Bose-Einstein condensation of a two-magnon bound state in a spin-one triangular lattice

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Abstract

Bose-Einstein condensation (BEC) of the **two-magnon bound state** at the saturation field is found in $Na_2BaNi(PO_4)_2$:

- The magnetic exchange model is established with inelastic neutron scattering experiments
- An exact solution of the model found stable two-magnon bound states and is further confirmed by an electron spin resonance (ESR) experiment
- Density Matrix Renormalized Group (DMRG) offer further evidence of the spin nematic (SN) phases below saturation field.

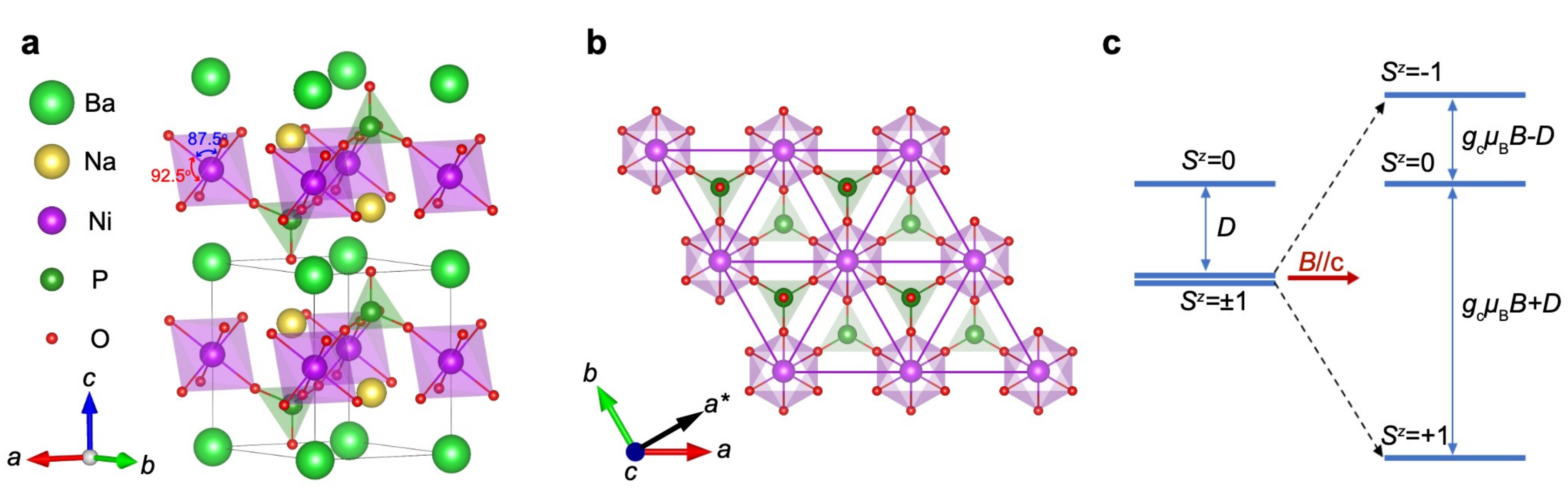
➢ Reference

J. Sheng, J.-W. Mei, L. Wang, W. Jiang, **L. Xu**, H. Ge, N. Zhao, T. Li, A. Candini, B. Xi, J. Zhao, Y. Fu, J. Yang, Y. Zhang, G. Biasiol, S. Wang, J. Zhu, P. Miao, X. Tong, D. Yu, R. Mole, L. Ma, Z. Zhang, Z. Ouyang, W. Tong, A. Podlesnyak, L. Wang, F. Ye, D. Yu, L. Wu and Z. Wang, Bose-Einstein condensation of a two-magnon bound state in a spin-one triangular lattice (2023), arXiv:2306.09695 [cond-mat].

