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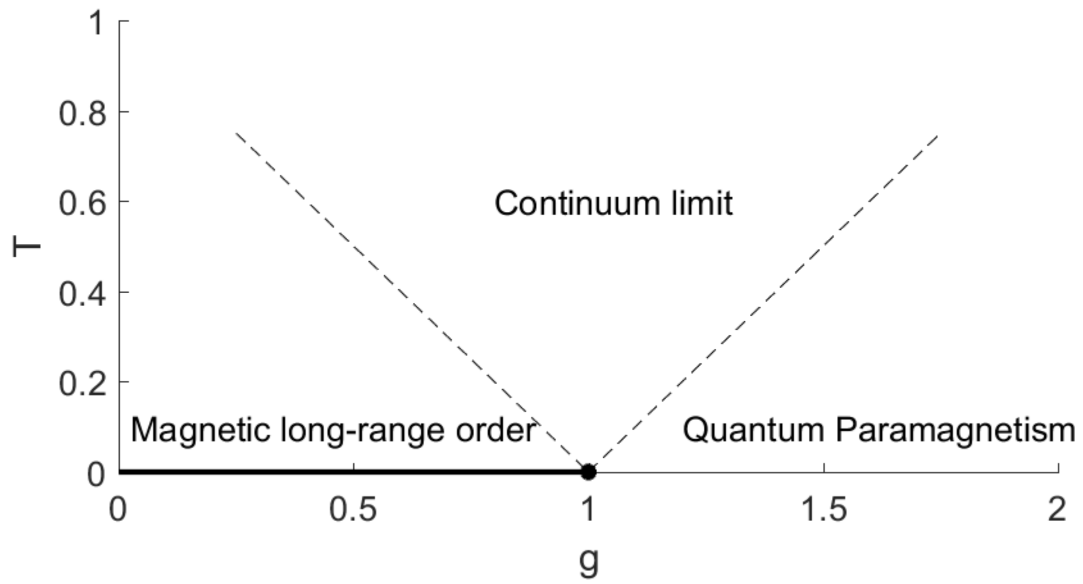

Quantum Criticality –

The transverse field Ising model

Emil Lytthans Boesen

Bachelor Thesis

Supervisor: Jens Paaske

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Abstract

In this thesis, critical behaviour of the classical and transverse quantum Ising model is analysed in zero and one dimension. This is done by evaluating the correlation function and correlation length, in each case, and finding the points where ξ diverges. In the zero-dimensional case, neither the quantum- or the classical model have any critical point. On the other hand, in one dimensional case, both classical and quantum model have phase transitions. Using the transfer matrix, the correlation length of the classical case is shown be have a quantum phase transition at zero field, the long-range order is achieved. In the quantum case, a Jordan-Wigner and a Bogoliubov transformation is used to diagonalize the Hamiltonian. The correlation function and length is then calculated by using the dynamics of domain walls in the limit $T \ll 2J(1-g)$. In analysis reveals an quantum critical point in $g_c = 1$ and the system experience long-rang order in the limit $T \ll 2J(1-g)$

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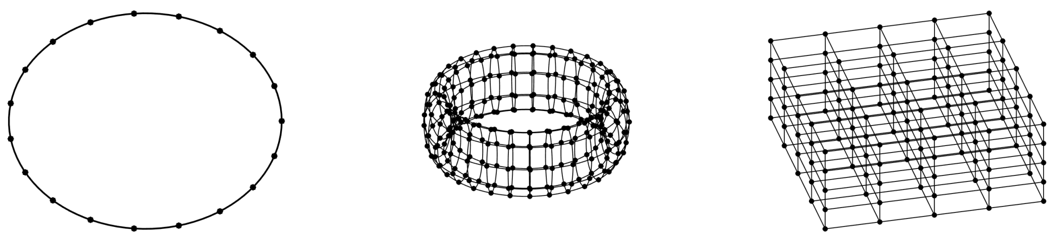
1 Introduction

In condensed matter- and high energy physics, a common model to describe interactions of many-particle system, is the Ising model. The model was first proposed by the German Physicist Ernst Ising [1] to describe theory of ferromagnets. Even though, the model was designed to describe magnets, it is also used as a toy model for studying integrable systems and qunatum critical behaviour in Theoretical Physics [2]. The Ising model was originally written as a classical model and has since been quantized to fit reality better. This new model is named the quantum Ising model and describes the interactions between spins on sites sitting in a d-dimensional grid with constant separation a and periodic boundary conditions. In one dimension, the Ising model describes a closed chain of N sites with perimeter L, fig 1a. Going a dimension up, the two dimensional grid takes the for of a cylinder joint at the ends, fig. 1b. Here, there are two different loops. One with N_x particles and perimeter L_x, and another with N_y particles and perimeter L_y. At last, in three dimensions, the grid takes the shape of a hypertorus in a four dimensional space. Along the x_i'th direction, the grid is periodic with length L_i and have N_i particles in each direction. The physical realization is last model is of course impossible, but should give the same results as a real grid with dimensions (L_x, L_y, L_z) for large system. The three scenarios are plotted in figure 1. In the Ising model, a given spin, at site i, interacts with the spin, at site j, with exchange energy $-J_{ij}$. If $J_{ij} > 0$, the interaction is called ferromagnetic, since its energetically favourable for the spins to align. In the other case, $J_{ij} < 0$, its energetically favourable for spins to anti-align, and the case is therefore called antiferromagnetic. A (QIM) of this kind is describes by the Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{ij} J_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z \tag{1.1}$$

in units where $\hbar = 1$. To make things simpler, the model is often limited to nearest neighbour interactions only. In other words $J_{ij} \neq 0$ if and only if site i and j are nearest neighbours. This model is called the nearest neighbour quantum Ising model and have hamiltonian

$$\hat{\mathcal{H}} = -J\sum_{<i,j>} \hat{\sigma}_i^z\hat{\sigma}_j^z \tag{1.2}$$



(a) $d = 1$ Ising Chain (b) $d = 2$ Ising Doughnut (c) $d = 3$ Ising Grid

Figure 1: The grid of an Ising model in $d = 1, 2, 3$ dimension with periodic boundary conditions. a) In one dimension, the sites is placed in a circle with perimeter L. b) In two dimensions, the sites make a sheath in the form of a closed cylinder. The cylinder has different perimeter, L_x and L_y, and number of particles N_x and N_y. c) In three dimensions, the sites makes a three dimensional grid. The periodic boundary conditions is not drawn here due to lack of dimensions.

where $\langle i,j\rangle$ refers to the sum over i and it's nearest neighbours j. In the ferromagnetic case, the ground state of this model has a two-fold degeneracy

$$|+\rangle \equiv \bigotimes_{i=1}^{N} |\uparrow\rangle \quad \text{and} \quad |-\rangle \equiv \bigotimes_{i=1}^{N} |\downarrow\rangle \tag{1.3}$$

with energy $E_0 = -2dJN$ and N being the total number of sites in the grid. Here $\{|\uparrow\rangle, |\downarrow\rangle\}$ are the eigenstates of the spin operator, $\hat{\sigma}^z$. In the ground state, all the spins align thereby creates a spontaneous magnetic field M. The direction of the field is either in the positive or negative z-direction is chosen by spontaneous symmetry breaking. The cause of this degeneracy is a Z_2 symmetric, generated by the transformation $\hat{U}(\theta) = \exp(i\theta \prod_j \hat{\sigma}^x_j)$ that maps the spin operators into negative of themselves

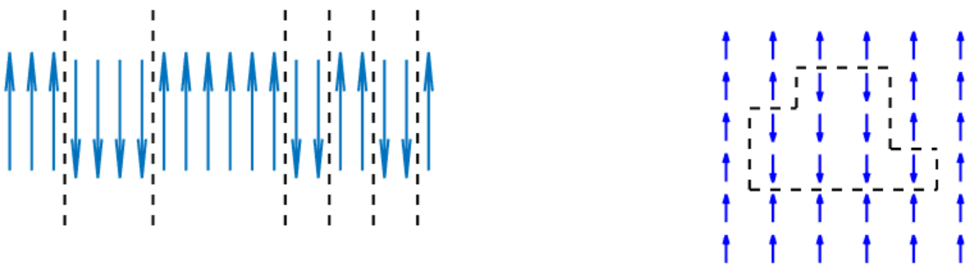
$$U : \hat{\sigma}^\alpha_i \to -\hat{\sigma}^\alpha_i \tag{1.4}$$

The Hamiltonian (1.2) is invariant under this transformation, which implies the degeneracy. The first excited states of the Ising model can be achieved by creating two domain walls in the grid, fig 2. These walls separates the grid into regions with different polarizations, creating wall domain with opposite magnetic field, compared to its neighbourhood. This weakens the magnetization M, and in the limit of many domain walls, the magnetization vanishes. In the antiferromagnetic case, these many domain wall states are the ground state, and the magnetization vanished completely for low temperatures T. Do to the translational invariance of the Ising model, a domain of a given size can moved around without any energy cost, which causes a big degeneracy is the energy spectrum. Even though, the Ising model described by the Hamiltonian (1.2) is completely solvable, and one can find every eigenstate of the Hamiltonian creating and moving around domain walls.

