Stability of Magnetization in Frustrated Heisenberg Lattices: A Linear Spin-Wave Approach With Duffy Regularization

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Abstract

A robust theoretical and computational framework is presented for analysing Heisenberg lattices in the next-nearest neighbour models. Built on the **Linear-Spin-Wave-Theory (LSWT) formalism**, the dispersion relation and staggered magnetization are studied as a function of the frustration parameter $\alpha = J_2/J_1$, where **Duffy regularization** is applied as an alternative to more complex numeric methods as Monte Carlo. Results are in agreement with the well known results on the instability of the magnetization in Heisenberg lattices (Chandra et al. 1988; Qian et al. 2024), finding the collapse region interval $0.378 \leq \alpha \leq 0.512$ for the 1/2-spin square lattice, where the LSWT also fails on predicting the dispersion relation due to the vanishing of magnetic ordering. This approach can be easily expanded to other geometries.

1. Introduction

Next-nearest neighbour Heisenberg lattice ($J_1 - J_2$ model):

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} \hat{S}_i \hat{S}_j + J_2 \sum_{\langle i,i' \rangle} \hat{S}_i \hat{S}_{i'} + J_2 \sum_{\langle j,j' \rangle} \hat{S}_j \hat{S}_{j'} \qquad (1)$$

- **Linear-Spin-Wave Theory (LSWT)** is introduced through the Holstein-Primakoff transformation, and considering a bipartite lattice, i.e., **antiferromagnetic (AFM)** ordering.
- **Diagonalization** is done by Fourier-transforming and applying a **Bogoliubov transformation**:

$$\hat{H} = NqJ_1(\alpha - 1/2)S(S+1) + \sum_{\mathbf{k} \in \mathrm{MBZ}} \omega_{\mathbf{k}} (\hat{\alpha}^\dagger_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}} + \hat{\beta}_{\mathbf{k}} \hat{\beta}^\dagger_{\mathbf{k}}) \qquad (2)$$

With the **dispersion relation**:

$$\omega_{\mathbf{k}} = qJ_1S\left[\sqrt{(1-\alpha(1-\eta_{\mathbf{k}}))^2 - \gamma_{\mathbf{k}}^2} - \alpha(1-\eta_{\mathbf{k}})(1-\alpha(1-\eta_{\mathbf{k}}))\right]$$

And the nearest and next-nearest factors defined as:

$$\gamma_{\mathbf{k}} = \frac{1}{q_1} \sum_{\delta} e^{i\mathbf{k}\cdot\delta} \quad ; \quad \eta_{\mathbf{k}} = \frac{1}{q_2} \sum_{\epsilon} e^{i\mathbf{k}\cdot\epsilon}$$

- **Frustrated magnetization** can be studied by computing the fluctuations around the AFM ground state:

$$\langle \hat{S}^z_i \rangle = \left(S + \frac{1}{2}\right) - \frac{1}{(2\pi)^d} \int d^d\mathbf{k} \frac{1-\alpha(1-\eta_{\mathbf{k}})}{\sqrt{q(1-\alpha(1-\eta_{\mathbf{k}}))^2 - \gamma_{\mathbf{k}}^2}}$$

With $q = q_2/q_1$.

2. Duffy Regularization of the MBZ

- **Duffy transformation** regularizes the singular vertices when computing the magnetization.
- MBZ symmetry (diamond) allows parameterization over the unit hypercube $[0,1]^d$, integrating over the upper hyper-triangle:

$$T_d = \left\{ \sum_{j=1}^{d} \frac{k_j}{k_j^{\max}} \leq 1,\ k_j \geq 0 \right\} \qquad (3)$$

- $\mathbf{k} \to \mathbf{k}(t_1, \ldots, t_d)$ with $t_1, \ldots, t_d \in [0,1]^d$, and the **Jacobian cancels out** the singular vertex, e.g. in d=2:

$$\int \frac{d^2\mathbf{k}}{|\mathbf{k}|} = 4\int_0^1 dt_1 \int_0^1 dt_2 \frac{\pi}{\sqrt{1+t_2^2}} = 4\pi \sinh^{-1}(1)$$

With $k_x = \pi t_1$ and $k_y = \pi t_1 t_2$.