Structure and Model

➢ Crystal and splitting energy levels

Ni^{2+}



➢ Hamiltonian

$$\mathcal{H}_{\mathrm{TL}} = J\sum_{\langle ij\rangle_{ab}}\left(S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z\right) - D\sum_i \left(S_i^z\right)^2$$

- Triangular lattice (TL)
- $S = 1$
- In-plane dominant
- XXZ model
- Easy-axis $J/D \sim 1/4$

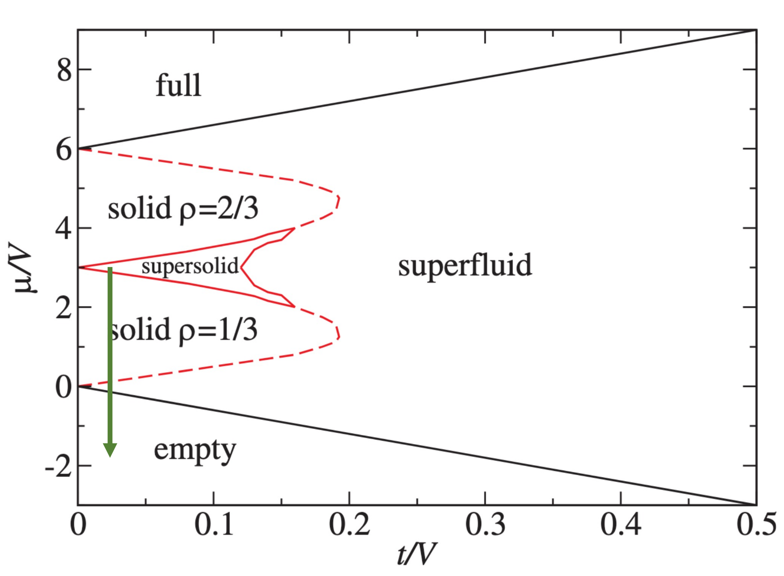
low-energy effective model,
project to the hard-core Bose-Hubbard model

$$\mathcal{H}_{\mathrm{eff}} = -t\sum_{\langle ij\rangle}\left(b_i^\dagger b_j + h.c.\right) + V\sum_{\langle ij\rangle} n_i n_j - \mu\sum_i n_i$$

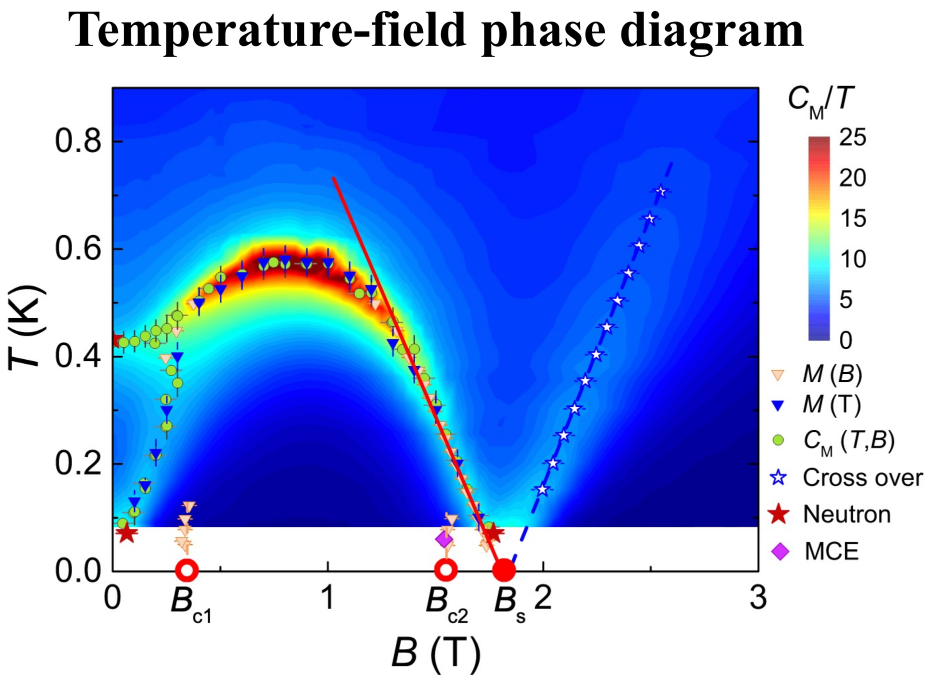
$$t = \frac{J^2}{2D}, V = \frac{2J^2}{D} + 4\Delta J, \mu = \frac{6J^2}{D} + 12\Delta J - 2g_c\mu_B B$$

➢ Phase diagram

Phys. Rev. Lett. 95, 127205 (2005).