This is all well and good until someone comes and turns on a magnetic field, $h^\alpha_i = Jg^\alpha_i$. This adds a new term to the Hamiltonian

$$\hat{\mathcal{H}} = -\sum_{<i,j>} J\hat{\sigma}^z_i\hat{\sigma}^z_j - J\sum_i g^\perp_i \hat{\sigma}^x_i + g^\parallel_i \hat{\sigma}^z_i \tag{1.5}$$

in units where $\mu_0 = 1$. Here $g^\alpha_i > 0$ is a dimensional coupling constant, which later will be used as order parameter to study critical points in the quantum Ising model. The new term breaks the Z_2 symmetry and mixes the eigenstates of the Hamiltonian. This new model is called the transverse field Ising model, and is, in most cases, not been solved.



(a) (b)

Figure 2: Example of domain walls is the one- and two dimensional quantum Ising model. The arrows indicate the spin direction, while the dashed lines indicated the domain walls

1.1 The classical Ising model i longitudinal field

When a problem is very hard to answer, it is sometimes beneficial to solve a simpler version of the original problem. Sometimes, the answer to the simpler version can then help one understand the harder problem. Therefore, the classical Ising model, the one from Ising's original paper, [1], is still useful and studied. In the classical model, spin operators are replaced by numbers, which can either plus of minus one

$$H_c = -J \sum_{<i,j>} m_i m_j - h \sum_i m_i \tag{1.6}$$

Here, $m_i \in \{-1, 1\}$ are just numbers and correspond to a classical spin in either a up or down state. Again, J is the interaction energy between spin and h is a longitudinal field. Unfortunately, the classical Ising model disagrees with the quantum model on crucial point. One problem is, that since the model is classical, quantum fluctuations doesn't exist, and the model is therefore static in time. Another problem is that the model cannot handle transverse fields. The model is therefore not only wrong, but cannot even mimic the quantum model correctly. Even then, the classical model is not completely useless. This is because, as we will see later, a classical field theory of dimension D can be maps into a quantum field theory in dimension d, via

$$D = d + 1 \tag{1.7}$$

This is accomplished by mapping one of the spacial dimensions of the classical model, into a complex time coordinate in the quantum field theory. In this way, the dynamics of a quantum field theory can be solved by solving a classical field theory in a higher dimension. The mapping is not exact, but works in some cases. The behaviour of the classical model can therefore be used to study the dynamics and phase transitions of the quantum model.

1.2 Quantum critical points and quantum phase transitions

A quantum critical point, in the context of condensed matter physics, is a point at $T = 0$, where the system changes characteristic in a non-analytical way. It is often the case, that one has a Hamiltonian, $H(g)$, that dependence on a parameter g. From this Hamiltonian, the partition function and free energy, of the system, can be calculated via

$$Z = \text{tr } e^{-\hat{\mathcal{H}}/T} = \sum_{a \in A} \langle a| \exp^{-\hat{\mathcal{H}}/T} |b\rangle \quad \text{and} \quad F = -T \ln Z \tag{1.8}$$

in units where $k_B = 1$. Here $A \subset \mathbb{H}$ is an arbitrary set of basis in the total ket-space $\mathbb{H}$ of the system. In an arbitrary basis, the exponential function of $-\hat{\mathcal{H}}/T$ is very hard to calculate. This is due to the definition of the exponential function for matrices, which involves an infinite number of matrix products

$$e^{\hat{A}} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n \tag{1.9}$$

In the eigenbasis of $\hat{\mathcal{H}}$, the matrix product simplifies greatly and the partition function just becomes a sum of Boltzmann factors

$$Z = \sum_{a \in A} e^{-E_a(g)/T} \tag{1.10}$$

From Z and F, most statistical objects can be calculated. When looking at the transverse field Ising model, (1.5), the order parameter is often the transverse magnetic field, h, and/or the temperature T. At critical points, the partition function will become non-analytical, and its high-order derivatives will diverge. When crossing these critical points, the system experience a quantum phase transition. The non-analytical behaviour of the system comes from the energy gap Δ, which is the energy difference between the first excited state of the system and the ground that, will vanish $\Delta \ll T$. If the non-analyticity happens for the second order derivative of the partition function, the phase transition is said to be of second order.

To study phase transitions, another interesting statistical object to look at, is the two-point spin correlation function $C(x_2, x_1; t_2, t_1)$. The correlation function tell how much a spin at position x_2 and time t_2 is correlated with the spin at position x_1 and time t_1. If there is a high probability for the spins will point in the same direction, when averaging over every allowed configuration, the spins are correlated strongly and $C \approx 1$. In the other limit, if the spin are random oriented, the spins are not correlated at all and $C = 0$. At last, if the spins are strongly correlated, but anti-align, the correlation function $C \approx -1$. To describe this, the correlation function is defined as

$$C(x,t) \equiv \langle \hat{\sigma}^z(x,t)\hat{\sigma}^z(0,0)\rangle = \begin{cases} \frac{1}{Z}\mathrm{tr}\left(e^{-\hat{\mathcal{H}}/T}\hat{\sigma}^z(x,t)\hat{\sigma}^z(0,0)\right) & \text{for} \quad t > 0 \\ 0 & \text{for} \quad t < 0 \end{cases} \tag{1.11}$$

where $x = x_2 - x_1$ and $t = t_2 - t_1$. Here, the translation- and time shift invariance of the Hamiltonian is used, so C only depends on the difference in space and time coordinates. Also, the correlation function is zero for $t < 0$ because of causality. In some cases, the equal-time correlation function, $C(x, 0)$ falls off exponentially in terms of separation $|x|$

$$C(x,0) \propto e^{-|x|/\xi} \tag{1.12}$$

Here ξ is called the correlation length and is often both temperature and field depended. For second-order phase transitions, the correlation length diverges, which results in the equal-time correlation function being constant $C(x,0) = \pm N_0^2$ for all separations $|x|$. The constant, $N_0 = \langle \hat{\sigma}_i^z \rangle$, at the critical point. The system therefore experience long-range order, where all spins in the grid are strongly correlated.

In this these, the phase transitions of the classical- and quantum Ising model in $d = 0, 1$ dimension, are studied using the method describes before.

2 Single Spin

Starting slow, the simplest case of the Ising model, is a single spin i a magnetic field h. The Ising model for this system can be solved for both the classical case and the quantum case. In this chapter, the the magnetization, magnetic susceptibility, and the correlation function is calculated for both the classical- and quantum case.

2.1 Single Classical spin in longitudinal field

Beginning with the classical model in longitudinal field, h, the Hamiltonian simply takes the form of

$$H_{\text{Classical}} = -hm \tag{2.1}$$

with $m \in \{-1, 1\}$. The energy difference, between the up- and down state, called the energy gap $\Delta = 2h$. From H, the partition function, free energy, and magnetization can then be calculated

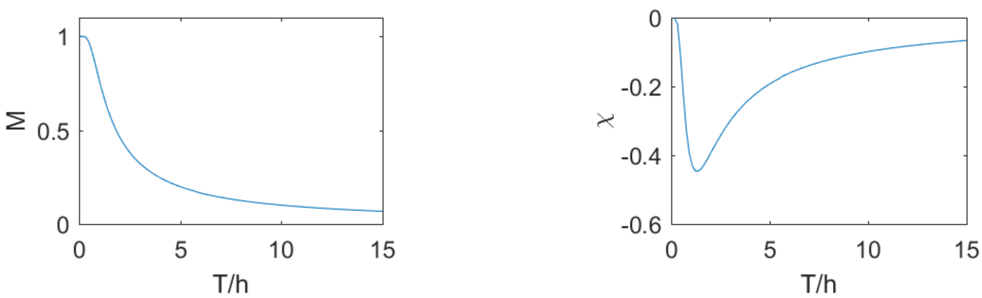
$$Z = \sum_{m\in\{-1,1\}} e^{-hm/T} = e^{-h/T} + e^{h/T} = 2\cosh(h/T) \tag{2.2}$$

$$F = -T\ln Z = -T\ln\left[2\cosh(h/T)\right] \tag{2.3}$$

$$M = -\frac{\partial F}{\partial h} = \tanh(h/T), \quad \chi = \frac{\partial M}{\partial h} = -\frac{1}{T\cosh^2(h/T)} \tag{2.4}$$

For low temperature, as also seen from fig. 3a, the spin mostly point along the h field, when gives the magnetization $M \approx 1$. As temperature increase, the energy gap $\Delta = 2h$ become less significant and the probability of being in the spin up and down state equals out $P_-/P_+ = e^{-\Delta/T} \overset{(T\to\infty)}{\to} 1$. The magnetization, M, therefore decreases, and in the limit of $T \gg \Delta$ it completely vanished. Looking at the susceptibility, it does not have any discontinuities, which implies no second order phase transition.

Because the classical model does not capture the quantum fluctuations, the time-correlation function does not depend on time. The spin, when measured in the m state will then stay there forever, and the model is static.



(a) (b)

Figure 3: Magnetization (a) and susceptibility (b) of a single classical Ising spin in a magnetic field h as a function of temperature.

