - 2c_i^\dagger c_i)(c_{j+1} + c_{j+1}^\dagger) \\ - (\frac{1-r}{2})(c_j - c_j^\dagger)(1 - 2c_i^\dagger c_i)(c_{j+1} - c_{j+1}^\dagger) + h(1 - 2c_j^\dagger c_j) \tag{83}$$

Using anticommutation relations

$$\begin{aligned} (1 - 2c_j^\dagger c_j)^2 &= 1 \\ (1 - 2c_j^\dagger c_j)c_j &= c_j \\ (1 - 2c_j^\dagger c_j)c_j^\dagger &= -c_j^\dagger \\ c_j(1 - 2c_j^\dagger c_j) &= -c_j \\ c_j^\dagger(1 - 2c_j^\dagger c_j) &= c_j^\dagger \end{aligned} \tag{84}$$

we reach the following form

$$-H_{XY} = \sum_{j=1}^{N} (\frac{1+r}{2})(-c_j + c_j^\dagger)(c_{j+1} + c_{j+1}^\dagger) \\ - (\frac{1-r}{2})(-c_j - c_j^\dagger)(c_{j+1} - c_{j+1}^\dagger) + h(1 - 2c_j^\dagger c_j) \tag{85}$$

or expanding the products

$$-H_{XY} = \sum_{j=1}^{N} (\frac{1+r}{2})[-c_j c_{j+1} - c_j c_{j+1}^\dagger + c_j^\dagger c_{j+1} + c_j^\dagger c_{j+1}^\dagger] \\ - (\frac{1-r}{2})[-c_j c_{j+1} + c_j c_{j+1}^\dagger - c_j^\dagger c_{j+1} + c_j^\dagger c_{j+1}^\dagger] + h(1 - 2c_j^\dagger c_j) \tag{86}$$

one can reach the simplest fermionic form of the Hamiltonian

$$-H_{XY} = \sum_{j=1}^{N} (-c_j c_{j+1}^\dagger + c_j^\dagger c_{j+1}) + r(-c_j c_{j+1} + c_j^\dagger c_{j+1}^\dagger) + h(1 - 2c_j^\dagger c_j) \tag{87}$$

2.2.2 Fourier Transformations

In the last form of the Hamiltonian, different sites are still exist. To eliminate these terms, we use Fourier Transformation to transfer our system to momentum space. We shall define gauge term b to indicate periodic—odd—where $b = 0$ and antiperiodic—even—where $b = 1/2$ fermions.

$$c_j = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}j(m+b)} \tilde{c}_m \tag{88a}$$

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}j(m+b)} \tilde{c}_m^\dagger \tag{88b}$$

$$\tilde{c}_m = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{-i\frac{2\pi}{N}j(m+b)} c_j \tag{88c}$$

$$\tilde{c}_m^\dagger = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} e^{i\frac{2\pi}{N}j(m+b)} c_j^\dagger \tag{88d}$$

where $\tilde{}$ specify the momentum space. We shall show firstly the derivation of each term and then derive the general form of the fourier transform.

$$\sum_{j=1}^{N} c_j c_{j+1} = \frac{1}{N} \sum_{j=1}^{N} \sum_{m,m'=0}^{N-1} e^{i\frac{2\pi}{N}j(m+b)} e^{i\frac{2\pi}{N}j(m'+b)} e^{i\frac{2\pi}{N}(m'+b)} \tilde{c}_m \tilde{c}_{m'} \tag{89a}$$

$$= \frac{1}{N} \sum_{m,m'=0}^{N-1} \sum_{j=1}^{N} e^{i\frac{2\pi}{N}j(m+m'+2b)} e^{i\frac{2\pi}{N}(m'+b)} \tilde{c}_m \tilde{c}_{m'} \tag{89b}$$

in order to simplify we are using

$$\sum_{j=1}^{N} e^{i\frac{2\pi}{N}j(m+m'+2b)} = N\delta_{m+m'+2b,N} \tag{90}$$

and one can reach the result

$$\sum_{j=1}^{N} c_j c_{j+1} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(N-m-b)} \tilde{c}_m \tilde{c}_{N-m-2b} \tag{91a}$$

$$= \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}(m+b)} \tilde{c}_m \tilde{c}_{N-m-2b} \tag{91b}$$

other terms can be derive in the same way. One can also use hermitian conjugate of the result. By keeping in mind $(AB)^\dagger = B^\dagger A^\dagger$

$$\sum_{j=1}^{N} (c_j c_{j+1})^\dagger = \sum_{m=0}^{N-1} (e^{-i\frac{2\pi}{N}(m+b)} \tilde{c}_m \tilde{c}_{N-m-2b})^\dagger \tag{92a}$$

$$\sum_{j=1}^{N} c_{j+1}^\dagger c_j^\dagger = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)} \tilde{c}_{N-m-2b}^\dagger \tilde{c}_m^\dagger \tag{92b}$$

$$\sum_{j=1}^{N} c_j^\dagger c_{j+1}^\dagger = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)} \tilde{c}_m^\dagger \tilde{c}_{N-m-2b}^\dagger \tag{92c}$$

last line is derived by using the fermionic commutation relation $\{c_m, c_n\} = 0$,

$$\tilde{c}_{N-m-2b}^\dagger \tilde{c}_m^\dagger = -\tilde{c}_m^\dagger \tilde{c}_{N-m-2b}^\dagger \tag{93a}$$

$$c_{j+1}^\dagger c_j^\dagger = -c_j^\dagger c_{j+1}^\dagger \tag{93b}$$

diagonal term in the hamiltonian can be derived as following

$$\sum_{j=1}^{N} c_j c_{j+1}^{\dagger} = \frac{1}{N}\sum_{j=1}^{N}\sum_{m,m'=0}^{N-1} e^{i\frac{2\pi}{N}j(m+b)}e^{-i\frac{2\pi}{N}j(m'+b)}e^{-i\frac{2\pi}{N}(m'+b)}\tilde{c}_m\tilde{c}_{m'}^{\dagger} \tag{94a}$$

$$= \frac{1}{N}\sum_{j=1}^{N}\sum_{m,m'=0}^{N-1} e^{i\frac{2\pi}{N}j(m-m')}e^{-i\frac{2\pi}{N}(m'+b)}\tilde{c}_m\tilde{c}_{m'}^{\dagger} \tag{94b}$$

$$= \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_m^{\dagger} \tag{94c}$$

taking the hermitian conjugate

$$\sum_{j=1}^{N}(c_j c_{j+1}^{\dagger})^{\dagger} = \sum_{m=0}^{N-1}(e^{-i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_m^{\dagger})^{\dagger} \tag{95a}$$

$$\sum_{j=1}^{N} c_{j+1}c_j^{\dagger} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_m^{\dagger} \tag{95b}$$

Using the fermionic commutation relation $\{c_m, c_n^{\dagger}\} = \delta_{m,n}$

$$\sum_{m=0}^{N-1}\tilde{c}_m\tilde{c}_m^{\dagger} = \sum_{m=0}^{N-1} 1 - \tilde{c}_m^{\dagger}\tilde{c}_m \tag{96}$$

$$\sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_m^{\dagger} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)} - e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m^{\dagger}\tilde{c}_m \tag{97}$$

Using the following series expansion

$$\sum_{m=0}^{N-1} ar^m = \frac{a\left(1-r^N\right)}{1-r} \tag{98}$$

$$\sum_{m=0}^{N-1} e^{imx} = \frac{1-e^{iNx}}{1-e^{ix}} \tag{99}$$

we can calculate

$$\sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)} = \frac{1-e^{N\left(i\frac{2\pi}{N}(m+b)\right)}}{1-e^{i\frac{2\pi}{N}(m+b)}} \tag{100a}$$

$$= \frac{1-e^{i2\pi(m+b)}}{1-e^{i\frac{2\pi}{N}(m+b)}} \tag{100b}$$

$$= \frac{1-1}{1-e^{i\frac{2\pi}{N}(m+b)}} = 0 \tag{100c}$$

the result is trivial but explain why we can switch the fermionic terms with negative sign.

$$\sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_m^\dagger = \sum_{m=0}^{N-1} -e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m^\dagger\tilde{c}_m \tag{101}$$

rewriting equation (95)

$$\sum_{j=1}^{N} c_{j+1}c_j^\dagger = -\sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m^\dagger\tilde{c}_m \tag{102a}$$

$$\sum_{j=1}^{N} c_j^\dagger c_{j+1} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}_m^\dagger\tilde{c}_m \tag{102b}$$

As can seen above calculations, one need to put attention to sign when reordering the terms

We shall generalize the Fourier Transform by assigning x and y integer constants which define the side interaction.

$$\sum_{j=1}^{N} c_{j+x}c_{j+y} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}\left[(x-y)(m+b)-yN\right]}\tilde{c}_m\tilde{c}_{N-m-2b} \tag{103}$$

in this context we can eliminate the term $e^{-i\frac{2\pi}{N}yN} = 1$. Then we have reached the general form of the fourier transformation for spin-1/2 chain models.

$$\sum_{j=1}^{N} c_{j+x}c_{j+y} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}\left[(x-y)(m+b)\right]}\tilde{c}_m\tilde{c}_{N-m-2b} \tag{104a}$$

$$\sum_{j=1}^{N} c^{\dagger}_{j+x}c^{\dagger}_{j+y} = \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}\left[(x-y)(m+b)\right]}\tilde{c}^{\dagger}_m\tilde{c}^{\dagger}_{N-m-2b} \tag{104b}$$

$$\sum_{j=1}^{N} c_{j+x}c^{\dagger}_{j+y} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}\left[(x-y)(m+b)\right]}\tilde{c}_m\tilde{c}^{\dagger}_m \tag{104c}$$

using fourier transformation in (104) we reach the followings

$$\sum_{j=1}^{N} c_j c_{j+1} = \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_{N-m-2b} \tag{105a}$$

$$\sum_{j=1}^{N} c_j c^{\dagger}_{j+1} = \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}^{\dagger}_m \tag{105b}$$

$$\sum_{j=1}^{N} c^{\dagger}_j c^{\dagger}_{j+1} = \sum_{m=0}^{N-1} e^{i\frac{2\pi}{N}(m+b)}\tilde{c}^{\dagger}_m\tilde{c}^{\dagger}_{N-m-2b} \tag{105c}$$

substituting these into equation (87) which we derived in the previous section

$$\begin{aligned} -H_{XY} = \sum_{m=0}^{N-1} & \left(e^{-i\frac{2\pi}{N}(m+b)} + e^{i\frac{2\pi}{N}(m+b)}\right)\tilde{c}^{\dagger}_m\tilde{c}_m \\ & + r\left(-e^{-i\frac{2\pi}{N}(m+b)}\tilde{c}_m\tilde{c}_{N-m-2b} + e^{i\frac{2\pi}{N}(m+b)}\tilde{c}^{\dagger}_m\tilde{c}^{\dagger}_{N-m-2b}\right) + Nh - 2h\tilde{c}^{\dagger}_m\tilde{c}_m \end{aligned} \tag{106}$$

Let us define $\Delta_m = \frac{2\pi}{N}(m+b)$. Using symmetry equations below and hyperbolic functions $e^{ix} + e^{-ix} = 2\cos x$ and $e^{ix} - e^{-ix} = 2\ i\sin x$.

$$\sum_m (2\cos\Delta_m)\, c_m^\dagger c_m = \frac{1}{2}\sum_m \left[2\cos\Delta_m c_m^\dagger c_m + 2\cos(-\Delta_m)\, c_{-m}^\dagger c_{-m}\right] \tag{107a}$$

$$\sum_{m=0}^{N-1} e^{-i\Delta_m}\tilde{c}_m\tilde{c}_{-m} = \frac{1}{2}\sum_{m=0}^{N-1}\left(e^{-i\Delta_m} - e^{i\Delta_m}\right)\tilde{c}_m\tilde{c}_{-m} \tag{107b}$$

$$= -i\sin\Delta_m\tilde{c}_m\tilde{c}_{-m} \tag{107c}$$

substituting these terms into equation (106) one can reach following form of the Hamiltonian

$$\begin{aligned} H_{XY} = -Nh - \sum_{m=0}^{N-1}\left[2\cos\left(\frac{2\pi}{N}(m+b)\right) - 2h\right]\tilde{c}_m^\dagger\tilde{c}_m \\ + ir\sin\left(\frac{2\pi}{N}(m+b)\right)\left(\tilde{c}_m\tilde{c}_{N-m-2b} + \tilde{c}_m^\dagger\tilde{c}_{N-m-2b}^\dagger\right) \end{aligned} \tag{108}$$

2.2.3 Bogoliubov Transformation

There are still non-diagonal terms $(\tilde{c}_m\tilde{c}_{N-m-2b} + \tilde{c}_m^\dagger\tilde{c}_{N-m-2b}^\dagger)$ in the hamiltonian. Bogoliubov transformation is a unitary transformation to mix these operators as holding CCR $\{y_i, y_j^\dagger\} = \delta_{ij}$. With the help of this transformation one can diagonalize the Hamiltonian by eliminating non-diagonal terms. Only for this section we use $\alpha = N - m - 2b$ and drop b terms for simplicity.

$$\begin{aligned} H = -Nh + \sum_{m=0}^{N-1}\tilde{c}_m^\dagger\tilde{c}_m\left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] + \tilde{c}_\alpha^\dagger\tilde{c}_\alpha\left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] \\ - ir\sin\left(\frac{2\pi}{N}(m+b)\right)\left[\tilde{c}_m\tilde{c}_\alpha + \tilde{c}_m^\dagger\tilde{c}_\alpha^\dagger\right] \end{aligned} \tag{109}$$

We define Bogoliubov angle θ_m and Bogoliubov fermions or quasiparticles γ_m

$$\tilde{c}_m = \cos\theta_m \gamma_m + i \sin\theta_m \gamma_\alpha^\dagger \tag{110a}$$
$$\tilde{c}_m^\dagger = \cos\theta_m \; \gamma_m^\dagger - i \sin\theta_m \; \gamma_\alpha \tag{110b}$$
$$\tilde{c}_\alpha = \cos\theta_\alpha \; \gamma_\alpha + i \sin\theta_\alpha \; \gamma_m^\dagger \tag{110c}$$
$$\tilde{c}_\alpha^\dagger = \cos\theta_\alpha \; \gamma_\alpha^\dagger - i \sin\theta_\alpha \; \gamma_m \tag{110d}$$

where fermionic canonical commutation relations (CCR)

$$\{\gamma_m, \gamma_m^\dagger\} = \gamma_m \gamma_m^\dagger + \gamma_m^\dagger \gamma_m = 1 \tag{111}$$
$$\{\gamma_m, \gamma_\alpha\} = \{\gamma_m^\dagger, \gamma_\alpha^\dagger\} = 0 \tag{112}$$

Let us keep in mind the trigonometric relations

$$\begin{aligned}
\theta_m &= -\theta_\alpha \\
\cos\theta_m &= \cos\theta_\alpha \\
\sin\theta_m &= -\sin\theta_\alpha \\
\sin(\theta_\alpha - \theta_m) &= \cos\theta_m \sin\theta_\alpha - \sin\theta_m \cos\theta_\alpha \\
\cos(\theta_m - \theta_\alpha) &= \cos\theta_m \cos\theta_\alpha + \sin\theta_m \sin\theta_\alpha \\
cos2\theta_m &= cos^2\theta_m - sin^2\theta_m \\
sin2\theta_m &= 2\sin\theta_m \cos\theta_m
\end{aligned}$$

Multiplying terms by keeping the order

$$\begin{aligned}
\tilde{c}_m \tilde{c}_\alpha = {} & \cos\theta_m \cos\theta_\alpha \; \gamma_m \; \gamma_\alpha + i \cos\theta_m \sin\theta_\alpha \; \gamma_m \; \gamma_m^\dagger \\
& + i \sin\theta_m \cos\theta_\alpha \; \gamma_\alpha^\dagger \gamma_\alpha \; - \sin\theta_m \sin\theta_\alpha \; \gamma_\alpha^\dagger \; \gamma_m^\dagger
\end{aligned} \tag{114a}$$

$$\begin{aligned}
\tilde{c}_m^\dagger \tilde{c}_\alpha^\dagger = {} & \cos\theta_m \cos\theta_\alpha \; \gamma_m^\dagger \; \gamma_\alpha^\dagger - i \sin\theta_\alpha \cos\theta_m \; \gamma_m^\dagger \; \gamma_m \\
& - i \sin\theta_m \cos\theta_\alpha \; \gamma_\alpha \; \gamma_\alpha^\dagger - \sin\theta_m \sin\theta_\alpha \; \gamma_\alpha \; \gamma_m
\end{aligned} \tag{114b}$$

$$\tilde{c}_\alpha^\dagger \tilde{c}_\alpha = cos^2\theta_\alpha \ \gamma_\alpha^\dagger \ \gamma_\alpha + i\cos\theta_\alpha \sin\theta_\alpha \ \gamma_\alpha^\dagger \ \gamma_m^\dagger - i\cos\theta_\alpha \sin\theta_\alpha \ \gamma_m \ \gamma_\alpha + \sin^2\theta_\alpha \ \gamma_m \ \gamma_m^\dagger \tag{114c}$$

$$\begin{aligned}\tilde{c}_m^\dagger \tilde{c}_m = {} & cos^2\theta_m \ \ \gamma_m^\dagger \ \ \gamma_m + i\sin\theta_m \cos\theta_m \ \ \gamma_m^\dagger \ \ \gamma_\alpha^\dagger \\ & - i\sin\theta_m \cos\theta_m \ \ \gamma_\alpha \ \ \gamma_m + \sin^2\theta_m \ \ \gamma_\alpha \ \ \gamma_\alpha^\dagger\end{aligned} \tag{114d}$$

