Cluster Mean Field Theory(CMFT) for quantum spin models

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Abstract

In this project, we employed cluster mean field theory (CMFT) to investigate phases in different quantum spin models, including $J_1 - J_2$ model and Compass Heisenberg model. By utilizing CMFT, we looked at the phases for these models by tracking the order parameters at the ground state. To validate our findings, we employed different theoretical approaches such as the Luttinger-Tisza method and Spin Wave Theory (SWT) to cross-verify our results obtained from CMFT. Our comparative analysis revealed good agreement between CMFT and these alternative methods, lending further support to the reliability and accuracy of CMFT in predicting phases in quantum spin models. Overall, our study highlights the utility of CMFT as a powerful tool for studying the rich phase behaviors in various quantum spin models, and provides a comprehensive analysis of its results in comparison with other theoretical approaches. This research contributes to the understanding of quantum spin systems and their phase diagrams, and opens up possibilities for further investigations in this field.

Cluster Mean Field Theory

- Interactions inside a cluster are treated exactly.
- Interactions between clusters are approximated by mean fields.

Heisenberg model Hamiltonian without presence of external magnetic field ($\hat{H} = J\sum_{c_{n\langle ij\rangle}} \mathbf{S}_{i,c_n}.\mathbf{S}_{j,c_n} + J\sum_{c_m \neq c_{n\langle ij\rangle}} \mathbf{S}_{i,c_n}.\mathbf{S}_{j,c_m}$) the intercluster spin-spin interaction terms are given by

$$\mathbf{S}_{i,c_n}.\mathbf{S}_{j,c_m} \approx \mathbf{S}_{i,c_n}\langle \mathbf{S}_{j,c_m}\rangle + \langle \mathbf{S}_{i,c_n}\rangle \mathbf{S}_{j,c_m} - \langle \mathbf{S}_{i,c_n}\rangle \langle \mathbf{S}_{j,c_m}\rangle$$

Using the above approximation the CMFT Hamiltonian for Heisenberg model is given by $\hat{H}_{CMFT} = \sum_{c_n} \hat{H}_{c_n}$ which gives

$$\hat{H}_{c_n} = J\sum_{\langle ij\rangle} \mathbf{S}_{i,c_n}.\mathbf{S}_{j,c_n} + \sum_{i=1}^{N} h_i \mathbf{S}_{i,c_n} (h_i\text{-intercluster mean field terms})$$

To solve the CMFT equations, we use open boundary conditions for the cluster.

AFM Heisenberg $J_1 - J_2$ model on a square lattice

The Hamiltonian is given by-$\hat{H} = J_1 \sum_{\langle ij\rangle} \mathsf{S}_i.\mathsf{S}_j + J_2 \sum_{\langle\langle ij\rangle\rangle} \mathsf{S}_i.\mathsf{S}_j$.