2.2 Single Quantum Spin in magnetic field

Things get more interesting in the quantum case. First of all, the model can now handle transverse fields, $h_\perp$, which gives a Hamiltonian of

$$\hat{\mathcal{H}} = -h_\parallel \hat{\sigma}^z - h_\perp \hat{\sigma}^x = -\begin{pmatrix} h_\parallel & h_\perp \\ h_\perp & h_\parallel \end{pmatrix} \tag{2.5}$$

writing the Hamiltonian in matrix notation. The eigenvalues with corresponding eigenstates can be calculated

$$E_\pm = \pm\sqrt{h_\parallel^2 + h_\perp^2} = \pm h \quad \text{with} \quad v_\pm = \frac{1}{\sqrt{2h}} \begin{pmatrix} \frac{h_\perp}{\sqrt{h \pm h_\parallel}} \\ \mp\sqrt{h \pm h_\parallel} \end{pmatrix} \tag{2.6}$$

Note here, that the eigenvalues of the quantum model is the same as in the classical case. Therefore, both models shares magnetization and susceptibility, as well as the lack of phase transitions. Another this is that since this is a quantum model, then or non-zero values of $h_\perp$, the spin operators does not commutate with the Hamiltonian, i.e. $\left[\hat{\sigma}^{z,x}, \hat{\mathcal{H}}\right] \neq 0$. In Heisenberg picture of Quantum Mechanics, the spin operators are therefore not constant in time, but rather follows the dynamics prescribed by

$$\frac{d\hat{\sigma}^\alpha}{dt} = \frac{1}{i\hbar}\left[\hat{\sigma}^\alpha, \hat{\mathcal{H}}\right] \neq 0 \tag{2.7}$$

This changes the time-correlation function, since the spin operators now is time dependent. This results in

$$C(t_1, t_2) = \frac{1}{Z}\text{tr}\left[e^{-\hat{\mathcal{H}}/T}\hat{\sigma}^z(t_2)\hat{\sigma}^z(t_1)\right] \qquad \text{for} \qquad t_2 \geq t_1 \tag{2.8}$$

where the operators $\hat{\sigma}_i^z(t)$ is the time-evolution of the spin operator along the z axis. For $t_1 > t_2$, the correlation is zero to account for causality. In Heisenberg picture, this is given by $\hat{\sigma}^z(t) = e^{i\hat{\mathcal{H}}t}\hat{\sigma}^z e^{-i\hat{\mathcal{H}}t}$ The correlation function can therefore be written as

$$\begin{aligned} C(t_2, t_1) &= \frac{1}{Z}\text{tr}\left[e^{-\hat{\mathcal{H}}/T}\left(e^{i\hat{\mathcal{H}}t_1}\hat{\sigma}^z e^{-i\hat{\mathcal{H}}t_1}\right)\left(e^{i\hat{\mathcal{H}}t_2}\tilde{\sigma}^z e^{-i\hat{\mathcal{H}}t_2}\right)\right] && (2.9) \\ &= \frac{1}{Z}\text{tr}\left[e^{-\hat{\mathcal{H}}/T(1+iT(t_2-t_1))}\hat{\sigma}^z e^{i\hat{\mathcal{H}}(t_2-t_1)}\hat{\sigma}^z\right] && (2.10) \end{aligned}$$

In the last equality, the cyclic invariance of the trace is used. Changing to the eigenbasis of $\hat{\mathcal{H}}$, the spin operator changes via the basis transformation, $\sigma^z \to S^{-1}\sigma^z S$ with transformation matrix S

$$S = \frac{1}{\sqrt{2h}}\begin{pmatrix} \frac{h_\perp}{\sqrt{h+h_\parallel}} & \frac{h_\perp}{\sqrt{h-h_\parallel}} \\ -\sqrt{h+h_\parallel} & \sqrt{h-h_\parallel} \end{pmatrix} \quad \text{and} \quad S^{-1} = \frac{1}{\sqrt{2h}}\begin{pmatrix} \frac{\sqrt{h+h_\parallel}(h-h_\parallel)}{h_\perp} & -\sqrt{h+h_\parallel} \\ \frac{\sqrt{h-h_\parallel}(h+h_\parallel)}{h_\perp} & \sqrt{h-h_\parallel} \end{pmatrix}$$

the spin operator in the new basis can then be calculated

$$\tilde{\sigma}^z = S^{-1}\sigma^z S = \frac{1}{h}\begin{pmatrix} -h_\parallel & h_\perp \\ h_\perp & h_\parallel \end{pmatrix} \tag{2.11}$$

Putting it all together, the time-correlation function of the single quantum spin can be calculated.

$$\begin{aligned} C(t_1, t_2) &= \frac{1}{Zh^2}\text{tr}\left[\begin{pmatrix} e^{ha} & 0 \\ 0 & e^{-ha} \end{pmatrix}\begin{pmatrix} -h_\parallel & h_\perp \\ h_\perp & h_\parallel \end{pmatrix}\begin{pmatrix} e^{-ihb} & 0 \\ 0 & e^{ihb} \end{pmatrix}\begin{pmatrix} -h_\parallel & h_\perp \\ h_\perp & h_\parallel \end{pmatrix}\right] && (2.12) \\ &= \frac{1}{Zh^2}\left[h_\parallel^2 e^{h(a-ib)} + h_\perp^2 e^{h(a+ib)} + h_\perp^2 e^{-h(a+ib)} + h_\parallel^2 e^{-h(a-ib)}\right] && (2.13) \end{aligned}$$

with $a = \frac{1+iT|t_2-t_1|}{T}$ and $b = |t_2 - t_1|$. Writing out a and b, the exponents reduces to

$$a - ib = \frac{1}{T} \quad \text{and} \quad a + ib = \frac{1}{T} + 2i|t_2 - t_1| \tag{2.14}$$

which results in a correlation function of

$$C(t_1, t_2) = \frac{h_\parallel^2}{h^2} + \frac{h_\perp^2}{h^2} \frac{\cosh\left(\frac{h(1-2iT|t_2-t_1|)}{T}\right)}{\cosh(h/T)} \tag{2.15}$$

This result can be rewritten as a scaling invariant function, $\tilde{\Phi}(y_1, y_2, y_3)$, with $y_1 = T|t_2 - t_1|$, $y_2 = \frac{2h_\parallel}{T}$, $y_3 = \frac{h_\perp}{T}$

$$\tilde{\Phi}_\sigma(y_1, y_2, y_3) = \frac{4y_3^2}{y_2^2 + 4y_3^2} + \frac{y_2^2}{y_2^2 + 4y_3^2} \frac{\cosh\left(\sqrt{y_2^2 + 4y_3^2}(1 - 2i|y_1|)/2\right)}{\cosh(\sqrt{y_2^2 + 4y_3^2}/2)} \tag{2.16}$$

Plotting the scaling function as a function of y_1 with y_2 and y_3, the function traces out an ellipse in the complex plane, fig 4. The ellipse has centre in $C = \frac{4y_3^2}{y_2^2+4y_3^2}$ and have semi-minor axis $a = \frac{y_2^2-4y_3^2}{y_2^2+4y_3^2}$ and semi-major axis $b = \frac{y_2}{y_2+4y_3^2}\tanh(L/\sqrt{y_2^2 + 4y_3^2})$. When varying y_1, the scaling function repeated it self for $y_1 \to y_1 + TP$. This means that the Single Quantum spin is 100% correlated to itself at a later time P. For the qunatum Ising spin, the period is given by

$$P = \frac{\pi}{\sqrt{h_\parallel^2 + h_\perp^2}} = \frac{\pi}{h} \tag{2.17}$$

which means that the time evolution of the single spin is periodic an angular frequency $\omega = 2h$. This is an already known result from classical Larmor precession, where a spin placed in a magnetic field B, precesses with angular frequency $\omega = \frac{eg}{2m}B$. In the zero temperature limit, $T \to 0$, the correlation function reduces to

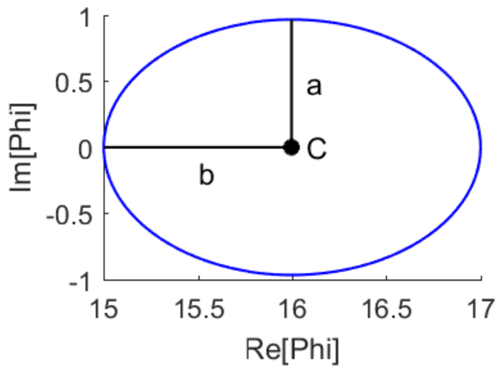


Figure 4: Plot of the Scaling invariant function $\tilde{\Phi}_\sigma(y_1, y_2, y_3)$ as a function of y_1 for fixed y_2 and y_3. The function traces out an ellipse in the complex plane with semi-major and -minor axis given by $a = \frac{y_2}{y_2+4y_3^2}\tanh\left(\frac{L}{\sqrt{y_2^2+y_3^2}}\right)$ and $b = \frac{4y_3^2-y_2^2}{y_2^2+4y_3^2}$, as well as having centre in $C = \frac{3y_3^2}{y_2^2+4y_3^2}$

$$C(|\Delta t|, 2h_\perp, h_\parallel) = \tilde{\Phi}_{T=0}\left(|\Delta t|, 2h_\perp, h_\parallel\right) = \frac{h_\parallel^2}{h^2} + \frac{h_\perp^2}{h^2} e^{-2ih|\Delta t|} \tag{2.18}$$

which traces out a circle in the complex plane with radius $R = \frac{h_\perp^2}{h^2}$ and centre $\frac{h_\parallel^2}{h^2}$. In the limit low perpendicular field limit $h_\perp \ll T$, the spin operator along z again commutated with the Hamiltonian. The quantum fluctuations therefore disappears and the quantum model is static just like the classical model. This can also be seen from the time-correlation function, that reduces to $C(t) = 1$ when $h_\perp \to 0$. The quantum model and classical model are therefore equal, when $h_\perp = 0$.

2.3 Subconclusion

In the classical single spin model, a magnetic field M is created spontaneously. The magnetic field is strongest in the low temperature limit $T \ll h$, but vanishes for $T/h \to \infty$. The classical model is also static, since correlation function $C(t) = 1$ is constant in time. Since the magnetic susceptibility, χ, is analytical for all values of T/h, no second order phase transitions are found in the classical model.

