XYZ-Ising Model: Phase Diagram

In this chapter, we study the phases of XYZ-Ising model at zero temperature as a function of coupling constants of Hamiltonian. Lieb, Schultz and Mattis studied this model where the interactions are alternately Ising and isotropic Heisenberg interactions [49]. They solved the model exactly in the sense that the ground state, all the elementary excitations and the free energy has been found.

4.1 The Hamiltonian

As we have mentioned in the chapter 3, the Hamiltonian is,

\[ H = \sum_{i}^{N} \left( J_x \sigma_{i,1}^{x} \sigma_{i,2}^{x} + J_y \sigma_{i,1}^{y} \sigma_{i,2}^{y} + J_z \sigma_{i,1}^{z} \sigma_{i,2}^{z} + \sigma_{i,2}^{z} \sigma_{i+1,1}^{z} \right) \] (4.1)

with \( \sigma_{N+1,1}^{z} = \sigma_{1,1}^{z} \).

Figure 4.1: The XYZ-Ising chain. There are two sites per unit cell. The \( x, y \) and \( z \) bonds are as indicated.
The fermionised Hamiltonian,

\[
H = \sum_{i=1}^{N} ((J_y - J_x u_i) i \xi_{i,1} \xi_{i,2} + J_z u_i) + \sum_{i=1}^{N-1} (i \xi_{i,2} \xi_{i+1,1}) + i \xi_{N,2} \xi_{1,1} \Sigma_x.
\]  

(4.2)

The XYZ-Ising model can be exactly solved as XY-Ising model has been solved for \(J_x = J_y = J/2\) in the last section.

### 4.2 Ground State in Extreme Limit of Coupling Constants

Let us discuss the ground state of XYZ-Ising model in extreme limits. When \(J_z\) is large then the Hamiltonian is expressed as

\[
H = J_z \sum_{i}^{N} \sigma_{i,1}^{z} \sigma_{i,2}^{z} = J_z \sum_{i}^{N} W_i.
\]

(4.3)

For large and positive (negative) \(J_z\), the Hamiltonian is minimum at \(W_i = -1(+1)\). Then, Hamiltonian becomes

\[
H = -(+)NJ_z.
\]

(4.4)

Therefore, for large and positive (negative) \(J_z\) the ground state belongs to \(W_i = -1(+1)\) sector as shown in figure 4.2.

Now let us consider another limit large \(J\). In this limit, the Hamiltonian is written as

\[
H = \frac{J}{2} \sum_{i}^{N} (\sigma_{i,1}^{x} \sigma_{i,2}^{x} + \sigma_{i,1}^{y} \sigma_{i,2}^{y})
\]

(4.5)

or, \(H = \frac{J}{4} \sum_{i}^{N} (\sigma_{i,1}^{+} \sigma_{i,2}^{-} + \sigma_{i,1}^{-} \sigma_{i,2}^{+})\).
The eigenstates are

\[ | \uparrow \uparrow \rangle, \]
\[ | \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle, \]
\[ | \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle, \]
and \[ | \downarrow \downarrow \rangle \]

with eigenvalues \( 0, \frac{J}{2}, -\frac{J}{2}, 0 \).

Therefore, spin singlet is the ground state of the model for large and positive \( J \) and spin triplet is the ground state for large and negative \( J \) as shown in figure (4.2).

Figure 4.2: The phase diagram of XYZ-Ising Model in \( J - J_z \) plane. The boundary of the figure indicates the extreme limits of \( J \) and \( J_z \). The blue, red and green line of the figure shows the range for large \( J \) and \( J_z \) in which the spin triplet (ST) state, spin singlet (SS) state and spin 1 antiferromagnetic (SPIN 1 AFM) state is the ground state respectively.

Let us find out the ground state in the limit of large \( J \) and \( J_z \). The Hamiltonian in this limit can be written as,

\[
H = \frac{J}{2} \sum_i \sigma_{i,1}^x \sigma_{i,2}^x + \sigma_{i,1}^y \sigma_{i,2}^y + J_z \sum_i \sigma_{i,1}^z \sigma_{i,2}^z. \]
The same eigenstates written in eqn.(4.6) are the eigenstates of the above Hamiltonian with eigenvalues $J_z, -J_z + \frac{J}{4}, -J_z - \frac{J}{4}$ and $J_z$ respectively.

