Competing magnetic interactions in a triangular lattice Heisenberg model motivated by $MnBi_2Te_4$ experiments

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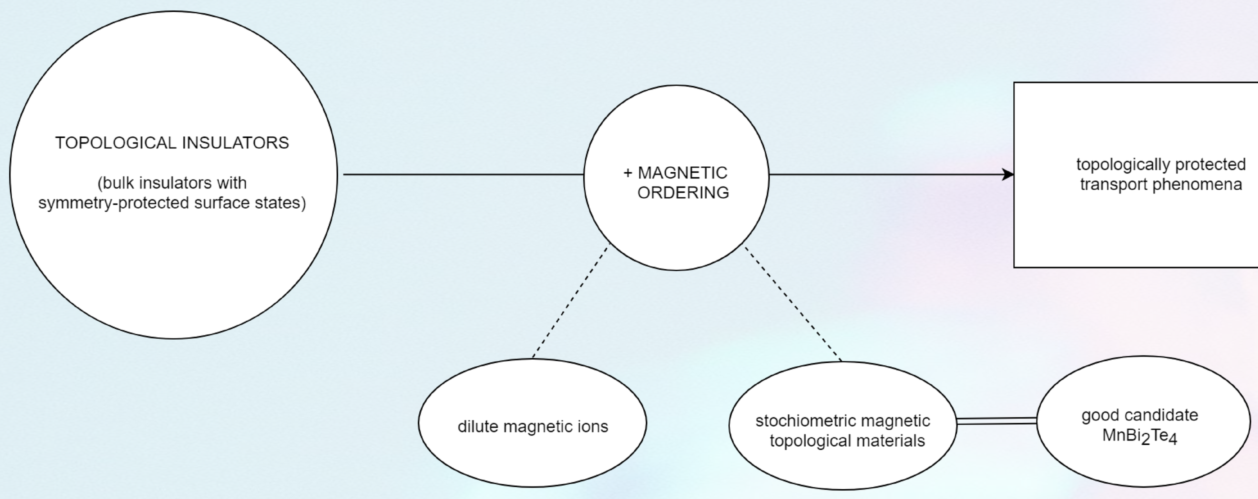
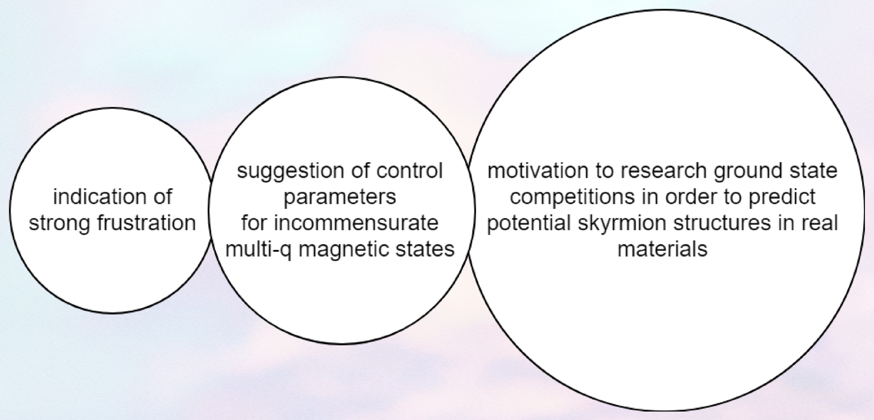
MOTIVATION

- Interplay between topological insulators and magnetism



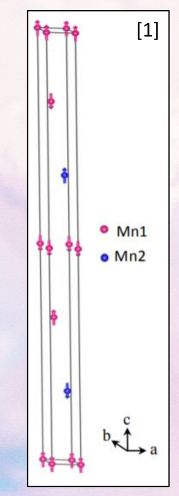
- $MnBi_2Te_4$ may be the first example of a stoichiometric antiferromagnetic topological insulator
- Experimental data have set the range for theoretical playground:

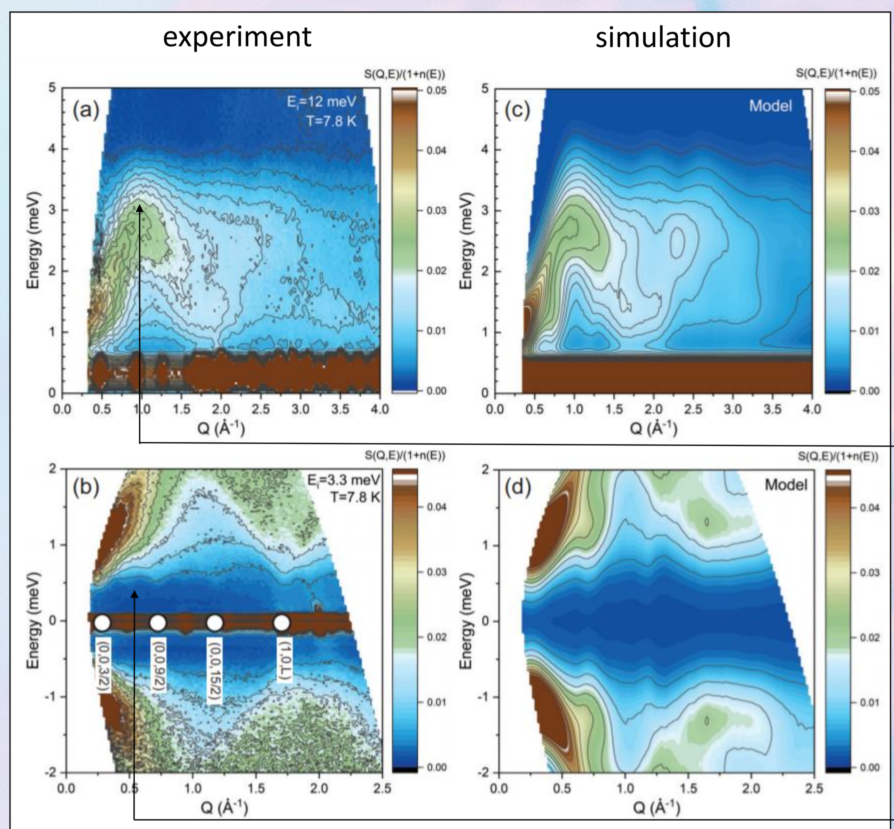


NEUTRON SCATTERING EXPERIMENTS ON $MnBi_2Te_4$

Neutron diffraction → determining magnetic crystal structure

Inelastic neutron scattering → study magnetic strucure within a layer





dispersing spin wave excitations reach a maximum energy near the Brillouin zone boundary of the triangular layer ($Q \approx 1\mathring{A}^{-1}$) and return to the smallest energy near the magnetic zone centers ($Q \approx 1.7\mathring{A}^{-1}$)

large spin gap ($\Delta \approx 1\ meV$) ⇒ strong Ising anisotropy

spin gap dispersion minima repeating at magnetic zone centers ⇒ relatively strong interlayer coupling

- Heisenberg model with interlayer coupling and single-ion anisotropy ($J_1, J_2, J_c, D_z > 0$)

$$H = -J_1 \sum_{\langle i,j \rangle \parallel} \boldsymbol{S}_i \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle \parallel} \boldsymbol{S}_i \boldsymbol{S}_j + J_c \sum_{\langle i,j \rangle \perp} \boldsymbol{S}_i \boldsymbol{S}_j - D_z \sum_i (S_i^z)^2$$

- Three free parameters for this model are determined within linear spin wave theory, from:
  - estimation of spin gap
  - observing magnetic field at which spin-flop transition occurs
  - fitting measured magnetic spectrum to the simulated one from energy cuts along momentum axis

THEORETICAL 2D MODEL

- Competing nearest and next nearest-neighbor interactions on a triangular lattice with easy-axis anisotropy under magnetic field ($J_1, J_2, h, D_z > 0$)

$$H = -J_1 \sum_{\langle i,j \rangle} \boldsymbol{S}_i \boldsymbol{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \boldsymbol{S}_i \boldsymbol{S}_j - h \sum_i S_i^z - D_z \sum_i (S_i^z)^2$$