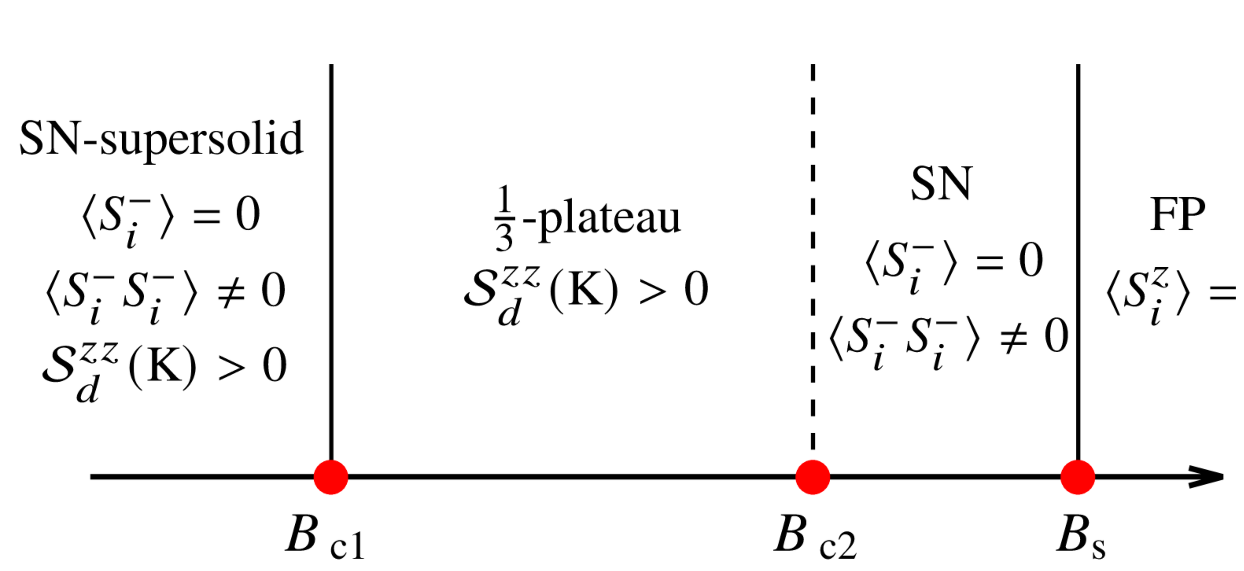
Temperature-field phase diagram



Schematic 0 K phase diagram

- B_{c1}, B_s : 2nd order transition
- B_{c2}: 1st order transition

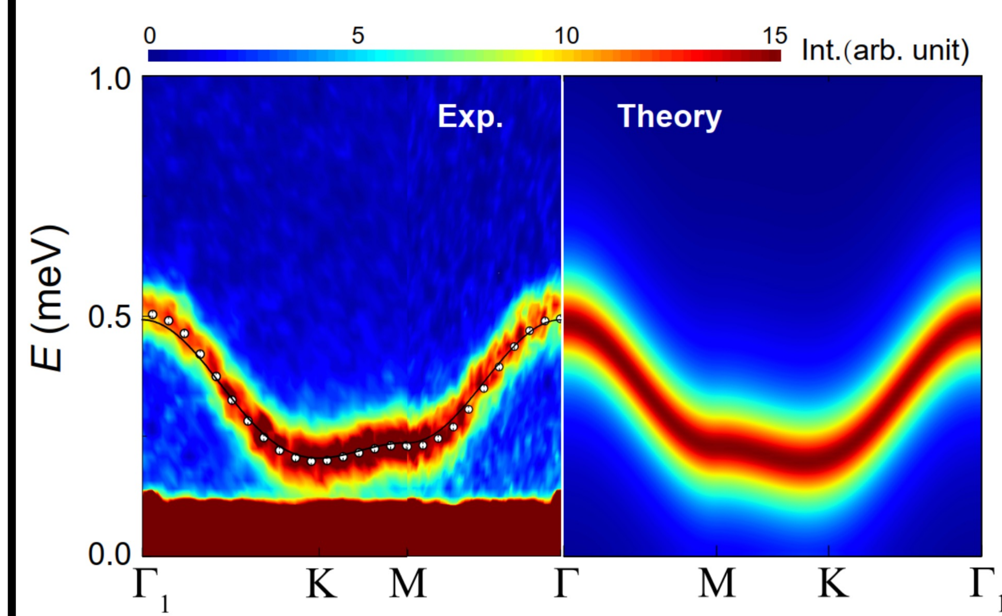
$$S_d^{zz}(\boldsymbol{k}) = \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}\langle S_i^z S_j^z\rangle$$



