Quantum fluctuations and the phase diagram of anisotropic dipolar magnets

Correlated Days, Ein Gedi, 06/2022

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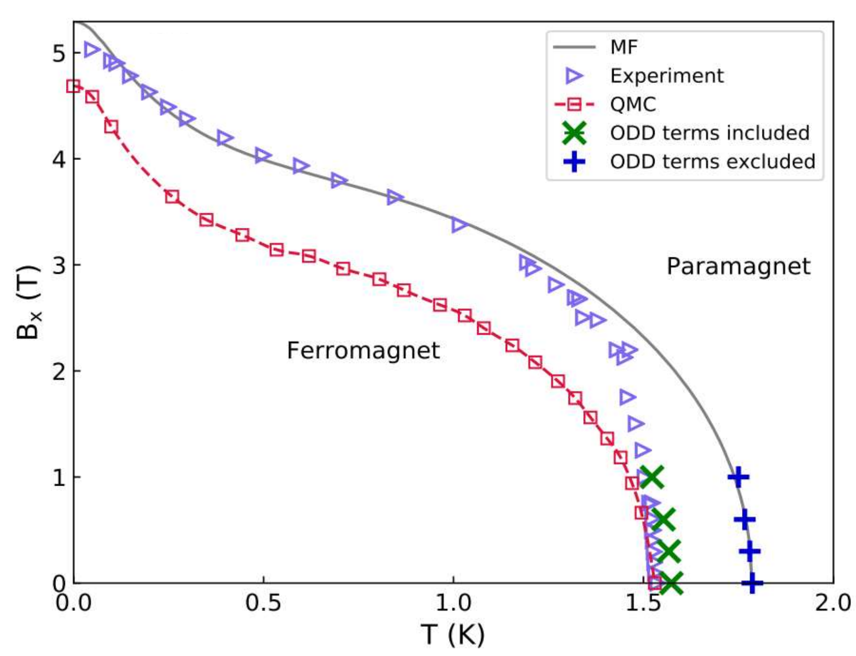
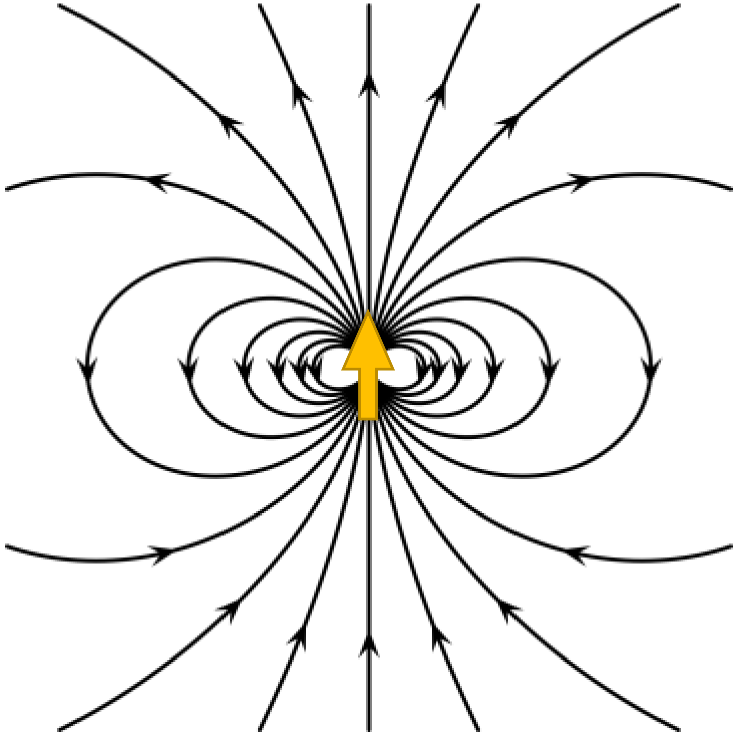
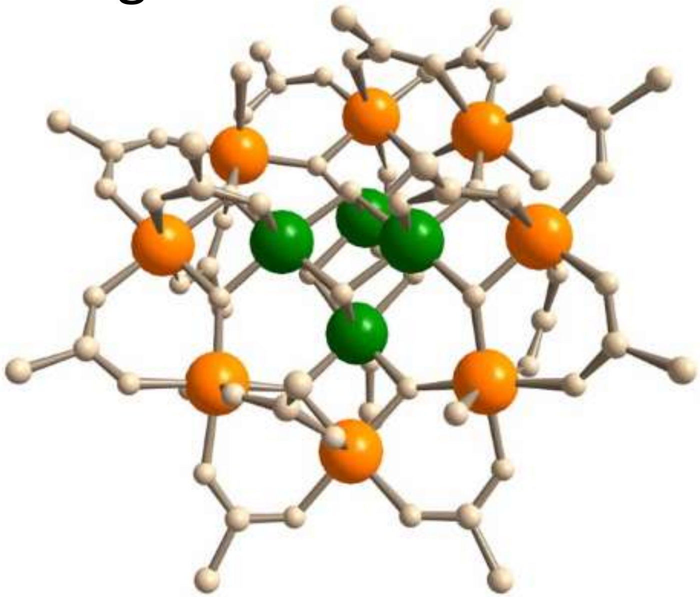