Adding non-diagonal terms

$$\begin{aligned}\tilde{c}_m \tilde{c}_\alpha + \tilde{c}_m^\dagger \tilde{c}_\alpha^\dagger = {} & \gamma_m \gamma_\alpha \left[\cos\theta_m \cos\theta_\alpha + \sin\theta_m \sin\theta_\alpha\right] \\ & + \gamma_m^\dagger \gamma_m \left[-i\left(\cos\theta_m \sin\theta_\alpha + \sin\theta_\alpha \cos\theta_m\right)\right] \\ & + \gamma_\alpha^\dagger \gamma_\alpha \left[i\left(\sin\theta_m \cos\theta_\alpha + \sin\theta_m \cos\theta_\alpha\right)\right] \\ & + \gamma_m^\dagger \gamma_\alpha^\dagger \left[\sin\theta_m \sin\theta_\alpha + \cos\theta_m \cos\theta_\alpha\right] \\ & + i\left[\cos\theta_m \sin\theta_\alpha - \sin\theta_m \cos\theta_\alpha\right]\end{aligned} \tag{115a}$$

and simplifying

$$\begin{aligned}\tilde{c}_m \tilde{c}_\alpha + \tilde{c}_m^\dagger \tilde{c}_\alpha^\dagger = {} & \left(\gamma_m \gamma_\alpha + \gamma_m^\dagger \gamma_\alpha^\dagger\right) cos(\theta_m - \theta_\alpha) + \gamma_m^\dagger \gamma_m \left(-2 \ i\cos\theta_m \sin\theta_\alpha\right) \\ & + \gamma_\alpha^\dagger \gamma_\alpha \left(2 \ \ i\sin\theta_m \cos\theta_\alpha\right) + isin\left(\theta_\alpha - \theta_m\right)\end{aligned} \tag{115b}$$

Writing Hamiltonian upon using Bogoliubov angle

$$
\begin{aligned}
H = -Nh + \sum_{m=0}^{N-1} \gamma_m^\dagger \gamma_m & \left[-\cos\left(\frac{2\pi}{N}(m+b)\right) cos^2\theta_m + hcos^2\theta_m \right. \\
& \left. + \cos\left(\frac{2\pi}{N}(m+b)\right) sin^2\theta_\alpha - hsin^2\theta_\alpha - 2r\sin\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_\alpha\cos\theta_m \right] \\
& + \gamma_\alpha^\dagger \gamma_\alpha \left[\cos\left(\frac{2\pi}{N}(m+b)\right) sin^2\theta_m - hsin^2\theta_m - \cos\left(\frac{2\pi}{N}(m+b)\right) cos^2\theta_\alpha \right. \\
& \left. + hcos^2\theta_\alpha + 2r\sin\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_m\cos\theta_\alpha \right] \\
& + \gamma_m \gamma_\alpha \left[-i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_m\cos\theta_m + ih\sin\theta_m\cos\theta_m \right. \\
& + i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_\alpha\cos\theta_\alpha - i\ h\cos\theta_\alpha\sin\theta_\alpha \\
& \left. - ir\sin\left(\frac{2\pi}{N}(m+b)\right) cos(\theta_m - \theta_\alpha) \right] \\
& + \gamma_m^\dagger \gamma_\alpha^\dagger \left[-i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_m\cos\theta_m + ih\sin\theta_m\cos\theta_m \right. \\
& + i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_\alpha\cos\theta_\alpha - i\ h\cos\theta_\alpha\sin\theta_\alpha \\
& \left. - i\ r\sin\left(\frac{2\pi}{N}(m+b)\right) cos(\theta_m - \theta_\alpha) \right] \\
& + hsin^2\theta_\alpha + hsin^2\theta_m - \cos\left(\frac{2\pi}{N}(m+b)\right) sin^2\theta_\alpha \\
& - \cos\left(\frac{2\pi}{N}(m+b)\right) sin^2\theta_m + r\sin\left(\frac{2\pi}{N}(m+b)\right) sin(\theta_\alpha - \theta_m)
\end{aligned}
\tag{116}
$$

using the fact that $\theta_m = -\theta_\alpha$

$$
\begin{aligned}
H = -Nh + \sum_{m=0}^{N-1} \left(\gamma_m^\dagger \gamma_m + \gamma_\alpha^\dagger \gamma_\alpha\right) \Bigg[&-\cos\left(\frac{2\pi}{N}(m+b)\right)\left(cos^2\theta_m - sin^2\theta_m\right) \\
&+ h\left(cos^2\theta_m - sin^2\theta_m\right) + r\sin\left(\frac{2\pi}{N}(m+b)\right)\sin 2\theta_m \Bigg] \\
+ \left(\gamma_m\gamma_\alpha + \gamma_m^\dagger\gamma_\alpha^\dagger\right) \Bigg[&-i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_m\cos\theta_m + ih\sin\theta_m\cos\theta_m \\
&- i\cos\left(\frac{2\pi}{N}(m+b)\right)\sin\theta_m\cos\theta_m + i\ h\cos\theta_m\sin\theta_m \\
&- i\ r\sin\left(\frac{2\pi}{N}(m+b)\right) cos2\theta_m \Bigg] \\
+ sin^2\theta_m \left[2h - 2\cos\left(\frac{2\pi}{N}(m+b)\right)\right] &- r\sin\left(\frac{2\pi}{N}(m+b)\right) sin2\theta_m
\end{aligned} \tag{117}
$$

lets define c as a constant

$$
c = sin^2\theta_m \left[2h - 2\cos\left(\frac{2\pi}{N}(m+b)\right)\right] - r\sin\left(\frac{2\pi}{N}(m+b)\right) sin2\theta_m \tag{118}
$$

cross terms should be equal to zero

$$
\begin{aligned}
&\left(\gamma_m\gamma_\alpha + \gamma_m^\dagger\gamma_\alpha^\dagger\right)\Bigg\{ isin2\theta_m \left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] \\
&\quad - i\ \ r\sin\left(\frac{2\pi}{N}(m+b)\right)\cos 2\theta_m \Bigg\} = 0
\end{aligned} \tag{119a}
$$

$$
sin2\theta_m \left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] = r\sin\left(\frac{2\pi}{N}(m+b)\right) cos2\theta_m \tag{119b}
$$

After calculations we reach the solution for Bogoliubov angle

$$\tan 2\theta_m = \frac{r \sin\left(\frac{2\pi}{N}(m+b)\right)}{h - \cos\left(\frac{2\pi}{N}(m+b)\right)} \tag{120a}$$

$$\sin 2\theta_m = \frac{r \sin\left(\frac{2\pi}{N}(m+b)\right)}{\sqrt{\left(r \sin\left(\frac{2\pi}{N}(m+b)\right)\right)^2 + \left(h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right)^2}} \tag{120b}$$

$$\cos 2\theta_m = \frac{h - \cos\left(\frac{2\pi}{N}(m+b)\right)}{\sqrt{\left(r \sin\left(\frac{2\pi}{N}(m+b)\right)\right)^2 + \left(h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right)^2}} \tag{120c}$$

$$\cos\theta_m = \sqrt{\frac{1+\cos 2\theta_m}{2}} \tag{120d}$$

$$\sin\theta_m = \sqrt{\frac{1-\cos 2\theta_m}{2}} \tag{120e}$$

we have used trigonometric identity in the last line $cos2\theta_m = 1 - 2sin^2\theta_m$ we simplify the diagonal part of the Hamiltonian

$$\begin{aligned} H = -Nh + \sum_{m=0}^{N-1} \left(\gamma_m^\dagger \gamma_m + \gamma_\alpha^\dagger \gamma_\alpha\right) \Bigg\{ cos2\theta_m \left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] \\ + r \sin\left(\frac{2\pi}{N}(m+b)\right) sin2\theta_m \Bigg\} + c \ (constant) \end{aligned} \tag{121}$$

using symmetry

$$\sum_{m=0}^{N-1} 2\ \gamma_m^\dagger \gamma_m = \gamma_m^\dagger \gamma_m + \gamma_\alpha^\dagger \gamma_\alpha \tag{122}$$

We derived diagonalized Hamiltonian

$$H = -Nh + \sum_{m=0}^{N-1} 2\ \gamma_m^\dagger \gamma_m \left\{ cos2\theta_m \left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right] \right. \\ \left. + r \sin\left(\frac{2\pi}{N}(m+b)\right) sin2\theta_m \right\} + c\ (constant) \tag{123}$$

$$c = sin^2\theta_m \left[2h - 2\cos\left(\frac{2\pi}{N}(m+b)\right)\right] - r\sin\left(\frac{2\pi}{N}(m+b)\right) sin2\theta_m \tag{124}$$

and expanding terms and substituting Bogoliubov angle (120)

$$c = h - cos\left(\frac{2\pi}{N}(m+b)\right) - \frac{\epsilon_m}{2} \tag{125}$$

where ϵ_m is the eigenvalue of the Hamiltonian

$$\epsilon_m = 2\sqrt{\left(r\sin\left(\frac{2\pi}{N}(m+b)\right)\right)^2 + \left(h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right)^2} \tag{126}$$

we collect all terms

$$H = -Nh + \sum_{m=0}^{N-1} \left\{ \epsilon_m \left(\gamma_m^\dagger \gamma_m - \frac{1}{2}\right) + \left[h - \cos\left(\frac{2\pi}{N}(m+b)\right)\right]\right\} \tag{127}$$

Last term and first term (Nh) cancels out. Thus, one arrives the diagonalized expression where $b = 0$, odd-number fermion (periodic) and $b = 1/2$ even-number fermion(antiperiodic)

$$H = \sum_{m=0}^{N-1} \epsilon_m^{(b)} \left(\gamma_m^{(b)\dagger}\gamma_m^{(b)} - \frac{1}{2}\right) \tag{128}$$

For correct energy spectrum one should consider odd and even number of fermion case separately. For the periodic boundary condition (odd-number-fermion $b = 0$)

$$E_m^{(0)}(r,h) = \epsilon_0^{(0)}\left(\langle\gamma_0^{(0)\dagger}\gamma_0^{(0)}\rangle - \frac{1}{2}\right) + \sum_{m=1}^{N-1}\epsilon_m^{(0)}\left(\langle\gamma_m^{(0)\dagger}\gamma_m^{(0)}\rangle - \frac{1}{2}\right) \tag{129}$$

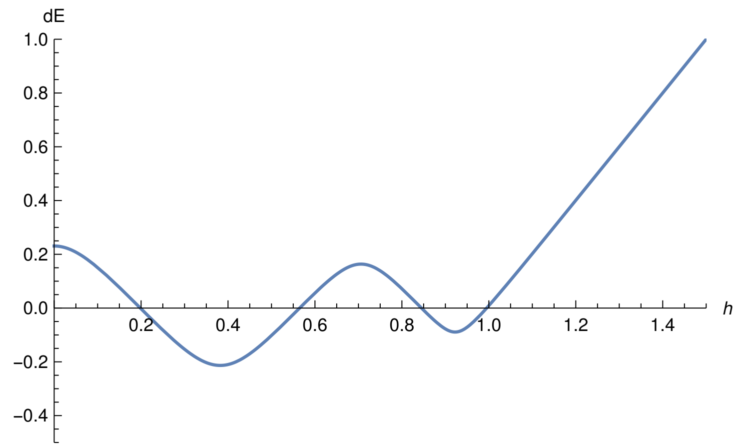

Figure 2: dE shows energy differences between two lowest state vs transverse magnetic field h where anisotropy $r = 0.1$ and total number of spin $N = 8$

and lowest state is $\langle \gamma_m^{(0)\dagger} \gamma_m^{(0)} \rangle = 0$ except $\langle \gamma_0^{(0)\dagger} \gamma_0^{(0)} \rangle = 1$ and $\epsilon_0^{(0)} = 2(h-1)$ Thus we obtain ground state energy where momentum index starts from $m = 1$

$$E_m^{(0)}(r,h) = (h-1) - \sum_{m=1}^{N-1} \sqrt{\left(r \sin\left(\frac{2\pi m}{N}\right)\right)^2 + \left(h - \cos\left(\frac{2\pi m}{N}\right)\right)^2} \tag{130}$$

For the antiperiodic boundary condition (even-number-fermion $b = 1/2$) $\langle \gamma_m^{(1/2)\dagger} \gamma_m^{(1/2)} \rangle = 0$ Therefore, ground state energy for even-fermion case

$$E_m^{(1/2)}(r,h) = -\sum_{m=1}^{N-1} \sqrt{\left(r \sin\left(\frac{2\pi}{N}(m+\frac{1}{2})\right)\right)^2 + \left(h - \cos\left(\frac{2\pi}{N}(m+\frac{1}{2})\right)\right)^2} \tag{131}$$

As can be concluded above calculations, there is a ground energy competition in this model. The ground state is switching between these two solutions when $h \leq 1$. As the energy gap vanishes, we expect an emergence of *quantum phase transition* and *spontaneous symmetry breaking*. As we consider thermodynamic limits $N \to \infty$ and $h > 1$ one can find energy difference between two lowest state becomes

$$dE = E_0^{(0)}(r,h) - E_0^{(1/2)}(r,h) = 2(h-1) \tag{132}$$

In the limit $h > 1$ degeneracy is lifted and dominated by $b = 1/2$ even-number-fermion case. We will be investigating Quantum Phase Transition by using Geometric Entanglement in the following sections.

2.2.4 Derivation of Ground State

Before starting derivation of Geometric Entanglement, we firstly give a quick derivation of the ground state of the model. Bogoliubov solution defined in the previous section (110) where $\theta_m = -\theta_{N-m-2b}$

$$\tilde{c}_m^{(b)} = \cos\theta_m^{(b)}\ \gamma_m^{(b)} + i\sin\theta_m^{(b)}\gamma_{N-m-2b}^{(b)\dagger} \tag{133a}$$
$$\tilde{c}_m^{b\dagger} = \cos\theta_m^{(b)}\ \gamma_m^{(b)\dagger} - i\sin\theta_m^{(b)}\ \gamma_{N-m-2b}^{(b)} \tag{133b}$$
$$\tilde{c}_{N-m-2b}^{(b)} = \cos\theta_m^{(b)}\ \gamma_{N-m-2b}^{(b)} - i\sin\theta_m^{(b)}\ \gamma_m^{(b)\dagger} \tag{133c}$$
$$\tilde{c}_{N-m-2b}^{(b)\dagger} = \cos\theta_m^{(b)}\ \gamma_{N-m-2b}^{(b)\dagger} + i\sin\theta_m^{(b)}\ \gamma_m^{(b)} \tag{133d}$$

Solving for γ_m and γ_{N-m-2b} terms

$$\gamma_m^{(b)} = c_m^{(b)}\cos\theta_m^{(b)} - i\sin\theta_m^{(b)}\ c_{N-m-2b}^{(b)\dagger} \tag{134a}$$
$$\gamma_{N-m-2b}^{(b)} = c_{N-m-2b}^{(b)}\cos\theta_m^{(b)} + i\sin\theta_m^{(b)}\ c_m^{(b)\dagger} \tag{134b}$$

The lowest state $\Psi_{1/2}(r,h)$ with even fermion case $b = 1/2$ has no Bogoliubov fermion in the ground state.

$$\gamma_m^{(1/2)}\left|\Psi_{1/2}\right\rangle_\gamma^m = \gamma_{N-m-1}^{(1/2)}\left|\Psi_{1/2}\right\rangle_\gamma^m = 0 \tag{135a}$$

$$c_m^{(1/2)}\left|\Omega\right\rangle = c_{N-m-1}^{(1/2)}\left|\Omega\right\rangle = 0 \tag{135b}$$

It can be written as linear combinations of fermionic vacuum states $|\Omega\rangle$ and a, b, c, d are constants.

$$|\Psi_{1/2}\rangle_{\gamma}^{m} = a\,|\Omega\rangle + b\; c_m^{\dagger}\,|\Omega\rangle + c\; c_{N-m-2b}^{\dagger}\,|\Omega\rangle + d\; c_m^{\dagger}\; c_{N-m-2b}^{\dagger}\,|\Omega\rangle \tag{136}$$

Let's recall commutation relations of fermions

$$\{c_i, c_j^{\dagger}\} = \delta_{ij} \tag{137}$$

$$c_i^2 = (c_i^{\dagger})^2 = 0 \tag{138}$$

it can be easily shown

$$c_{N-m-2b}\; c_m^{\dagger}\; c_{N-m-2b}^{\dagger} = -c_m^{\dagger} + (c_m^{\dagger}\; c_{N-m-2b}^{\dagger}\; c_{N-m-2b}) \tag{139a}$$

$$c_m\; c_m^{\dagger}\; c_{N-m-2b}^{\dagger} = c_{N-m-2b}^{\dagger} + (c_m^{\dagger}\; c_{N-m-2b}^{\dagger}\; c_m) \tag{139b}$$

collecting all terms together

$$\begin{aligned}
&\gamma_m^{(1/2)}\,|\Psi_{1/2}\rangle_{\gamma}^{m} = \Big(a\cos\theta_m c_m\,|\Omega\rangle - i\;\, a\sin\theta_m c_{N-m-2b}^{\dagger}\,|\Omega\rangle\Big) \\
&+ \Big(b\cos\theta_m c_m\;\; c_m^{\dagger}\,|\Omega\rangle - i\;\, b\sin\theta_m c_{N-m-2b}^{\dagger}\;\; c_m^{\dagger}\,|\Omega\rangle\Big) \\
&+ \Big(c\cos\theta_m c_m\;\; c_{N-m-2b}^{\dagger}\,|\Omega\rangle - i\;\, c\sin\theta_m (c_{N-m-2b}^{\dagger})^2\,|\Omega\rangle\Big) \\
&+ \Big(d\cos\theta_m\; c_m\; c_m^{\dagger}\; c_{N-m-2b}^{\dagger}\,|\Omega\rangle - i\;\, d\sin\theta_m\; c_{N-m-2b}^{\dagger}\; c_m^{\dagger}\; c_{N-m-2b}^{\dagger}\,|\Omega\rangle\Big) = 0
\end{aligned} \tag{140}$$