In the quantum model of the single spin in magnetic field $(h_\perp, h_\|)$, the magnetization and magnetic susceptibility is the same as in the classical case. The correlation function here is not a constant, but instead traces out an ellipse in the complex plane. The angular frequency, for which the ellipse is draws, $\omega = 2h = \sqrt{h_\|^2 + h_\perp^2}$, which agrees with the result from classical Larmor precession. In the low perpendicular field limit $h_\perp \ll T$, the correlation function $C(t) = 1$ is constant in time.

The classical- and quantum model is therefore equal in the limit of $h_\perp \ll T$

3 Classical Ising chain

Going a dimension up the classical Ising chain is analysed here. The Hamiltonian of the chain is written as

$$H = -\sum_{j=1}^{N} [J m_j m_{j+1} + h m_j] \tag{3.1}$$

with J being the spin-spin exchange energy, h being a longitudinal field, and N being the number of sites in the chain. Notice that the J here defined to be twice as big as the J in 3.1 Here, the time-correlation function is still constant and the model is static. However, the spacial, equal-time correlation function $C(x,0)$ is not. To see this, one first need the partition function

3.1 Calculating the partition function using transfer matrix

To calculating the correlation function of the system, one first need to calculate the partition function. To do that, one normally diagonalizes the Hamiltonian first. This is not a trivial task though. Because the matrix that has to be diagonalized, has $2^N \times 2^N$ entrenches, where N is the number of particles, then, for large systems, the task is to hard for even the best computers. The method of diagonalizing H can therefore not be used to calculate the partition function. Instead, the transfer matrix method is used. Here, the sum in the Boltzmann factors is split up into products

$$Z = \sum_{m_j \in \{-1,1\}} e^{\sum_{j=1}^{N} \frac{J m_j m_{j+1} + h m_j}{T}} = \sum_{m_j \in \{-1,1\}} \prod_{j=1}^{N} T_{m_j m_{j+1}} \tag{3.2}$$

Here, the matrix $T_{ab} = \exp[(Jab + ha)/T]$ is a 2-by-2 matrix called the transfer matrix, and depends both on the state of the j'th and the $j+1$'th state. Because of translation invariance of the Ising model, the Transfer matrix is the same all sites, which results in Z being the trace of a matrix product

$$Z = \sum_{m_1 \in \{-1,1\}} \left(T^N\right)_{m_1 m_1} = \mathrm{tr}\left[T^N\right] \tag{3.3}$$

In the diagonal basis of T, the partition function simplifies to

$$Z = \lambda_+^N + \lambda_-^N \quad \text{with} \quad \lambda_\pm = e^{J/T}\cosh(h/T) \pm \left(e^{2J/T}\sinh^2(h/T) + e^{-2J/T}\right) \tag{3.4}$$

Here, $\lambda_\pm$ is two eigenvalues of T. A thing that will become important later, it the fact that $\lambda_+ > \lambda_- > 0$ in the ferromagnetic case $J > 0$. This is guaranteed since $J > 0$ implies $e^{-4J/T} < 1$, which further implies $\sqrt{\sinh^2(h/T) + e^{-4J/T}} < \sqrt{\sinh^2(h/T) + 1} = \cosh(h/T)$. Using this, the eigenvalues in (3.4) are guaranteed to satisfy

$$\lambda_\pm > e^{J/T}\left(\cosh(h/T) - \cosh(h/T)\right) = 0 \tag{3.5}$$

3.2 Correlation function

To study the order in the classical chain, the equal-time correlation function between the ℓ'th and the ℓ''th site, $C(\ell - \ell')$ is studied. Just as before with the partition function, the transfer matrix T is used.

$$C(\ell-\ell') \equiv \langle m_\ell m_{\ell'} \rangle = \frac{1}{Z} \sum_{m_j \in \{-1,1\}} \prod_{j=1}^{N} T_{m_j m_{j+1}} m_\ell m_{\ell'} \tag{3.6}$$

To rewrite the correlation function in terms of matrix products, the numbers m_ℓ and $m_{\ell'}$ are written as the matrix

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z \tag{3.7}$$

which coincidentally is the third Pauli matrix. This is not because of any quantum effect. Remember, this is a pure classical model. It just happens to be a Pauli matrix that describes the number m_ℓ in this context. Writing this out, and using the cyclic structure of the trace, the correlation function can be written as the following

$$C(x) = \frac{1}{Z} \sum_{m_1, m_{\ell'} m_\ell} \left(T^{\ell'-1}\right)_{m_1, m_{\ell'}} \sigma^z_{m_\ell m_\ell} \left(T^{\ell-\ell'}\right)_{m_{\ell'}, m_\ell} \sigma^z_{m_\ell m_\ell} \left(T^{N-\ell+1}\right)_{m_\ell, m_1} \tag{3.8}$$

$$= \frac{1}{Z} \mathrm{tr}\left[T^{\ell'-1} \sigma^z T^{\ell-\ell'} \sigma^z T^{N-\ell+1}\right] = \frac{1}{Z} \mathrm{tr}\left[T^{\ell'} \sigma^z T^{\ell-\ell'} \sigma^z T^{N-\ell}\right] \tag{3.9}$$

Again, to simplify calculations, the basis is change to the eigenbasis of T_{ab}, which transforms the spin matrix σ^z into

$$\tilde{\sigma}^z = S^{-1} \sigma^z S = \frac{1}{\delta} \begin{pmatrix} \alpha - \Sigma & \alpha - \lambda_- \\ \lambda_+ - \alpha & \Sigma - \alpha \end{pmatrix} \tag{3.10}$$

with $\alpha = e^{\frac{J+h}{T}}$, $\delta = (\lambda_+ - \lambda_-)/2 = \sqrt{e^{J/T} \sinh^2(h/T) + e^{-2J/T}}$, and $\Sigma = (\lambda_+ + \lambda_-)/2 = e^{J/T} \cosh(h/T)$. Inserting this into the correlation function, one gets

$$C(\ell-\ell') = \frac{1}{Z\delta^2} \Big(\lambda_+^N (\alpha - \Sigma)^2 + \lambda_+^{N-\ell+\ell'} \lambda_-^{\ell-\ell'} (\alpha - \lambda_-)(\lambda_+ - \alpha) + \lambda_+^{\ell-\ell'} \lambda_-^{N-\ell+\ell'} (\alpha - \lambda_-)(\lambda_+ - \alpha) + \lambda_-^N (\Sigma - \alpha)^2 \Big) \tag{3.11}$$

Using that $Z = \lambda_+^N + \lambda_-^N$, the fraction be split up into an constant term and a term depending on the separation of the two sites

$$C(\ell-\ell') = \frac{(\alpha-\Sigma)^2}{\delta^2} + \frac{(\alpha-\lambda_-)(\lambda_+-\alpha)}{\delta^2} \frac{\left(\frac{\lambda_+}{\lambda_-}\right)^{-(\ell-\ell')} + \left(\frac{\lambda_+}{\lambda_-}\right)^{-(N-(\ell-\ell'))}}{1 + \left(\frac{\lambda_+}{\lambda_-}\right)^N} \tag{3.12}$$

Doing the same calculation for $\ell < \ell'$, reveals a similar result, The only difference is $\ell - \ell'$ is replaced by $\ell' - \ell$. The separation can therefore be replaced by with $|\ell - \ell'|$ without loss of generality. Since the correlation function is varying exponentially, one can write it in terms of $e^{x/\xi}$, where $x = a(l - l')$ and ξ being a correlation length. To do this, one can rewrite λ_+/λ_- as $\exp \ln(\lambda_+/\lambda_-)$.

$$C(x) = \frac{(\alpha-\Sigma)^2}{\delta^2} + \frac{(\alpha-\lambda_-)(\lambda_+-\alpha)}{\delta^2} \frac{e^{-|x|/\xi} + e^{-(L-|x|)/\xi}}{1 + e^{-L/\xi}} \tag{3.13}$$

In doing so, the correlation length, ξ comes out in a natural way as

$$\frac{1}{\xi} = \frac{1}{a} \ln\left(\frac{\cosh(h/T) + \sqrt{\sinh^2(h/T) + e^{-4J/T}}}{\cosh(h/T) - \sqrt{\sinh^2(h/T) + e^{-4J/T}}} \right) \tag{3.14}$$

Since $\lambda_+ > \lambda_- > 0$ in the ferromagnetic case, $J < 0$, the correlation length is always real and positive. At last, using the definitions of Σ, δ, and α, the fractions in eq. (3.13), simplifies

$$\frac{(\alpha-\Sigma)^2}{\delta^2} = \frac{\left(e^{(J+h)/T} - e^{J/T}\cosh(h/T)\right)^2}{e^{2J/T}(\sinh^2(h/T)+e^{-4J/T})} = \frac{\sinh^2(h/T)}{\sinh^2(h/T)+e^{-4J/T}} \tag{3.15}$$

$$\frac{(\alpha-\lambda_-)(\lambda_+-\alpha)}{\delta^2} = \frac{e^{-4J/T}}{\sinh^2(h/T)+e^{-4J/T}} \tag{3.16}$$

Also, the factor with exponential terms in (3.13) can be rewritten as a fraction of hyperbolic cosine terms

$$\frac{e^{-|x|/\xi}+e^{-(L-|x|)/\xi}}{1+e^{-L/\xi}} = \frac{e^{(L-2|x|)/2\xi}+e^{-(L-2|x|)/2\xi}}{e^{L/2\xi}+e^{-L/2\xi}} = \frac{\cosh\left(\frac{L-2|x|}{2\xi}\right)}{\cosh\left(\frac{L}{2\xi}\right)} \tag{3.17}$$

Using all this, the correlation function reduces to

$$C(x) = \frac{\sinh^2(h/T)}{\sinh^2(h/T)+e^{-4J/T}} + \frac{e^{-4J/T}}{\sinh^2(h/T)+e^{-4J/T}}\frac{\cosh\left(\frac{L-2|x|}{2\xi}\right)}{\cosh\left(\frac{L}{2\xi}\right)} \tag{3.18}$$

Note that the maximum distance that two spin can be from each other is $L/2$ because of the periodic boundary conditions. Plotting for fixed temperature, fig. 5, the correlation function is positive for all separation and field. All spins therefore tends to point in the same direction, creating a non-zero spontaneous magnetic field, M. For increasing temperatures, the correlation function decreases and the magnetization gets weaker.