We have shown the zero temperature phase diagram of the model in figure 4.2 in extreme limit. In the first quadrant of figure (4.2) where $J > 0$, $J_z > 0$, spin singlet state is the ground state for large $J, J_z$ as shown in figure (4.2). In the second quadrant of figure (4.2) where $J > 0$ and $J_z < 0$, spin one antiferromagnet, $|\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\rangle$, is the ground state for $|J_z| > \frac{|J|}{8}$ for large $J$ and $J_z$ and spin singlet state is ground state for $|J_z| > \frac{|J|}{8}$ for large $J$ and $J_z$. In the third quadrant of figure (4.2) where $J < 0$ and $J_z < 0$, spin triplet state is the ground state for $|J_z| < \frac{|J|}{8}$ for large $J$ and $J_z$ and spin one antiferromagnetic state is ground state for $|J_z| > \frac{|J|}{8}$ for large $J$ and $J_z$. In the fourth quadrant of figure (4.2) where $J < 0$ and $J_z > 0$, spin triplet is the ground state for large $J$ and $J_z$.

### 4.3 The Ground States in all defect sectors

As we have shown in the last chapter the zero defect sector of Hamiltonian consists of both periodic and anti-periodic boundary condition. The ground state energy of zero defect sector $GSE_{zds}$ under anti-periodic and periodic boundary condition is given by,

$$GSE_{zds} = -NJ_z - \sum_{n=1}^{N} \sqrt{J^2 + 1 - 2J \cos\left(\frac{2n + \alpha\pi}{N}\right)},$$

where $\alpha = 1$ and 0 belongs to anti-periodic and periodic boundary condition respectively.

Using this expression, we calculated numerically the ground state energy of zero defect sector under anti-periodic and periodic boundary condition for $J$ and $J_z$ from -100 to 100, as shown in figure 4.3(a) and figure 4.3(c). The ground state energy under anti-periodic or periodic boundary condition is minimum for small $J$ and large positive $J_z$ and large $|J|$. In figure 4.3(b) and figure 4.3(d) the sign of ground state energy has been shown under anti-periodic and periodic boundary condition.

It was already shown in the last chapter, closed chain becomes $n_D$ decoupled
open chain for \( n_D \) defect sectors. There can be various partitions of \( N \) for \( n_D \) defect sectors. Therefore, instead of finding the ground state energy of \( n_D \) defect sector we calculate the ground state energy for each partition of \( N \). Let us consider \( \{ L_i \} \) as the partition of \( N \) belonging to \( n_D \) defect sectors. Then,

\[
\sum_{i=1}^{n_D} L_i = N \tag{4.9}
\]

Then, the ground state energy \( GSE_{\{L_i\}} \) of partition \( \{L_i\} \) is given by

\[
GSE_{\{L_i\}} = -(N - 2n_D)J_z - \sum_{i=1}^{n_D} \sum_{n=1}^{L_i} \sqrt{J^2 + 1 - 2J \cos \left( \frac{n\pi}{L_i + 1} \right)} \tag{4.10}
\]

The ground state energy of various defect sectors is plotted in \( J - J_z \) plane for \( J \) and \( J_z \) from -100 to 100 for \( N=10 \) unit cells. There are 42 partitions for various defect sectors of 10 unit cells.

The ground state energy of zero defect sector under periodic and anti-periodic boundary condition are equal.

The ground state energy of 1 defect sector for partition 10 is shown in the figure 4.3(e). The ground state energy is minimum at large negative \( J_z \) and large \( |J| \).

The ground state energy of 2 defect sector for the partitions \((9, 1), (8, 2), (7, 3), (6, 4) \) and \((5, 5) \) is shown in the figure 4.4(a) and 4.4(b). The ground state energy is minimum at large positive \( J_z \) and large \( |J| \) for all partitions of 2 defect sector.