Solving equation for each fermion operator we find $b = c = 0$ and;

$$\Big[(-i\;\, a\sin\theta_m + d\cos\theta_m)\; c_{N-m-2b}^{\dagger}\Big]\,|\Omega\rangle = 0 \tag{141a}$$

$$\frac{d}{a} = i\;\, tan\theta_m \tag{141b}$$

Substituting constants into equation (136) where $d = i\sin\theta_m$ and $a = \cos\theta_m$ we get the ground state for antiperiodic boundary even-fermion case where vacuum state $|\Omega\rangle$

$$|\Psi_{1/2}\rangle = \prod_{m=0}^{m<\frac{N-1}{2}} \left(\cos\theta_m + i\sin\theta_m \; c_m^\dagger \; c_{N-m-1}^\dagger\right)|\Omega\rangle \tag{142a}$$

$$|\Psi_{1/2}\rangle = \prod_{m=0}^{m<\frac{N-1}{2}} \cos\theta_m \; e^{i \; tan\theta_m \; c_m^\dagger \; c_{N-m-1}^\dagger}|\Omega\rangle \tag{142b}$$

For the periodic conditions (odd-fermions) the lowest state is $\gamma_0^{(0)} = c_0^{(0)}$ fermion where there is no Bogoliubov fermions in the state $|\Phi\rangle$

$$|\Psi_0\rangle \equiv \gamma_0^{(0)\dagger}|\Phi\rangle = \tilde{c}^{(0)\dagger}|\Phi\rangle \tag{143}$$

repeating same calculations we reach the ground state for odd-fermion case.

$$|\Psi_0\rangle = \prod_{m=0}^{m<\frac{N}{2}} \left(\cos\theta_m + i\sin\theta_m \; c_m^\dagger \; c_{N-m}^\dagger\right)|\Omega\rangle \tag{144a}$$

$$|\Psi_0\rangle = \prod_{m=0}^{m<\frac{N}{2}} \cos\theta_m \; e^{i \; tan\theta_m \; c_m^\dagger \; c_{N-m}^\dagger}|\Omega\rangle \tag{144b}$$

For simplicity, after this point we will consider only $b = 1/2$ even-fermion case.

2.2.5 Geometric Entanglement

Geometric Entanglement is a method for quantifying entanglement in the multipartite system [70]. The derivative of the entanglement present sudden changes near the critical point in the spin chain problems. We have given the development of the method in the section (1.1) In this part, we will derive the overlap of the ground state and general product state per site and per block.

2.2.5.a) Geometric Entanglement per site

Product of single spin state $|\Phi_1\rangle = (a|\uparrow\rangle + b|\downarrow\rangle)^{\otimes N}$ can be written in fermionic language by applying the Jordan-Wigner transformation we derived in section (2.2.1)

$$|\Phi_1\rangle = \otimes_{i=1}^{N} \left(a + b\sigma_i^-\right)|\uparrow\uparrow\ldots\uparrow\rangle \tag{145}$$

$$= \prod_{i=1}^{N}\left[a + b\prod_{j=1}^{i-1}(1-2c_j^\dagger c_j)c_i^\dagger\right]|\Omega\rangle \tag{146}$$

$|\Omega\rangle$ is the vacuum with no c fermions. Using CCR and $c_i|\Omega\rangle = 0$

$$|\Phi_1\rangle = \prod_{i=1}^{N}\left(a + b\ c_i^\dagger\right)|\Omega\rangle = a^N\prod_{i=1}^{N}e^{b'c_i^\dagger}|\Omega\rangle \tag{147}$$

$$= a^N e^{\sum_{i=1}^{N} b'c_i^\dagger} e^{\sum_{i<j}(b')^2 c_i^\dagger c_j^\dagger} \tag{148}$$

where we have defined $b' = b/a$ and use BCH formula for $A^2 = B^2 = 0$ and $\{A,B\} = 0$ and $e^A e^B = e^{A+B}e^{[A,B]/2} = e^{A+B}e^{AB}$ for reaching the last line

$$\prod_{i=1}^{N}e^{b'c_i^\dagger} = e^{\sum_{i=1}^{N} b'c_i^\dagger} e^{\sum_{i<j}(b')^2 c_i^\dagger c_j^\dagger} \tag{149}$$

for even fermion case (b=1/2), by using Fourier transform

$$\sum_{j\le l} c_j^\dagger c_l^\dagger = \frac{1}{N}\sum l = 1^N \sum_{j=1}^{l}\sum_{m,m'=0}^{N-1} e^{-i\frac{2\pi}{N}j(m'+\frac{1}{2})-i\frac{2\pi}{N}l(m'+\frac{1}{2}}) \tilde{c}_m^\dagger \tilde{c}_{m'}^\dagger \tag{150a}$$

$$= \frac{1}{N}\sum_{m,m'=0}^{N-1}\sum l = 1^N \sum_{j=1}^{l} e^{-i\frac{2\pi}{N}(m+\frac{1}{2})}\frac{1-e^{-i\frac{2\pi}{N}l(m+\frac{1}{2})}}{1-e^{-i\frac{2\pi}{N}(m+\frac{1}{2})}}e^{-i\frac{2\pi}{N}l(m'+\frac{1}{2})}\tilde{c}_m^\dagger \tilde{c}_{m'}^\dagger \tag{150b}$$

noting that

$$\sum_{l=1}^{N} e^{-i\frac{2\pi}{N}l(m'+\frac{1}{2})} = e^{-i\frac{2\pi}{N}(m'+\frac{1}{2})}\frac{1-e^{-i\frac{2\pi}{N}N(m'+\frac{1}{2})}}{1-e^{-i\frac{2\pi}{N}(m'+\frac{1}{2})}} \tag{151a}$$

$$= \frac{2e^{-i\frac{2\pi}{N}(m'+\frac{1}{2})}}{1-e^{-i\frac{2\pi}{N}(m'+\frac{1}{2})}} = \frac{e^{-i\frac{\pi}{N}(m'+\frac{1}{2})}}{isin\frac{\pi}{N}(m'+\frac{1}{2})} \tag{151b}$$

$$\sum_{l=1}^{N} e^{-i\frac{2\pi}{N}l(m+m'+1)} = N\delta_{m+m'+1,N} \tag{151c}$$

we find

$$\begin{aligned}\sum_{j\le l} c_j^\dagger c_l^\dagger = \frac{1}{N}\sum_{m,m'=0}^{N-1} \frac{e^{-i\frac{\pi}{N}(m+\frac{1}{2})}}{isin\frac{\pi}{N}(m+\frac{1}{2})}\frac{e^{-i\frac{\pi}{N}(m'+\frac{1}{2})}}{isin\frac{\pi}{N}(m'+\frac{1}{2})}\tilde{c}_m^\dagger\tilde{c}_{m'}^\dagger \\ -\sum_{m=0}^{N-1}\frac{e^{-i\frac{\pi}{N}(m+\frac{1}{2})}}{isin\frac{\pi}{N}(m+\frac{1}{2})}\tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger\end{aligned} \tag{152}$$

the first term vanishes since m and m' are symmetric. expanding second term

$$\sum_{j\le l} c_j^\dagger c_l^\dagger = -\frac{1}{2}\sum_{m=0}^{N-1}\left[\frac{e^{-i\frac{\pi}{N}(m+\frac{1}{2})}}{isin\frac{\pi}{N}(m+\frac{1}{2})} - \frac{e^{-i\frac{\pi}{N}(N-m-\frac{1}{2})}}{isin\frac{\pi}{N}(N-m-\frac{1}{2})}\right]\tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger \tag{153}$$

$$= \sum_{m=0}^{N-1} i\cot\frac{\pi(m+\frac{1}{2})}{N}\tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger \tag{154}$$

and collection all terms in the initial product state

$$|\Phi_1\rangle = a^N e^{\sum_{i=1}^{N} b'c_i^\dagger} e^{(b')^2\sum_{m=0}^{N-1} i\cot\frac{\pi(m+\frac{1}{2})}{N}\ \tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger}|\Omega\rangle \tag{155}$$

Simplifying $c_i^2 = 0$ and $(\sum_{i=1}^{N} b'c_i^\dagger)^2 = 0$ and using exponential expansion

$$e^{\sum_{i=1}^{N} b'c_i^\dagger} = 1 + \sum_{i=1}^{N} b'c_i^\dagger \tag{156}$$

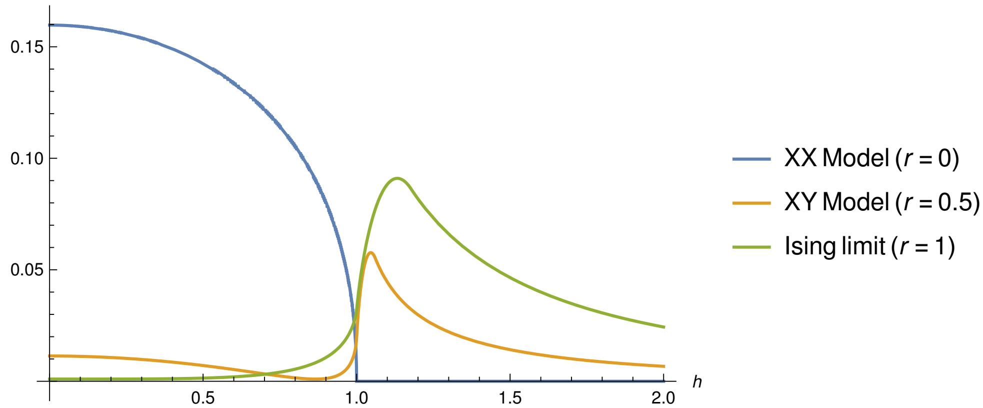

Figure 3: XY model global entanglement per site vs transverse magnetic field (h) in the thermodynamic limit where $N = 1000$

and choosing a and b normalizable constants where ξ is arbitrary term

$$a = cos\ \frac{\xi}{2} \tag{157a}$$

$$b = sin\ \frac{\xi}{2} \tag{157b}$$

we reach the general product state which is written in the same form as the ground state with respect to $\tilde{c}$ fermions in the momentum space for even N

$$|\Phi_1(\xi)\rangle = \left(1 + \tan\frac{\xi}{2}\sum_{i=1}^{N} c_i^\dagger\right)\prod_{m=0}^{m<\frac{N-1}{2}}\left(cos^2\ \frac{\xi}{2} + i\sin^2\ \frac{\xi}{2}\cot\frac{\pi(m+\frac{1}{2})}{N}\ \tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger\right) \tag{158}$$

let us remember the ground state we derived in equation (142)

$$|\Psi_{1/2}\rangle = \prod_{m=0}^{m<\frac{N-1}{2}}\left[\cos\theta_m + i\sin\theta_m\tilde{c}_m^\dagger\tilde{c}_{N-m-1}^\dagger\right]|\Omega\rangle \tag{159}$$

and we arrive the overlap for even N

$$\langle\Psi_{1/2}|\Phi(\xi)\rangle = \prod_{m=0}^{m<\frac{N-1}{2}} \left(\cos\theta_m \cos^2\frac{\xi}{2} + \sin\theta_m \sin^2\frac{\xi}{2} \cot\frac{\pi(m+\frac{1}{2})}{N}\right) \tag{160}$$

recalling the geometric entanglement

$$\Lambda_{max}(\Psi) \equiv \max_{\Phi} \langle\Phi|\Psi\rangle \tag{161a}$$

$$E_{log_2}(\Psi) \equiv -log_2\ \Lambda^2_{max}(\Psi) \tag{161b}$$

Entanglement density can be defined as following for even number of N particle

$$\mathcal{E} \equiv \frac{E_{log_2}(\Psi)}{N} \tag{162}$$

2.2.5.b) Geometric Entanglement per block

One can also consider block entanglement in the multipartite systems. In this section we will derive geometric entanglement per block which consist $L = 2$. We begin with writing product state

$$|\phi^{[2i-1,2i]}\rangle = a\,|\uparrow\rangle_{2i-1} \otimes |\uparrow\rangle_{2i} + b\,|\uparrow\rangle_{2i-1} \otimes |\downarrow\rangle_{2i} + c\,|\downarrow\rangle_{2i-1} \otimes |\uparrow\rangle_{2i} + d\,|\downarrow\rangle_{2i-1} \otimes |\downarrow\rangle_{2i} \tag{163a}$$

$$= \left(a + \mathbb{1} \otimes \mathbb{1} + b\mathbb{1} \otimes \sigma^- + c\sigma^- \otimes \mathbb{1} + d\sigma^- \otimes \sigma^-\right) |\uparrow\rangle_{2i-1} \otimes |\uparrow\rangle_{2i} \tag{163b}$$

mapping to fermionic picture by Jordan Wigner transformation

$$a + b\sigma^-_{2i} + c\sigma^-_{2i-1} + d\sigma^-_{2i-1} \otimes \sigma^-_{2i} \tag{164}$$

$$= a + b\prod_{j=1}^{2i-1}(1 - 2c^\dagger_j c_j)c^\dagger_{2i} + c\prod_{j=1}^{2i-2}(1 - 2c^\dagger_j c_j)c^\dagger_{2i-1} + dc^\dagger_{2i-1}(1 - 2c^\dagger_{2i-1}c_{2i-1})c^\dagger_{2i} \tag{165}$$

Total product state becomes where $|\Omega\rangle$ is vacuum state with no c fermions and N is even

$$|\Phi\rangle = \prod_{i=1}^{N/2} \left[a + b \prod_{j=1}^{2i-1} (1 - 2c_j^\dagger c_j) c_{2i}^\dagger + c \prod_{j=1}^{2i-2} (1 - 2c_j^\dagger c_j) c_{2i-1}^\dagger + d c_{2i-1}^\dagger c_{2i}^\dagger \right] |\Omega\rangle \tag{166}$$

using the fact that $c\,|\omega\rangle = 0$ and defining $b' = b/a$

$$\begin{aligned}
|\Phi\rangle &= \prod_{i=1}^{N/2} \left[a + b c_{2i}^\dagger + c c_{2i-1}^\dagger + d c_{2i-1}^\dagger c_{2i}^\dagger \right] |\Omega\rangle \\
&= a^{N/2} \prod_{i=1}^{N/2} \left[1 + b' c_{2i}^\dagger + c' c_{2i-1}^\dagger + d' c_{2i-1}^\dagger c_{2i}^\dagger \right] |\Omega\rangle \\
&= a^{N/2} \prod_{i=1}^{N/2} e^{[b' c_{2i}^\dagger + c' c_{2i-1}^\dagger + d' c_{2i-1}^\dagger c_{2i}^\dagger]} |\Omega\rangle \\
&= a^{N/2} \left[\prod_{i=1}^{N/2} e^{[b' c_{2i}^\dagger + c' c_{2i-1}^\dagger} \right] \left[\prod_{i=1}^{N/2} e^{d' c_{2i-1}^\dagger c_{2i}^\dagger]} \right] |\Omega\rangle \\
&= a^{N/2} \left[\prod_{i=1}^{N/2} e^{[b' c_{2i}^\dagger + c' c_{2i-1}^\dagger} \right] \left[e^{d' \sum_{i=1}^{N/2} c_{2i-1}^\dagger c_{2i}^\dagger]} \right] |\Omega\rangle
\end{aligned} \tag{167}$$

one can arrive the product state in the fermionic picture

$$|\Phi\rangle = a^{N/2} e^{\sum_{i=1}^{N/2} b' c_{2i}^\dagger + c' c_{2i-1}^\dagger} e^{\sum_{i<j} (b' c_{2i}^\dagger + c' c_{2i-1}^\dagger)(b' c_{2j}^\dagger + c' c_{2j-1}^\dagger)} e^{d' \sum_{i=1}^{N/2} c_{2i-1}^\dagger c_{2i}^\dagger} |\Omega\rangle \tag{168}$$