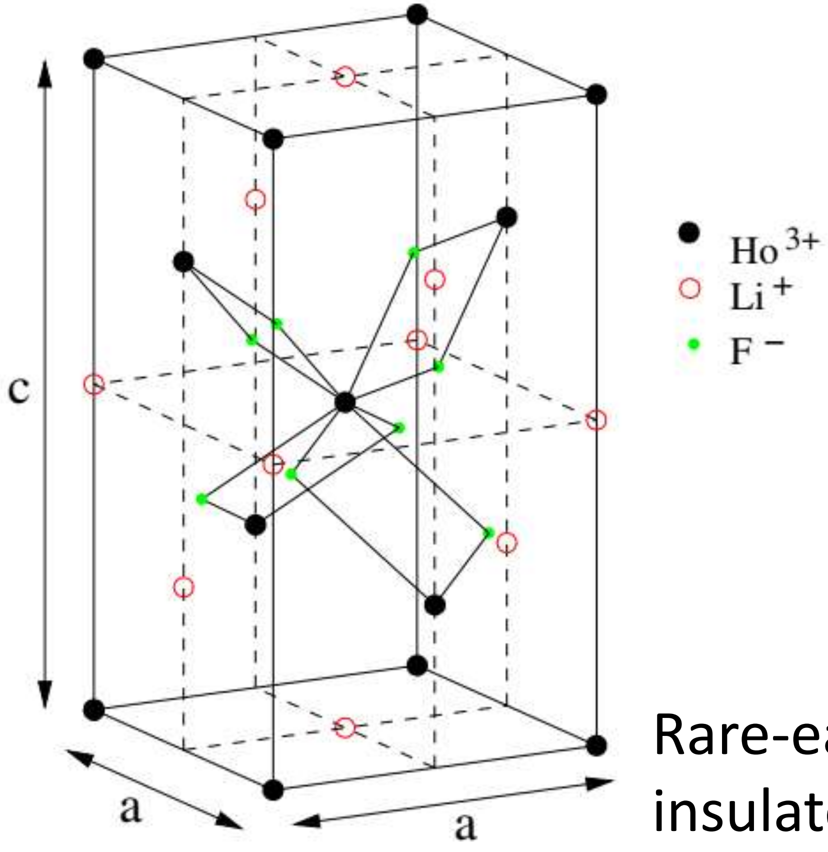
TD, J. C. Andresen, and M. Schechter, Phys. Rev. B **105**, L180413 (2022)

Introduction



Single molecule magnets



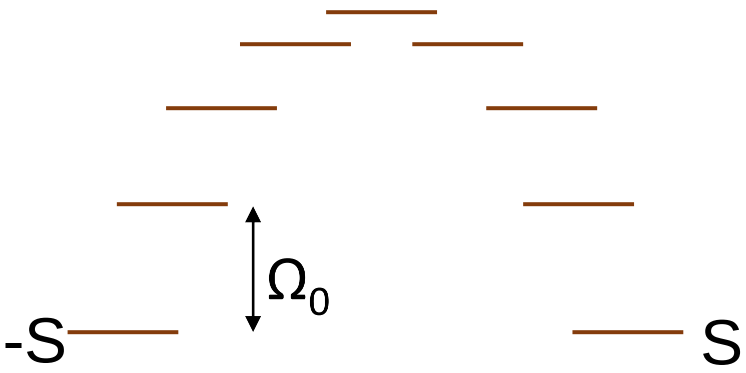


Rare-earth magnetic insulators

Anisotropic dipolar systems

Magnetic insulators, large spin, strong lattice anisotropy, dominant dipolar interaction

$$H_{\mathrm{cf}} = -D \sum_i {S_i^z}^2$$



$$H_D = H_{\mathrm{cf}} - \sum_{ij} V_{ij}^{\mu\nu} S_i^{\mu} S_j^{\nu}$$

$$H_{\mathrm{Ising}} = -\sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z$$