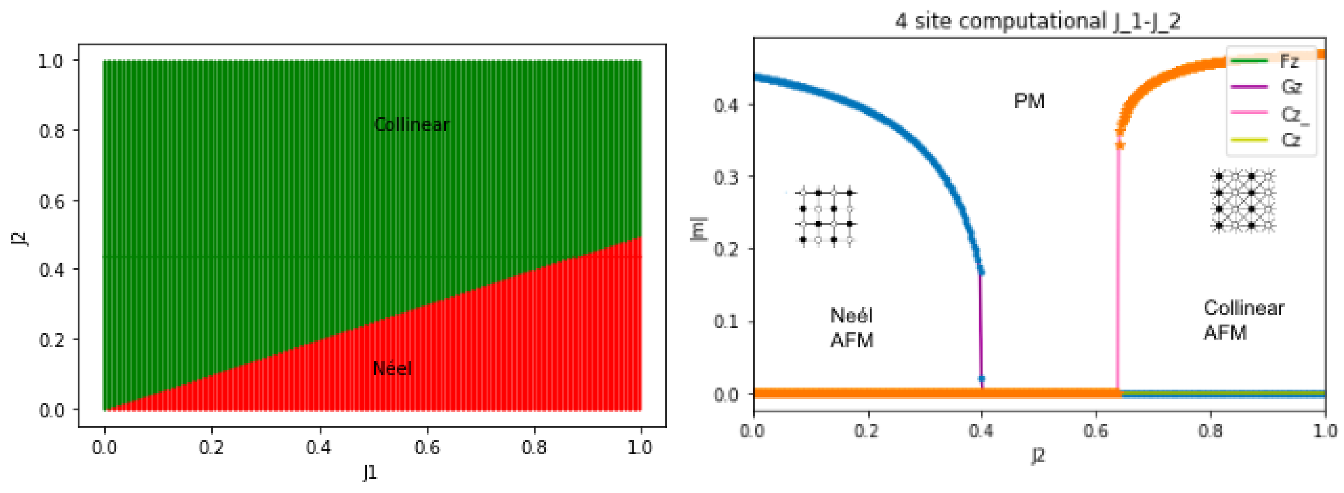


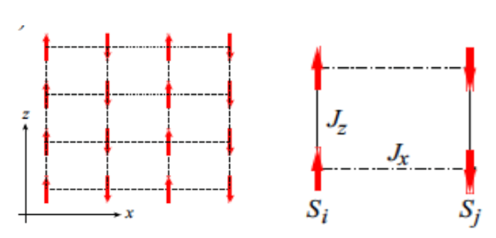
Figure 1. 1. Left-Classical Phase Diagram 2. Right - $|m|$ vs J_1/J_2 for AFM Heisenberg $J_1 - J_2$ model on a square lattice obtained by CMFT

The square-lattice S = 1/2 Heisenberg model with only nearest-neighbor interactions $J_1 > 0$ has an antiferromagnetic ground state.

- In (a) Néel order for $J_2/J_1 < 0.4 - 0.42$.(classical $E_g = -\frac{J_1}{2} + \frac{J_2}{2}$ per site)
- In (b)$0.4 < J_2/J_1 < 0.6$ (approximately) the ground state may be a columnar VBS,
- For $J_2/J_1 > 0.6$, the ground state has collinear (striped) magnetic order, as shown in (c)(classical $E_g = -\frac{J_2}{2}$ per site).

Compass Heisenberg model on a square lattice

The Hamiltonian is given by - $\hat{H} = \sum_{\langle ij\rangle^x} J_x S_i^x S_j^x + \sum_{\langle ij\rangle^z} J_z S_i^z S_j^z + I\sum_{\langle ij\rangle} \mathsf{S}_i.\mathsf{S}_j$



ϕ	α	$E_0(\phi)$	ϕ	α	$E_0(\phi)$
F_z	z	$\frac{J_z}{4} + \frac{I}{2}$	G_z	z	$-\frac{J_z}{4} - \frac{I}{2}$
F_x	x	$\frac{J_x}{4} + \frac{I}{2}$	G_x	x	$-\frac{J_x}{4} - \frac{I}{2}$
F_y	y	$\frac{I}{2}$	G_y	y	$-\frac{I}{2}$
C_z	z	$\frac{J_z}{4}$	C_x	x	$\frac{J_x}{4}$
C_z'	z	$-\frac{J_z}{4}$	C_x'	x	$-\frac{J_x}{4}$

Figure 2. 1. Left-Compass Heisenberg model on a square lattice 2. Right - Classification of ordered phases of the CH model.

