Quantum phases from semi-classical Monte Carlo

Exploring the phases of $J_1 - J_2$ Heisenberg model

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$J_1 - J_2$ Heisenberg model

Quantum spin model with nearest neighbor and next nearest neighbor coupling

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

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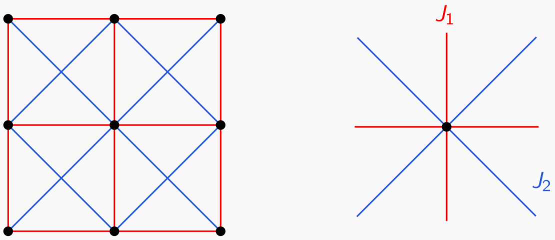

Figure 1: Lattice structure

Quantum phases at $T = 0$

- a Néel-ordered phase ((π, π) AFM) for $J_2/J_1 \lesssim 0.4$.
- a quantum paramagnetic phase ($0.4 \lesssim J_2/J_1 \lesssim 0.6$).
- a collinear-ordered phase ($(\pi, 0)$ or $(0, \pi)$ AFM) for $J_2/J_1 \gtrsim 0.6$.

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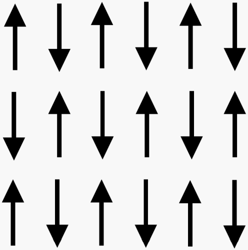
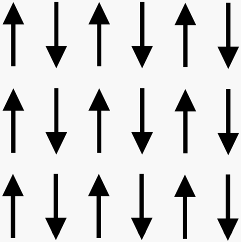


(a) Néel (π, π) AFM



(b) Collinear $(\pi, 0)$ AFM

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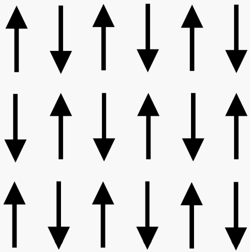

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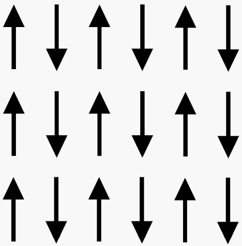
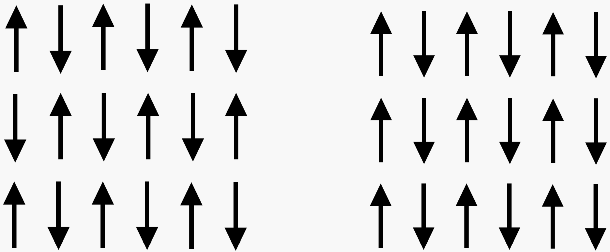


(b) Collinear $(\pi, 0)$ AFM

Quantum phases at $T = 0$

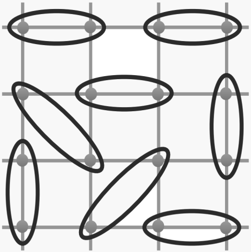
- a Néel-ordered phase ((π,π) AFM) for $J_2/J_1 \lesssim 0.4$.
- a spin liquid phase ($0.4 \lesssim J_2/J_1 \lesssim 0.6$).
- a collinear-ordered phase ($(\pi,0)$ or $(0,\pi)$ AFM) for $J_2/J_1 \gtrsim 0.6$.



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

Spin liquid phase

- Spin liquid $\sim$ a sea of singlet-triplet dimers.
- A purely "quantum" effect.



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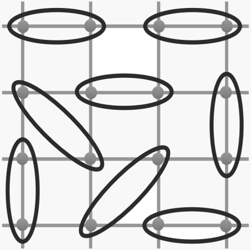

Figure 3: Spin liquid phase.

Question: Emergent spin liquid by adding "quantum fluctuations" on top of a classical model?

Semi-classical mapping

$$\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j = \underbrace{\hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j} + \hat{Z}_i \hat{Z}_j$$

$\hat{X}_i \hat{X}_j + \hat{Y}_i \hat{Y}_j \sim$ acts like a fluctuation in the Z basis.