Anisotropic dipolar systems

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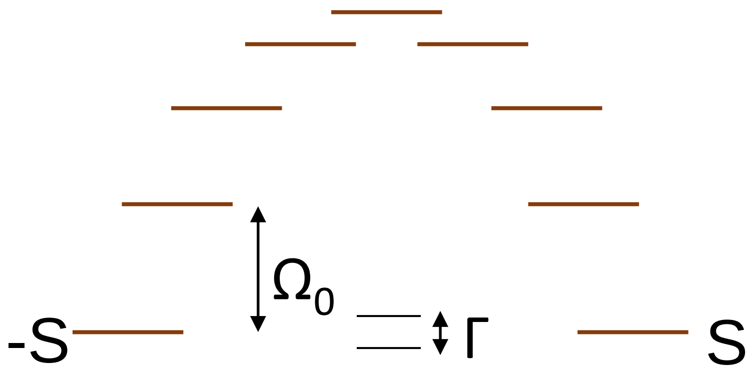
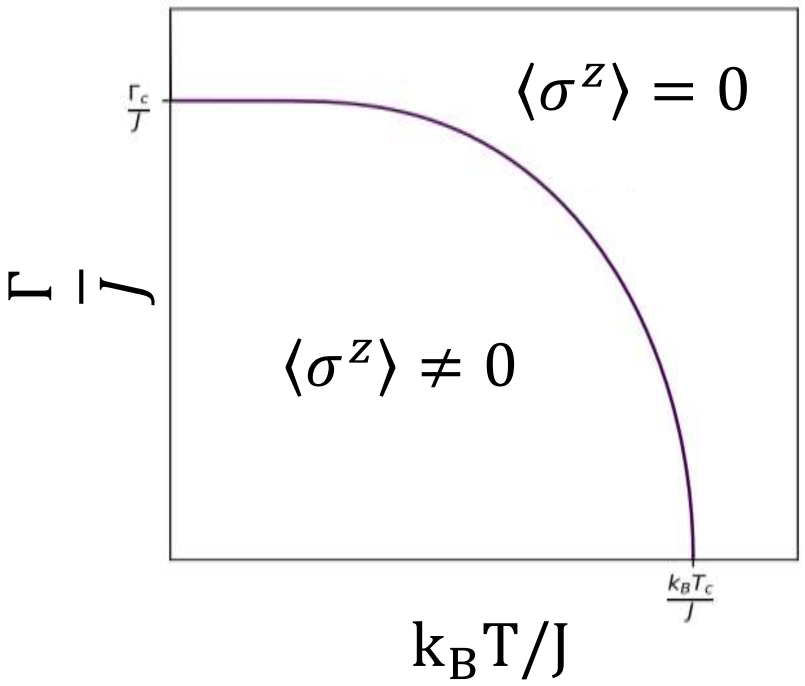


$$H_D = H_{\mathrm{cf}} - \sum_{ij} V_{ij}^{\mu\nu} S_i^\mu S_j^\nu - \Delta \sum_i S_i^x$$

$$H_{\mathrm{Ising}} = -\sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$$

$$\Gamma \propto \Delta^{2S}$$



Mean field (MF) phase diagram

of transverse field Ising model (TFIM)

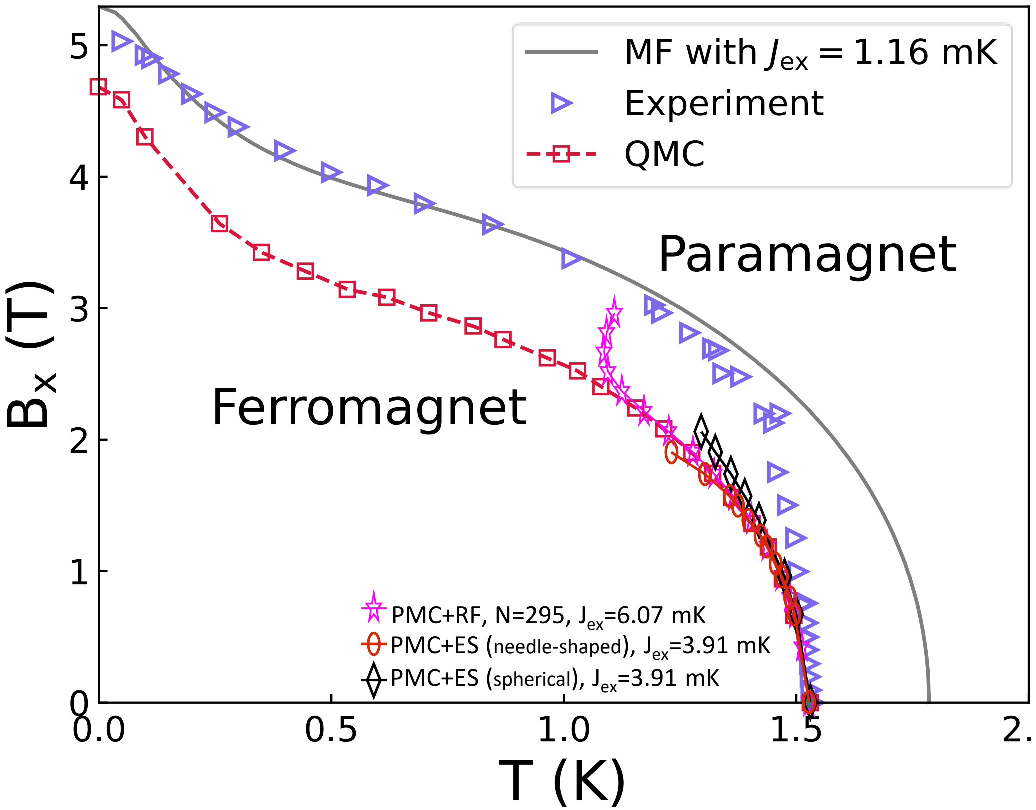
$LiHoF_4$ – the archetypal Ising magnet?