3. Results

Spectrum analysis of the frustrated AFM square lattice

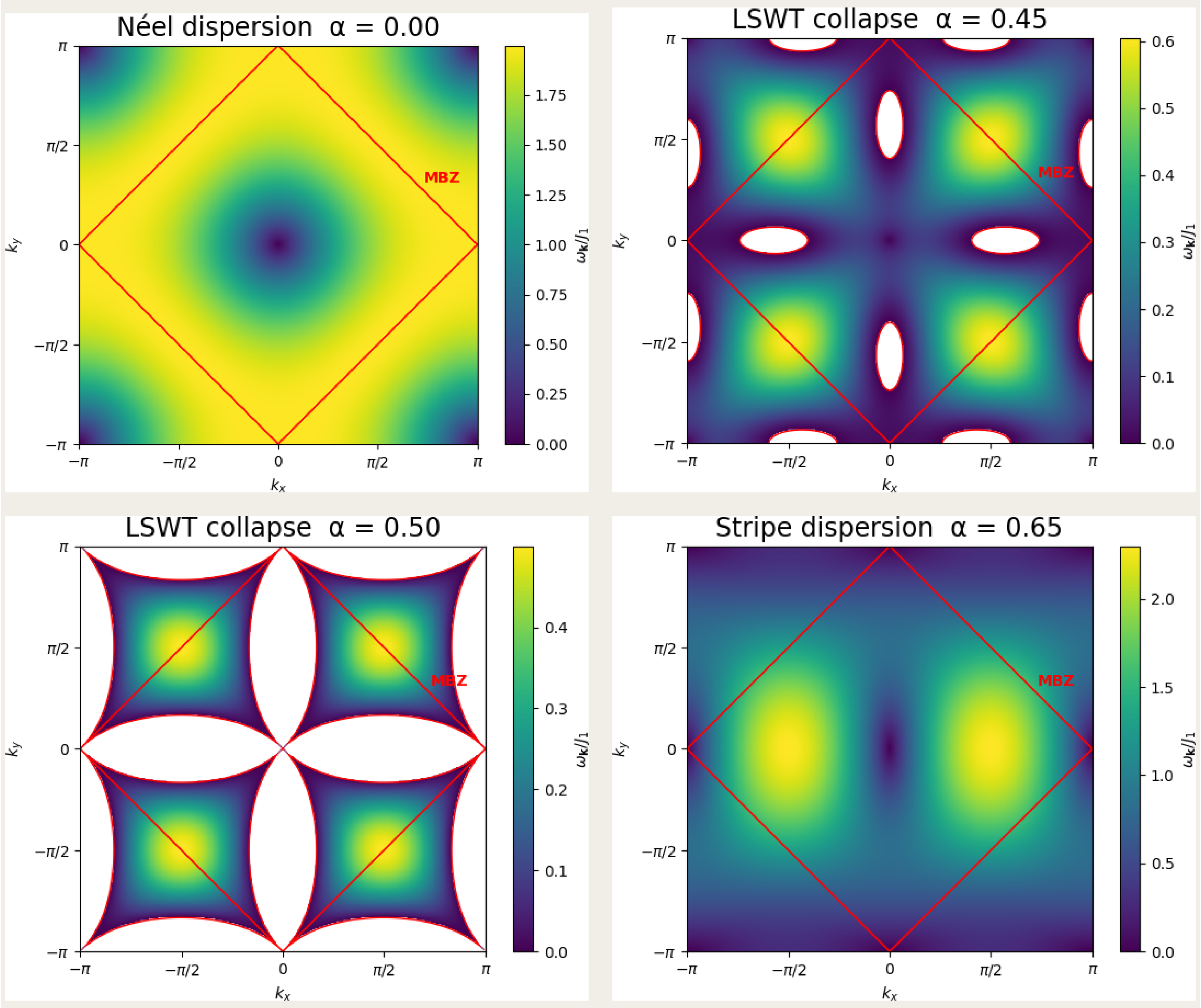

Figure 1. Dispersion relation for different fixed values of frustration.