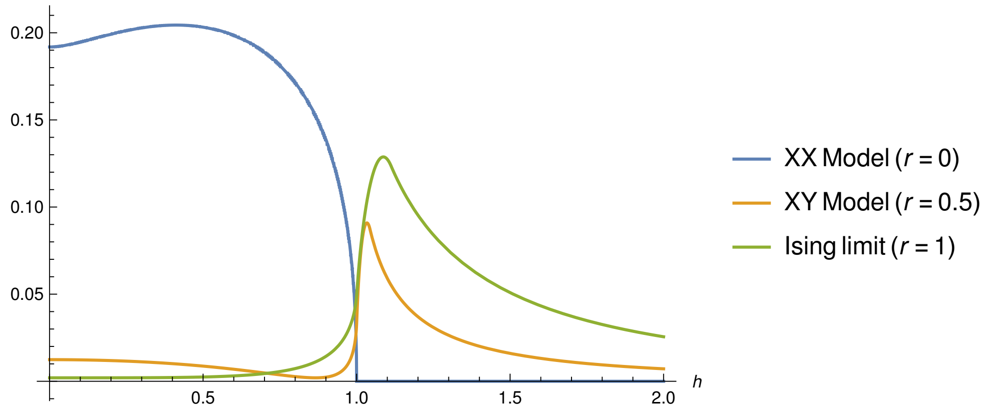

Figure 4: XY model global entanglement per block vs transverse magnetic field (h) in the thermodynamic limit

expanding the terms and evaluating fourier transform we arrive the overlap for even N

$$\langle\Psi|\Phi\rangle = \chi_N \prod_{m=0}^{m<(N/2-1)/2} a^2 \cos\theta_m \cos\theta_{\frac{N}{2}-m-1} + d^2 \sin\theta_m \sin\theta_{\frac{N}{2}-m-1} + \cos\theta_{\frac{N}{2}-m-1} \sin\theta_m \left[\frac{b^2+c^2}{2}\cot\frac{2\pi}{N}(m+\frac{1}{2}) + b\, c\cot\frac{2\pi}{N}(m+\frac{1}{2})\cos\frac{2\pi}{N}(m+\frac{1}{2}) + a\ d\sin\frac{2\pi}{N}(m+\frac{1}{2})\right] + \cos\theta_m \sin\theta_{\frac{N}{2}-m-1}\left[-\frac{b^2+c^2}{2}\cot\frac{2\pi}{N}(m+\frac{1}{2}) + b\ c\cot\frac{2\pi}{N}(m+\frac{1}{2})\cos\frac{2\pi}{N}(m+\frac{1}{2}) + a\ d\sin\frac{2\pi}{N}(m+\frac{1}{2})\right] \tag{169}$$

with

$$\chi_N = 1 \text{ for } N/4 = \text{integer}$$
$$\chi_N = a\cos\theta_{\frac{1}{2}(\frac{N}{2}-1)} + d\sin\theta_{\frac{1}{2}(\frac{N}{2}-1)} \text{ for } N/2 = \text{odd integer}$$

One can choose normalizable arbitrary constants $a^2+b^2+c^2+d^2=1$

$$a = \cos\gamma$$
$$b = \cos\alpha \sin\beta \sin\gamma$$
$$c = \sin\alpha \sin\beta \sin\gamma$$
$$d = \cos\beta \sin\gamma$$

Thus, geometric entanglement per block will be

$$\Lambda_{max}(\Psi) \equiv \underset{\Phi}{max} \langle\Phi|\Psi\rangle \tag{170a}$$
$$E_{log_2}(\Psi) \equiv -log_2\ \Lambda^2_{max}(\Psi) \tag{170b}$$
$$\mathcal{E} \equiv \frac{E_{log_2}(\Psi)}{N} \tag{170c}$$

2.2.6 Quantum Phase Transition

Quantum Phase Transition has been discussed in details in the first section. Here, we will investigate quantum phase transition by looking at global entanglement and its derivative near the quantum critical point for the XY spin chain model and its limits such as XX and Ising model. Most of the case, the field derivative of the entanglement diverges near the critical point. Let us start with the Figure (5)

One can easily spot the fluctuation in the entanglement density near the critical point $h = 1$. As can be also seen on the Figure (3). One can observe that in the XX limit ($r = 0$) entanglement density decrese to 0 as $h = 1$ On the other hand in the Ising and XY model one can see a change in entanglement near the critical point.

In order to notice sharp changes near critical point, one need to examine the field derivative of the entanglement on the Figure (6) and Figure (7). XY Model exhibit following phases; ordered oscillatory, ferromagnetic and paramagnetic. Ordered oscillatory ends on the line $r^2 + h^2 = 1$ as Ferromagnetic phase starts. In the critical point, Quantum Phase Transition occurs, and the system becomes Paramagnetic.

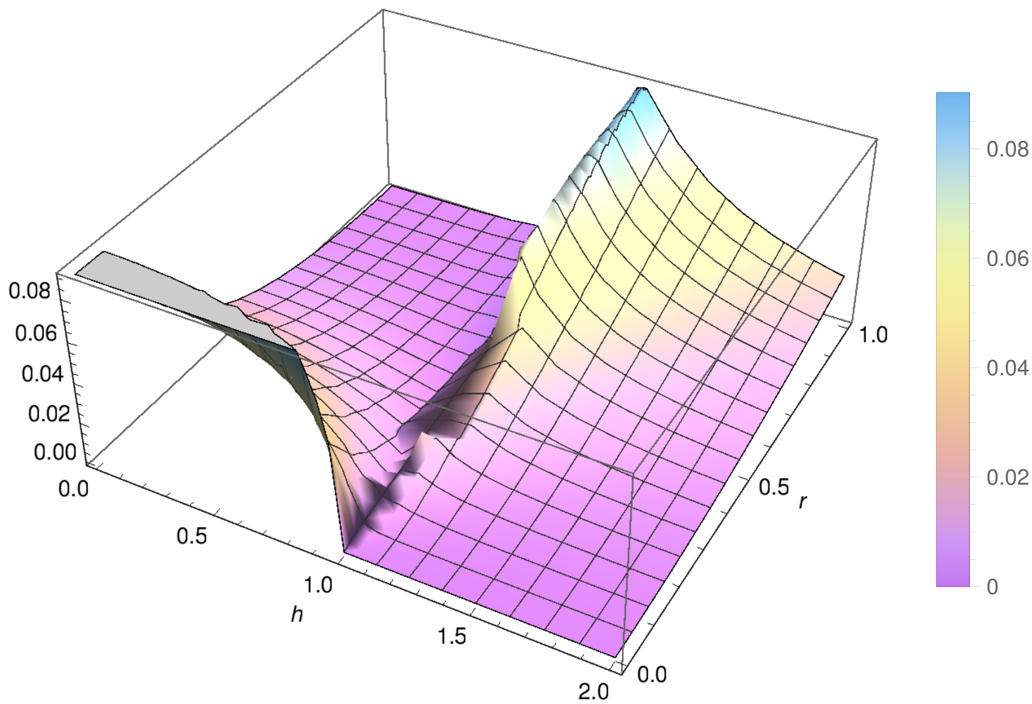

Figure 5: Entanglement density per site vs transverse magnetic field (h) vs anisotropy (r) in the thermodynamic limit where $N = 1000$

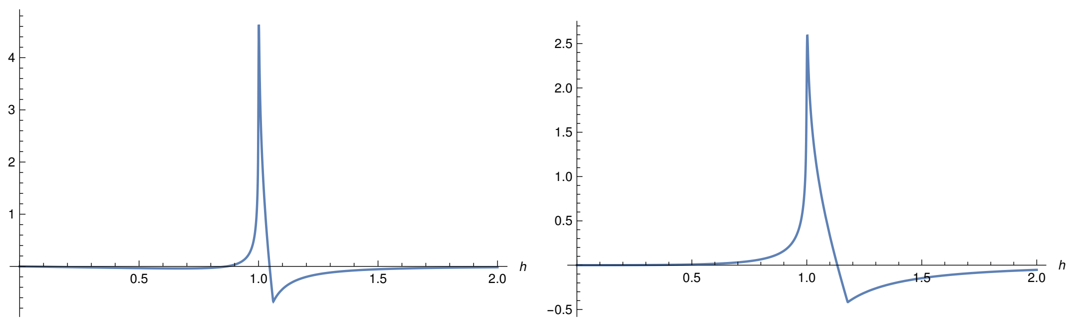

Figure 6: Derivative of Entanglement Density. XY Model r=0.5 (left panel) and Ising Limit r=1 (right panel)

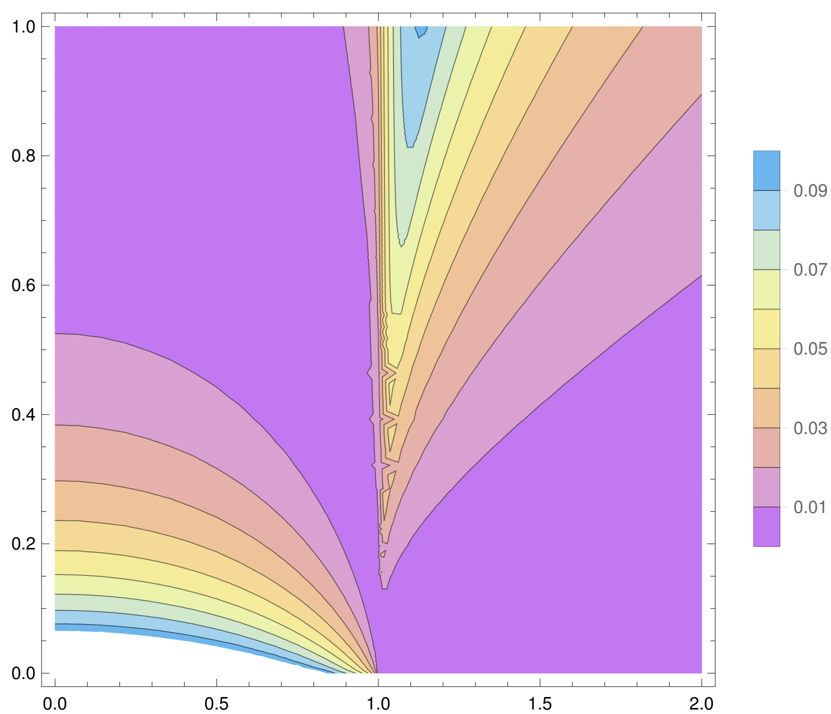

Figure 7: Contour plotting of Entanglement density vs transverse magnetic field (h) vs anisotropy (r) in the thermodynamic limit where $N = 1000$

2.3 XY Model with three-site interaction

The motivation of this section is examining QPT and quantum entanglement with next-nearest interaction Hamiltonian in the transverse field. One can suspect that extra σ_z term in the triangular lattice might have change some of the properties of the system. We will give an exact solution of the Hamiltonian and examine global entanglement and quantum phase transition. We will follow the same steps as in the previous section.

2.3.1 Diagonolization of Hamiltonian

Let us define the Hamiltonian. We use H_{XzY} for labeling to show three-site interaction.

$$H_{XzY} = -\sum_{j=1}^{N}(\frac{1+r}{2})\sigma^x_{j-1}\sigma^z_j\sigma^x_{j+1} + (\frac{1-r}{2})\sigma^y_{j-1}\sigma^z_j\sigma^y_{j+1} + h\sigma^z_j \tag{171}$$

As one can see, there is an extra σ^z term in the X and Y blocks. Applying Jordan-Wigner transformation which we defined in equation (75), we have

$$\begin{aligned}
\sigma^x_{j-1}\sigma^z_j\sigma^x_{j+1} &= \prod_{i=1}^{j-2}(1-2c^\dagger_i c_i)(c_{j-1}+c^\dagger_{j-1})(1-2c^\dagger_j c_j)\prod_{i=1}^{j}(1-2c^\dagger_i c_i)(c_{j+1}+c^\dagger_{j+1}) \\
&= \prod_{i=1}^{j-2}(1-2c^\dagger_i c_i)(c_{j-1}+c^\dagger_{j-1})\prod_{i=1}^{j-1}(1-2c^\dagger_i c_i)(c_{j+1}+c^\dagger_{j+1}) \\
&= (c_{j-1}+c^\dagger_{j-1})(1-2c^\dagger_{j-1}c_{j-1})(c_{j+1}+c^\dagger_{j+1}) \\
&= (-c_{j-1}+c^\dagger_{j-1})(c_{j+1}+c^\dagger_{j+1}) \\
&= -c_{j-1}c_{j+1} - c_{j-1}c^\dagger_{j+1} + c^\dagger_{j-1}c_{j+1} + c^\dagger_{j-1}c^\dagger_{j+1}
\end{aligned} \tag{172}$$

and for the next block

$$
\begin{aligned}
\sigma^y_{j-1}\sigma^z_j\sigma^y_{j+1} &= -\prod_{i=1}^{j-2}(1-2c_i^\dagger c_i)(c_{j-1}-c_{j-1}^\dagger)\prod_{i=1}^{j-1}(1-2c_i^\dagger c_i)(c_{j+1}-c_{j+1}^\dagger) \\
&= -(c_{j-1}-c_{j-1}^\dagger)(1-2c_{j-1}^\dagger c_{j-1})(c_{j+1}-c_{j+1}^\dagger) \\
&= (c_{j-1}+c_{j-1}^\dagger)(c_{j+1}-c_{j+1}^\dagger) \\
&= c_{j-1}c_{j+1}-c_{j-1}c_{j+1}^\dagger+c_{j-1}^\dagger c_{j+1}-c_{j-1}^\dagger c_{j+1}^\dagger
\end{aligned}
\tag{173}
$$

Substituting into Hamiltonian (171), we reach the fermionic form

$$
-H_{XzY} = \sum_{j=1}^{N}(-c_{j-1}c_{j+1}^\dagger + c_{j-1}^\dagger c_{j+1}) + r(-c_{j-1}c_{j+1}+c_{j-1}^\dagger c_{j+1}^\dagger) + h(1-2c_j^\dagger c_j)
\tag{174}
$$

Further applying Fourier transformation in equation (104), we obtain

$$
\begin{aligned}
-H_{XzY} = \sum_{m=0}^{N-1} &\left(e^{-i\frac{2\pi}{N}2(m+b)} + e^{i\frac{2\pi}{N}2(m+b)}\right)\tilde{c}_m^\dagger \tilde{c}_m \\
&+ r\left(-e^{-i\frac{2\pi}{N}2(m+b)}\tilde{c}_m\tilde{c}_{N-m-2b} + e^{i\frac{2\pi}{N}2(m+b)}\tilde{c}_m^\dagger\tilde{c}_{N-m-2b}^\dagger\right) \\
&+ Nh - 2h\tilde{c}_m^\dagger\tilde{c}_m
\end{aligned}
\tag{175}
$$

Next using symmetry equation (107), we arrive at

$$
\begin{aligned}
H_{XzY} = -Nh - \sum_{m=0}^{N-1}&\left\{\left[2\cos\left(\frac{2\pi}{N}2(m+b)\right) - 2h\right]\tilde{c}_m^\dagger\tilde{c}_m \right.\\
&\left. + i\ r\sin\left(\frac{2\pi}{N}2(m+b)\right)\left(\tilde{c}_m\tilde{c}_{N-m-2b}+\tilde{c}_m^\dagger\tilde{c}_{N-m-2b}^\dagger\right)\right\}
\end{aligned}
\tag{176}
$$

2.3.2 Geometric Entanglement and QPT

In the Appendix (A) we present a general Bogoliubov solution for bilinear Hamiltonian. H_{XzY} can be easily solved by substituting into equation (A-8).

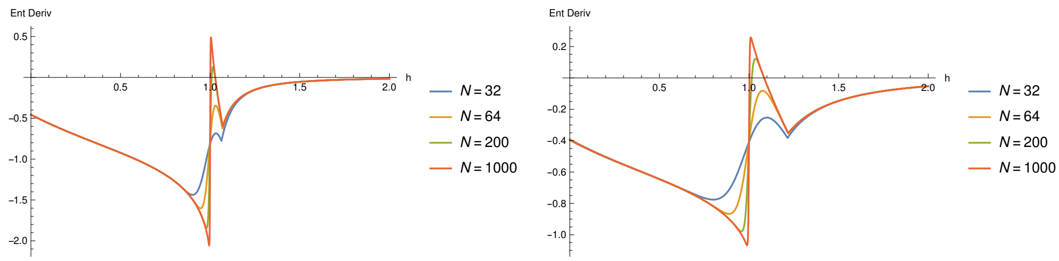

Figure 8: Derivative of Entanglement Density. XzY Model r=0.5 (left panel) and Ising Limit r=1 (right panel)

The solution of Bogoliubov fermions is as follows

$$\tan 2\theta_m = \frac{r \sin\left(\frac{2\pi}{N}2(m+b)\right)}{h - \cos\left(\frac{2\pi}{N}2(m+b)\right)} \tag{177a}$$

$$\sin 2\theta_m = \frac{r \sin\left(\frac{2\pi}{N}2(m+b)\right)}{\sqrt{\left(r \sin\left(\frac{2\pi}{N}2(m+b)\right)\right)^2 + \left(h - \cos\left(\frac{2\pi}{N}2(m+b)\right)\right)^2}} \tag{177b}$$

$$\cos 2\theta_m = \frac{h - \cos\left(\frac{2\pi}{N}2(m+b)\right)}{\sqrt{\qquad}} \tag{177c}$$

One notices the same form of solution except twice momentum as in the XY model (120). This similarity will be investigated in the next section.

One can see the change in global entanglement near the critical point. It is also important to notice that disorder line $r^2 + h^2 = 1$ in the XY model, does not exist in this model. At the point $h = 1$, QPT emerges between ferromagnet and paramagnet phases. As can be seen in Figure 8, the derivative of the entanglement shows divergence near the critical point.