- Full microscopic Hamiltonian (J=8, I=7/2):

$$H = \sum_i H_{\mathrm{cf}}(\boldsymbol{J}_i) - g_L\mu_B \sum_i B_x J_i^x + \frac{1}{2}(g_L\mu_B)^2 \sum_{i\neq j} V_{ij}^{\mu\nu} J_i^\mu J_j^\nu + J_{\mathrm{ex}} \sum_{\langle i,j\rangle} \boldsymbol{J}_i \cdot \boldsymbol{J}_j + A \sum_i (\boldsymbol{I}_i \cdot \boldsymbol{J}_i)$$

- The only free parameter, J_{ex}, can be used to tune $T_c(B_x = 0)$

- Something missing!



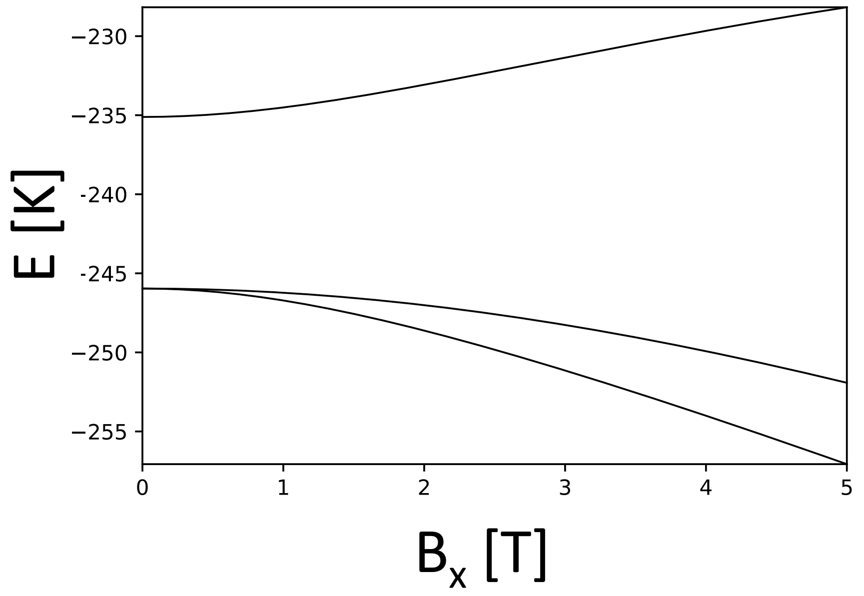
▷ Experiment (x=1)
— MF (J_{ex} = 1.16 mK)
□ QMC (J_{ex} = 3.91 mK)

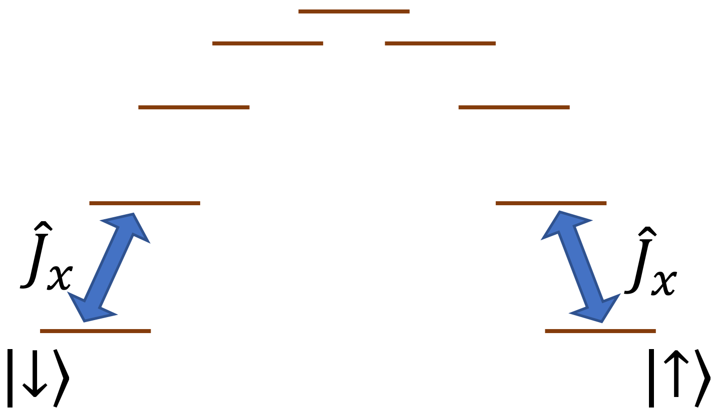
Chakraborty et al., PRB 70, 144411 (2004)
Tabei et al., PRB 78, 184408 (2008)
Babkevich et al., PRB 94, 174443 (2016)