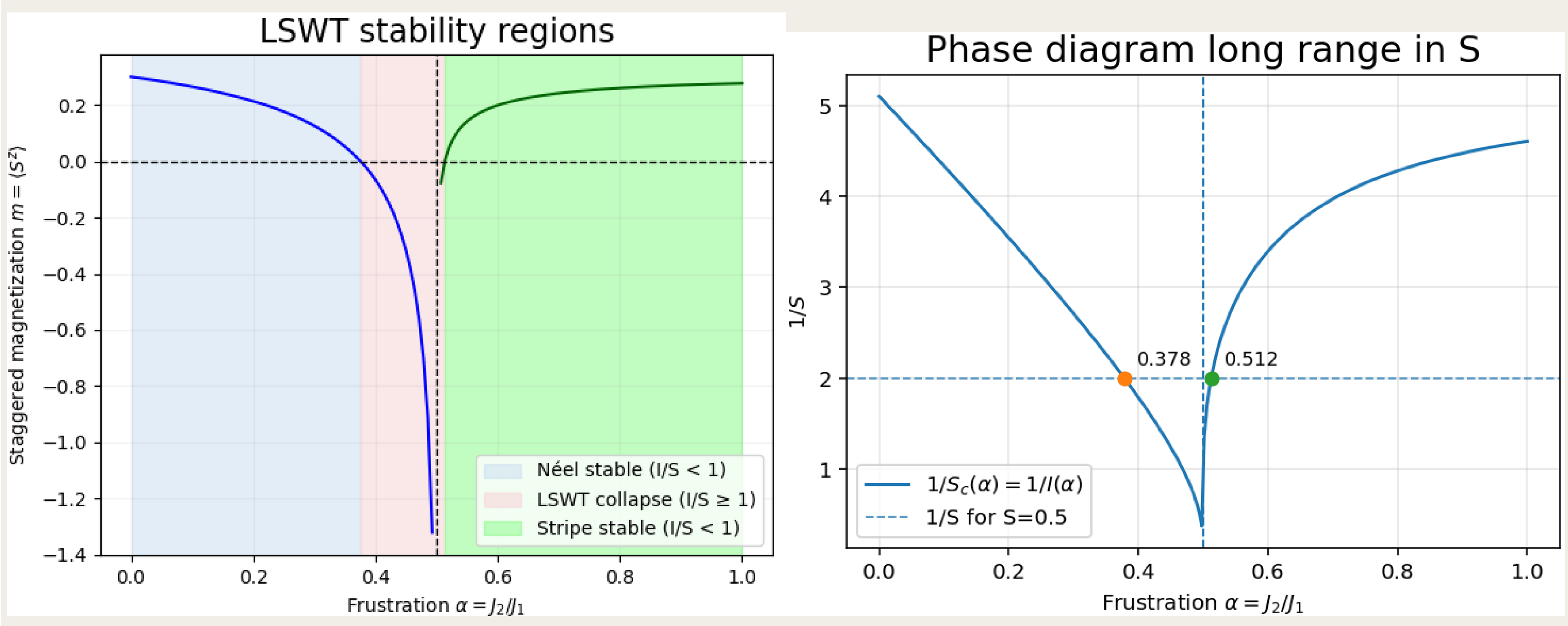

Figure 2. (Left) Staggered magnetization for S=1/2 and d=2. (Right) Long-range S phase diagram (in high agreement with (Chandra et al. 1988)).

4. Outcomes and perspectives

- The LSWT approach with Duffy regularization is a robust technique to study frustration in Heisenberg lattices.
- This approach can be easily extended to different geometries.

References

- Qian, X. and M. Qin (2024). "Absence of spin liquid phase in the J 1- J 2 Heisenberg model on the square lattice". In: *Physical Review B* 109.16, p. L161103.
- Chandra, P. and B. Doucot (1988). "Possible spin-liquid state at large S for the frustrated square Heisenberg lattice". In: *Physical Review B* 38.13, p. 9335.