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$\implies$ **Proposal:** $\hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \approx \underbrace{\hat{Z}_i \hat{Z}_j}_{\text{Ising}} +$ quantum fluctuations

$\therefore$ Semi-classical mapping of $J_1 - J_2$ Heisenberg model to a $J_1 - J_2$ classical Ising and add quantum fluctuations on top of it!

$$H = J_1 \sum_{\langle i,j \rangle} \hat{Z}_i \hat{Z}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \hat{Z}_i \hat{Z}_j + \text{q.f.}$$

Quantum fluctuations

Source of quantum fluctuations: quantum dimer formation.

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For a two-site Heisenberg interaction $J\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2$, we get the following singlet-triplet basis

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

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

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Energy eigenvalues

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

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

Quantum fluctuations (contd.)

Energy of the dimer $$\langle E \rangle = \frac{3J}{4}\left(\frac{e^{-\beta J}-1}{3e^{-\beta J}+1}\right)$$

Magnetization of the dimer $$\langle \vec{M} \rangle = 0.$$

Quantum fluctuations (contd.)

Energy of the dimer $\langle E \rangle = \frac{3J}{4}\left(\frac{e^{-\beta J} - 1}{3e^{-\beta J} + 1}\right)$

Magnetization of the dimer $\langle \vec{M} \rangle = 0.$

Encode the *quantum effects* of the dimer as a *semi-classical dimer*.

Semi-classical dimer $\langle \boldsymbol{i}, \boldsymbol{j} \rangle$

$$M_{\text{dimer}}(T) = 0, \qquad E_{\text{dimer}}(T) = \frac{3J}{4}\left(\frac{e^{-J/T} - 1}{3e^{-J/T} + 1}\right).$$

Semi-classical model

Two different degrees of freedom/units in the lattice:

- Classical **Ising spin** Hamiltonian:

$$E = J_1 \sum_{\langle i,j \rangle} S_i S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i S_j$$

- Semi-classical **dimer** $\langle i,j \rangle$ (source of quantum fluctuations):

$$S_i = S_j = 0, \qquad E_J(T) = \frac{3J}{4}\left(\frac{e^{-J/T} - 1}{3e^{-J/T} + 1}\right)$$

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Combine the dynamics using a Markov chain Monte Carlo simulation!

Markov chain process now includes two different types of steps-

- random spin flips moves $(1-p)$.
- dimer creation/annihilation moves (p).

Standard Metropolis acceptance $\longrightarrow P_{\text{accept}} = \min[1, e^{-\beta\Delta E}]$

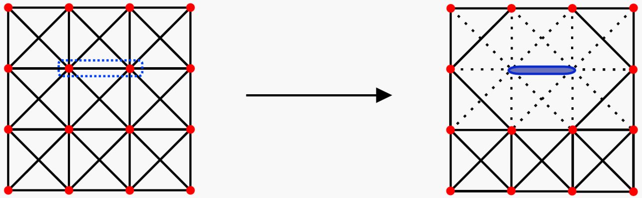


Figure 5: Dimer creation on $\langle i, j\rangle$ with $S_i = S_j = 0$ and $E = E_J(T)$.

Order parameters

Three order parameters for four different phases:

- Staggered magnetizaton (π, π)

$$m_{(\pi,\pi)} = \frac{1}{L^2} \sum_{i=1}^{L^2} (-1)^{i_x + i_y} \, S_i$$

- Staggered magnetizaton $(\pi, 0)$ and $(0, \pi)$

$$m_{(\pi,0)} + m_{(0,\pi)} = \frac{1}{L^2} \sum_{i=1}^{L^2} \left[(-1)^{i_x} + (-1)^{i_y} \right] S_i$$

- Number of dimers

$$N_{\text{dimers}} = N_{J_1 \text{ dimers}} + N_{J_2 \text{ dimers}}$$

Lattice geometry: 10×10

Phases:

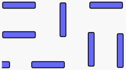
(π, π) AFM

↑↓↑↓↑↓
↓↑↓↑↓↑

$(\pi, 0)$ AFM

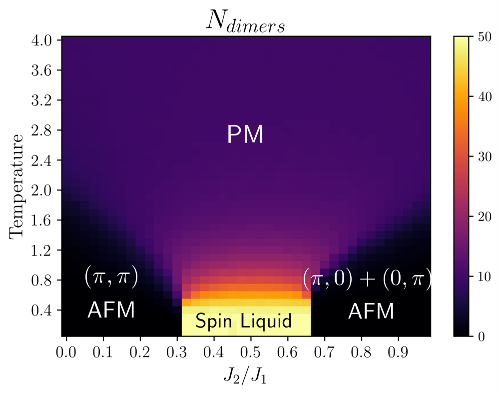
↑↓↑↓↑↓
↑↓↑↓↑↓

Spin Liquid



PM

↑↑↓↑↓↓
↓↑↑↓↑↓



Quantum phase transition

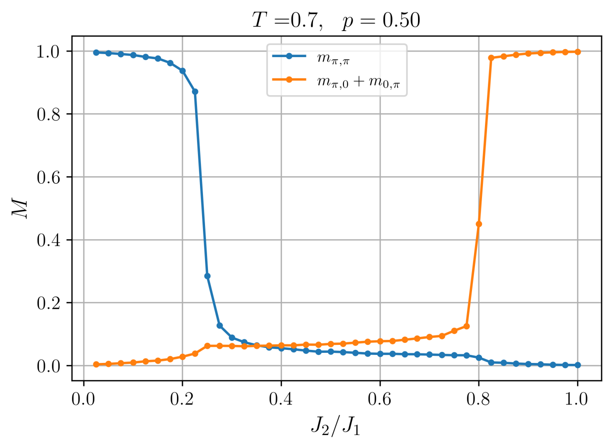


Figure 7: SL$\rightarrow$ $(\pi, 0) + (0, \pi)$ AFM transition is first-order, whereas the (π, π) AFM $\rightarrow$ SL transition is second-order.

Results ($p = 0.15$)

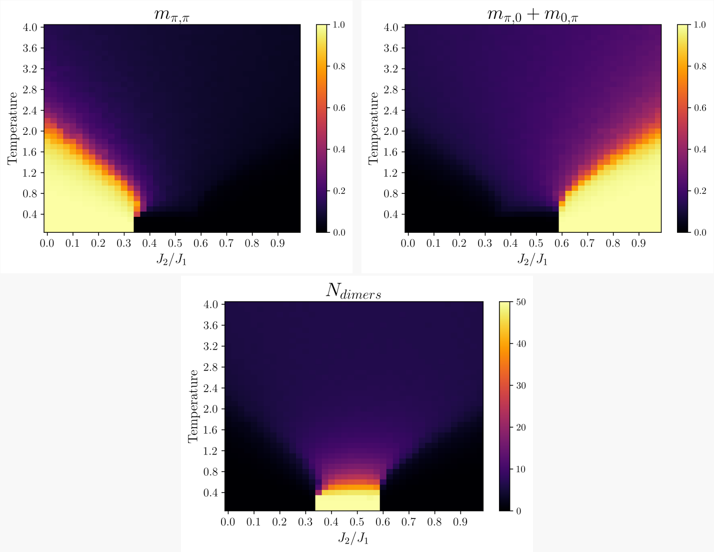


Figure 8: Order parameters at $p = 0.15$

Results ($p = 0.25$)

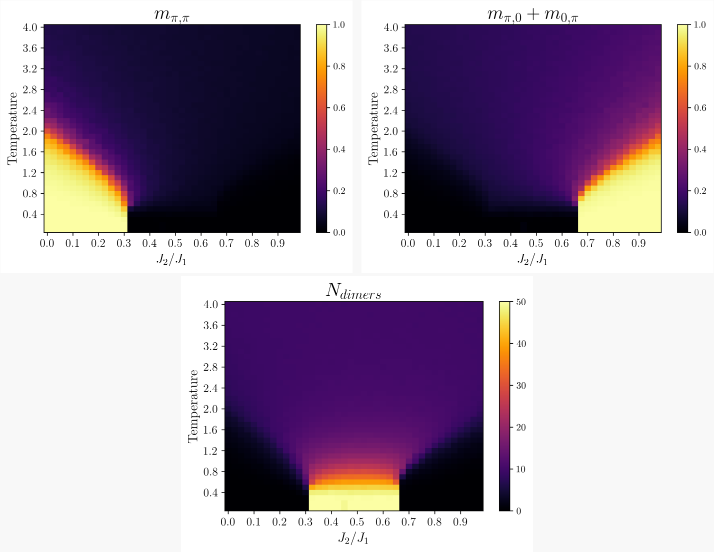


Figure 9: Order parameters at $p = 0.25$

Results ($p = 0.50$)