Off-diagonal dipolar (ODD) terms

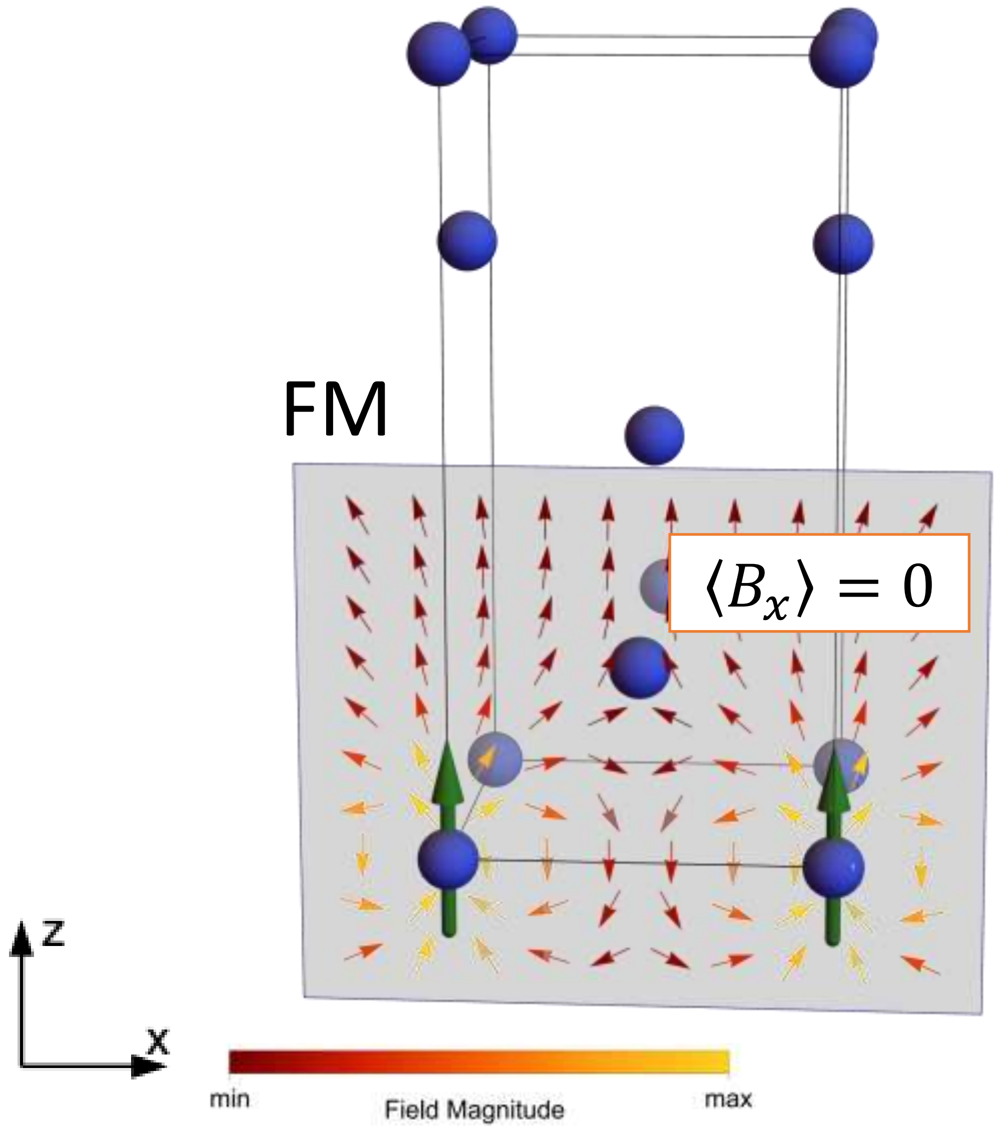
- Terms of the form $V_{ij}^{zx}\langle J_i^z\rangle J_j^x$
- Effectively act as internal transverse magnetic fields
- Decrease the energy of spin j regardless of its state
- Neglected in TFIM due to projection
- Vanish due to symmetry *in FM phase*