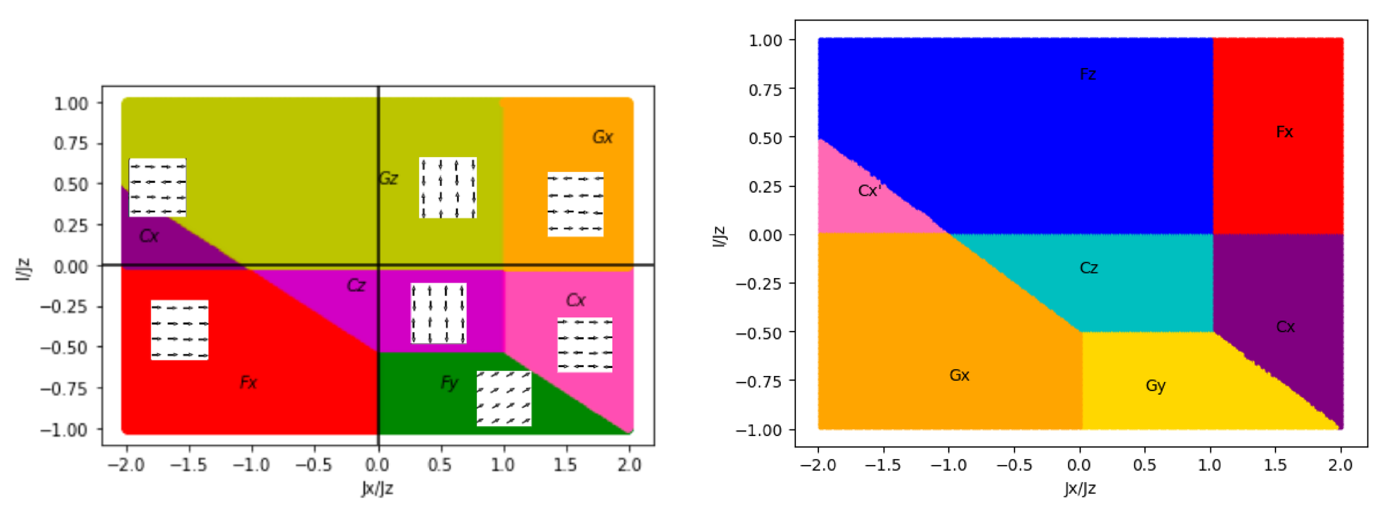


Figure 3. 1. Left-Classical ground state AFM Phase Diagram 2. Right - Classical ground state FM Phase Diagram.

with S_i^α being $\frac{\sigma_i^\alpha}{2}$,where σ_is are the Pauli matrices, $\vec{S_i} = S_i^x, S_i^y, S_i^z$ and two types of nearest neighbour interactions along bonds in the 2D lattice: (i) the frustrated compass interactions J_x, J_z which couple S_i^α components along α-oriented bonds (the two axes are labelled α = x, z), and (ii) Heisenberg interactions of amplitude I.

- To draw the classical ground state phase diagram the ground-state energies E_0 associated to these different phases are compared.
- For each phase, the index $\alpha \in x, y, z$ denotes the easy axis or spin direction favored, while the capital letter in α indicates the type of spatial structure or correlation pattern, i.e., G for Neel-type AF phase, F for FM phase, and C for columnar or C-type AF order.

Results for Compass Heisenberg Model

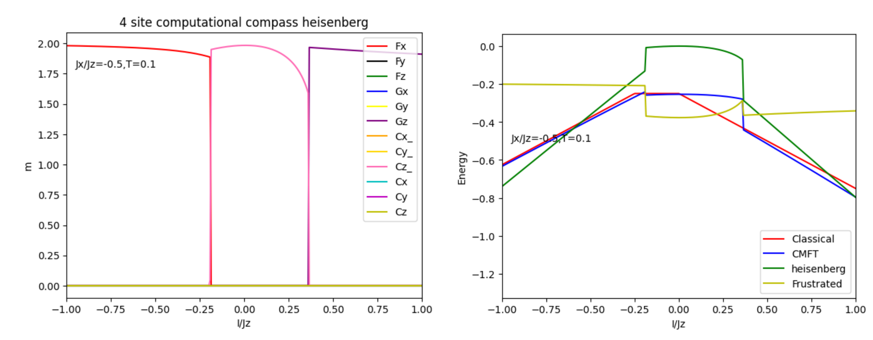


Figure 4. 1. Magnetization vs I/J_z for fixed J_x/J_z value 2. Corresponding energy comparison between classical and CMFT Hamiltonians