The ground state energy of 3 defect sector for the partitions \((8, 1, 1), (7, 2, 1), (6, 3, 1), (6, 2, 2), (5, 4, 1), (5, 3, 2), (4, 4, 2) \) and \((4, 3, 3) \) is shown in the figure 4.4(b), 4.5(a) and 4.5(b). The ground state energy is minimum at large positive \( J_z \) and large \( J \) for first, second and third partitions. For fourth, fifth, sixth, seventh partitions, the ground state energy is minimum at large positive \( J \) and \( J_z \). For last partition \((4, 3, 3) \), the ground state energy is minimum at large positive \( J_z \) and large \( |J| \).

The ground state energy of 4 defect sector for the partitions \((7, 1, 1, 1), (6, 2, 1, 1), (5, 3, 1, 1), (5, 2, 2, 1), (4, 4, 1, 1), (4, 3, 2, 1), (4, 2, 2, 2), (3, 3, 3, 1) \) and \((3, 3, 2, 2) \) is shown in the figure 4.5(b), 4.6(a) and figure 4.6(b). The ground state energy is minimum at large positive \( J_z \) and large \( J \) for first 7 partitions. For
other partitions (3, 3, 3, 1) and (3, 3, 2, 2), the ground state energy is minimum for large positive $J$ and $J_z$.

The ground state energy of 5 defect sector for the partitions (6, 1, 1, 1, 1), (5, 2, 1, 1, 1), (4, 3, 1, 1, 1), (4, 2, 2, 1, 1), (3, 3, 2, 1, 1), (3, 2, 2, 1, 1) and (2, 2, 2, 2, 2) is shown in the figure 4.6(b), 4.7(a) and 4.7(b). The ground state energy is minimum at large positive $J$ for first two partitions. For all other partitions of 5 defect sectors, ground state is minimum at large $|J|$.

The ground state energy of 6 defect sector for the partitions (5, 1, 1, 1, 1, 1), (4, 2, 1, 1, 1, 1), (3, 3, 1, 1, 1, 1), (3, 2, 2, 1, 1, 1), (2, 2, 2, 1, 1, 1) is shown in the figure 4.7(b) and 4.8(a). The ground state energy is minimum at large negative $J_z$ and large $J$ for first three partitions. For other partitions of 6 defect sector, the ground state energy is minimum for large negative $J_z$ and large positive $J$.

The ground state energy of 7 defect sector for the partitions (4, 1, 1, 1, 1, 1, 1), (3, 2, 1, 1, 1, 1, 1) and (2, 2, 2, 1, 1, 1, 1) is shown in the figure 4.8(a) and 4.8(b). The ground state energy is minimum at large negative $J_z$ and large positive $J$ for first and second partitions. For third partition, the ground state is minimum at large negative $J_z$ and large $|J|$.

The ground state energy of 8 defect sector for the partitions (3, 1, 1, 1, 1, 1, 1, 1) and (2, 2, 1, 1, 1, 1, 1, 1) is shown in the figure 4.8(b). The ground state energy is minimum at large negative $J_z$ and large $|J|$ for both partitions of 8 defect sector.

The ground state energy of 9 defect sector for the partition (2, 1, 1, 1, 1, 1, 1, 1, 1) is shown in the figure 4.8(b). The ground state energy is minimum at large negative $J_z$ and large $|J|$. The ground state energy of full defect sector is minimum at large negative $J_z$ and large $|J|$. In the figure 4.9(b), the sign of ground state energy is plotted for $J$ and $J_z$ from -100 to 100.

Among all these ground states of various defect sectors, we find that the ground state energy of zero defect sector is minimum for positive $J_z$. 

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4.4 Zero Temperature Phase Diagram

For each $J$ and $J_z$, we calculate the ground state numerically in all partitions of the model and plot the zero temperature phase diagram as shown in figure (4.4). In order to plot the phase diagram, we found out the minimum energy for each partition for each $J$ and $J_z$ and calculated numerically the first order derivative of $E$ with respect to $J$ for each $J$ and $J_z$. For all those values of $J$ and $J_z$, wherever we found a discontinuity in the first derivative of ground state energy, we plot those values of $J$ and $J_z$ in $J - J_z$ plane. For $J_z < 0$, we find that the system undergoes through a first order phase transition and for $J_z > 0$, the system undergoes through topological phase transition in the model because it is characterised by winding number. The fact that zero defect sector is ground state sector for $J_z > 0$ makes it easier to analyse the phase transition for $J_z > 0$.