Results

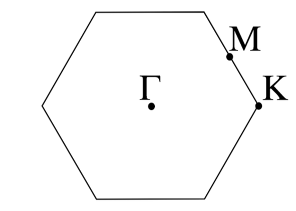
➢ One-magnon dispersion

$$E_1(\boldsymbol{k}) = 2J\left(\cos k_x + 2\cos\frac{k_x}{2}\cos\frac{\sqrt{3}k_y}{2}\right) - 6\Delta J + D + g_c\mu_B B$$



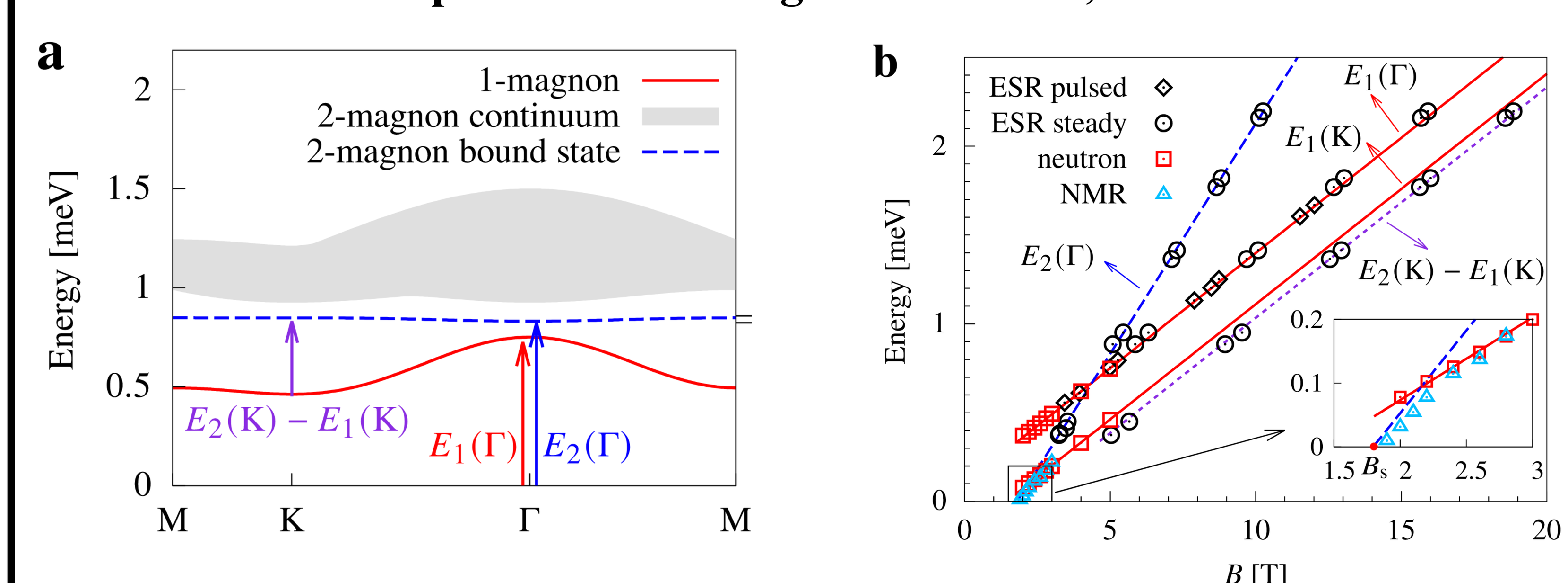
INS intensity

- $T = 60$ mK, $B = 5$ T
- one-magnon BEC is below the experimentally observed critial point ($B_s \approx 1.8$ T)



➢ Lippmann-Schwinger equation

Solution of the spin-1 model along with neutron, ESR and NMR data



Two-magnon state $|\boldsymbol{r}_1, \boldsymbol{r}_2\rangle = 1/2 S_{r_1}^- S_{r_2}^- |\mathrm{FP}\rangle$

- The first excitation agrees with $E_2(\boldsymbol{\Gamma})$.,
- The second excitation along the line $E_2(\mathbf{K}) - E_1(\mathbf{K})$, corresponding to a transition from the 1-magnon band to the 2-magnon bound state.