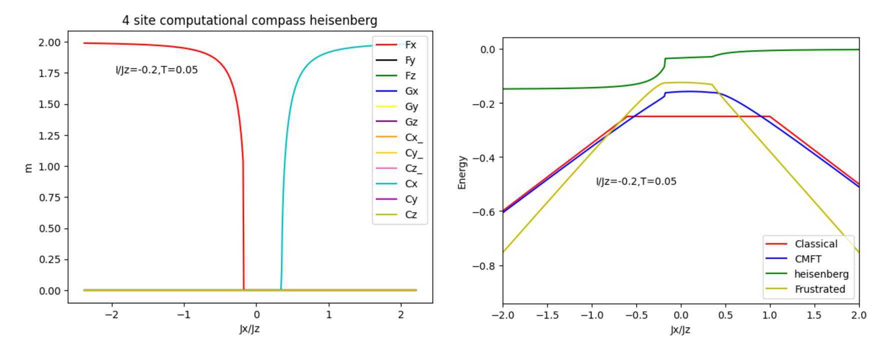


Figure 5. 1. Magnetization vs J_x/J_z for fixed I/J_z value 2. Corresponding energy comparison between classical and CMFT Hamiltonians

Spin Wave Theory for Compass Heisenberg model

The Holstein Primakoff transformation $S_{\vec{r}}^z = S - a_{\vec{r}}^\dagger a_{\vec{r}} = S - n_{\vec{r}}, \quad S_{\vec{r}}^+ = \sqrt{2S}\sqrt{1 - \frac{a_{\vec{r}}^\dagger a_{\vec{r}}}{2S}} a_{\vec{r}}$.(suitable for F_z phase) for CH model gives the Hamiltonian in k space as below after fourier transform

$$H_{LSW}(k) = S\sum_k \left\{ \frac{J_x}{2}\cos k_x \left(a_k a_{-k} + a_k a_k^+ + a_k^+ a_k + a_k^+ a_{-k}^+\right) - 2J_z a_k^+ a_k + 4\left[-I a_k^+ a_k + \frac{I(cos(k_x) + cos(k_z))}{4}\left(a_k^+ a_{-k}^+ + a_k a_{-k}\right)\right]\right\}$$

Which gives us the the following dispersion relation after bogulioubov transformation

$$\omega_{Fz}(\vec{k}) = 2S\sqrt{\left(2\left|J_z + 2I\right| + I_{\vec{k}} + J_{kx}\right)^2 - J_{kx}^2}, \left\{J_{kx}, I_{\vec{k}}\right\} = \left\{J_x \cos k_x, 2I\left(\cos k_x + \cos k_z\right)\right\}$$

In the same way other dispersion relations for different phases are given as $\omega_{Cz}(\vec{k}) = 2S\sqrt{(2\left|J_z\right| + J_{kx} + I_{kz})^2 - (J_{kx} + I_{kx})^2}, \{J_{k\alpha}, I_{k\alpha}\} = \{J_\alpha \cos k_\alpha, 2I\cos k_\alpha\}$.

$$\omega_{Gy}(\vec{k}) = 2S\sqrt{(I_0 + J_{kz} - J_{kx})^2 - \left(I_{\vec{k}} + J_{kx} + J_{kz}\right)^2},$$

$$\omega_{Gz}(\vec{k}) = 2S\sqrt{(2J_z + 4I + J_{kx})^2 - \left(J_{kx} + I_{\vec{k}}\right)^2}.$$

