Generic nearest-neighbour square-kagome model: XXZ and Dzyaloshinskii-Moriya interactions

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I. Highlights

The main results of the research work performed over this year can be summarized as (a) a step-by-step determination of the generic nearest-neighbour Hamiltonian on a square-kagome lattice, (b) group theoretical determination of the possible ground state phases for this Hamiltonian, and (c) numerical verification of the phases for the XXZ model with Dzyaloshinskii-Moriya interactions which is a specific case of the generic Hamiltonian.

II. Introduction

Our present work sits at the frontier of the ideas of unconventional phenomena, spin liquids, and chiral phases in geomerticaly frustrated lattices like honeycomb, kagome, square-kagome etc. In this project, we explore the zero-temperature magnetic phases for the generic nearest-neighbour Hamiltonian allowed by the symmetry of the square-kagome lattice for classical Heisenberg spins. The square-kagome lattice being made of corner sharing blocks of shape illustrated in Fig.1, the most general form of nearest-neighbour Hamiltonian can be broken down into a sum over all such building blocks.

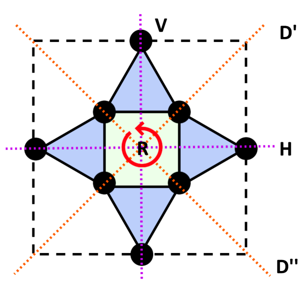

Fig. 1. Symmetries in a square-kagome lattice

Now, the lattice has $\mathbf{D_4}$ point-group symmetry and the Hamiltonian must respect all the lattice symmetries. This strongly constrains the form of possible exchange interactions. Taking into account all these constraints, we found that there are only eight independent coupling parameters in the Hamiltonian allowed by the square-kagome symmetry. The structure of the coupling matrices indicate that the system supports local XYZ model with out-of-plane Dzyaloshinskii-Moriya (DM) interactions. Lack of inversion symmetry in square-kagome lattice also assures the possibility of existence of DM interaction in the lattice. Using group theoretical analysis we obtained the possible ground state spin configurations for this general model. We are yet to determine the order parameters that classify these ground state phases, explore the ideas of exotic properties and unconventional phenomena in those phases, and study their excitation spectra. As a verification of the theory we numerically studied a specific case where the Hamiltonian reduces to XXZ model with out-of-plane Dzyaloshinskii-Moriya couplings and obtained the zero-temperature classical phase diagram. We found the theory to be consistent with the numerical results.

III. The $\mathbf{D_4}$ symmetry group and ground state spin configurations

In order to diagonalize the Hamiltonian, and obtain the order parameters that characterize the ground state phases, we employed representation theory for the point-group operations to a general model of anisotropic nearest-neighbour exchange interactions on the square-kagome lattice. There are 8 spin vectors in a unit cell having in total 24 components. So we considered a 24-dimensional reducible representation Γ of the $\mathbf{D_4}$ symmetry group. The group is of order eight and its elements are $\{e, R_{\frac{\pi}{2}}, R_{\pi}, R_{\frac{3\pi}{2}}, D', D'', V, H\}$, where e is the identity, $R_{\frac{\pi}{2}}, R_{\pi}, R_{\frac{3\pi}{2}}$ are rotation by $\frac{\pi}{2}, \pi$, and $\frac{3\pi}{2}$ about the highest symmetry axis, D', D'' are reflections about the two diagonals and V, H are reflections about the edge bisectors of the dashed square illustrated in Fig.1 respectively. There are five classes denoted by $E = \{e\}, C_4 = \{R_{\frac{\pi}{2}}, R_{\frac{3\pi}{2}}\}, C_2 = \{R_{\pi}\}, C_2' = \{D', D''\}, C_2'' = \{V, H\}$, and the character table for this symmetry group is given by

D_4	γ_I	E	$2C_4$	C_2	$2C_2'$	$2C_2''$
Γ_1	2	1	1	1	1	1
Γ_2	4	1	1	1	-1	-1
Γ_3	3	1	-1	1	1	-1
Γ_4	3	1	-1	1	-1	1
Γ_5	6	2	0	-2	0	0
Γ		24	0	0	-2	-2

The last row in the table corresponds to the characters of the reducible representation Γ. The representation Γ can be decomposed in terms of the irreducible representations (irreps) Γ_I $(I = 1, 2, ..., 5)$ as $\Gamma = \bigoplus_I \gamma_I \Gamma_I$ with γ_I being the number of times the I-th irrep appears in the sum. The basis spin configurations of these irreps provide the order parameters necessary to diagonalize the Hamiltonian. The resulting basis configurations $\tilde{\Gamma}_{I\alpha}$ with $\alpha = a, b, c, ...$ that we have obtained are illustrated in Fig.2. Note that, in determining these configurations, we also obtained some basis vectors that do not respect the unit-length spin constraint. Those unphysical cofigurations are not listed in Fig.2, but they are necessary to span the entire space of order parameters.