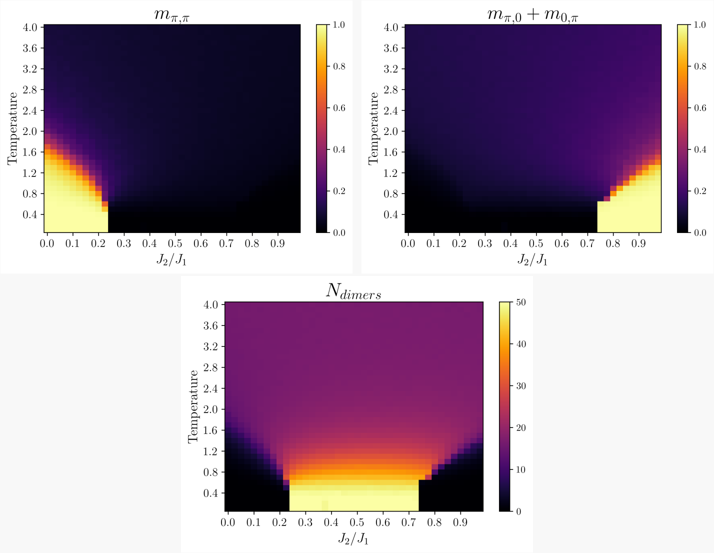


Figure 10: Order parameters at $p = 0.50$

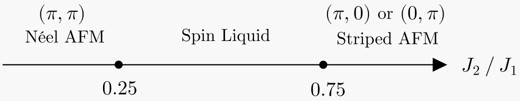


Figure 11: $T = 0$ phase structure argued from an energetic viewpoint.

Entropic stabilization

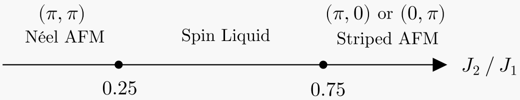


Figure 11: $T = 0$ phase structure argued from an energetic viewpoint.

- Broader SL region, but meta-stable at very small temperatures!
- AFM state entropically more favorable than a dimerized SL (even at extremely small temperatures).

Entropic stabilization (contd.)

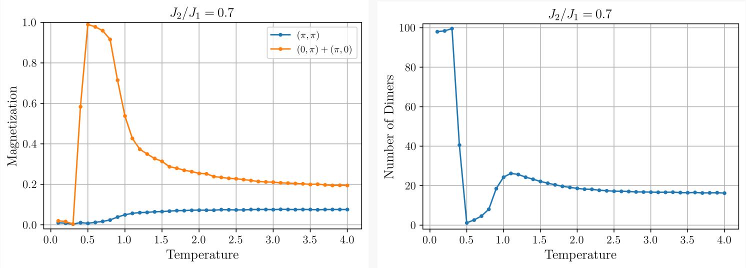


Figure 12: Entropic stabilization of AFM and destabilization of the spin liquid state.

- Entropic stabilization pushes the boundaries of the phases,
- can be tuned via the parameter p to tune the phase transition points.

Summary

Conclusions:

- $J_1 - J_2$ Heisenberg $\xrightarrow{\text{semi-classical}}$ $J_1 - J_2$ Ising model $+$ dimer fluctuations.
- Quantum phases do emerge as a semi-classical correction!

Future direction:

- Tune p to maximises the Monte Carlo acceptance ratios.
- Address critical properties of the model.
- Dimer structure factor as a direct indicator for the SL phase.
- Extension of the "semi-classical" method to other lattice geometries and spin models.

References

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