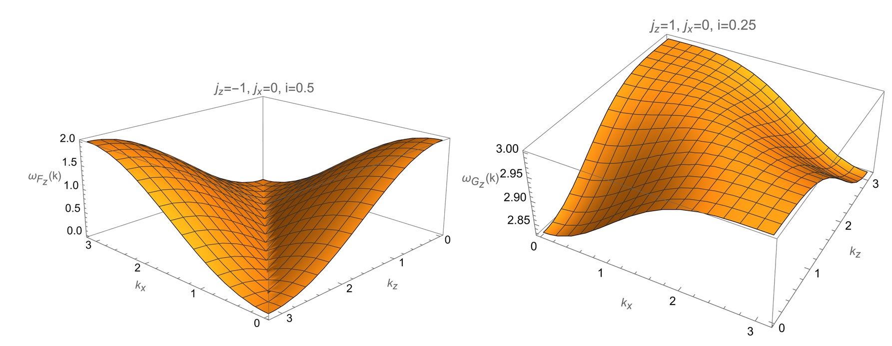


Figure 6. 1. Dispersion relation for F_z as a ground state in FM CH model 2. Dispersion relation for G_z as a ground state in AFM CH model

Luttinger Tisza for Compass Heisenberg model

Basic ingredients: -Find solutions for $x/y/z$ components which has to fulfill $\left(S_i^x\right)^2 + \left(S_i^y\right)^2 + \left(S_i^z\right)^2 = 1$ ('strong' condition)

-Relax this to 'weak' condition $\sum_i \left(S_i^x\right)^2 + \left(S_i^y\right)^2 + \left(S_i^z\right)^2 = N$.

-Minimize with weak constraint: $\sum_{ij} J_{ij}\vec{S}_i\vec{S}_j - \lambda\left(\sum_i \left|\vec{S}_i\right|^2 - N\right)$

- Derivative: $\sum_\delta J_\delta \vec{S}_{i+\delta} - 2\lambda\vec{S}_i = 0$

- Ansatz: $\vec{S}_i = \vec{u}\mathrm{e}^{i\vec{q}\vec{r}_i} \sum_\delta J_\delta \vec{u}\mathrm{e}^{i\vec{q}\left(\vec{r}_i + \vec{\delta}\right)} = 2\lambda\vec{u}\mathrm{e}^{i\vec{q}\vec{r}_i} \Rightarrow \underbrace{\sum_\delta J_\delta \mathrm{e}^{i\vec{q}\vec{\delta}}}_{=J_{\vec{q}}} = \tilde{\lambda}$

For CH model

$$H = \frac{1}{\sqrt{N}}\sum_{i,j,q}(J_x e^{-iq_x}\tilde{S}_q^x\tilde{S}_q^x + J_z e^{-iq_z}\tilde{S}_q^z\tilde{S}_q^z + I(e^{-iq_x}(\tilde{S}_q^x\tilde{S}_q^x + \tilde{S}_q^y\tilde{S}_q^y + \tilde{S}_q^z\tilde{S}_q^z) + e^{-iq_z}(\tilde{S}_q^x\tilde{S}_q^x + \tilde{S}_q^y\tilde{S}_q^y + \tilde{S}_q^z\tilde{S}_q^z)))$$

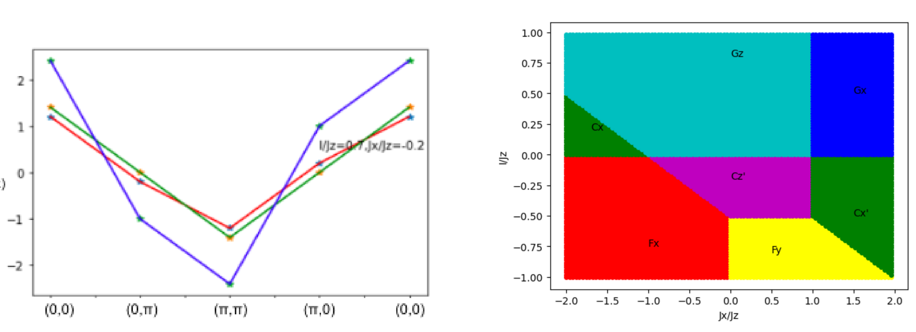


Figure 7. 1. Energy eigenspectrum calculated using Luttinger-Tisza method for the Brillouin zone points (0,0),(0,π),(π,0),(π, π): the red, green, blue line denotes the eigenspectrum corresponding the x, y, z component of spin operators in k space respectivel 2. Phase diagram obtained by luttinger tisza method

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References

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