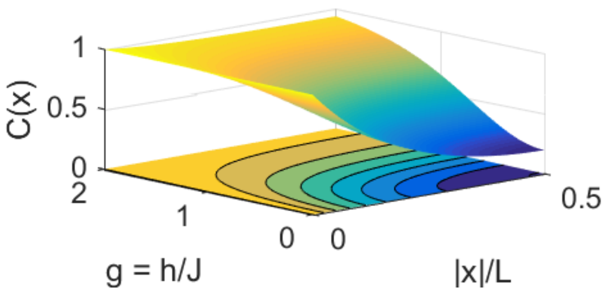


Figure 5: Plot of the correlation function of the classical Ising chain for $T/J = 100$

3.3 Quantum Critical Point

Looking at the correlation function of the classical Ising chain, eq. (3.14), the square root term equals zero and the eigenvalues of T_{ab} is equal.

$$\sqrt{\sinh^2(h/T)+e^{-4J/T}} = 0 \tag{3.19}$$

When this happens, the correlation function diverges and the system experience long-range order. Clearly, since $\sinh(x) =$, when $x = 0$ and $\exp(-2J/T) \to 0$, for $T \to 0$. The quantum critical point, where the system experience long-rang order, must therefore be in the point $(h_c, T_c) = (0, 0)$. In the neighbourhood of the quantum critical point, $h \ll T \ll J$, the eigenvalues of the transfer matrix, eq. 3.4, reduces to

$$\lambda_\pm \approx e^{J/T} \pm e^{-J/T} = \begin{cases} 2\cosh(J/T) & \text{for} \quad + \\ 2\sinh(J/T) & \text{for} \quad - \end{cases} \tag{3.20}$$

which further reduces the correlation length, eq. (3.4), to

$$\frac{a}{\xi} = \ln\left(\frac{\lambda_+}{\lambda_-}\right) \approx \ln\coth(J/T) \tag{3.21}$$

Since $T \ll J$, the correlation function diverges in an exponential way,

$$\frac{\xi}{a} = \left[\ln\left(1 + e^{-2J/T}\right) - \ln\left(1 - e^{-2J/T}\right)\right]^{-1} \approx \frac{1}{2}e^{2J/T} \gg 1 \tag{3.22}$$

and the system experience long range order. Note here, if the low-temperature limit, $T \ll J$, is taken first, the correlation length approaches zero. This is okay, since the correlation still approaches $C(x) = 1$ for all distances.

$$C(x) \approx 1 - e^{-\frac{2|x|h}{aT}} \to 1 \quad \text{for} \quad T \to 0 \tag{3.23}$$

The system therefore still experience long-range.

3.4 Mapping from classical chain to Single Quantum Spin

As said in the intro, a quantum field theory is dimension d is equivalent to a quantum field theory in dimension $D = d + 1$. One should therefore expect the classical Ising chain to be equivalent the dynamics of the single quantum spin. This can be done here, by mapping the space-coordinate $|x|$ into a complex a complex time coordinate, $\tau = it$ and the length of the chain L into the temperature of the quantum spin T_Q. Doing this via the transformation

$$|x| \to it, \quad L \to \frac{1}{T_Q}, \quad \sinh\left(\frac{h}{T}\right) \to h_{\parallel}, \quad e^{-2J/T} \to h_{\perp} \tag{3.24}$$

The space-correlation function is then successfully mapped into the complex-time correlation function, if and only if

$$\frac{1}{2\xi} \to h_Q = \sqrt{h_{\parallel}^2 + h_{\perp}^2} \tag{3.25}$$

which happens in the quantum limit $h \ll T \ll J$.

3.5 Antiferromagnet

One thing that is worth mentioning, is what happens to the correlation function in the Antiferromagnetic case, $J < 0$. Here, $\exp(-4J/T) > 1$, which implies

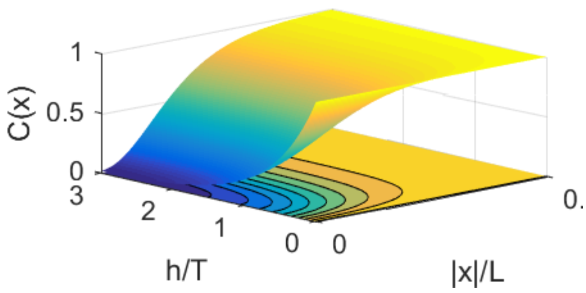
$$\sqrt{\sinh^2(h/T) + e^{-4J/T}} > \cosh(h/T) \Rightarrow \lambda_- < 0 \tag{3.26}$$

Still, the absolute value of the ratio of the eigenvalues, $|\lambda_+/\lambda_-|$ is still greater than one. To avoid any negative or complex correlation lengths, the correlation length is therefore redefined as

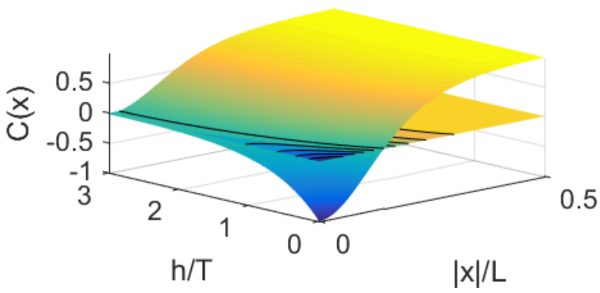
$$\xi = \frac{1}{a}\ln\left|\frac{\lambda_+}{\lambda_-}\right| \tag{3.27}$$

which results in multiple sign changes in the correlation function, (3.17). Looking only at the x dependent terms of C, every exponential term changes their sign

$$\frac{(-1)^{|x|/a}e^{-|x|/\xi} + (-1)^{N+\frac{|x|}{a}}e^{-(L-|x|)/\xi}}{1 + (-1)^N e^{-L/\xi}} = (-1)^{|x|/a}\frac{\mathrm{Th}\left(\frac{L-2|x|}{2\xi}, N\right)}{\mathrm{Th}\left(\frac{L}{2\xi}, N\right)} \tag{3.28}$$



(a) Even separation



(b) Odd separations

Figure 6: Plot of the correlation function for the classical antiferromagntic chain for both even and odd separations. Both graphs are drawn for $T = 3J$, Notice in the odd case, the correlation function takes negative values

Here, $\mathrm{Th}(x, n)$ is a function that changes between $\cosh(x)$ and $\sinh(x)$ when n changes from being even or odd.

$$\mathrm{Th}(x,n) \equiv \begin{cases} \cosh(x) & \text{for even n} \\ \sinh(x) & \text{for odd n} \end{cases} \tag{3.29}$$

For large x, $\mathrm{Th}(x, n)$ is same for even and odd n. Putting it all together, the correlation function of the antiferromagnet reduces to

$$C(x) = \frac{\sinh^2(h/T)}{\sinh^2(h/T) + e^{-4J/T}} + (-1)^{|x|/a} \frac{e^{-4J/T}}{\sinh^2(h/T) + e^{-4J/T}} \frac{\mathrm{Th}\left(\frac{L-2|x|}{2\xi}, N\right)}{\mathrm{Th}\left(\frac{L}{2\xi}, N\right)} \tag{3.30}$$

Now the correlation function can both be positive and negative, 6. Notice that in the odd-separation case, 6b, the correlation can take negative values. What is happening here, is the spins anti-aligning with their nearest neighbour, and creating two sub grids with opposite polarization.

3.6 Subconclusion

When analysing the classical Ising chain in a magnetic field, h, the equal-time correlation function $C(x, t)$ can be calculated by used the transfer matrix method. In the ferromagnetic case, $J > 0$, the correlation function is positive for all values of separations, fields, and temperatures. The chain therefore creates a spontaneous magnetic field, M which weakens when temperature increases.

The classical Ising chain also has a quantum critical point at $h_c = 0$, where long-range order appear is the chain. In this region, the classical Ising chain can be mapped into the time correlation function of a single quantum spin. This is done by mapping the spacial-coordinate of the classical model into a complex time coordinate of the quantum model.