➢ U(1) symmetric Density Matrix Renormalization Group (DMRG)

- in-plane dipolar structure factor

$$S_d^\perp(\boldsymbol{k}) = \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}\langle S_i^x S_j^x + S_i^y S_j^y\rangle$$

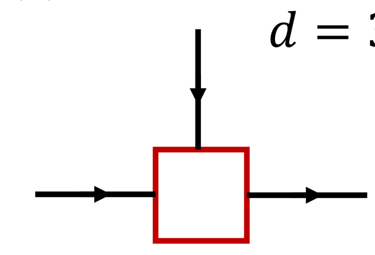
- in-plane quadrupolar structure factor

$$S_q^\perp(\boldsymbol{k}) = \frac{1}{N}\sum_{i,j} e^{-i\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}\langle Q_i^{x^2-y^2} Q_j^{x^2-y^2} + Q_i^{xy} Q_j^{xy}\rangle$$

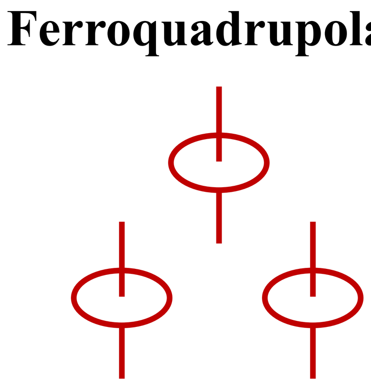
$$Q_i^{x^2-y^2} \equiv S_i^x S_i^x - S_i^y S_i^y,\ Q_i^{xy} \equiv S_i^x S_i^y + S_i^y S_i^x$$