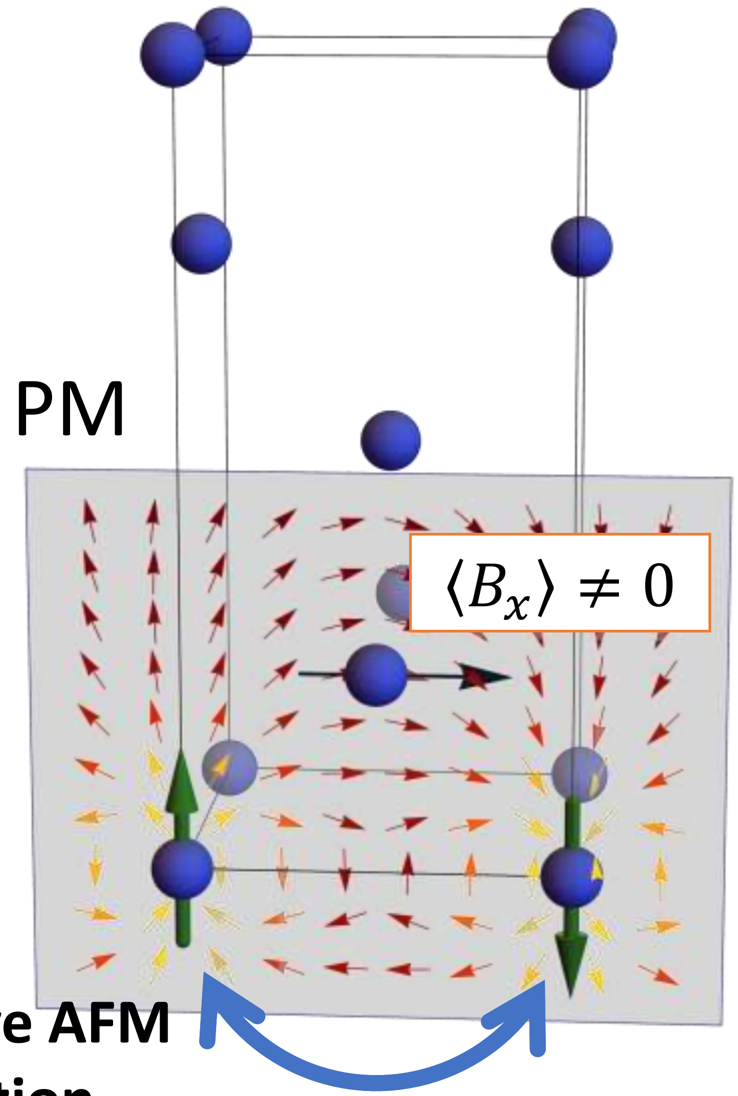
➢Energetically disfavor ferromagnetic order





ODD terms and the phase diagram - example





Effective AFM interaction

Studied Hamiltonian – Monte Carlo Simulation

- Starting from the full microscopic Hamiltonian we keep ODD terms
- Approximation: for each spin, each of the other N-1 spins are projected not *one* of their single-site states — neglecting quantum many body effects
- Effective Hamiltonian
- Hybrid quantum-classical Monte Carlo

$$H_{\mathrm{eff}} = \sum_i H_{\mathrm{cf}}(\boldsymbol{J}_i) - g_L \mu_B \sum_i \langle \boldsymbol{B}_i \rangle \cdot \boldsymbol{J}_i$$

