Chapter 1

Semi-classical treatment of the $J_1 - J_2$ Heisenberg model

The 2-dimensional $J_1 - J_2$ Heisenberg model with nearest (J_1) and next-nearest neighbor (J_2) interactions on a square lattice is an archetypal example of a strongly correlated and frustrated spin model. Although the model is conceptually simple and easy to write down, it exhibits rich and interesting physics owing to the interplay between frustration and quantum fluctuations. The model is known to exhibit two phases with quasi-classical long range antiferromagnetic (AFM) order at $T = 0$ (Fig. 1.1), namely, a Néel-ordered phase ((π, π) AFM) for $J_2/J_1 \lesssim 0.4$, and a stripe-ordered phase (($\pi, 0$) or ($0, \pi$) AFM) for $J_2/J_1 \gtrsim 0.6$. These two AFM states are separated by an intermediate quantum paramagnetic state ($0.4 \lesssim J_2/J_1 \lesssim 0.6$), also known as the *spin liquid* phase [1]. These phase transitions can be readily studied using state-of-the-art Quantum Monte Carlo or Exact Diagonalization calculations, but these methods require large amounts of computational resources. In this chapter, we will present a semi-classical approach to study the spin-1/2 $J_1 - J_2$ Heisenberg model where we treat a part of the Hamiltonian as a source of *quantum fluctuations* and encode them in a semi-classical manner in combination with classical Monte Carlo simulations, thereby reducing the computational cost required.

1.1 The Hamiltonian

With the nearest and the next-nearest neighbor coupling constants being J_1 and J_2, respectively, the Hamiltonian for the quantum spin-1/2 $J_1 - J_2$ Heisenberg model is given by

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \tag{1.1.1}$$

where $\langle i, j \rangle$ denotes a nearest neighbor links and $\langle\langle i, j \rangle\rangle$ denotes the next-nearest neighbor links (Fig. 1.2). Further, the spin-1/2 operators are defined as $\hat{\vec{S}} = (\hbar/2)\vec{\sigma}$, and we'll set $\hbar = 1$ for our purposes.

$$\hat{\vec{S}} = \frac{1}{2}\vec{\sigma} \tag{1.1.2}$$

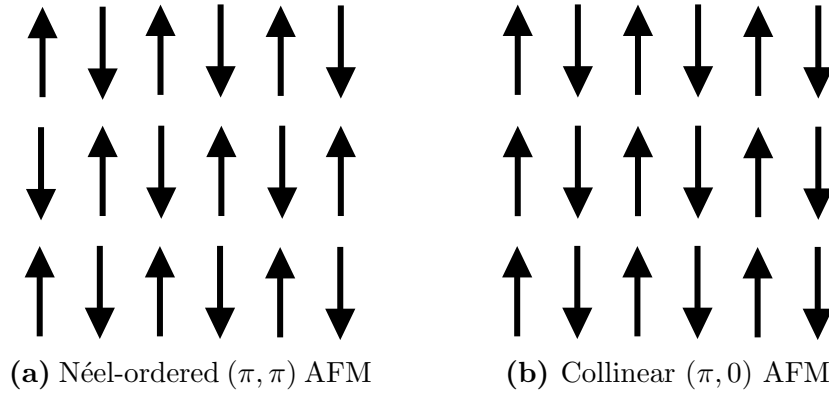**(a)** Néel-ordered (π, π) AFM   **(b)** Collinear $(\pi, 0)$ AFM

Figure 1.1: Anti-Ferromagnetic phases of the $J_1 - J_2$ Heisenberg Model

Therefore, in terms of Pauli operators, the Hamiltonian can be written as

$$\hat{H} = \frac{J_1}{4} \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j + \frac{J_2}{4} \sum_{\langle\langle i,j \rangle\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \tag{1.1.3}$$

Since the Hamiltonian contains σ^x (or $\hat{X}$), σ^y (or $\hat{Y}$), as well as σ^z (or $\hat{Z}$) terms, the energy eigenstates of the Hamiltonian (consequently, the ground state) will never be an eigenstate of either $\hat{X}, \hat{Y}$ or $\hat{Z}$. Let us look at this statement from another perspective – consider the interaction term

$$\vec{\sigma}_i \cdot \vec{\sigma}_j = \hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j + \hat{Z}_i \hat{Z}_j \tag{1.1.4}$$