In order to show that the system has a first order phase transition we plot the ground state energy versus $J$ for $J_z = -2$ and $J_z = -4$ as shown in figure (4.10). The ground state energy has two kinks which indicates that first order derivative is discontinuous.

In order to show that the system has a topological phase transition for $J_z > 0$, we compute winding number. In order to compute the winding number we calculate Berry’s phase. The winding number $\nu$ is related to Berry’s phase $\phi$ by

$$\nu = \frac{\phi}{\pi}.$$  \hspace{1cm} (4.11)

The Berry’s phase for Hamiltonian $H(R)$ is given by

$$\phi = \phi_t - \phi_0 = \int_{R(0)}^{R(t)} \langle \Psi| i\partial_R |\Psi \rangle dR,$$  \hspace{1cm} (4.12)

where parameters $R_1, R_2, ..., R_N$ are components of a vector $R$.

For our case, Hamiltonian $H$ is function of only one parameter $k$ which runs from $0$ to $\pi$ as we have mentioned in chapter 3. Therefore,

$$\phi = \int_0^\pi \langle \Psi| i\partial_k |\Psi \rangle dk$$  \hspace{1cm} (4.13)
From eqn. (3.40) in chapter 3 we write the two component wave function,

\[ |\Psi_{k,1}\rangle = \begin{bmatrix} e^{i\alpha_k} \\ 1 \end{bmatrix} \]  

(4.14)

and \[ |\Psi_{k,2}\rangle = \begin{bmatrix} 1 \\ e^{-i\alpha_k} \end{bmatrix}. \]  

(4.15)

The integrand \[ \langle \Psi^\dagger | i\partial_k | \Psi \rangle \] is then given by,

\[ \langle \Psi^\dagger | i\partial_k | \Psi \rangle = \begin{bmatrix} e^{-i\alpha_k} & 1 \end{bmatrix} i\partial_k \begin{bmatrix} e^{i\alpha_k} \\ 1 \end{bmatrix} = -\frac{\partial\alpha_k}{\partial k}. \]  

(4.16)

Therefore, the berry’s phase is given by,

\[ \phi = -\int_0^\pi \frac{\partial\alpha_k}{\partial k} dk \]
\[ = -\int_0^\pi d\alpha_k \]
\[ = -(\alpha(\pi) - \alpha(0)). \]  

(4.17)

In chapter 3, we have shown in figure (3.3) and (3.4) that \( \alpha(0) = 0 \) and \( \alpha(\pi) = 0 \) for |J| > 1 and \( \alpha(0) = 0 \) and \( \alpha(\pi) = \pi \) for |J| < 1. Therefore, the Berry’s phase \( \phi \) is given by,

\[ \phi = 0 \] for \( |J| > 1 \)
and \( \phi = -\pi \) for \( |J| < 1. \)  

(4.18)

Now, we calculate the winding number from eqn. (4.11),

\[ \nu = 0 \] for \( |J| > 1, \)
\[ \nu = -1 \] and for \( |J| < 1. \)  

(4.19)

Therefore, the winding number takes different values for both cases |J| > 1 and |J| < 1 which characterises the phase transition shown in figure (4.4).

For \( J_z > 0 \), the zero defect sector is the ground state sector of the Hamiltonian.
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So, for $J_z > 0$, we can calculate first order derivative substituting $E_G = GSE_{zds}$ from eqn. (4.10). From eqn. (4.10), we can write,

$$\frac{\partial E_G}{\partial J} = -\frac{1}{N} \sum_{n=1}^{N} \frac{J - \cos\left(\frac{2n\pi}{N}\right)}{\sqrt{J^2 + 1 - 2J \cos\left(\frac{2n\pi}{N}\right)}}$$

$$\frac{\partial^2 E_G}{\partial J^2} = -\frac{1}{N} \sum_{n=1}^{N} \frac{\sin^2\left(\frac{2n\pi}{N}\right)}{\left\{J^2 + 1 - 2J \cos\left(\frac{2n\pi}{N}\right)\right\}^{3/2}}$$  \hspace{1cm} (4.20)