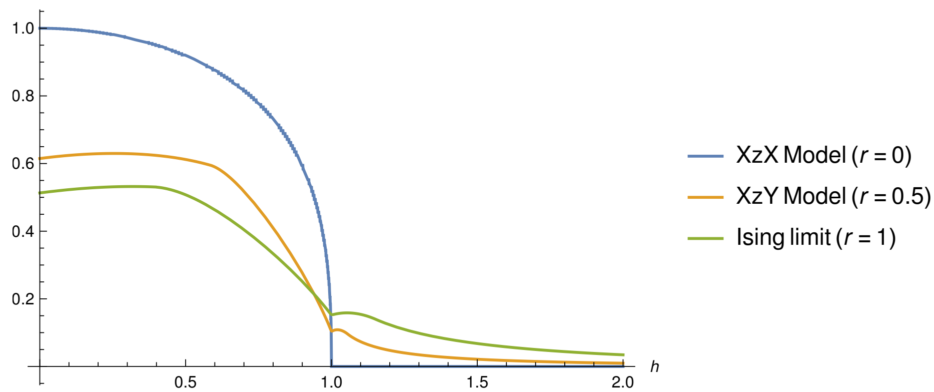

Figure 9: Entanglement density per site vs transverse magnetic field (h) in the thermodynamic limit where $N = 1000$

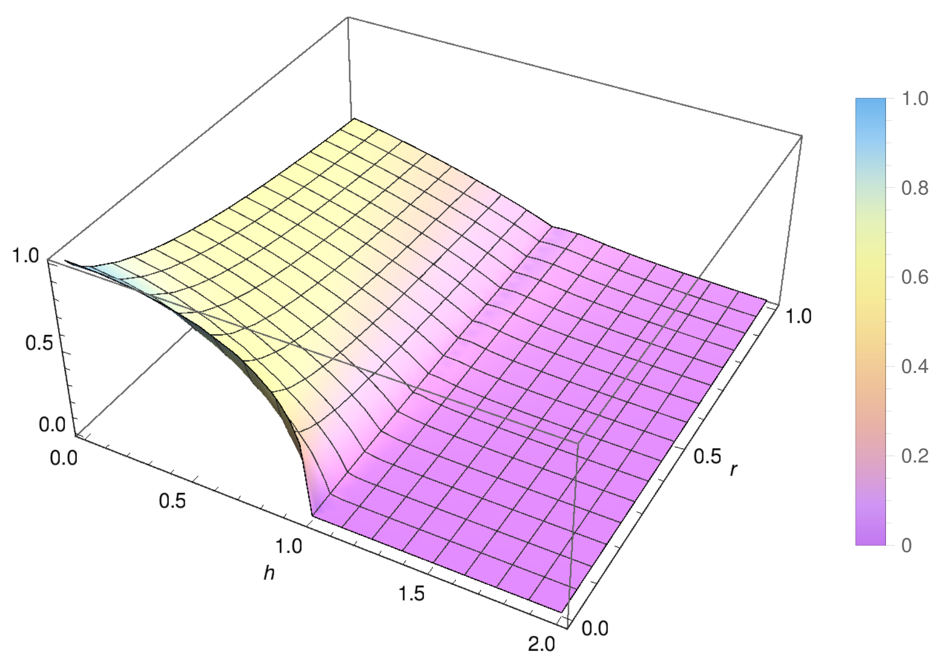

Figure 10: Entanglement density per site vs transverse magnetic field (h) vs anisotropy (r) in the thermodynamic limit where $N = 1000$

2.4 XY Model with n-site interaction

Often interaction in the spin chains problems are treated in nearest neighbor or three-site interaction. However, generalizing this model to n-site interaction can be useful for seeing overall features of the model and even can give some strange features which we will examine in this section. We shall define the Hamiltonian in a way that n shows the number of σ_z terms in the each block where $0 \leq n < N$. One can simply take $n = 0$ to have original XY Model and $n = 1$ to reach H_{XzY} or XY model with three-site interaction.

2.4.1 Diagonolization of Hamiltonian

We start with the definition of the Hamiltonian

$$H_{XnY} = -\sum_{j=1}^{N} \Bigg((\frac{1+r}{2})\sigma_{j-1}^{x}\sigma_{j}^{z}\sigma_{j+1}^{z}...\sigma_{j+n-1}^{z}\sigma_{j+n}^{x} + (\frac{1-r}{2})\sigma_{j-1}^{y}\sigma_{j}^{z}\sigma_{j+1}^{z}...\sigma_{j+n-1}^{z}\sigma_{j+n}^{y} + h\sigma_{j}^{z} \Bigg) \tag{178}$$

Applying Jordan-Wigner transformation, we transform the n-site terms to

$$
\begin{aligned}
\sigma^x_{j-1}\sigma^z_j\sigma^z_{j+1}\dots\sigma^z_{j+n-1}\sigma^x_{j+n} &= \prod_{i=1}^{j-2}(1-2c_i^\dagger c_i)(c_{j-1}+c_{j-1}^\dagger)(1-2c_j^\dagger c_j) \\
&(1-2c_{j+1}^\dagger c_{j+1})\dots(1-2c_{j+n-1}^\dagger c_{j+n-1}) \\
&\prod_{i=1}^{j+n-1}(1-2c_i^\dagger c_i)(c_{j+n}+c_{j+n}^\dagger) \\
&= \prod_{i=1}^{j-2}(1-2c_i^\dagger c_i)(c_{j-1}+c_{j-1}^\dagger) \\
&\prod_{i=1}^{j-1}(1-2c_i^\dagger c_i)(c_{j+n}+c_{j+n}^\dagger) \\
&= (c_{j-1}+c_{j-1}^\dagger)(1-2c_{j-1}^\dagger c_{j-1})(c_{j+n}+c_{j+n}^\dagger) \\
&= (-c_{j-1}+c_{j-1}^\dagger)(c_{j+n}+c_{j+n}^\dagger) \\
&= -c_{j-1}c_{j+n}-c_{j-1}c_{j+n}^\dagger+c_{j-1}^\dagger c_{j+n}+c_{j-1}^\dagger c_{j+n}^\dagger
\end{aligned} \tag{179}
$$

and

$$
\begin{aligned}
\sigma^y_{j-1}\sigma^z_j\sigma^y_{j+1}\dots\sigma^z_{j+n-1}\sigma^x_{j+n} &= -\prod_{i=1}^{j-2}(1-2c_i^\dagger c_i)(c_{j-1}-c_{j-1}^\dagger)(1-2c_j^\dagger c_j) \\
&(1-2c_{j+1}^\dagger c_{j+1})\dots(1-2c_{j+n-1}^\dagger c_{j+n-1}) \\
&\prod_{i=1}^{j+n-1}(1-2c_i^\dagger c_i)(c_{j+n}-c_{j+n}^\dagger) \\
&= -(c_{j-1}-c_{j-1}^\dagger)(1-2c_{j-1}^\dagger c_{j-1})(c_{j+n}-c_{j+n}^\dagger) \\
&= (c_{j-1}+c_{j-1}^\dagger)(c_{j+n}-c_{j+n}^\dagger) \\
&= c_{j-1}c_{j+n}-c_{j-1}c_{j+n}^\dagger+c_{j-1}^\dagger c_{j+n}-c_{j-1}^\dagger c_{j+n}^\dagger
\end{aligned} \tag{180}
$$

Substituting them into the Hamiltonian (178), we have

$$-H_{XnY} = \sum_{j=1}^{N} (\frac{1+r}{2})(-c_{j-1}c_{j+n} - c_{j-1}c_{j+n}^{\dagger} + c_{j-1}^{\dagger}c_{j+n} + c_{j-1}^{\dagger}c_{j+n}^{\dagger}) + (\frac{1-r}{2})(c_{j-1}c_{j+n} - c_{j-1}c_{j+n}^{\dagger} + c_{j-1}^{\dagger}c_{j+n} - c_{j-1}^{\dagger}c_{j+n}^{\dagger}) + h(1-2c_j^{\dagger}c_j) \tag{181}$$

which is then simplified to

$$-H_{XnY} = \sum_{j=1}^{N} (-c_{j-1}c_{j+n}^{\dagger} + c_{j-1}^{\dagger}c_{j+n}) + r(-c_{j-1}c_{j+n} + c_{j-1}^{\dagger}c_{j+n}^{\dagger}) + h(1-2c_j^{\dagger}c_j) \tag{182}$$

Using Fourier transformation formulas which we found in (104) for the n-site interaction, we have

$$\begin{aligned} -H_{XnY} = \sum_{m=0}^{N-1} & \left(e^{-i\frac{2\pi}{N}(n+1)(m+b)} + e^{i\frac{2\pi}{N}(n+1)(m+b)}\right)\tilde{c}_m^{\dagger}\tilde{c}_m \\ & + r\left(-e^{-i\frac{2\pi}{N}(n+1)(m+b)}\tilde{c}_m\tilde{c}_{N-m-2b} + e^{i\frac{2\pi}{N}(n+1)(m+b)}\tilde{c}_m^{\dagger}\tilde{c}_{N-m-2b}^{\dagger}\right) \\ & + Nh - 2h\tilde{c}_m^{\dagger}\tilde{c}_m \end{aligned} \tag{183}$$

Using symmetry equations (107), we have

$$\begin{aligned} H_{XnY} = -Nh - \sum_{m=0}^{N-1} & \left\{ \left[2\cos\left(\frac{2\pi}{N}(n+1)(m+b)\right) - 2h \right] \tilde{c}_m^{\dagger}\tilde{c}_m \right. \\ & \left. + i\ r\sin\left(\frac{2\pi}{N}(n+1)(m+b)\right)\left(\tilde{c}_m\tilde{c}_{N-m-2b} + \tilde{c}_m^{\dagger}\tilde{c}_{N-m-2b}^{\dagger}\right) \right\} \end{aligned} \tag{184}$$

It is convenient to define

$$\Theta_n^{(b)} = \frac{2\pi}{N}(n+1)(m+b) \tag{185}$$

$$H_{XnY} = -Nh - \sum_{m=0}^{N-1} \left(2\cos\Theta_n - 2h\right) \tilde{c}_m^\dagger \tilde{c}_m + i \ r \sin\Theta_n \left(\tilde{c}_m \tilde{c}_{N-m-2b} + \tilde{c}_m^\dagger \tilde{c}_{N-m-2b}^\dagger\right) \tag{186}$$

Using the matrix form of the Bogoliubov transformation $(A-8)$ one can easily diagonalize the Hamiltonian and derive solution of the generalized XY model in the n-site interaction. This model also can be solved exactly and the structure looks very similar to XY model.

Here we present n-th nearest neighbor interaction solution

$$\tan 2\theta_m = \frac{r\sin\Theta_n}{h-\cos\Theta_n} \tag{187a}$$

$$\sin 2\theta_m = \frac{r\sin\Theta_n}{\sqrt{(r\sin\Theta_n)^2 + (h-\cos\Theta_n)^2}} \tag{187b}$$

$$\cos 2\theta_m = \frac{h-\cos\Theta_n}{\sqrt{(r\sin\Theta_n)^2 + (h-\cos\Theta_n)^2}} \tag{187c}$$

Eventually we obtain the diagonalized Hamiltonian,

$$H = \sum_{m=0}^{N-1} \epsilon_m^{(b)} \left(\gamma_m^{(b)\dagger}\gamma_m^{(b)} - \frac{1}{2}\right) \tag{188}$$

where ϵ_m is the eigenvalue of the Hamiltonian

$$\epsilon_m^{(b)} = 2\sqrt{(r\sin\Theta_n)^2 + (h-\cos\Theta_n)^2} \tag{189}$$

and

$$\gamma_m^{(b)} = c_m^{(b)}\cos\theta_m - i\sin\theta_m^{(b)} \ c_{N-m-2b} \tag{190}$$

The ground state energy for the periodic boundary condition (odd-number-fermion $b = 0$)

$$E_m^{(0)}(r,h) = (h-1) - \sum_{m=1}^{N-1} \sqrt{\left(r\sin\Theta_n^{(0)}\right)^2 + \left(h - \cos\Theta_n^{(0)}\right)^2} \tag{191}$$

and antiperiodic boundary condition (even-number-fermion $b = 1/2$)

$$E_m^{(1/2)}(r,h) = -\sum_{m=1}^{N-1} \sqrt{\left(r\sin\Theta_n^{(1/2)}\right)^2 + \left(h - \cos\Theta_n^{(1/2)}\right)^2} \tag{192}$$

We note that one can vary the number of σ_z terms to obtain other models without having to solve them again:

$n \to 0$	XY model
$n \to 1$	XY model with three-site interaction (XzY) model
$n \to \frac{N}{2} - 2$	halfway interaction

We shall examine the features of *halfway interaction* in the context of quantum phase transition and geometric entanglement in the next section.

2.4.2 Mapping to 2D Classical Ising Model

Before moving to next section, we will investigate the two-dimensional classical duality of one-dimensional XY model with n-site interaction. It has been shown many times by several authors that one-dimensional quantum XY Model can be mapped to two-dimensional square-lattice Ising model in the transverse field by choosing proper constants [19] [71] [72].

In the section (2.1.1) we have given the brief derivation of transfer matrix solution of 2D Square-lattice Ising Model. (59). One can study the derivation of eigenvalues and eigenvectors of the transfer matrix by using Jordan-Wigner, Fourier and Bogoliubov transformation [9]. In this part we will present the solution of this model.

$$V_1 = (2sinh2K_1)^{M/2} \;\; e^{-2K_1' \;\tau^x}$$
$$V_2 = e^{K_2 \sum \tau_m^z \tau_{m+1}^z + H \sum \tau_m^z}$$
$$Z = tr\left(V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}}\right)^N = trV^N$$

and H_V is diagonalized Hamiltonian with ϵ_k energy eigenvalues

$$V = V_1^{\frac{1}{2}} V_2 V_1^{\frac{1}{2}} \tag{193a}$$
$$V = exp\left(-\sum_k \epsilon_k \gamma_k^\dagger \gamma_k\right) = exp\left(-H_V\right) \tag{193b}$$
$$cosh\;\epsilon_k = cosh2K_1' \cosh 2K_2 - cosk \sinh 2K_1' \sinh 2K_2 \tag{193c}$$

The XY model solution of Bogoliubov fermions has the same form as the V matrix with proper constants [73].

$$\tan 2\theta_k^V = \frac{\sin k \sinh 2K_2}{\sinh 2K_1' \cosh 2K_2 \cos k \cosh 2K_1' \sinh 2K_2} \tag{194}$$
$$\tan 2\theta_k^{XnY} = \frac{r \sin \Theta}{h - \cos \Theta} \tag{195}$$

where Θ in the second equation is

$$\Theta(n) = \frac{2\pi}{N}(n+1)(m+b) \tag{196}$$

Thus $[H_{XnY}, H_V] = 0$ if we choose r and h in the following form

$$h = \frac{\tanh 2K_1'}{\tanh 2K_2} \tag{197}$$
$$r = \frac{1}{cosh2K_1'} \tag{198}$$

In the case $n = 0$, it reduces to the XY Model. It has been known that

1D quantum XY model is mapped to 2D Square-lattice Ising Model. An interesting point here is that as we change the number of σ_z term (n), this mapping looks still valid since h and r terms are not coupled with Θ. Thus, one can naively think that where $n = 1 \rightarrow$ XzY model should also correspond to same 2D square-lattice Ising model. It can also be shown that any Hamiltonian with n-site interaction in the XY Model should obey the following commutation relations $[H_{XnY}, H_V] = 0$

2.4.3 Geometric Entanglement and QPT

In this section, we will continue with XnY model which we developed in the previous section and examine the effects of *halfway interaction*. One specific point ($n = N/2 - 1$) is interesting in this model since in this point characteristic of Θ changes. It affects the solution of Bogoliubov fermions by vanishing some of the *sin* and *cos* terms depending on periodic/antiperiodic boundary conditions ($b = 0/b = \frac{1}{2}$). Recalling the solution of XY model with n-th nearest neighbors interaction

$$\tan 2\theta_m = \frac{r \sin \Theta}{h - \cos \Theta} \tag{199a}$$

where

$$\Theta(n) = \frac{2\pi}{N}(n+1)(m+b) \tag{200}$$

with a simple algebra one can show the solution of this interaction for even-fermion case (b=1/2)

$$\tan 2\theta_m^{(1/2)} = \frac{r \sin\left[\pi\left(m + \frac{1}{2}\right)\right]}{h - \cos\left[\pi\left(m + \frac{1}{2}\right)\right]} \tag{201a}$$

$$\tan 2\theta_m = \frac{(-1)^m r}{h} \tag{201b}$$

and for odd-fermion case (b=0)

$$\tan 2\theta_m^{(0)} = \frac{r \sin[\pi m]}{h - \cos[\pi m]} = 0 \tag{202a}$$

plotting global entanglement and derivative of the entanglement in the halfway interaction, it can be seen that there is no divergence near the critical point. There can be two reasons for this result. Firstly, this method might not be able to detect the entanglement. However, in the next graph one can see the entanglement measurement for $r = 0.5$ and $r = 1$ case. Thus it is not the explanation. Second reason, Quantum Phase Transition do not exist where particles have interaction with the opposite side of the circle in the cyclic boundary conditions.

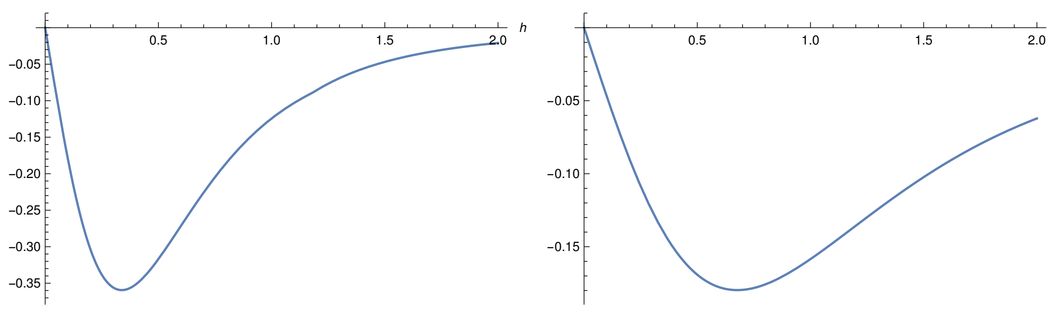

Figure 11: Derivative of Entanglement Density for halfway interaction in the XnY model where r=0.5 (left panel) and Ising Limit r=1 (right panel)

One can naturally think that this interaction is not possible in the real lattice. In this point, we would like to point out that n and N are arbitrary numbers, and halfway interaction occurs also in the small systems such as $n = 3$ while $N = 8$. On the other hand, as we investigate other interactions, we find out that quantum phase transition exists except the halfway interaction. For instance, when $n = 52$ while $N = 100$, we can see discontinuity near the critical point. Therefore, derivative of the entanglement does not diverge near the critical point if and only if $n = N/2 - 1$ for even number of particles.