Let's start by considering the $\hat{Z}$ eigenstates $\{|\uparrow\rangle, |\downarrow\rangle\}$. In this basis, the $\hat{Z}_i \hat{Z}_j$ term measures the alignment between sites i and j. On the other hand, the action of the $\hat{X}_i \hat{X}_j$ and $\hat{Y}_i \hat{Y}_j$ is to flip the states (with additional phase factors), hence acting like a *quantum fluctuation*. Therefore, we propose that if we can model an *effective semi-classical* process to simulate the quantum fluctuations in this system, then we can write the interaction term as

$$\vec{\sigma}_i \cdot \vec{\sigma}_j = \hat{Z}_i \hat{Z}_j + \mathcal{E}(Q)_{ij} \tag{1.1.5}$$

where $\mathcal{E}(Q)_{ij}$ is our notation for effective quantum fluctuations between site i and j. We can write our Hamiltonian in a similar fashion

$$\hat{H} = \frac{J_1}{4} \sum_{\langle i,j \rangle} \left[\hat{Z}_i \hat{Z}_j + \mathcal{E}(Q)_{ij} \right] + \frac{J_2}{4} \sum_{\langle\langle i,j \rangle\rangle} \left[\hat{Z}_i \hat{Z}_j + \mathcal{E}(Q)_{ij} \right] \tag{1.1.6}$$

Since we are treating the quantum fluctuations $\mathcal{E}(Q)_{ij}$ in a semi-classical manner, the Hamiltonian (1.1.6) is now diagonal in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis just like a classical Ising model. Hence, we can replace $\hat{Z}$ with a classical Ising spin $s_i \in \{\pm 1\}$

$$E = \frac{J_1}{4} \sum_{\langle i,j \rangle} [s_i s_j + \mathcal{E}(Q)_{ij}] + \frac{J_2}{4} \sum_{\langle\langle i,j \rangle\rangle} [s_i s_j + \mathcal{E}(Q)_{ij}] \tag{1.1.7}$$
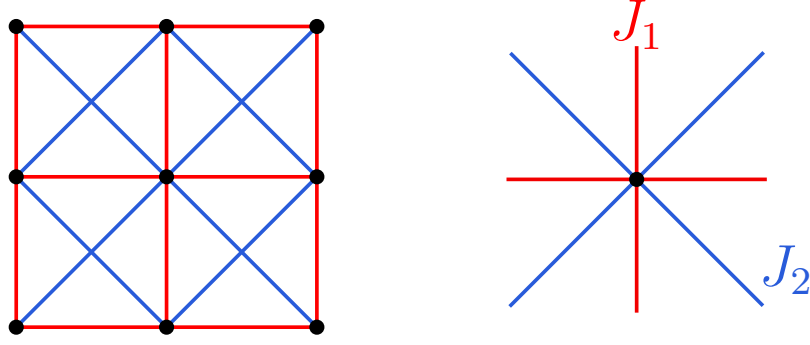
Figure 1.2: $J_1 - J_2$ Heisenberg model lattice structure. The bonds in red represent the J_1 (nearest neighbor) interaction and the bonds in blue represent the J_2 (next-nearest neighbor) interactions.

Therefore, in an effective limit, we propose to simplify the $J_1 - J_2$ Heisenberg model to a **$J_1 - J_2$ classical Ising model with quantum fluctuations** (Eq. (1.1.7)). If modelled correctly, these quantum fluctuations should give rise to the same phase diagram as obtained through a thorough Quantum Monte Carlo treatment.

1.2 Quantum fluctuations

To analyze the source of quantum fluctuations in the $J_1 - J_2$ Heisenberg model, we'll start with a simple two-site interaction Hamiltonian. Let's say our two-site Hamiltonian $\hat{h}$ is given by

$$\hat{h} = J\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \tag{1.2.1}$$

where i and j denote the only two neighboring sites. One can view this as the interaction term appearing in an *addition of angular momentum* problem where $\hat{\vec{M}} = \hat{\vec{S}}_i + \hat{\vec{S}}_j$. Then the interaction term looks like

$$\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \frac{\left(\hat{\vec{M}}^2 - \hat{\vec{S}}_i^2 - \hat{\vec{S}}_j^2\right)}{2} \tag{1.2.2}$$