U(1) tensor

$d = 3$

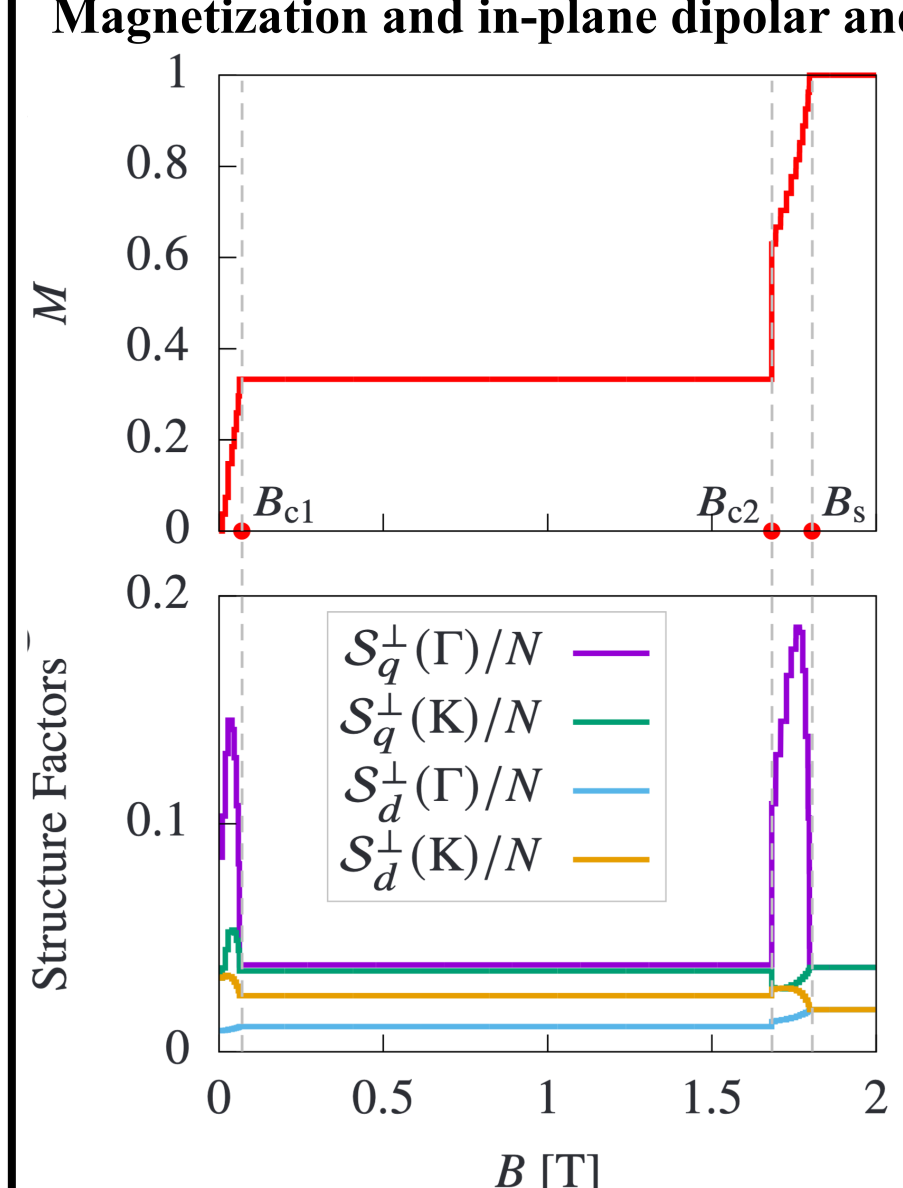


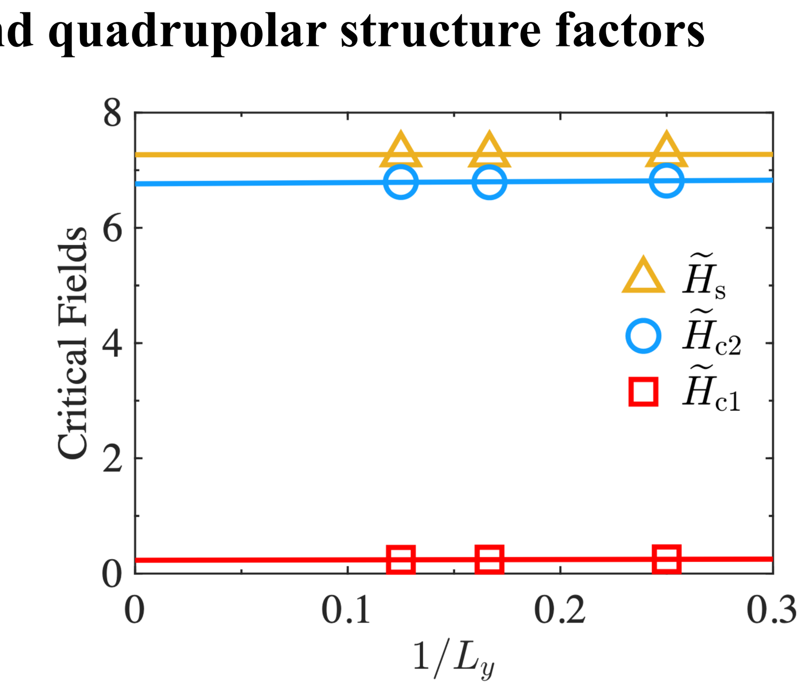
Ferroquadrupolar



- 9×6 TL torus for magnetization and structure factor,
- 6×4, 9×6, and 12×8 TL cylinder for extrapolation to the thermodynamic limit,
- U(1) tensor is used to improve the performance of the simulation,
- $E(S_z, \tilde{H}) = E(S_z, 0) - \tilde{H}S_z, \tilde{H} = g_c\mu_B B$.

Magnetization and in-plane dipolar and quadrupolar structure factors





- For $B < B_{c1}$ and $B_{c2} < B < Bs$, the ferroquadrupolar order is dominant in these SN phases,
- B_{c1} (B_{c2}) is a second (first) order transition,
- Extrapolation of critical fields agree well with the experiment.