Now, a general spin configuration $\tilde{S}$ allowed by the square-kagome lattice symmetries can be expressed in this basis as

$$\tilde{S} = \sum_{I\alpha} m_{I\alpha}\tilde{\Gamma}_{I\alpha}$$

where $I = 1, 2, ..., 5$, and $\alpha = a, b, c, ...$ with $m_{I\alpha}$ being the order parameter of configuration $\Gamma_{I\alpha}$. Expressing the Hamiltonian in terms of these order parameters as

$$\mathcal{H} = \sum_{I\alpha} \lambda_{I\alpha}(\{J_i\}) m_{I\alpha}^2$$

leads a straight forward determination of the possible ground state configurations for a particular set of coupling parameters $\{J_i\}$. For a uniform lattice, we obtain the ground state just by saturating the order parameter ($m_{I\alpha} = 1$) for which the coefficient $\lambda_{I\alpha}$ is a minimum. The method we have developed is quite general and can be applied for arbitrary interactions allowed by the square-kagome lattice symmetry. However, for concreteness, we focused our attention to the XXZ model with out-of-plane DM interactions for numerical verification.

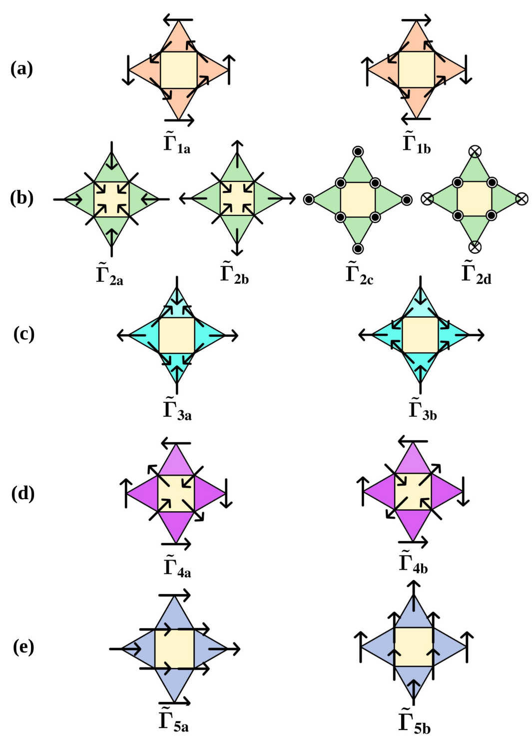

Fig. 2. (a), (b), (c), (d), and (e) are basis spin configurations for irreducible representations Γ_1 to Γ_5 respectively. Note that, there are more symmetry-allowed spin configurations that fail to respect the unit-length spin constraint, and thus considered unphysical and hence are not shown.

IV. Phase diagram for XXZ and DM interactions in a square-kagome lattice

We performed a classical Monte Carlo simulation based on Metropolis algorithm to obtain the phase diagram of the system with nearest-neighbour XXZ and Dzyaloshinskii-Moriya interactions in the classical limit. In our simulation we minimized the local Hamiltonian for a single Heisenberg spin with temperature annealing and checked for total energy convergence of the system in each case. The MC simulation yields a rich phase diagram of five distinct classical phases as a function of XXZ anisotropy parameter Δ and strength of DM interaction D as illustrated in Fig.3. The ground state phases that we obtained are consistent with the theoretical predictions of spin configurations as shown in Fig.2. The phases $\tilde{\Gamma}_{2c}$ (green triangle) and $\tilde{\Gamma}_{5a/5b}$ (blue circle) are out-of-plane and in-plane ferromagnetic configurations respectively. The phases $\tilde{\Gamma}_{2b}$ (purple square) and $\tilde{\Gamma}_{4b}$ (red diamond) are some chiral phases that are yet to be analyzed. The phase named X (black star) consists of non-coplanner spin configurations which can be explained by basis spin configurations beyond those listed in Fig.2. We are yet to theoretically determine the exact range of the coupling parameters for which a particular ground state configuration arises. Then we will analyze each of these phases and study their excitation spectrum, in particular the magnon exciations, by employing spin-wave analysis. The work is in progress and we expect to finish the work in a few months. We hope that the present work will serve as a classical foundation to further connect the network of quantum spin liquids in square-kagome lattice.

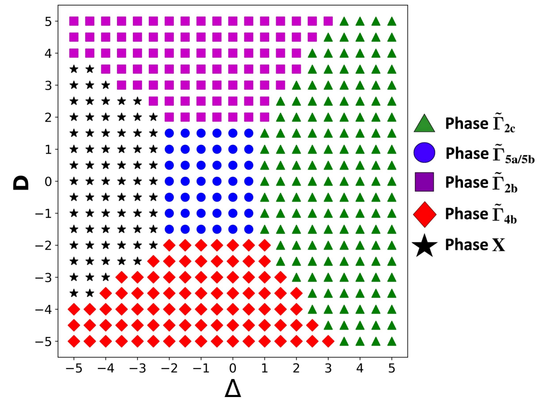

Fig. 3. Phase diagram obtained by classical Monte Carlo simulation of the XXZ model with out-of-plane DM interactions in square-kagome lattice. Simulations were performed for clusters of $N = 6L^2$ classical spins with linear dimension $L = 10$ unit cells.