We can show analytically that at $J = 1$, the second order derivative blows up. At $J=1$, the eqn. (4.20) becomes,

$$\frac{\partial^2 E_G}{\partial J^2} = -\frac{1}{N} \sum_{n=1}^{N} \frac{\sin^2\left(\frac{2n\pi}{N}\right)}{\left\{4 \sin^2\left(\frac{n\pi}{N}\right)\right\}^{3/2}}$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \frac{4 \sin^2\left(\frac{n\pi}{N}\right) \cos^2\left(\frac{n\pi}{N}\right)}{\left\{8 \sin^3\left(\frac{n\pi}{N}\right)\right\}}$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \frac{\cos^2\left(\frac{n\pi}{N}\right)}{\left\{2 \sin\left(\frac{n\pi}{N}\right)\right\}}$$

$$= \infty$$  \hspace{1cm} (4.21)

because at $n = N$, the denominator becomes zero.

Similarly, we can show that at $J=-1$ also, the second order derivative of ground state energy blows up. At $J=-1$, the eqn. (4.20) becomes,

$$\frac{\partial^2 E_G}{\partial J^2} = -\frac{1}{N} \sum_{n=1}^{N} \frac{\sin^2\left(\frac{2n\pi}{N}\right)}{\left\{4 \cos^2\left(\frac{n\pi}{N}\right)\right\}^{3/2}}$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \frac{4 \sin^2\left(\frac{n\pi}{N}\right) \cos^2\left(\frac{n\pi}{N}\right)}{\left\{8 \cos^3\left(\frac{n\pi}{N}\right)\right\}}$$

$$= -\frac{1}{N} \sum_{n=1}^{N} \frac{\sin^2\left(\frac{n\pi}{N}\right)}{\left\{2 \cos\left(\frac{n\pi}{N}\right)\right\}}$$

$$= \infty$$  \hspace{1cm} (4.22)

because at $n = N/2$, the denominator becomes zero.

Thus, at $J = \pm 1$, the model has second order phase transition for $J_z > 0$. In
figure (4.12), we plot the first order and second order derivative of energy versus 
$J$ for $J = -2$ to 2.
(a) The color variation shows the magnitude of ground state energy of zero defect sector in $J - J_z$ plane under anti-periodic boundary condition.

(b) The color variation shows the sign of ground state energy of zero defect sector in $J - J_z$ plane under anti-periodic boundary condition.

(c) The color variation shows the magnitude of ground state energy of zero defect sector in $J - J_z$ plane under periodic boundary condition.

(d) The color variation shows the magnitude of ground state energy of zero defect sector in $J - J_z$ plane under periodic boundary condition.

(e) The color variation shows the magnitude of ground state energy of one defect sector in $J - J_z$ plane.

Figure 4.3:
Figure 4.4: The ground state energy is plotted for various partitions of $N=10$ shown in the light green patch (for example (9, 1), (8, 2) etc). The color variation of the graph shows the magnitude of ground state energy.
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Figure 4.5: The ground state energy is plotted for various partitions of $N=10$ shown in the light green patch. The color variation of the graph shows the magnitude of ground state energy.
Figure 4.6: The ground state energy is plotted for various partitions of $N=10$ shown in the light green patch. The color variation of the graph shows the magnitude of ground state energy.
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Figure 4.7: The ground state energy is plotted for various partitions of N=10 shown in the light green patch. The color variation of the graph shows the magnitude of ground state energy.
Figure 4.8: The ground state energy is plotted for various partitions of $N=10$ shown in the light green patch. The color variation of the graph shows the magnitude of ground state energy.
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Figure 4.9: The ground state energy is plotted in full defect sector in $J - J_z$ plane. The color variation of the graph in figure (a) shows the magnitude of the ground state energy and in figure (b) sign of the ground state energy.

Figure 4.10: The ground state energy versus $J$ is plotted for $J_z = -2$ in figure (a) and for $J_z = -4$ in figure (b). The kink in the ground state energy shows the first order transition.
Figure 4.11: The red line in the phase diagram shows the first order transition and green line shows the topological phase transition at $J = \pm 1$ described by the order parameter winding number.

Figure 4.12: The first and second order derivative of the ground state energy is plotted in $J - J_z$ plane for $J_z > 0$ in figure (a) and figure (b).