As can be shown using the Clebsch-Gordan coefficients calculation, the eigenstates of the $\hat{\vec{M}}^2$ and the $\hat{M}_z$ operator are the singlet and triplet states

$$\left.\begin{aligned} |s = 1;\, m_s = +1\rangle &= |\uparrow\uparrow\rangle \\ |s = 1;\, m_s = -1\rangle &= |\downarrow\downarrow\rangle \\ |s = 1;\, m_s = 0\rangle &= (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} \end{aligned}\right\} s = 1 \text{ (triplet)} \tag{1.2.3a}$$

$$\left.\begin{aligned} |s = 0;\, m_s = 0\rangle &= (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2} \end{aligned}\right\} s = 0 \text{ (singlet)} \tag{1.2.3b}$$

The energy eigenvalues of the singlet and triplet states are accordingly given by

$$\hat{h}\,|s=1\rangle = \frac{+J}{4}\,|s=1\rangle \quad \rightarrow \text{ triplet} \tag{1.2.4a}$$

$$\hat{h}\,|s=0\rangle = \frac{-3J}{4}\,|s=0\rangle \quad \rightarrow \text{ singlet} \tag{1.2.4b}$$

At $T = 0$, the two-site *dimer* state is simply the entangled singlet state $|s = 0; m_s = 0\rangle$ with an energy of $-3J/4$. Since entangled singlet dimer states are a purely quantum phenomena, we propose them to be the source of quantum fluctuations at $T = 0$.

However, at finite temperatures $T \neq 0$, the mixed state of the system is described through the thermal density matrix

$$\hat{\rho} = \frac{e^{-\beta\hat{h}}}{\text{Tr}(e^{-\beta\hat{h}})} \tag{1.2.5}$$

Using $\hat{\rho}$, we can compute the thermal expectation value of the energy

$$\langle E \rangle = \frac{\sum_i e^{-\beta E_i} E_i}{\sum_i e^{-\beta E_i}} = \frac{3J}{4}\left(\frac{e^{-\beta J} - 1}{3e^{-\beta J} + 1}\right) \tag{1.2.6}$$

Similarly, we can also compute the expectation value of the net magnetization which corresponds to the operator $\hat{\vec{M}} = \hat{\vec{S}}_i + \hat{\vec{S}}_j$, and it is a straightforward exercise to show that

$$\langle \vec{M} \rangle = 0 \tag{1.2.7}$$

which means that the two-site interaction acts like a *zero magnetization* dimer.

Since the entangled mixed-state (combination of singlet and triplet states) in the two-site Hamiltonian is a purely quantum effect, we can attribute the *quantum fluctuations* in our model to the *dimers*. Therefore, we propose to model the quantum fluctuations between site i and j as a *classical analog* of dimers

$$\textbf{Semi-classical dimer } \langle \boldsymbol{i}, \boldsymbol{j} \rangle \rightarrow \quad M(T) = 0, \quad E_J(T) = \frac{3J}{4}\left(\frac{e^{-J/T} - 1}{3e^{-J/T} + 1}\right). \tag{1.2.8}$$

Hence, in addition to the classical Ising spin flip dynamics in our effective model, we have also introduced *dimer* degrees of freedom (to compensate for quantum fluctuations) which can be created or destroyed to minimize the free energy F of the system.

1.3 Semi-classical Monte Carlo

Till now, we have proposed two important simplifications of the quantum $J_1 - J_2$ Heisenberg model, i.e.,

1. the quantum model is equivalent to a combination of $J_1 - J_2$ Ising model and some effective quantum fluctuations.

2. the quantum fluctuations can be modelled semi-classically by semi-classical dimers with zero magnetization and a temperature dependent energy $E(T)$ (Eq. (1.2.8)).

To *incorporate* the semi-classical dimers with the $J_1 - J_2$ Ising model, we design a Metropolis Markov chain Monte Carlo algorithm with dimer creation and annihilation steps as Metropolis proposals. Roughly speaking, the Metropolis proposals consist of both spin flips and dimer creation-annihilation steps on the $J_1 - J_2$ Ising lattice, and we expect the effects of the quantum fluctuations to revive in this semi-classical Monte Carlo simulation. A semi-classical Monte Carlo sweep is then defined as follows:

1. Randomly choose a site i on the lattice.

2. Check if the site i is a part of the dimer or a free spin.

3. If site i is a free spin, then we have two possible moves:

   – With a probability p, propose a spin flip $\sigma_i \to -\sigma_i$.
   – With a probability $1 - p$, propose the formation of a semi-classical dimer with another nearest or next-nearest neighbor free spin.