4 Qunatum Ising chain

To complete the picture of Ising chains, the time has come to analyse the transverse field quantum Ising chain. Here, the general quantum Ising model, eq. (1.5), takes the form

$$\hat{\mathcal{H}} = -J\sum_{j=1}^{M}\left[\hat{\sigma}_j^x\hat{\sigma}_{j+1}^x + g\hat{\sigma}_j^x\right] \tag{4.1}$$

Again, the J here is twice as big as in the J in eq. (1.5). Also, note that the Hamiltonian here is rotated 90° compared to the Hamiltonian (3.1). The reason why is because it simplifies the calculations of the correlation function without changing the underlying physics of the model. As describes in the introduction, the Ising model can be excited by creating domain wall on the chain, fig 7a. Because of the translational invariance of $\hat{\mathcal{H}}$, a domain can then be moved around without any energy cost, as long as the number of domains is unchanged. The transverse field Ising model has, as described later, a phase transition at $g_c = 1$. But before this can be analysed, the Hamiltonian must be diagonalized.

4.1 Fermionic transformations

To help describe the nature of the chain, a Jordan-Wigner transformation can be used, [3]. This maps the vector space $\mathbb{H}$, consisting of all spin states of the QIC, into a Fock space, $\mathbb{F}$, of spinless fermions. It does that by mapping a spin up state into the Fock state of zero fermions, $n = 0$, and the spin down state into the $n = 1$ state. In doing so, the annihilation operator, of the fermions are defined as

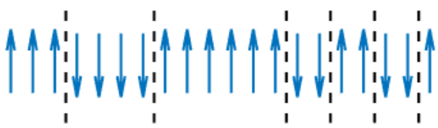
$$\hat{c}_i = \left(\prod_{j=1}^{i-1}\hat{\sigma}_j^z\right)\hat{\sigma}_i^+ \tag{4.2}$$

Looking at the chain in fig. 7a, the transformed version of the states, takes the form of fig. 7b. Since the particles are fermions, they must satisfy the following anti-commutator relations

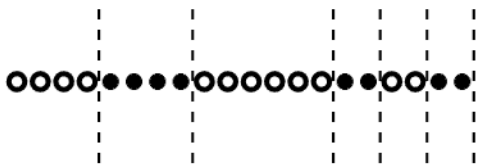
$$\left\{\hat{c}_i, \hat{c}_j^\dagger\right\} = \delta_{ij}\hat{\mathbb{I}} \quad \text{and} \quad \{\hat{c}_i, \hat{c}_j\} = \left\{\hat{c}_i^\dagger, \hat{c}_j^\dagger\right\} = \hat{\mathbf{0}} \tag{4.3}$$

From the fermion operators, the spin operators can be written as

$$\hat{\sigma}_i^z = \hat{\mathbb{I}} - 2\hat{c}_i^\dagger\hat{c}_i \quad \text{and} \quad \hat{\sigma}_i^x = \prod_{j=1}^{i-1}(\hat{\mathbb{I}} - 2\hat{c}_j^\dagger\hat{c}_j)(\hat{c}_i + \hat{c}_i^\dagger) \tag{4.4}$$



(a)



(b)

Figure 7: a) Example of the configuration of a small quantum Ising chain. The chain is separated into 7 domains by 6 domain walls. b) The Jordan-Wigner transformed version of a). Here, • marks a site holding a fermion, while ∘ marked a site with no fermions. In both figures, the dashed line marks the domain walls on the chain.

Using this, the Hamiltonian takes the form of

$$\hat{\mathcal{H}} = -J\sum_{j=1}^{M}\left[\hat{c}_j^\dagger\hat{c}_{j+1} + \hat{c}_{j+1}^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_{j+1}^\dagger + \hat{c}_{j+1}\hat{c}_j - 2g\hat{c}_j^\dagger\hat{c}_j + g\hat{\mathbb{I}}\right] \tag{4.5}$$

Since the Hamiltonian has terms such as $c_j^\dagger c_{j+1}^\dagger$, which violates fermion number, particles can be created spontaneously by flipping spins in pairs. This means that when a pair of domain walls are created, they will move in opposite directions as time evolves, which has been verified experimentally, [4]. To describe the motion of domain walls, the momentum operators, $\hat{c}_k$ are introduced as the discrete fourie transformation of the fermionic operators

$$\hat{c}_k = \frac{1}{\sqrt{N}}\sum_{j=1}^{N}\hat{c}_j e^{-ikr_j} \tag{4.6}$$

For a chain of length $L = Na$, the possible momentum states k is limited to

$$k = \frac{2\pi n}{a} \quad \text{with} \quad n \in \mathbb{Z} \quad \text{and} \quad -\frac{\pi}{L} < k < \frac{\pi}{L} \tag{4.7}$$

Using the inverse Fourie transformation, the Hamiltonian can be rewritten in terms of the momentum operators

$$\hat{\mathcal{H}} = J\sum_k\left(2\left[g - \cos(ka)\right]\hat{c}_k^\dagger\hat{c}_k + i\sin(ka)\left[\hat{c}_{-k}^\dagger\hat{c}_k^\dagger + \hat{c}_{-k}\hat{c}_k\right] - g\hat{\mathbb{I}}\right) \tag{4.8}$$

The Hamiltonian still violates fermion number conservation. To avoid this, a Bogoliubov transformation can be used, which transforms the Hamiltonian into a new Fock space, where fermion number is conserved. In the new space, the new fermionic momentum operators, $\hat{\gamma}_k$, are defined as

$$\hat{\gamma}_k = u_k\hat{c}_k - iv_k\hat{c}_{-k}^\dagger \tag{4.9}$$

Here, $u_k = \cos(\theta_k/2)$ and $v_k = \sin(\theta_k/2)$ with angle, θ_k defined by the relation

$$\tan\theta_k = \frac{\sin(ka)}{g - \cos(ka)} \tag{4.10}$$

The new fermion operators also have to satisfy the same anti-commutator relation as the Jordan-Wigner operators. Putting it all together, the Hamiltonian in the new Fock space, is now diagonalized

$$\hat{\mathcal{H}} = \sum_k \epsilon_k(\hat{\gamma}_k^\dagger\hat{\gamma}_k - 1/2\hat{\mathbb{I}}) \tag{4.11}$$

with dispersion

$$\epsilon_k = 2J\sqrt{1 + g^2 - 2g\cos(ka)} \geq 0 \tag{4.12}$$

For small values of k, ϵ_k approaches $\approx 2J|1-g| = |\Delta|$, which is the energy required to create a momentum fermion on the chain. In the limit of $g \to 1$, the energy gap closes, and fermions can be created spontaneously. The transverse field quantum Ising chain therefore has a quantum critical point at $g_c = 1$.

4.2 Correlation function, correlation length and equilibration time

To study phase transitions of the quantum Ising model at $g_c = 1$, the equal-time correlation function is to be calculated. Using the Jordan-Wigner operators $\hat{c}_j$, the correlation function between the i'th and the $i+n$'th can be calculated

$$C(x,0) = C(an,0) = \langle \hat{\sigma}_i^x \hat{\sigma}_{i+n}^x \rangle = \left\langle (\hat{c}_i^\dagger - \hat{c}_i) \prod_{j=i+1}^{i+n-1} \left[(\hat{c}_j^\dagger + \hat{c}_j)(\hat{c}_j^\dagger - \hat{c}_j) \right] (\hat{c}_{i+n}^\dagger + \hat{c}_{i+n}) \right\rangle \quad (4.13)$$

Here, $\hat{\sigma}_j^x$ is factored into $(\hat{c}_j^\dagger + \hat{c}_j)(\hat{c}_j^\dagger - \hat{c}_j)$. Using Wick's theorem, which states

$$\langle y_1 y_2, \cdots, y_{2n} \rangle = \sum_P \langle y_{P1} y_{P2} \rangle \cdots \langle y_{P(2n-1)} y_{P2n} \rangle \quad (4.14)$$

where P sum over all possible combinations y_i and y_j pair, the correlation function, in the limit of large separations, can been calculated. This will not be done here, but has done by other [7]. The result being a correlation function defined

$$C(x,0) = zT^{1/4} G_I(\Delta/T) \exp\left(-\frac{|x|T}{c} F_I(\Delta/T) \right) \quad (4.15)$$

with $c = 2Ja$, $z = J^{-1/4}$, and G_I and F_I being scaling invariant function, defined by the integrals

$$F_I(s) = |s|\theta(-s) + \frac{1}{\pi} \int_0^\infty dy \ln \coth\left(\frac{\sqrt{y^2+s^2}}{2} \right) \quad (4.16)$$

$$\ln G_I(s) = \int_s^1 \frac{dy}{y} \left[\left(\frac{dF_I(y)}{dy} \right)^2 - \frac{1}{4} \right] + \int_1^\infty \frac{dy}{y} \left(\frac{dF_I(y)}{dy} \right)^2 \quad (4.17)$$

In eq. (4.15), the correlation function comes out to be

$$\xi^{-1} = \frac{T}{c} F(\Delta/T) \quad (4.18)$$

which can be evaluated in different limits. This is done in appendix B for three different limits, which have result

$$\xi = \begin{cases} \sqrt{\frac{\pi c^2}{2T\Delta}} e^{\Delta/T} & \text{for} \quad T \ll \Delta, 0 < \Delta \\ \frac{c}{|\Delta|} & \text{for} \quad T \ll |\Delta|, 0 > \Delta \\ \frac{4T}{c\pi} & \text{for} \quad T \gg |\Delta| \end{cases} \quad (4.19)$$

From the limits of the correlation function, the transverse field quantum Ising chain is separated into three regions. The first being the magnetically order side, $T \ll \Delta$, where ξ diverges when $T \to 0$ and thereby creating long-range order. In the second region, $T \ll -\Delta$, the correlation length is analytical when $T \to 0$. The chain will here act like a paramagnet [7], but will not be explored in this thesis.