We present a contour map for the derivative of the entanglement vs n-site

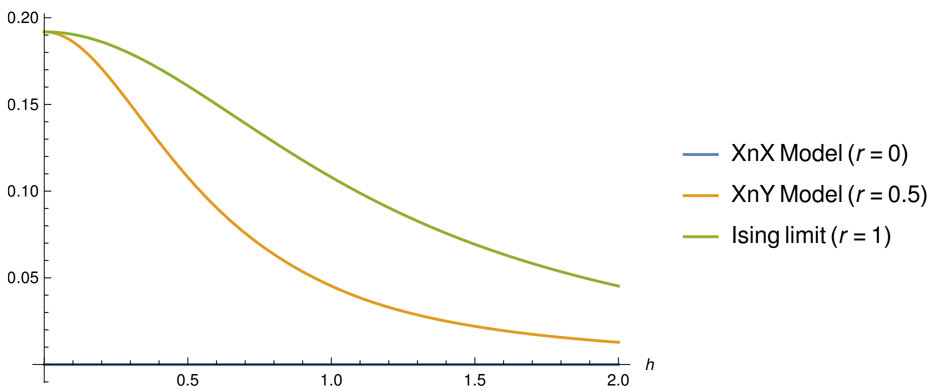

Figure 12: Entanglement Density for halfway interaction in the XnY model in the thermodynamic limit where $N = 1000$

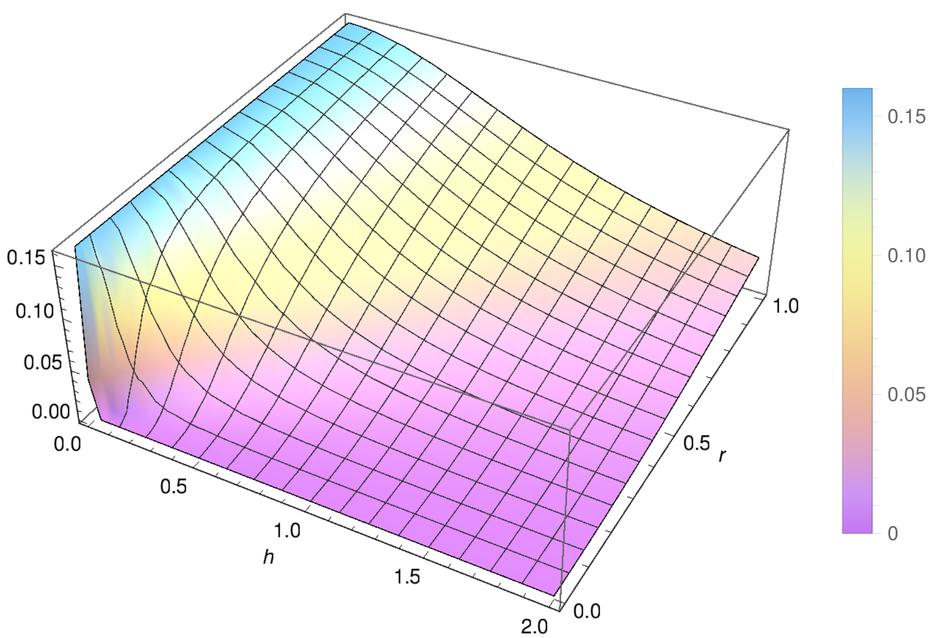

Figure 13: Entanglement density of halfway interaction vs transverse magnetic field (h) vs anisotropy (r) in the thermodynamic limit where $N = 1000$

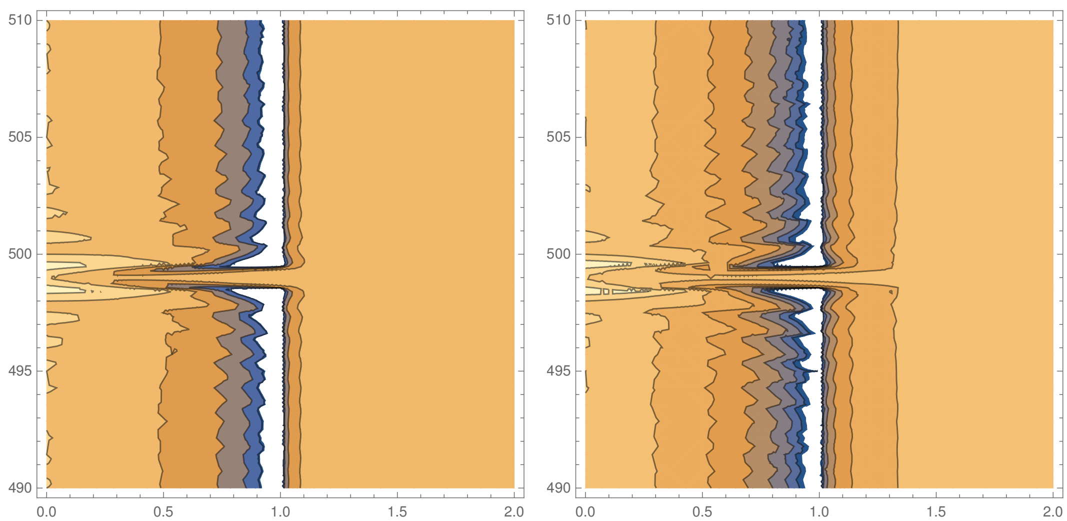

Figure 14: Derivative of Entanglement Density for halfway interaction. XnY Model r=0.5 (left panel) and Ising Limit r=1 (right panel) where n=490-510 and N=1000. At the halfway interaction (N=499) there is no discontinuity in the derivative of the entanglement therefore QPT do not emerge

interaction on the figure (14) As one can easily see in the halfway interaction (n=49 in this case) derivative of entanglement is continuous function as other points are not. Therefore, halfway interaction is like spin coupling between opposite pairs which we do not expect the quantum phase transition.

3 Generalized Cluster-XY Model

In this section, we introduce a new form of the generalized Cluster-XY Hamiltonian. Similar Hamiltonian has been presented by Suzuki [30]. However, this Hamiltonian is more convenient and efficient regarding the size of the diagonalized matrix. By using this model, one can derive the exact solution of the many suitable bilinear spin systems without applying any transformation. Then one can examine global entanglement and quantum phase transition easily. In the next part, we will give several examples of this model and investigate the Quantum Phase Transition for each of them.

3.1 Diagonolization of Hamiltonian

We begin with defining the Hamiltonian. One needs to pay attention six arbitrary quantities in this model. $N^{(x)}$ and $N^{(y)}$ are the number of X and Y blocks in the Hamiltonian. For example, one can build a Hamiltonian with several X blocks and only one Y block in the transverse field. $J_l^{(x)}$ and $J_{l'}^{(y)}$ are the lists of coupling constants for each block. Thus, one can choose the strength of each block separately. At last, one can choose any number of site interaction for each block separately. $n_l^{(x)}$ and $n_{l'}^{(y)}$ are list of σ_z terms for each block. One should pay attention that the number of term in the $J_l^{(x)}$ & $J_{l'}^{(y)}$ and $n_l^{(x)}$ & $n_{l'}^{(y)}$ can not exceed X & Y. The Hamiltonian is

$$H_{CXY} = -\sum_{j=1}^{N}\left(\sum_{l=1}^{N^{(x)}} J_l^{(x)}\sigma_{j-1}^{x}\sigma^{z}\ldots\sigma^{z}\sigma_{j+n_l^{(x)}}^{x} + \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)}\sigma_{j-1}^{y}\sigma^{z}\ldots\sigma^{z}\sigma_{j+n_{l'}^{(y)}}^{y} + h\sigma_j^z\right) \tag{203}$$

Applying Jordan-Wigner transformation and simplifying, we arrive at

$$
\begin{aligned}
H_{CXY} = -\sum_{j=1}^{N} \Bigg[& \sum_{l=1}^{N^{(x)}} J_l^{(x)} \left(c_{j-1}^\dagger c_{j+n_l^{(x)}} + c_{j-1}^\dagger c_{j+n_l^{(x)}}^\dagger - c_{j-1} c_{j+n_l^{(x)}} - c_{j-1} c_{j+n_l^{(x)}}^\dagger \right) \\
& + \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \left(c_{j-1}^\dagger c_{j+n_{l'}^{(y)}} - c_{j-1}^\dagger c_{j+n_{l'}^{(y)}}^\dagger + c_{j-1} c_{j+n_{l'}^{(y)}} - c_{j-1} c_{j+n_{l'}^{(y)}}^\dagger \right) \\
& + h(1 - 2c_j^\dagger c_j) \Bigg]
\end{aligned}
\tag{204}
$$

Mapping to momentum space, we have

$$
\begin{aligned}
H_{CXY} = -Nh - \sum_{m=0}^{N-1} \sum_{l,l'=1}^{X,Y} \Bigg[& \left(J_l^{(x)} e^{i\frac{2\pi}{N}(m+b)(1+n_l^{(x)})} + J_{l'}^{(y)} e^{i\frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)})} \right) c_m^{(b)\dagger} c_m^{(b)} \\
& + \left(-J_l^{(x)} e^{-i\frac{2\pi}{N}(m+b)(1+n_l^{(x)})} + J_{l'}^{(y)} e^{-i\frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)})} \right) c_m^{(b)} c_{N-m-2b}^{(b)} \\
& - \left(J_l^{(x)} e^{-i\frac{2\pi}{N}(m+b)(1+n_l^{(x)})} + J_{l'}^{(y)} e^{-i\frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)})} \right) c_m^{(b)} c_m^{(b)\dagger} \\
& + \left(J_l^{(x)} e^{i\frac{2\pi}{N}(m+b)(1+n_l^{(x)})} - J_{l'}^{(y)} e^{i\frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)})} \right) c_m^{(b)\dagger} c_{N-m-2b}^{(b)\dagger} \\
& - 2h c_m^{(b)\dagger} c_m^{(b)} \Bigg]
\end{aligned}
\tag{205}
$$

Similar to earlier discussion, we define Θ for simplicity,

$$
\Theta_l^{(x)} = \frac{2\pi}{N}(m+b)(1+n_l^{(x)}) \tag{206a}
$$

$$
\Theta_{l'}^{(y)} = \frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)}) \tag{206b}
$$

Recall the fermionic commutation relations $\{c_i, c_j^\dagger\} = \delta_{ij}$ and apply the symmetry we reach,

$$H_{CXY} = -Nh - \sum_{m=0}^{N-1} \sum_{l,l'=1}^{X,Y} \Big\{ c_m^{(b)\dagger} c_m^{(b)} \left(2\ J_l^{(x)} \cos\Theta_l^{(x)} + 2\ J_{l'}^{(y)} \cos\Theta_{l'}^{(y)} - 2h\right) \\ + i\left(J_l^{(x)} \sin\Theta_l^{(x)} - J_{l'}^{(y)} \sin\Theta_{l'}^{(y)}\right)\left[c_m^{(b)} c_{N-m-2b}^{(b)} + c_m^{(b)\dagger} c_{N-m-2b}^{(b)\dagger}\right]\Big\} \tag{207}$$

After Bogoliubov transformation (A-8), we have

$$H_{CXY} = -\sum_{m=0}^{N-1} \sum_{l,l'=1}^{X,Y} \Big\{ \left(\gamma_{N-m-2b}^{(b)\dagger} \gamma_{N-m-2b}^{(b)} + \gamma_m^{(b)\dagger} \gamma_m^{(b)}\right) \Big[-hcos2\theta_m^{(b)} \\ + J_l^{(x)} \cos\left(2\theta_m^{(b)} + \Theta_l^{(x)}\right) + J_{l'}^{(y)} \cos\left(2\theta_m^{(b)} - \Theta_{l'}^{(y)}\right)\Big] \\ - i\left(\gamma_m^{(b)} \gamma_{N-m-2b}^{(b)} + \gamma_m^{(b)\dagger} \gamma_{N-m-2b}^{(b)\dagger}\right)\Big[h \sin 2\theta_m^{(b)} - J_l^{(x)} \sin\left(2\theta_m^{(b)} + \Theta_l^{(x)}\right) \\ - J_{l'}^{(y)} \sin\left(2\theta_m^{(b)} - \Theta_{l'}^{(y)}\right)\Big] + h\ \cos 2\theta_m^{(b)} + h(N-1) \\ + 2\sin\theta_m^{(b)}\left[J_l^{(x)} \sin\left(\theta_m^{(b)} + \Theta_l^{(x)}\right) + J_{l'}^{(y)} \sin\left(\theta_m^{(b)} - \Theta_{l'}^{(y)}\right)\right]\Big\} \tag{208}$$

Equating non-diagonal terms to zero, we obtain

$$h \sin 2\theta_m^{(b)} - J_l^{(x)}\left[\sin 2\theta_m^{(b)} \cos\left(\Theta_l^{(x)}\right) + cos2\theta_m^{(b)} \sin\left(\Theta_l^{(x)}\right)\right] \\ - J_{l'}^{(y)}\left[sin2\theta_m^{(b)} \cos\left(\Theta_{l'}^{(y)}\right) - cos2\theta_m^{(b)} \sin\left(\Theta_{l'}^{(y)}\right)\right] = 0 \tag{209}$$

Solving for θ_m, we obtain the result

$$\beta_m = \sum_{l=1}^{N^{(x)}} J_l^{(x)} \sin\left(\Theta_l^{(x)}\right) - \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \sin\left(\Theta_{l'}^{(y)}\right) \tag{210}$$

$$\alpha_m = h - \sum_{l=1}^{N^{(x)}} J_l^{(x)} \cos\left(\Theta_l^{(x)}\right) - \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \cos\left(\Theta_{l'}^{(y)}\right) \tag{211}$$

$$\tan 2\theta_m = \frac{\beta_m}{\alpha_m} \tag{212}$$

Finally, we reach the diagonalized Hamiltonian,

$$H = \sum_{m=0}^{N-1} \epsilon_m \left(\gamma_m^\dagger \gamma_m - \frac{1}{2} \right) \tag{213}$$

where ϵ_m is the eigenvalue of the Hamiltonian

$$\epsilon_m = 2\sqrt{(\beta_m)^2 + (\alpha_m)^2} \tag{214}$$

and and

$$\gamma_m = c_m \cos\theta_m - i \sin\theta_m \; c_{N-m-2b} \tag{215}$$

One should also pay attention to b gauge term which can be $b = 0$ (odd-fermion case, periodic boundary conditions) or $b = 1/2$ (even-fermion case, antiperiodic boundary conditions).

3.2 Geometric Entanglement and QPT

In this part, we present several examples of the Hamiltonian we developed in the previous section. The requested Hamiltonian may not be in the H_{CXY} but one can easily obtain the same form by operating rotation matrix on spin states.

$$\begin{aligned} H_{CXY} = -\sum_{j=1}^{N} \Bigg(& \sum_{l=1}^{N^{(x)}} J_l^{(x)} \sigma_{j-1}^x \sigma^z \ldots \sigma^z \sigma_{j+n_l^{(x)}}^x \\ & + \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \sigma_{j-1}^y \sigma^z \ldots \sigma^z \sigma_{j+n_{l'}^{(y)}}^y + h\sigma_j^z \Bigg) \end{aligned} \tag{216}$$

Let us recall the solution for this Hamiltonian

$$\Theta_l^{(x)} = \frac{2\pi}{N}(m+b)(1+n_l^{(x)}) \tag{217a}$$

$$\Theta_{l'}^{(y)} = \frac{2\pi}{N}(m+b)(1+n_{l'}^{(y)}) \tag{217b}$$

$$\beta_m = \sum_{l=1}^{N^{(x)}} J_l^{(x)} \sin\left(\Theta_l^{(x)}\right) - \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \sin\left(\Theta_{l'}^{(y)}\right) \tag{217c}$$

$$\alpha_m = h - \sum_{l=1}^{N^{(x)}} J_l^{(x)} \cos\left(\Theta_l^{(x)}\right) - \sum_{l'=1}^{N^{(y)}} J_{l'}^{(y)} \cos\left(\Theta_{l'}^{(y)}\right) \tag{217d}$$

$$\epsilon_m = 2\sqrt{(\beta_m)^2 + (\alpha_m)^2} \tag{217e}$$

and

$$\tan 2\theta_m = \frac{\beta_m}{\alpha_m} \tag{218a}$$

$$\sin 2\theta_m = \frac{(\beta_m)}{\sqrt{(\beta_m)^2 + (\alpha_m)^2}} \tag{218b}$$

$$\cos 2\theta_m = \frac{(\alpha_m)}{\sqrt{(\beta_m)^2 + (\alpha_m)^2}} \tag{218c}$$

$$\cos\theta_m = \sqrt{\frac{1+\cos 2\theta_m}{2}} \tag{218d}$$

$$\sin\theta_m = sgn(\beta_m)\sqrt{\frac{1-\cos 2\theta_m}{2}} \tag{218e}$$

where X and Y are the number of X and Y blocks in the Hamiltonian and $J_l^{(x)}$ and $J_{l'}^{(y)}$ are the list of coupling constants for each block and $n_l^{(x)}$ and $n_{l'}^{(y)}$ are list of σ_z terms or site interaction for each X or Y block.