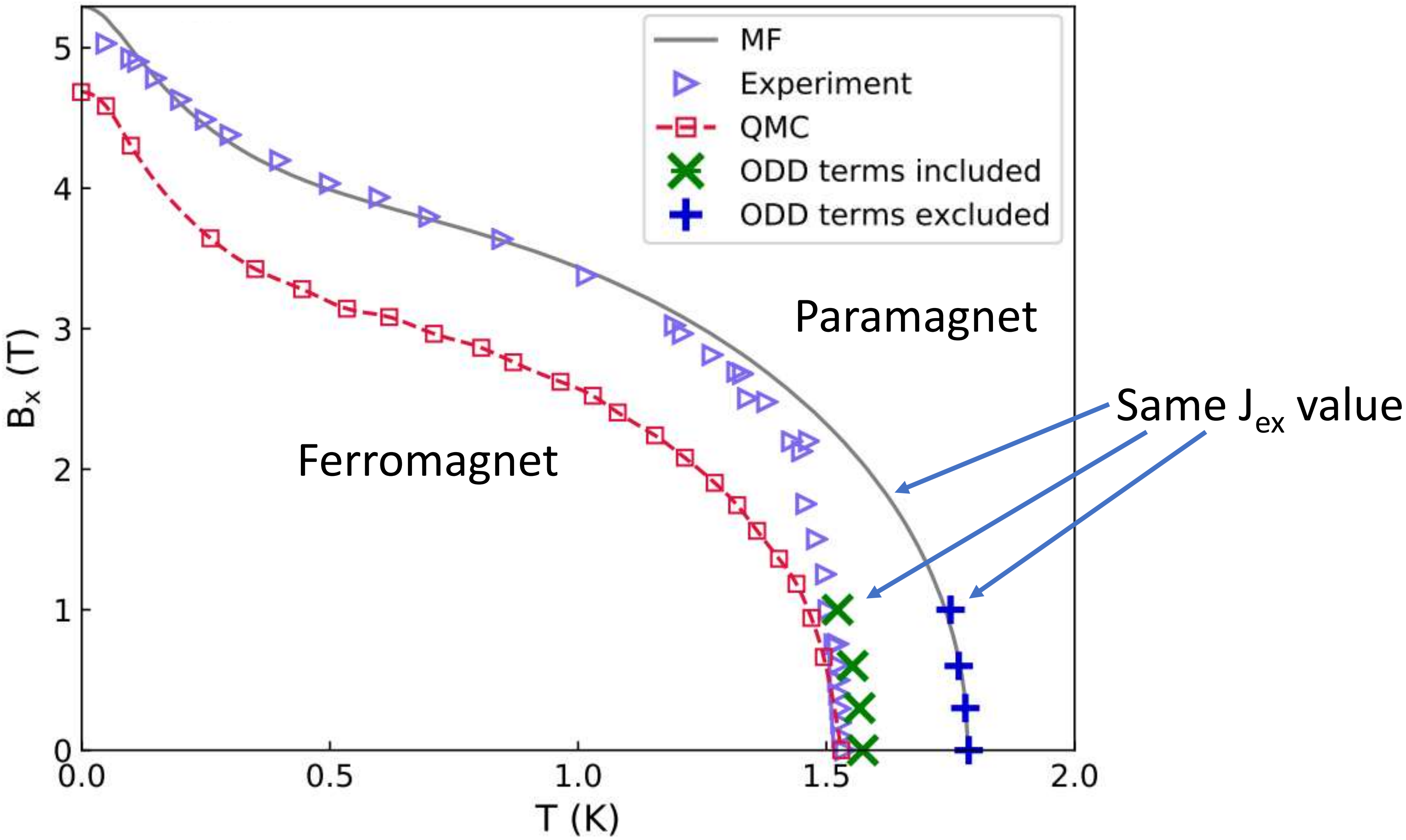
$$B_i^x = B_x - g_L \mu_B \sum_{j \neq i} V_{ij}^{zx} J_j^z$$

$$B_i^y = -g_L \mu_B \sum_{j \neq i} V_{ij}^{zy} J_j^z$$

$$B_i^z = -\frac{1}{2} g_L \mu_B \sum_{j \neq i} V_{ij}^{zz} J_j^z - \frac{J_{\mathrm{ex}}}{2 g_L \mu_B} \sum_{j \in N.N.} J_j^z$$