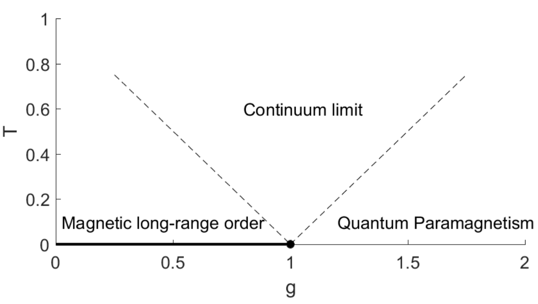


Figure 8: Phase diagram of the transverse quantum Ising chain. The diagram is separated in three regions.

4.3 Magnetically ordered phase

In the low temperature, positive field limit, $\Delta > 0$, $T \ll \Delta$, the thermal energy is mush smaller that the energy gap, and fermions cannot be created spontaneously. The chain, should therefore be in the ground state with no fermions in the Bogoliubov Fock space, $|0\rangle_B$. Since the chain has a temperature, T, thermal excitations can excite particles with momenta k and relativistic dispersion $\epsilon_k^2 \approx \Delta^2 + c^2k^2$. These particles will then move around the chain with constant momenta and collide as classical particles. From the dynamics of these particles, the equal-time correlation function can be calculated. This is done by considering n of these particles on the chain. Each particle is created with a momentum probability density of

$$\rho \approx \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-(\Delta+\frac{c^2k^2}{2\Delta})/T} \overset{\left(u=\frac{ck}{\sqrt{2\Delta T}}\right)}{=} \sqrt{\frac{\Delta T}{2c^2}} \frac{1}{\pi} e^{-\Delta/T} \int_{-\infty}^{\infty} due^{-u^2} = \sqrt{\frac{\Delta T}{2c^2\pi}} e^{-\Delta/T} \tag{4.20}$$

which is equal to $\frac{n}{L}$. Looking at one of these particle, since the Ising chain is translational invariant, the probability of finding the particle in an interval of $|x|$ is $p = |x|/L$. Here L is the length of the chain. Looking at two spins at point 0 and x, the spin product $\hat{\sigma}^x(x)\hat{\sigma}^x(0)$ depends on the number of particles, j, in the interval $I = [0, x]$. For an even number of particles, the two spins point mostly in the same direction, $\hat{\sigma}^x(x)\hat{\sigma}^x(0) = N_0^2 > 0$, where N_0 is field dependent. For an odd j, the sign is flipped and $\hat{\sigma}^x(x)\hat{\sigma}^x(0) = -N_0^2 < 0$. The correlation function is therefore given by

$$C(x,0) = N_0^2 \sum_{j=1}^{n} (-1)^j p_j(|x|) \tag{4.21}$$

where $p_j(|x|)$ is the probability of finding j particles in the interval $I = [0, x]$. In this case, the problem of finding p_j is simple counting problem, which has answer

$$p_j = \binom{n}{j} \left(\frac{|x|}{L}\right)^j \left(1 - \frac{|x|}{L}\right)^{n-j} = \binom{n}{j} \left(\frac{|x|\rho}{n}\right)^j \left(1 - \frac{|x|\rho}{n}\right)^{n-j} \tag{4.22}$$

Using this, the equal-time correlation function can be calculated for $|x| \ll L$

$$C(x,0) = N_0^2 \sum_{j=0}^{n} \left(\frac{-|x|\rho}{n}\right)^j \left(1 - \frac{|x|\rho}{n}\right)^{n-j} = N_0 \left(1 - \frac{2|x|}{\rho n}\right)^n \approx N_0^2 e^{-\frac{2|x|}{\rho}} \tag{4.23}$$

In this picture, the correlation length ξ is given by

$$\xi = \frac{1}{2\rho} = \sqrt{\frac{c^2\pi}{2\Delta T}} e^{\Delta/T} \tag{4.24}$$

which is the same answer given by the integral (A.5). From the integrals, the constant $N_0 = \sqrt{z}\Delta^{1/8}$. Since this method works so well at describing the equal-time correlations, one should expect it to work just as well to describe the time evolution of C. For a particle, which at time $t = 0$ was inside the interval $|x|$ and has momentum k, the probability of still being in the interval at time $t > 0$ is

$$p^k(t) = \frac{|x - v_k t|}{L} \tag{4.25}$$

Here, $v_k = \partial_k \epsilon_k$ is the velocity of the particle. Averaging over all momenta, the the probability of a particle initially created in the interval $[0, x]$, will have probability $p(t)$ of still being inside $[0, x]$ at time t. The probability is calculated by averaging p^k over all momenta weighed by the probability of the particle having momentum k

$$p(t) = \frac{1}{\rho} \int \frac{dk}{2\pi} e^{-\epsilon_k/T} \frac{|x - v_k t|}{L} \tag{4.26}$$

Inserting this values into (4.21), correlation function takes the form of

$$C(x,t) = N_0^2 e^{-2pN} = N_0^2 R(x,t) \tag{4.27}$$

with

$$R(x,t) = \exp\left(-\frac{1}{\pi} \int_{-\infty}^{\infty} dk e^{-\epsilon_k/T} |x - v_k t| \right) \tag{4.28}$$

and $N_0^2 = z G_I(s)$. In the limit magnetic limit,

$$\ln G_I(s \gg 1) \approx \int_1^s \frac{1}{4y} dy + \int_s^\infty \frac{4y^2 - 4y + 2}{2\pi y^2} e^{-2y} dy \approx \frac{1}{4} \ln s \Rightarrow G_I(s) = s^{1/4} \tag{4.29}$$

The correlation function of the quantum Ising chain, in the limit $0 < T \ll \Delta$, is

$$C(x,0) = z \Delta^{1/4} e^{-|x|/\xi} = N_0^2 e^{-|x|/\xi} \tag{4.30}$$

with $N_0 = \frac{\Delta^{1/8}}{J^{1/8}} = (2(1-g))^{-1/8}$. Looking at the equal-distance correlation function, $C(0,t)$, one can define a equilibrium time τ_ϕ. This is the time scale for which the system returns to equilibrium after a local, thermal perturbation. τ_ϕ can be found by looking at how $R(0,t)$ restores as a function of time

$$\frac{1}{\tau_\phi} = \frac{1}{\pi} \int_{-\infty}^{\infty} dk e^{-\epsilon_k/T} |\partial_k \epsilon_k| = -\frac{2T}{\pi} \int_0^\infty dk \frac{d}{dk} e^{-\epsilon_k/T} = \frac{2T}{\pi} e^{-\Delta/T} \tag{4.31}$$

A useful quantify to have in mind later is the ratio between the equilibrium time τ_ϕ and the correlation length ξ

$$\frac{\tau_\phi}{\xi} = \sqrt{\frac{\Delta}{2Tc^2}} \tag{4.32}$$

This will be used to rewrite correlation function in a scaling invariant way. In general, the integral (4.28) can be calculated by separating the integral into two

$$I = \int_{-\infty}^{k_0} dk e^{-\epsilon_k/T} (x - v_k t) + \int_{k_0}^{\infty} dk e^{-\epsilon_k/T} (v_k t - x) \tag{4.33}$$

where k_0 is the momentum that satisfy $\partial_k \epsilon_k t = x$ and is given by

$$k_0 = \frac{x\Delta}{\sqrt{c^2 t^2 + x^2}} \tag{4.34}$$

Looking only at the term involving x, the integrals can be solved by combining the two and expanding ϵ_k

$$I_x = x \left[\int_{-\infty}^{k_0} dk e^{-\epsilon_k/T} - \int_{k_0}^{\infty} dk e^{-\epsilon_k/T} \right] = x \int_{-k_0}^{k_0} dk e^{-\epsilon_k/T} \tag{4.35}$$

$$\overset{\left(u = \frac{ck}{\sqrt{2\Delta T}}\right)}{\approx} x \sqrt{\frac{\Delta T}{2c^2}} e^{-\Delta/T} \int_{-\frac{ck_0}{\sqrt{2\Delta T}}}^{\frac{ck_0}{\sqrt{2\Delta T}}} du e^{-u^2} = \frac{x\pi}{\xi} \operatorname{erf}\left(\frac{ck_0}{\sqrt{2\Delta T}} \right) \tag{4.36}$$

Here $\text{erf}(x) \in]-1,0[$ is the error function. Using the ratio (??) as well as eq. (4.34), this input of the error function can be rewritten is a scaling invariant way

$$\frac{ck_0}{\sqrt{2\Delta T}} = \frac{\Delta x}{\sqrt{c^2t^2+x^2}\sqrt{2\Delta T}} = \sqrt{\frac{\Delta}{2Tc^2}}\frac{\frac{x}{t}}{\sqrt{1+\left(\frac{x}{ct}\right)^2}} \approx \frac{\bar{x}}{\bar{t}\sqrt{\pi}} \tag{4.37}$$

The other terms in (4.28) can also be calculated

$$I_k = t\left[-\int_{-\infty}^{k_0} dk e^{-\epsilon_k/T}\partial_k\epsilon_k + \int_{k_0}^{\infty} dk e^{-\epsilon_k/T}\partial_k\epsilon_k\right] = -2tT\int_{k_0}^{\infty} dk\frac{d}{dk}e^{-\epsilon_k/T} \tag{4.38}$$

$$= 2tTe^{-\sqrt{\Delta^2+c^2k_0^2}/T} \approx \pi\bar{t}e^{-\frac{\bar{x}^2}{\pi\bar{t}^2}} \tag{4.39}$$

Setting in all together, the function $R(x,t)$ can be written as a scaling invariant function $\Phi_R(x/\xi, t/\tau_\phi)$, given by

$$\ln\Phi_R(\bar{x},\bar{t}) = -\bar{x}\ \text{erf}\left(\frac{\bar{x}}{\sqrt{\pi}\bar{t}}\right) - \bar{t}e^{-\frac{\bar{x}^2}{\pi\bar{t}^2}} \tag{4.40}$$

As seen in eq. (4.20) and (4.31), when $T \to 0$, both the correlation length, ξ, and the equilibrium time, τ_ϕ diverges. As seen in the plot 9, the scaling function approaches 1 and the chain experience long-range order in both space and time

$$C(x,t) = N_0^2 = \left(\frac{\Delta}{J}\right)^{1/4} \tag{4.41}$$

The transverse field quantum Ising model, therefore has a quantum phase transition at $T = 0$ and $g < g_c = 1$. When $g > g_c = 1$, the critical behaviour disappears.