One can substitute this solution into geometric entanglement per site/block equation without performing any transformation. Recalling geometric entanglement per site [70] derived from the overlap

$$\langle\Psi_{1/2}|\Phi(\xi)\rangle = \prod_{m=0}^{m<\frac{N-1}{2}} \left(\cos\theta_m \cos^2\frac{\xi}{2} + \sin\theta_m \sin^2\frac{\xi}{2}\cot\frac{\pi(m+\frac{1}{2})}{N}\right) \tag{219}$$

and for geometric entanglement per block, the overlap is

$$\langle\Psi_{1/2}|\Phi\rangle = \chi_N \prod_{m=0}^{m<(N/2-1)/2} \Bigg\{ a^2 \cos\theta_m \cos\theta_{\frac{N}{2}-m-1} + d^2 \sin\theta_m \sin\theta_{\frac{N}{2}-m-1} +$$
$$\cos\theta_{\frac{N}{2}-m-1} \sin\theta_m \left[\frac{b^2+c^2}{2} \cot\frac{2\pi}{N}(m+\frac{1}{2}) + b\ c \cot\frac{2\pi}{N}(m+\frac{1}{2}) \cos\frac{2\pi}{N}(m+\frac{1}{2}) \right.$$
$$\left. + a\ \ d \sin\frac{2\pi}{N}(m+\frac{1}{2}) \right] + \cos\theta_m \sin\theta_{\frac{N}{2}-m-1} \left[-\frac{b^2+c^2}{2} \cot\frac{2\pi}{N}(m+\frac{1}{2}) \right.$$
$$\left. + b\ \ c \cot\frac{2\pi}{N}(m+\frac{1}{2}) \cos\frac{2\pi}{N}(m+\frac{1}{2}) + a\ \ d \sin\frac{2\pi}{N}(m+\frac{1}{2}) \right] \Bigg\} \tag{220}$$

with

$$\chi_N = 1 \text{ for } N/4 = \text{integer}$$
$$\chi_N = a\cos\theta_{\frac{1}{2}(\frac{N}{2}-1)} + d\sin\theta_{\frac{1}{2}(\frac{N}{2}-1)} \text{ for } N/2 = \text{odd integer}$$

and

$$a = \cos\gamma$$
$$b = \cos\alpha \sin\beta \sin\gamma$$
$$c = \sin\alpha \sin\beta \sin\gamma$$
$$d = \cos\beta \sin\gamma$$

Entanglement density ($\mathcal{E}$) for the number of N particle is obtained from

$$\Lambda_{max}(\Psi) \equiv \max_{\Phi} \langle\Phi|\Psi\rangle \tag{221a}$$
$$E_{log_2}(\Psi) \equiv -log_2\ \Lambda^2_{max}(\Psi) \tag{221b}$$
$$\mathcal{E} \equiv \frac{E_{log_2}(\Psi)}{N} \tag{221c}$$

3.2.1 XY model and XY Model with n-site interaction

In this part, we present the solution of the anisotropic XY model in the transverse field and XY model with n-site interaction by using the method we derived earlier. In these models, there are one X and Y block and r is the anisotropy constant. We introduce the following quantities that characterize the model:

$$N^{(x)} = 1 \tag{222a}$$

$$N^{(y)} = 1 \tag{222b}$$

$$J_l^{(x)} = \{(1+r)/2\} \tag{222c}$$

$$J_{l'}^{(y)} = \{(1-r)/2\} \tag{222d}$$

$$n_l^{(x)} = \{0\} \tag{222e}$$

$$n_{l'}^{(y)} = \{0\} \tag{222f}$$

Putting these terms into H_{CXY} (203), we get XY Model

$$H_{XY} = -\sum_{j=1}^{N}\left[\frac{1+r}{2}\sigma_{j-1}^{x}\sigma_{j}^{x} + \frac{1-r}{2}\sigma_{j-1}^{y}\sigma_{j}^{y} + h\sigma_{j}^{z}\right] \tag{223}$$

$$\tan 2\theta_m^{(b)} = \frac{(\frac{1+r}{2})\sin\left(\Theta_l^{(x)}\right) - (\frac{1-r}{2})\sin\left(\Theta_{l'}^{(y)}\right)}{h - (\frac{1+r}{2})\cos\left(\Theta_l^{(x)}\right) - (\frac{1-r}{2})\cos\left(\Theta_{l'}^{(y)}\right)} \tag{224a}$$

$$\tan 2\theta_m^{(b)} = \frac{r\sin\left(\Theta_l^{(x)}\right)}{h - \cos\left(\Theta_l^{(x)}\right)} \tag{224b}$$

where

$$\Theta_l^{(x)} = \Theta_{l'}^{(y)} = \frac{2\pi}{N}(m+b) \tag{225}$$

Likewise, we can solve the H_{XnY} model with using following terms

$$N^{(x)} = 1 \tag{226a}$$
$$N^{(y)} = 1 \tag{226b}$$
$$J_l^{(x)} = \{(1+r)/2\} \tag{226c}$$
$$J_{l'}^{(y)} = \{(1-r)/2\} \tag{226d}$$
$$n_l^{(x)} = \{n\} \tag{226e}$$
$$n_{l'}^{(y)} = \{n\} \tag{226f}$$

$$H = -\sum_{j=1}^{N} \left[\frac{1+r}{2} \sigma_{j-1}^x \sigma^z \dots \sigma^z \sigma_{j+n}^x + \frac{1-r}{2} \sigma_{j-1}^y \sigma^z \dots \sigma^z \sigma_{j+n}^y + h\sigma_j^z \right] \tag{227}$$

We can also build different numbers of site interaction for each block, such as n-site interaction for X block and m-site interaction for Y block

$$N^{(x)} = 1 \tag{228a}$$
$$N^{(y)} = 1 \tag{228b}$$
$$J_l^{(x)} = \{(1+r)/2\} \tag{228c}$$
$$J_{l'}^{(y)} = \{(1-r)/2\} \tag{228d}$$
$$n_l^{(x)} = \{n\} \tag{228e}$$
$$n_{l'}^{(y)} = \{m\} \tag{228f}$$

$$H = -\sum_{j=1}^{N} \left[\frac{1+r}{2} \sigma_{j-1}^x \sigma^z \dots \sigma^z \sigma_{j+n}^x + \frac{1-r}{2} \sigma_{j-1}^y \sigma^z \dots \sigma^z \sigma_{j+m}^y + h\sigma_j^z \right] \tag{229}$$

3.2.2 GHZ-Cluster transition

In this part, we present GHZ-Cluster state which studied by Wolf et al. [74]. This time we choose $X = 2$ and a list of $J_l^{(x)}$ since we need two X blocks and $Y = 1$ even though we do not have Y block. We are choosing the strength $J_{l'}^{(y)} = n_{l'}^{(y)} = 0$ in order to eliminate Y block. As one can see we assign different value for h to build desired Hamiltonian. Here we give the parameters

$$h = (1+g)^2 \tag{230a}$$
$$N^{(x)} = 2 \tag{230b}$$
$$N^{(y)} = 1 \tag{230c}$$
$$J_l^{(x)} = \{-2(g^2-1), -(g-1)^2\} \tag{230d}$$
$$J_{l'}^{(y)} = \{0\} \tag{230e}$$
$$n_l^{(x)} = \{0, 1\} \tag{230f}$$
$$n_{l'}^{(y)} = \{0\} \tag{230g}$$

after a rotation of the Hamiltonian ($\sigma_x \to \sigma_z$) we reach

$$H = -\sum_{j=1}^{N}[2(g^2-1)\sigma_{j-1}^x\sigma_j^x + (g-1)^2\sigma_{j-1}^x\sigma^z\sigma_{j+1}^x - (1+g)^2\sigma_j^z] \tag{231}$$

where $g = 0$ for GHZ state $g = -1$ for cluster state.

Next figures show the global entanglement [75] upon using the solution which we derived in the previous section equation (217). The first figure shows the global entanglement per site (blue) and per block (orange, L=2) of GHZ states ($g = 0$). One can examine the derivative of the entanglement to see the divergence near the critical point.

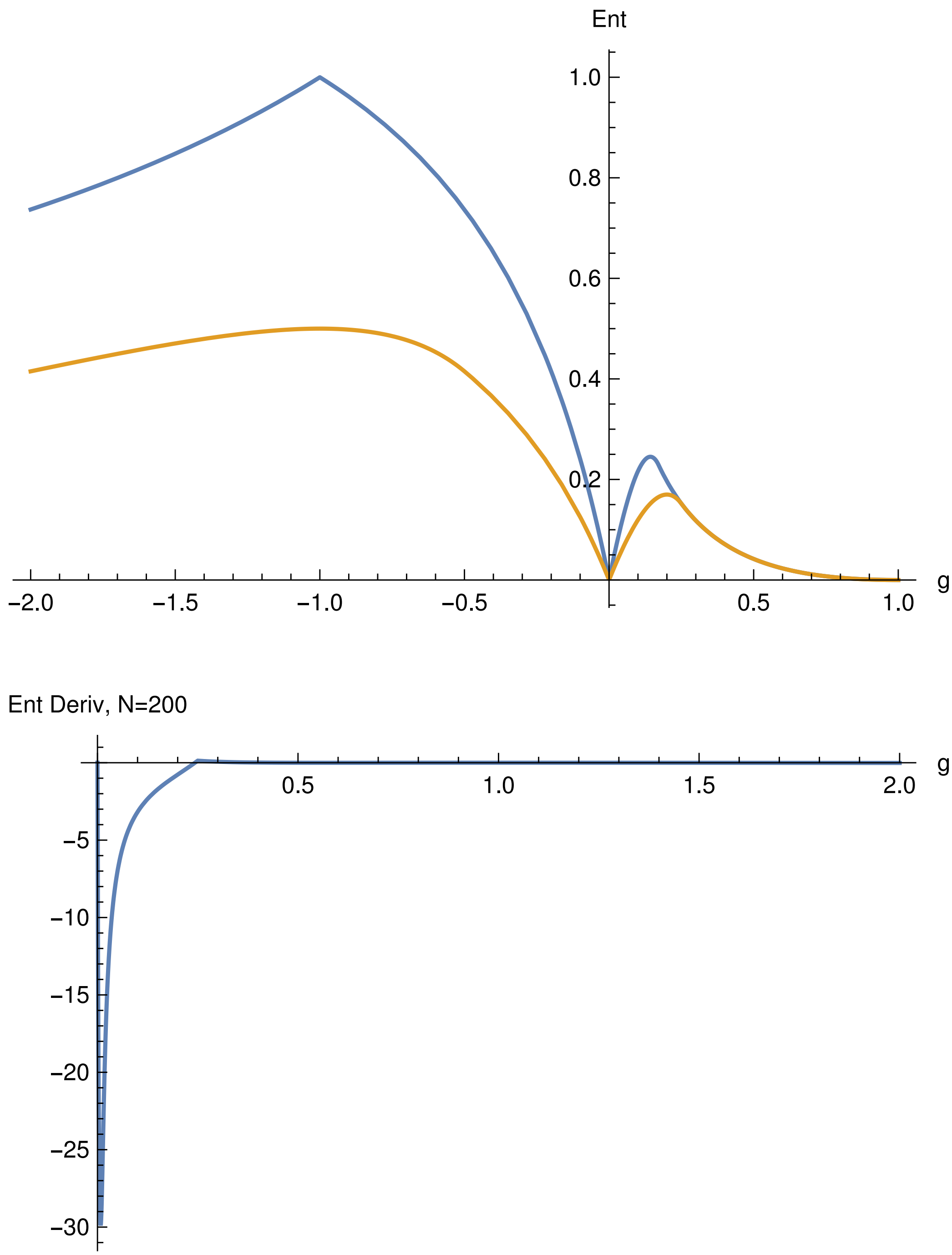

Figure 15: Geometric Entanglement per site (orange) and per block (blue, L=2) for GHZ-Cluster state (first). Derivative of the Entanglement per site (second) where N=200

3.2.3 SPT-Antiferromagnetic transition

At last, we examine quantum phase transition between a symmetry protected topological order and an antiferromagnetic phase [76] by using the same method we derived. We choose one X and one Y block. We set $h = 0$ to eliminate transverse field term. Parameters of the model considered is as follows

$$h = 0 \tag{232a}$$
$$N^{(x)} = 1 \tag{232b}$$
$$N^{(y)} = 1 \tag{232c}$$
$$J_l^{(x)} = \{1\} \tag{232d}$$
$$J_{l'}^{(y)} = \{\lambda\} \tag{232e}$$
$$n_l^{(x)} = \{1\} \tag{232f}$$
$$n_{l'}^{(y)} = \{0\} \tag{232g}$$

Thus the Hamiltonian

$$H = -\sum_{j=1}^{N} \sigma_{j-1}^x \sigma^z \sigma_{j+1}^x + \lambda \sum_{j=1}^{N} \sigma_{j-1}^y \sigma_j^y$$

As can be seen from the following plot, the quantum phase transition occurs at $\lambda = 1$

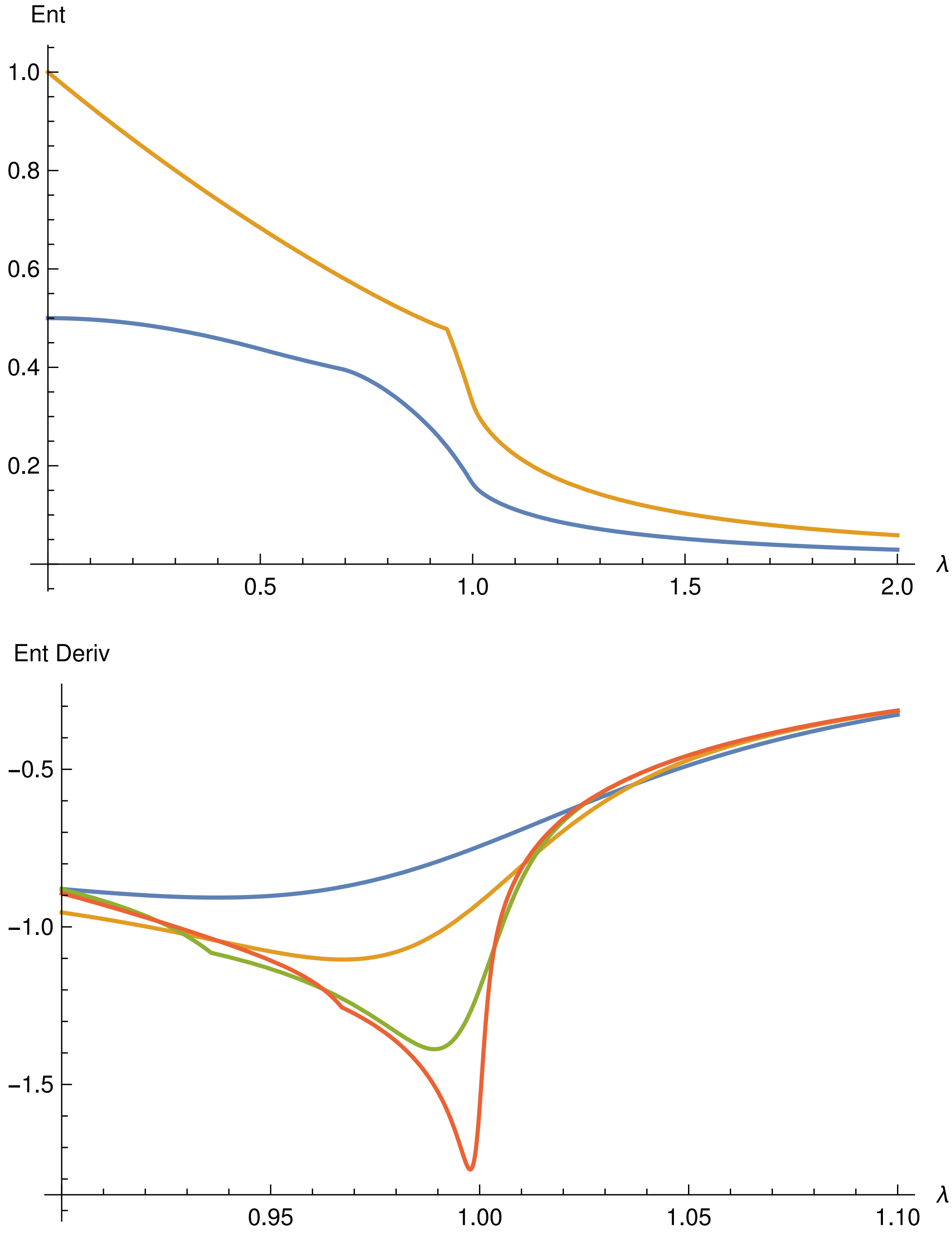

Figure 16: Geometric Entanglement per site (blue) and per block (orange) for SPT-Antiferromagnetic phase (first). Derivative of the Entanglement (second) where Blue: N=32, Orange: N=64, Green: N=200, Red: N=1000

4 Conclusion and Outlook

In this work, we have given a detailed treatment to diagonalization of the one-dimensional anisotropic XY model in the transverse field. We firstly presented Jordan-Wigner transformation and derived Fourier transformation and Bogoliubov transformation for generalized XY model with n-site interaction. Further, we introduced a geometric measure of entanglement per site/block for quantifying entanglement in the multipartite system. We examined global entanglement near the quantum critical point and investigated quantum phase transition in several models.

Later, we introduced the Quantum XY model with n-site interaction and obtained the energy eigenvalues for the general model. We specifically examined three-site interaction and show the emergence of quantum phase transition. Later we discussed halfway interaction and realized that field derivative of the global entanglement is continuous near the quantum critical point. We also discussed duality between one dimensional quantum XY model with n-site interaction and two dimensional Square-lattice Ising model.