4. If the site i is involved in a dimer (not a free spin), then propose the annihilation of the dimer and create two new random Ising spins.

5. Calculate the change in energy ΔE.

6. Accept the proposed move with a probability of $\min\left[e^{-\beta \Delta E}, 1\right]$.

7. Steps 1 to 6 are then repeated $\mathcal{N} = L^2$ times.

The probability p is changed so as to tune the ratio of random spin-flip dynamics with dimer-formation dynamics. We will discuss the specifics of these parameters in the upcoming sections.

1.4   Dimer dynamics in Monte Carlo

In this section, we will outline the idea behind the physics of creation and annihilation of dimers. The Monte Carlo dynamics is controlled by the change in energies. Hence, it is helpful to calculate the relevant expressions.

Since the semi-classical dimer is a zero magnetization unit, it implies that the contribution of the neighbor interaction $S_i S_j = 0$ if i or j are part of a dimer. This can be encoded by **setting $S_i = 0$ if site i is making a dimer with one of its neighbors**.

On the basis of this setup, we can calculate the changes in energy in a dimer creation or annihilation process. Let's say a dimer is created between sites $i = (i_x, i_y)$ and $j = (j_x, j_y)$.
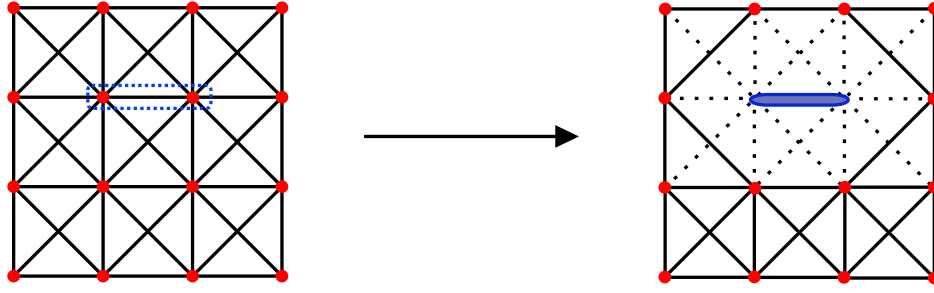
Figure 1.3: Semi-classical dimer formation on $\langle i, j \rangle$ with $S_i = S_j = 0$ and $E = E(T)$.

The change in energy due to dimer creation is then given by

$$\Delta E_{\mathrm{c}} = + E_J(T) - \frac{J_1}{4} \left[S_{(i_x, i_y)} \sum_{\vec{\delta} \in \{(0, \pm 1), (\pm 1, 0)\}} S_{(i_x, i_y) + \vec{\delta}} \quad + S_{(j_x, j_y)} \sum_{\vec{\delta} \in \{(0, \pm 1), (\pm 1, 0)\}} S_{(j_x, j_y) + \vec{\delta}} \right]$$

$$- \frac{J_2}{4} \left[S_{(i_x, i_y)} \sum_{\vec{\delta} \in \{(1, \pm 1), (-1, \pm 1)\}} S_{(i_x, i_y) + \vec{\delta}} \quad + S_{(j_x, j_y)} \sum_{\vec{\delta} \in \{(1, \pm 1), (-1, \pm 1)\}} S_{(j_x, j_y) + \vec{\delta}} \right] + \frac{J}{4} S_{(i_x, i_y)} S_{(j_x, j_y)}$$

where J is equal to J_1 or J_2 depending on whether the dimer is formed with the nearest or next-nearest neighbor, respectively, and the Ising spin configuration $\{S_{(x,y)}\}$ is the set of values before the dimer is formed.

Similarly, the change in energy due to annihilation of the dimer between sites i and j and creation of two free spins is given by

$$\Delta E_{\mathrm{a}} = - E_J(T) + \frac{J_1}{4} \left[S'_{(i_x, i_y)} \sum_{\vec{\delta} \in \{(0, \pm 1), (\pm 1, 0)\}} S'_{(i_x, i_y) + \vec{\delta}} \quad + S'_{(j_x, j_y)} \sum_{\vec{\delta} \in \{(0, \pm 1), (\pm 1, 0)\}} S'_{(j_x, j_y) + \vec{\delta}} \right]$$

$$+ \frac{J_2}{4} \left[S'_{(i_x, i_y)} \sum_{\vec{\delta} \in \{(1, \pm 1), (-1, \pm 1)\}} S'_{(i_x, i_y) + \vec{\delta}} \quad + S'_{(j_x, j_y)} \sum_{\vec{\delta} \in \{(1, \pm 1), (-1, \pm 1)\}} S'_{(j_x, j_y) + \vec{\delta}} \right] - \frac{J}{4} S'_{(i_x, i_y)} S'_{(j_x, j_y)}$$

where again J is equal to J_1 or J_2 depending on whether it was a nearest or next-nearest neighbor dimer, respectively, and the spin configuration $\{S'_{(x,y)}\}$ is the set of values after the two new random spins are formed in place of the dimer.