- Ansatz:
  Ordered ground states will only have few dominant $\boldsymbol{q}$-vectors. [2]

$$\Rightarrow \quad q = \arccos\left[\frac{1}{2}\left(1 - \frac{J_1}{J_2}\right)\right]$$

nontrivial amplitude q depends only on the ratio of J_1 and J_2 and not on h and D_z

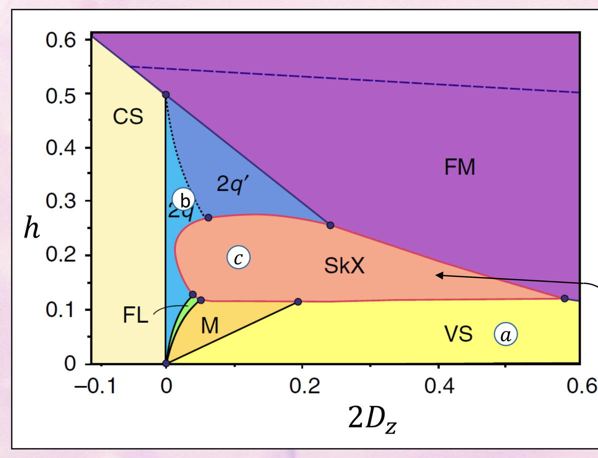
- Classical threshold for which any spin structure becomes ferromagnetic: $\frac{J_2}{J_1} \le \frac{1}{3}$

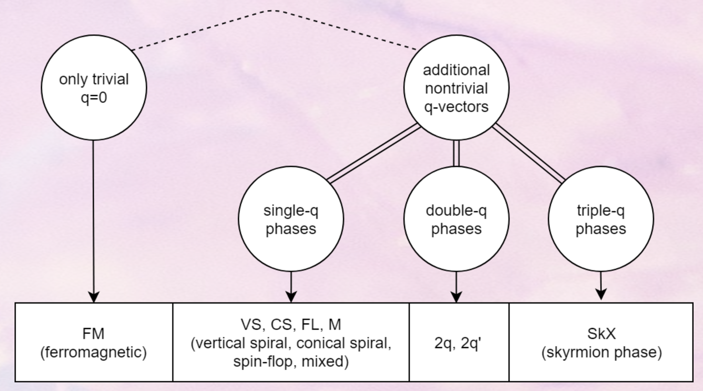
$\Rightarrow$ we are interested to study ground state phase diagram for: $\frac{1}{3} \le \frac{J_2}{J_1} \le \frac{1}{2}$

- In particular, we want to study experimentally expected skyrmion/spiral state for $\frac{J_2}{J_1} \approx \frac{1}{3}, D_z \in (0.3, 1)$

PHASE DIAGRAM

- This model for $\frac{J_2}{J_1} = \frac{1}{2}$ has been studied extensively. [3]
- Phase diagram shows different phases which can be classified based on the number of dominant $\boldsymbol{q}$-vectors:





they can be further distinguished by the relative strengths of amplitudes related to different q-vectors and their modulations

STRUCTURE FACTOR

- One way to identify different phases is by structure factor components. In our case it is especially useful as structure factor is a quantity that can be measured by neutron scattering experiments.

$$S^{ab}(\boldsymbol{q}) = \frac{1}{N^2} \sum_{i,j} S_i^a S_j^b e^{i\boldsymbol{q}(\boldsymbol{r}_i - \boldsymbol{r}_j)}, \qquad \{a,b\} \in \{x,y,z\}$$

where spin orientation in real space in the state characterized with α nontrivial phases is:

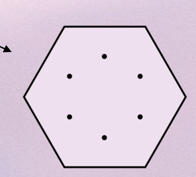
$$\boldsymbol{S}_i = \boldsymbol{A}_0 + \frac{1}{2} \sum_{\alpha=1}^{3} \left(\boldsymbol{A}_\alpha e^{i\boldsymbol{q}_\alpha \boldsymbol{x}_i} + c.c.\right) + higher\ harmonics, \qquad \boldsymbol{A}_0 = (0, 0, A_0^z)$$