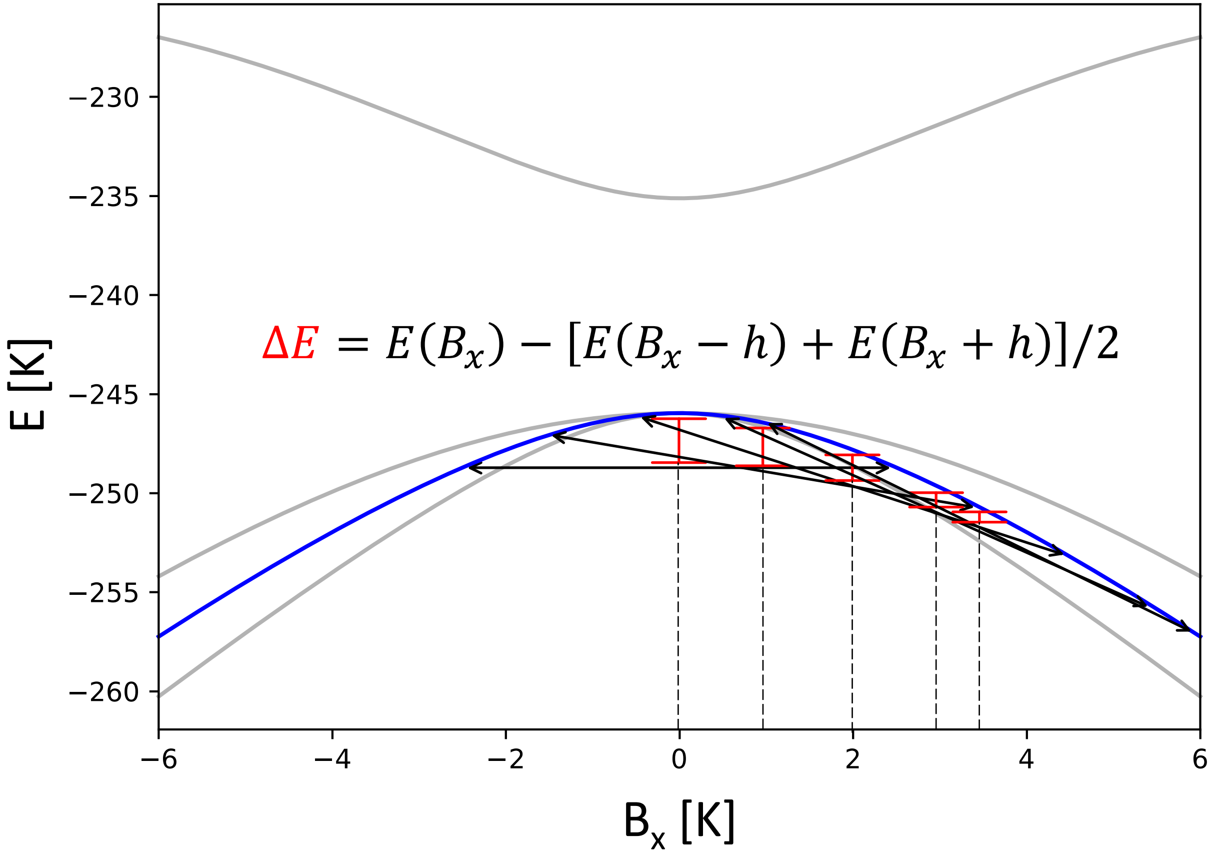
$(J_{\mathrm{ex}} = 1.16\ \mathrm{mK})$

Numerical results

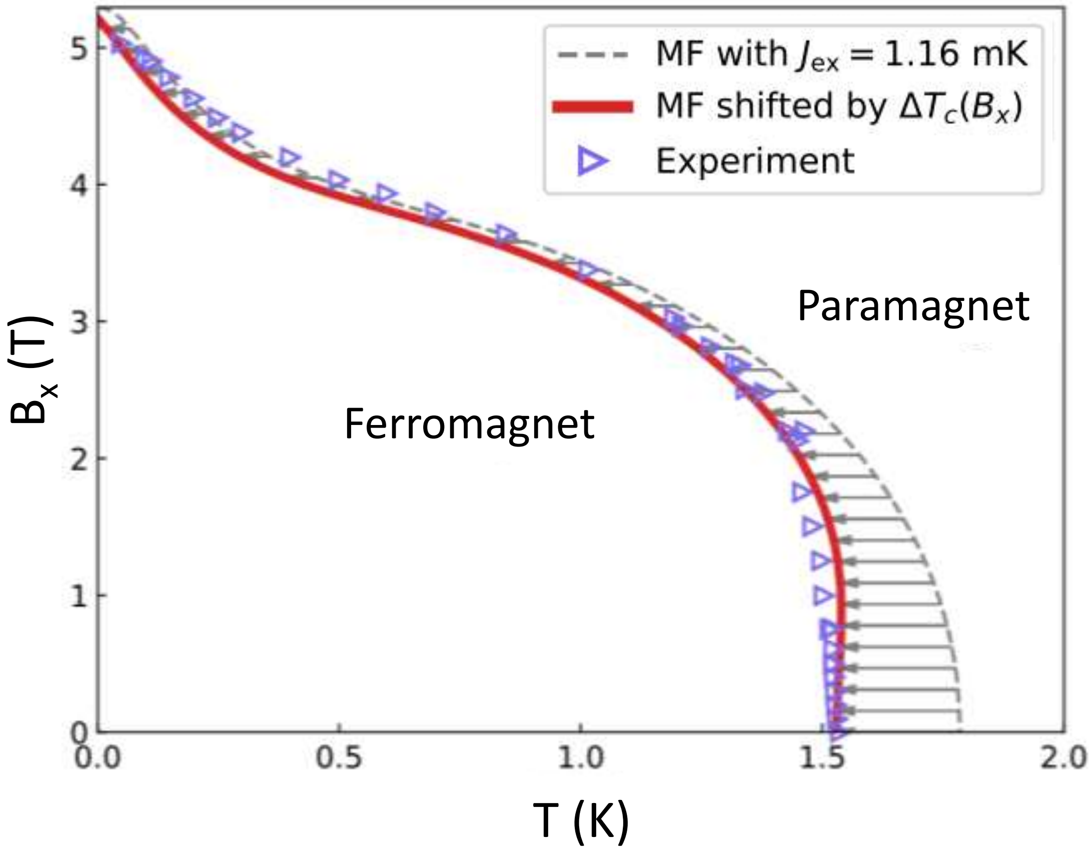


Can it explain the full phase boundary line?

ΔE is an estimation of energy difference between the PM and FM phases



Further, assume $\Delta T_c \propto \Delta E$



Conclusions

- Quantum fluctuations induced by off-diagonal dipolar terms affect even the classical phase transition of dipolar Ising systems
- The effect diminishes with increasing external B_x
- Description of anisotropic dipolar systems by the Ising model essentially insufficient

Thank you!