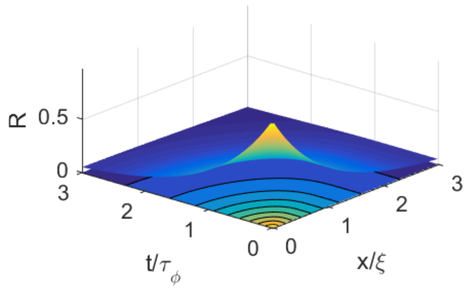


Figure 9: Plot of the scaling invariant function $\Phi_R(x,y)$ as a function function x/ξ and t/τ_ϕ

4.4 Subconclusion

In analysing the transverse field quantum Ising chain, the Hamiltonian is diagonalized by first using a Jordan-Wigner transformation and then using Bogoliubov transformation. This transforms the a Hamiltonian to describe fermions moving around a chain with momenta k. The dispersion relation of these fermions are approximately relativistic, and corresponds to a domain wall moving between sites. The minimal energy for creating a fermion, $|\Delta| = 2J|1-g|$, which vanishes at $g_c = 1$. The transverse field quantum Ising model, therefore has a critical point transition at $g_c = 1$.

In the fermion picture, the correlation function $C(x,t)$ can be calculated as the result of a simple counting problem, and shown be a scaling function. From this, the correlation and equilibration time can be found and shown to diverge in the low temperature, positive gap limits $T \ll \Delta$, revealing a quantum phase transition at $g < g_c$. Here, the scaling function is equal to one, and long-range order appears both in space and time.

5 Conclusion

In the classical single spin model, a magnetic field M is created spontaneously. The magnetic field is strongest in the low temperature limit $T \ll h$, but vanishes for $T/h \to \infty$. The classical model is also static, since correlation function $C(t) = 1$ is constant in time. Since the magnetic susceptibility, χ, is analytical for all values of T/h, no second order phase transitions are found in the classical model. In the quantum model of the single spin in magnetic field $(h_\perp, h_\parallel)$, the magnetization and magnetic susceptibility is the same as in the classical case. The correlation function here is not a constant, but instead traces out an ellipse in the complex plane. The angular frequency, for which the ellipse is draws, $\omega = 2h = \sqrt{h_\parallel^2 + h_\perp^2}$, which agrees with the result from classical Larmor precession. In the low perpendicular field limit $h_\perp \ll T$, the correlation function $C(t) = 1$ is constant in time. The classical- and quantum model is therefore equal in the limit of $h_\perp \ll T$

When analysing the classical Ising chain in a magnetic field, h, the equal-time correlation function $C(x,t)$ can be calculated by used the transfer matrix method. In the ferromagnetic case, $J > 0$, the correlation function is positive for all values of separations, fields, and temperatures. The chain therefore creates a spontaneous magnetic field, M which weakens when temperature increases. The classical Ising chain also has a quantum critical point at $h_c = 0$, where long-range order appear is the chain. In this region, the classical Ising chain can be mapped into the time correlation function of a single quantum spin. This is done by mapping the spacial-coordinate of the classical model into a complex time coordinate of the quantum model.

In analysing the transverse field quantum Ising chain, the Hamiltonian is diagonalized by first using a Jordan-Wigner transformation and then using Bogoliubov transformation. This transforms the a Hamiltonian to describe fermions moving around a chain with momenta k. The dispersion relation of these fermions are approximately relativistic, and corresponds to a domain wall moving between sites. The minimal energy for creating a fermion, $|\Delta| = 2J|1-g|$, which vanishes at $g_c = 1$. The transverse field quantum Ising model, therefore has a critical point transition at $g_c = 1$. In the fermion picture, the correlation function $C(x,t)$ can be calculated as the result of a simple counting problem, and shown be a scaling function. From this, the correlation and equilibration time can be found and shown to diverge in the low temperature, positive gap limits $T \ll \Delta$, revealing a quantum phase transition at $g < g_c$. Here, the scaling function is equal to one, and long-range order appears both in space and time.

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A Different limits of the correlation length ξ for QIC

In the quantum Ising model, the correlation function depends on the two functions, F_I and G_I. The functions are defined in terms of the integrals

$$F_I(s) = |s|\theta(-s) + \frac{1}{\pi}\int_0^\infty dy \, \ln\coth\left(\frac{\sqrt{y^2+s^2}}{2}\right) \tag{A.1}$$

$$\ln G_I(s) = \int_s^1 \frac{dy}{y}\left[\left(\frac{dF_I(y)}{dy}\right)^2 - \frac{1}{4}\right] + \int_1^\infty \frac{dy}{y}\left(\frac{dF_I(y)}{dy}\right)^2 \tag{A.2}$$

where $\theta(x)$ is the heavy-side function. In the context of the quantum Ising model, $s = \frac{\Delta}{T}$, where $\Delta = 2J(1-g)$ is the energy gap between the ground state and first excited state of the Hamiltonian and T is the temperature. In the three different limits, $T \ll \Delta$, $T \ll -\Delta$, and $T \gg |\Delta|$, the correlation length can be calculated by approximating the integral the limits.

A.1 Magnetic order phase: $T \ll \Delta$

In this region, $s = \Delta/T \gg 1$. Using this, the function $F_I(s)$ takes the form of

$$F_I(s \gg 1) \approx \frac{1}{\pi}\int_0^\infty dy \ln\coth\left(\frac{s}{2} + \frac{y^2}{4\sqrt{s}}\right) \tag{A.3}$$

$$= \frac{1}{\pi}\int_0^\infty dy \ln\left(1 + e^{-s}e^{-\frac{y^2}{2s}}\right) - \ln\left(1 - e^{-s}e^{-\frac{y^2}{2s}}\right) \tag{A.4}$$

$$\approx \frac{2}{\pi}e^{-s}\int_0^\infty dy\, e^{-\frac{y^2}{2s}} = \frac{1}{\pi}\sqrt{2s\pi}e^{-s} = \sqrt{\frac{2s}{\pi}}e^{-s} \tag{A.5}$$

In the first approximation, $\sqrt{1+x^2} = 1 + x^2/2 + o(x^4)$ is used, and in the second approximation, $\ln(1+x) = x + o(x^2)$ is used. Inserting this into $A.6$ the correlation length is given by

$$\xi_c \approx \sqrt{\frac{\pi c^2}{2T\Delta}}e^{\Delta/T} \tag{A.6}$$

A.2 Paramagnetic phase: $\Delta < 0$ and $T \ll |\Delta|$

In this limit, the correlations length get an extra term compared to the classical correlation length, (A.6)

$$F(s \ll -1) = -s + \frac{1}{\pi}\int_0^\infty dy \ln\coth\left(\frac{\sqrt{y^2+s^2}}{2}\right) \approx -s + \frac{c}{T}\xi_c^{-1} \tag{A.7}$$

which gives a correlation length of

$$\xi \approx \frac{1}{\frac{-\Delta}{c} + \xi_c^{-1}} \overset{(T\to 0)}{\to} \frac{c}{|\Delta|} \tag{A.8}$$

A.3 Continuum limit: $T \gg |\Delta|$

In this limit, $|s| \ll 1$, which gives a F_I of

$$F(|s| \ll 1) \approx \frac{1}{\pi}\int_0^\infty dy \ln\coth\left(\frac{y}{2}\right) = \frac{1}{\pi}\int_0^\infty dy \ln\left(\frac{1+e^{-y}}{1-e^{-y}}\right) \tag{A.9}$$

$$\approx \frac{2}{\pi}\sum_{n=0}^{\infty}\int_0^\infty \frac{dy}{2n+1}e^{-(2n+1)y} = \frac{2}{\pi}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2} \tag{A.10}$$

In the in first approximation, $s \approx 0$ is used. In the second approximation, the logarithm is expanded in terms of e^{-y} which gives an integral, which evaluated gives an infinity sum of a odd fraction squared. The sum luckily converges to $\frac{\pi^2}{8}$ and the correlation length is

$$\xi = \frac{4T}{c\pi} \tag{A.11}$$

A.4 Summary

In summary, the correlation function of the quantum Ising model is given by

$$\xi = \begin{cases} \sqrt{\frac{\pi c^2}{2T\Delta}} e^{\Delta/T} & \text{for} \quad T \ll \Delta, 0 < \Delta \\ \frac{c}{|\Delta|} & \text{for} \quad T \ll |\Delta|, 0 > \Delta \\ \frac{4T}{c\pi} & \text{for} \quad T \gg |\Delta| \end{cases} \tag{A.12}$$