1.5   Classical expectation

Before moving to numerical Monte Carlo simulations to aid our calculations, it is helpful to develop a first-order intuition of the change in physics which occurs by the introduction of semi-classical dimers. Let us consider the $T = 0$ ground state situation. We expect three different type of orders in our system − the Néel-ordered (π, π) AFM phase, the $(\pi, 0)$ or $(0, \pi)$ AFM phase, and the spin liquid phase (all dimer state). At $T = 0$, the

(π, π)
Néel AFM   Spin Liquid

$(\pi, 0)$ or $(0, \pi)$
Striped AFM

$J_2 \, / \, J_1$

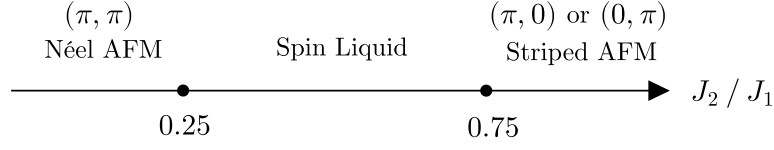0.25   0.75

Figure 1.4: Ground State

system attains the minimum energy state. Therefore, we can compare the energies (per site) of the three phases to find regions of stability.

For the Néel-ordered (π, π) AFM phase, we have a staggered magnetization along both the axes, and $S_i S_j = -1$ for all the bonds. Therefore, the energy per site is given by

$$E_{(\pi,\pi)} = \frac{J_1}{2}\left(\frac{J_2}{J_1} - 1\right) \tag{1.5.1}$$

Similarly, for the $(\pi, 0)$ or $(0, \pi)$ staggered AFM phase, we have $S_i S_j = -1$ for the next-nearest neighbor links $\langle\langle i, j \rangle\rangle$ and $S_i S_j = \pm 1$ for the nearest neighbours $\langle i, j \rangle$, i.e., keeps fluctuating between ± 1, hence cancelling the contribution.

$$E_{(\pi,0) \text{ or } (0,\pi)} = \frac{J_1}{2}\left(-\frac{J_2}{J_1}\right) \tag{1.5.2}$$

Finally, for the completely dimerized (spin liquid) phase, the energy per site is given by

$$E_{\text{SL}} = \frac{J_1}{2}\left[-\frac{3}{4}(f) - \frac{3}{4}\frac{J_2}{J_1}(1-f)\right]$$

where f is the fraction of nearest neighbor dimers. Since we are mainly interested in the regime $J_2/J_1 \in [0, 1]$, the parameter value $f = 1$ gives the minimum energy per site

$$E_{\text{SL}} = \frac{J_1}{2}\left(-\frac{3}{4}\right) \tag{1.5.3}$$

Therefore, on comparing the energies, it is straightforward to see that the classical expectation of the phase boundaries at $T = 0$ is given as

$$0 \leq \frac{J_2}{J_1} \leq 0.25 \qquad \longrightarrow \quad (\pi, \pi) \text{ AFM}$$

$$0.25 \leq \frac{J_2}{J_1} \leq 0.75 \qquad \longrightarrow \quad \text{Spin Liquid phase}$$

$$0.75 \leq \frac{J_2}{J_1} \qquad \longrightarrow \quad (\pi, 0) \text{ or } (0, \pi) \text{ AFM}$$

Therefore, **exactly** at $T = 0$, the phase transition in our effective model occurs at the points $J_2/J_1 = 0.25$ and $J_2/J_1 = 0.75$. However, as we'll discuss later, even a small temperature of $T \sim \mathcal{O}(\texttt{1.0e-4})$ can lead to the entropic stabilization of the fully dimerized

configuration and can play a huge role in extending the boundaries of the spin liquid phase to bring the semi-classically derived critical points closer to the quantum results.

1.6 Results