- Among other phases, skyrmion phase which is characterized with equal amplitudes of the three fundamental modulations, is especially of our interest:

$$\boldsymbol{A}_\alpha = A e^{i\varphi_\alpha}(-i \sin\chi_\alpha, i\cos\chi_\alpha, 1), \qquad \chi_\alpha = \chi + \frac{2\pi}{3}(\alpha - 1), \qquad \alpha \in \{1,2,3\}$$

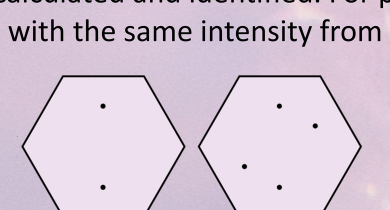
which leads to structure factor components, e.g. $S^{xx}(\boldsymbol{q})$:

$$S^{xx}(\boldsymbol{q}) = \frac{A_{1x}^2}{4}\left(\delta_{\boldsymbol{q}=\boldsymbol{q}_1} + \delta_{\boldsymbol{q}=-\boldsymbol{q}_1}\right) + \frac{A_{2x}^2}{4}\left(\delta_{\boldsymbol{q}=\boldsymbol{q}_2} + \delta_{\boldsymbol{q}=-\boldsymbol{q}_2}\right) + \frac{A_{3x}^2}{4}\left(\delta_{\boldsymbol{q}=\boldsymbol{q}_3} + \delta_{\boldsymbol{q}=-\boldsymbol{q}_3}\right), \qquad A_{\alpha x} = A e^{i\phi,\alpha} \sin\chi_\alpha$$



theoretically predicted plotted structure factor in first Birllouin zone agrees with numerical results;
the relative ratio between the peak intensities depends on the magnitudes of modulations in momentum space

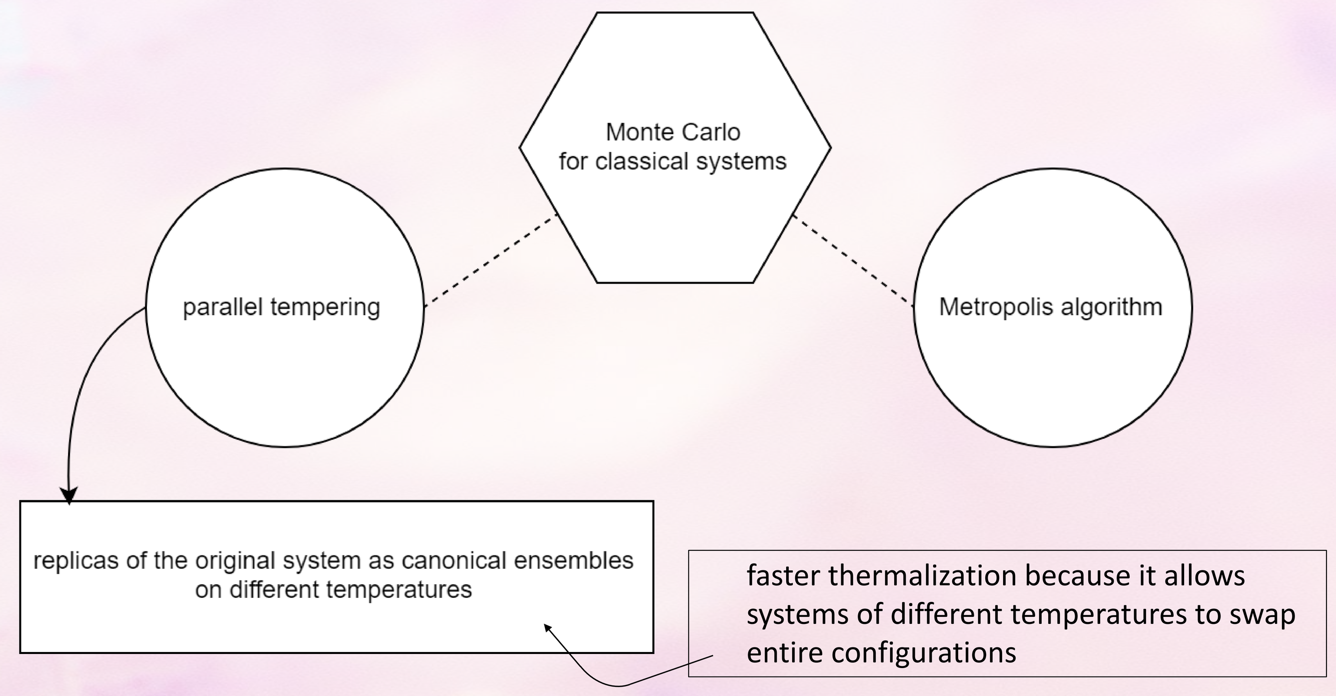
- In the same way, other phases are calculated and identified. For perfect single-q and double-q phases for specified q-vectors contribution with the same intensity from all vectors, $S^{xx}(\boldsymbol{q})$ factors are:



- However, structure factor approach is limited for $\frac{J_2}{J_1} \approx \frac{1}{3}$ when $q \to 0$!
- Other approaches needed!

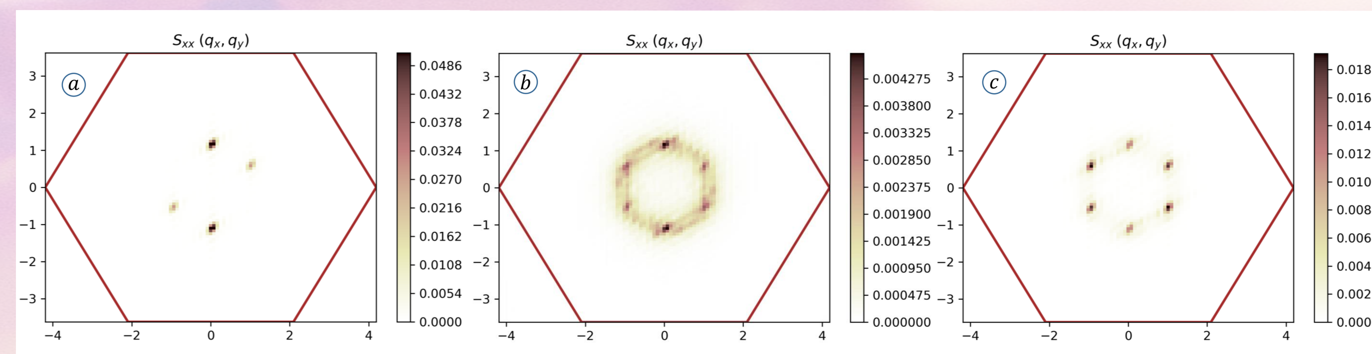
MONTE CARLO SIMULATION

- Classical Monte Carlo simulation with Metropolis algorithm and parallel tempering:



NUMERICAL RESULTS

- Numerically we identify the different phases looking at the structure factor of our MC simulations, averaged over the different realizations.
- The calculation is performed on triangular lattice with periodic boundary conditions.
- Presented graphs are obtained for 32×32 lattices with 10^6 MC steps at temperatures much lower than ordering temperature.



single-q phase double-q phase triple-q phase

More features included, but agreements with theoretical prediction and previous publications! [2]

ONGOING WORK

- Systematical numerical approach (MC + structure factor) to further study ground state competition for:

$$\frac{1}{3} \le \frac{J_2}{J_1} \le \frac{1}{2}$$

- We are experimentally primarily interested in exploring the appearance and stability of skyrmion phase for strong easy-axis anisotropies

$\Rightarrow$ Analytical approach (exact calculation + numerical minimization of the energy for scalar field) in the vicinity of skyrmion phase for larger easy-axis anisotropies

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