In the last section, we introduced a generalized Cluster-XY Hamiltonian which one can examine quantum entanglement and quantum phase transition of many suitable bilinear Hamiltonian by defining quantities that characterize the model. We also presented several examples such as QPT between GHZ-Cluster phase and SPT-Antiferromagnetic phase.

For the future work, we shall examine global entanglement and quantum phase transition in two-dimensional models and attempt to generalize Cluster-XY Hamiltonian for higher spin problems.

References

[1] Hans Bethe. Zur theorie der metalle. *Zeitschrift für Physik*, 71(3-4):205–226, 1931.

[2] Ernst Ising. Beitrag zur theorie des ferromagnetismus. *Zeitschrift für Physik*, 31(1):253–258.

[3] Ian Affleck, Tom Kennedy, Elliott H. Lieb, and Hal Tasaki. Rigorous results on valence-bond ground states in antiferromagnets. *Phys. Rev. Lett.*, 59:799–802, Aug 1987.

[4] J. Hubbard. Electron Correlations in Narrow Energy Bands. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 276(1365):238–257, 1963.

[5] Wilhelm Lenz. Beitrag zum verständnis der magnetischen erscheinungen in festen körpern. *Z. Phys.*, 21:613–615, 1920.

[6] H. A. Kramers and G. H. Wannier. Statistics of the two-dimensional ferromagnet. part i. *Phys. Rev.*, 60:252–262, Aug 1941.

[7] Lars Onsager. Crystal statistics. I. A two-dimensional model with an order-disorder transition. *Physical Review*, 65(3-4):117–149, 1944.

[8] T. D. Lee and C. N. Yang. Statistical theory of equations of state and phase transitions. ii. lattice gas and ising model. *Phys. Rev.*, 87:410–419, Aug 1952.

[9] T. D. Schultz, D. C. Mattis, and E. H. Lieb. Two-dimensional Ising model as a soluble problem of many fermions, 1964.

[10] Barry M. McCoy and Tai Tsun Wu. The Two-Dimensional Ising Model, 1973.

[11] Elliott Lieb, Theodore Schultz, and Daniel Mattis. Two soluble models of an antiferromagnetic chain. *Annals of Physics*, 16(3):407–466, 1961.

[12] Barry M McCoy. Spin correlation functions of the x- y model. *Physical Review*, 173(2):531, 1968.

[13] Eytan Barouch, Barry M. McCoy, and Max Dresden. Statistical mechanics of the XY model. I. *Physical Review A*, 2(3):1075–1092, 1970.

[14] Eytan Barouch and Barry M McCoy. Statistical mechanics of the x y model. ii. spin-correlation functions. *Physical Review A*, 3(2):786, 1971.

[15] Rodne J Baxter. Exactly solvable models in statistical mechanics, 1982.

[16] Alexander R Its, Bai-Qi Jin, and Vladimir E Korepin. Entanglement in the xy spin chain. *Journal of Physics A: Mathematical and General*, 38(13):2975, 2005.

[17] F. Verstraete, M. Popp, and J. I. Cirac. Entanglement versus correlations in spin systems. *Phys. Rev. Lett.*, 92:027901, Jan 2004.

[18] Antonella De Pasquale and Paolo Facchi. XY model on the circle: Diagonalization, spectrum, and forerunners of the quantum phase transition. *Physical Review A - Atomic, Molecular, and Optical Physics*, 80(3):1–14, 2009.

[19] Masuo Suzuki. Relationship among Exactly Soluble Models of Critical Phenomena. I. *Progress of Theoretical Physics*, 46(5):1337–1359, 1971.

[20] Jiannis K. Pachos and Martin B. Plenio. Three-spin interactions in optical lattices and criticality in cluster hamiltonians. *Physical Review Letters*, 93(5):1–4, 2004.

[21] Ping Lou, Wen Chin Wu, and Ming Che Chang. Quantum phase transition in spin-1/2 XX Heisenberg chain with three-spin interaction. *Physical Review B - Condensed Matter and Materials Physics*, 70(6):064405, 2004.

[22] V. Derzhko, O. Derzhko, and J. Richter. Exact solution of a spin-1/2 XX chain with three-site interactions in a random transverse field: Influence of randomness on the quantum phase transition. *Physical Review B*, 83(17):174428, 2011.

[23] I. Titvinidze and G. I. Japaridze. Phase diagram of the spin S = 1/2 extended XY model. *European Physical Journal B*, 32(3):383–393, 2003.

[24] Juan I Cirac and Peter Zoller. Quantum computations with cold trapped ions. *Physical review letters*, 74(20):4091, 1995.

[25] A Imamog, David D Awschalom, Guido Burkard, David P DiVincenzo, Daniel Loss, M Sherwin, A Small, et al. Quantum information processing using quantum dot spins and cavity qed. *Physical Review Letters*, 83(20):4204, 1999.

[26] Konstantin Konstantinovich Likharev. *Dynamics of Josephson junctions and circuits*. Gordon and Breach science publishers, 1986.

[27] Mohamed Azzouz. Interchain-coupling effect on the one-dimensional spin-1/2 antiferromagnetic heisenberg model. *Phys. Rev. B*, 48:6136–6140, Sep 1993.

[28] O. Derzhko, T. Verkholyak, R. Schmidt, and J. Richter. Square-lattice s=1/2 XY model and the Jordan – Wigner fermions: the ground-state and thermodynamic properties. *Physica A*, 320:407 – 428, 2003.

[29] John Bardeen, Leon N Cooper, and J Robert Schrieffer. Theory of superconductivity. *Physical Review*, 108(5):1175, 1957.

[30] M Suzuki. The dimer problem and the generalized x-model. *Physics Letters A*, 34(6):338–339, 1971.

[31] Erwin Schrödinger. Discussion of probability relations between separated systems. In *Mathematical Proceedings of the Cambridge Philosophical Society*, volume 31, pages 555–563. Cambridge Univ Press, 1935.

[32] Albert Einstein, Boris Podolsky, and Nathan Rosen. Can quantum-mechanical description of physical reality be considered complete? *Physical review*, 47(10):777, 1935.

[33] John S Bell. On the einstein podolsky rosen paradox, 1964.

[34] John F. Clauser, Michael A. Horne, Abner Shimony, and Richard A. Holt. Proposed experiment to test local hidden-variable theories. *Phys. Rev. Lett.*, 23:880–884, Oct 1969.

[35] Alain Aspect, Philippe Grangier, and Gérard Roger. Experimental tests of realistic local theories via bell's theorem. *Phys. Rev. Lett.*, 47:460–463, Aug 1981.

[36] Dagmar Bruss. Characterizing entanglement. *Journal of Mathematical Physics*, 43(9):4237–4251, 2002.

[37] Michael Nielsen and Isaac L. Chuang. Quantum Computation and Quantum Information, 2000.

[38] Charles H Bennett, Gilles Brassard, Claude Crépeau, Richard Jozsa, Asher Peres, and William K Wootters. Teleporting an unknown quantum state via dual classical and einstein-podolsky-rosen channels. *Physical review letters*, 70(13):1895, 1993.

[39] Peter W Shor. Algorithms for quantum computation: Discrete logarithms and factoring. In *Foundations of Computer Science, 1994 Proceedings., 35th Annual Symposium on*, pages 124–134. IEEE, 1994.

[40] Lov K Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the twenty-eighth annual ACM symposium on Theory of computing*, pages 212–219. ACM, 1996.

[41] Artur K Ekert. Quantum cryptography based on bell's theorem. *Physical review letters*, 67(6):661, 1991.

[42] Charles H Bennett, David P DiVincenzo, John A Smolin, and William K Wootters. Mixed State Entanglement and Quantum Error Correction. *Physical Review A*, 54(1):7, 1996.

[43] Luigi Amico, Rosario Fazio, Andreas Osterloh, and Vlatko Vedral. Entanglement in many-body systems. *Reviews of Modern Physics*, 80(2):517–576, 2008.

[44] Ingo Peschel. Special review: entanglement in solvable many-particle models. *Brazilian Journal of Physics*, 42(3-4):267–291, 2012.

[45] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight. Quantifying Entanglement. *Physical Review Letters*, 78(12):2275–2279, 1997.

[46] Dieter Heiss. *Fundamentals of quantum information: quantum computation, communication, decoherence and all that*, volume 587. Springer, 2008.

[47] Juan Ignacio Cirac. *Fundamentals of Quantum Information: Quantum Computation, Communication, Decoherence and All That*, chapter Quantum Information: Entanglement, Purification, Error Correction, and Quantum Optical Implementations, pages 199–239. Springer Berlin Heidelberg, Berlin, Heidelberg, 2002.

[48] Daniel M Greenberger, Michael A Horne, and Anton Zeilinger. Going beyond bell's theorem. In *Bell's theorem, quantum theory and conceptions of the universe*, pages 69–72. Springer, 1989.

[49] William K Wootters. Entanglement of formation of an arbitrary state of two qubits. *Physical Review Letters*, 80(10):2245, 1998.

[50] William K Wootters. Entanglement of formation and concurrence. *Quantum Information & Computation*, 1(1):27–44, 2001.

[51] Abner Shimony. Degree of entanglement. *Annals of the New York Academy of Sciences*, 755:675, 1995.

[52] H. Barnum and N. Linden. Monotones and invariants for multi-particle quantum states. *J. Phys. A: Math. Theor.*, 34:6787, 2001.

[53] Tzu-Chieh Wei and Paul M. Goldbart. Geometric measure of entanglement and applications to bipartite and multipartite quantum states. *Phys. Rev. A*, 68:042307, Oct 2003.

[54] Tzu-Chieh Wei, Smitha Vishveshwara, and Paul M. Goldbart. Global geometric entanglement in transverse-field XY spin chains: finite and infinite systems. *arXiv preprint*, page 36, 2010.

[55] Ching Yu Huang and Feng Li Lin. Multipartite entanglement measures and quantum criticality from matrix and tensor product states. *Physical Review A - Atomic, Molecular, and Optical Physics*, 81(3):1–9, 2010.

[56] Subir Sachdev. *Quantum Phase Transitions 2nd*. 2nd edition, 2011.

[57] Tobias J. Osborne and Michael a. Nielsen. Entanglement, Quantum Phase Transitions, and Density Matrix Renormalization. *Quantum Information Processing*, 1(April):45–53–53, 2002.

[58] Huihuo Zheng. Entanglement in quantum phase transition. pages 1–10, 2012.

[59] Matthias Vojta. Quantum phase transitions. *Rep. Prog. Phys.*, 66:2069–2110, 2003.

[60] Jeffrey Goldstone, Abdus Salam, and Steven Weinberg. Broken symmetries. *Physical Review*, 127(3):965–970, 1962.

[61] E Castellani. On the meaning of symmetry breaking. *Symmetries in Physics: Philosophical Reflections*, 2003.

[62] Shigetoshi Katsura. Statistical mechanics of the anisotropic linear Heisenberg model. *Physical Review*, 127(5):1508–1518, 1962.

[63] Román Orús and Tzu Chieh Wei. Visualizing elusive phase transitions with geometric entanglement. *Physical Review B - Condensed Matter and Materials Physics*, 82(15):1–6, 2010.

[64] Holstein Primakoff and T Holstein. Many-body interactions in atomic and nuclear systems. *Physical Review*, 55(12):1218, 1939.

[65] Pascual Jordan and Eugene Paul Wigner. über das paulische äquivalenzverbot. In *The Collected Works of Eugene Paul Wigner*, pages 109–129. Springer, 1993.

[66] Michael Nielsen. The Fermionic canonical commutation relations and the Jordan-Wigner transform. *Michaelnielsen.Org*, pages 1–8, 2005.

[67] Pierre Pfeuty. The one-dimensional ising model with a transverse field. *ANNALS of Physics*, 57(1):79–90, 1970.

[68] J. Oitmaa and a. von Brasch. Spin-1 Ising model in a transverse crystal field. *Physical Review B*, 67(17):1–4, 2003.

[69] HW Capel. On the possibility of first-order phase transitions in ising systems of triplet ions with zero-field splitting. *Physica*, 32(5):966–988, 1966.

[70] Tzu-Chieh Wei, Dyutiman Das, Swagatam Mukhopadyay, Smitha Vishveshwara, and Paul M Goldbart. Global entanglement and quantum criticality in spin chains. *Physical Review A*, 71(6):060305, 2005.

[71] Masuo Suzuki. Relationshio between d-Dimensional Quantal Spin Systems and (d+1)-Dimensional Ising Systems. 56(5):1454–1469, 1976.

[72] SL Sondhi, SM Girvin, JP Carini, and D Shahar. Continuous quantum phase transitions. *Reviews of Modern Physics*, 69(1):315, 1997.

[73] Marek M. Rams, Valentin Zauner, Matthias Bal, Jutho Haegeman, and Frank Verstraete. Truncating an exact matrix product state for the XY model: Transfer matrix and its renormalization. *Physical Review B - Condensed Matter and Materials Physics*, 92(23):8, 2015.

[74] Michael M Wolf, Gerardo Ortiz, Frank Verstraete, and J Ignacio Cirac. Quantum phase transitions in matrix product systems. *Physical review letters*, 97(11):110403, 2006.

[75] Tzu-Chieh Wei. Entanglement under the renormalization-group transformations on quantum states and in quantum phase transitions. *Physical Review A*, 81(6):062313, 2010.

[76] W Son, L Amico, R Fazio, A Hamma, S Pascazio, and V Vedral. Quantum phase transition between cluster and antiferromagnetic states. *EPL (Europhysics Letters)*, 95(5):50001, 2011.

[77] John Chalker. Quantum Theory of Condensed Matter Overall scheme Anderson insulator. *Quantum*, pages 1–12, 2009.

A Bogoliubov Transformation in the Matrix Form

In this part, we present generalised matrix form of the Bogoliubov transformation for the bilinear Hamiltonians. Hamiltonian can be written in two ways [77]

For real β

$$H = \lambda\left(c_1^\dagger c_1 + c_2^\dagger c_2\right) + \beta\left(c_1^\dagger c_2^\dagger + c_2 c_1\right) \tag{A-1}$$

We define the Bogoliubov angle where $\{\gamma_i, \gamma_j^\dagger\} = \delta_{ij}$

$$\tilde{c}_1 = \cos\theta\ \gamma_1 + i\sin\theta\ \gamma_2^\dagger \tag{A-2a}$$

$$\tilde{c}_1^\dagger = \cos\theta\ \gamma_1^\dagger - i\sin\theta\ \gamma_2 \tag{A-2b}$$

$$\tilde{c}_2 = \cos\theta\ \gamma_2 - i\sin\theta\ \gamma_1^\dagger \tag{A-2c}$$

$$\tilde{c}_2^\dagger = \cos\theta\ \gamma_2^\dagger + i\sin\theta\ \gamma_1 \tag{A-2d}$$

writing the Bogoliubov transformation in the matrix form

$$\begin{pmatrix} c_1 \\ c_2^\dagger \end{pmatrix} = \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2^\dagger \end{pmatrix} \tag{A-3}$$

we can write Hamiltonian (A-1) in the matrix form

$$H = \frac{1}{2}\begin{pmatrix} c_1^\dagger & c_2 & c_2^\dagger & c_1 \end{pmatrix} \begin{pmatrix} \lambda & \beta & 0 & 0 \\ \beta & -\lambda & 0 & 0 \\ 0 & 0 & \lambda & -\beta \\ 0 & 0 & -\beta & -\lambda \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} + \lambda \tag{A-4}$$

calculating upper 2×2 block and doing the same calculation for other block

$$\begin{pmatrix} \cos\theta & -i\sin\theta \\ -i\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \lambda & \beta \\ \beta & -\lambda \end{pmatrix} \begin{pmatrix} \cos\theta & i\sin\theta \\ i\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix} \tag{A-5}$$

$$= \begin{pmatrix} \gamma_1^\dagger & \gamma_2 \end{pmatrix} \begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix} \begin{pmatrix} \gamma_1 \\ \gamma_2^\dagger \end{pmatrix} \tag{A-6}$$

diagonalized Hamiltonian can be written where $\epsilon = \sqrt{\lambda^2 + \beta^2}$

$$H = \epsilon \left(\gamma_1^\dagger \gamma_1 + \gamma_2^\dagger \gamma_2 \right) + \lambda - \epsilon \tag{A-7}$$

For complex β

$$H = \lambda \left(c_1^\dagger c_1 + c_2^\dagger c_2 \right) + \beta \left(c_1^\dagger c_2^\dagger - c_2 c_1 \right) \tag{A-8}$$

we can write Hamiltonian (A-8) in the matrix form

$$H = \frac{1}{2} \begin{pmatrix} c_1^\dagger & c_2 & c_2^\dagger & c_1 \end{pmatrix} \begin{pmatrix} \lambda & \beta & 0 & 0 \\ -\beta & -\lambda & 0 & 0 \\ 0 & 0 & \lambda & -\beta \\ 0 & 0 & \beta & -\lambda \end{pmatrix} \begin{pmatrix} c_1 \\ c_2^\dagger \\ c_2 \\ c_1^\dagger \end{pmatrix} + \lambda \tag{A-9}$$

invoking the same method, we reached diagonalized Hamiltonian where $\epsilon' = \sqrt{\lambda^2 - \beta^2}$

$$H = \epsilon' \left(\gamma_1^\dagger \gamma_1 + \gamma_2^\dagger \gamma_2 \right) + \lambda - \epsilon' \tag{A-10}$$