Thermodynamic properties of the spin-1/2 Ising-Heisenberg model on a triangle-hexagon lattice

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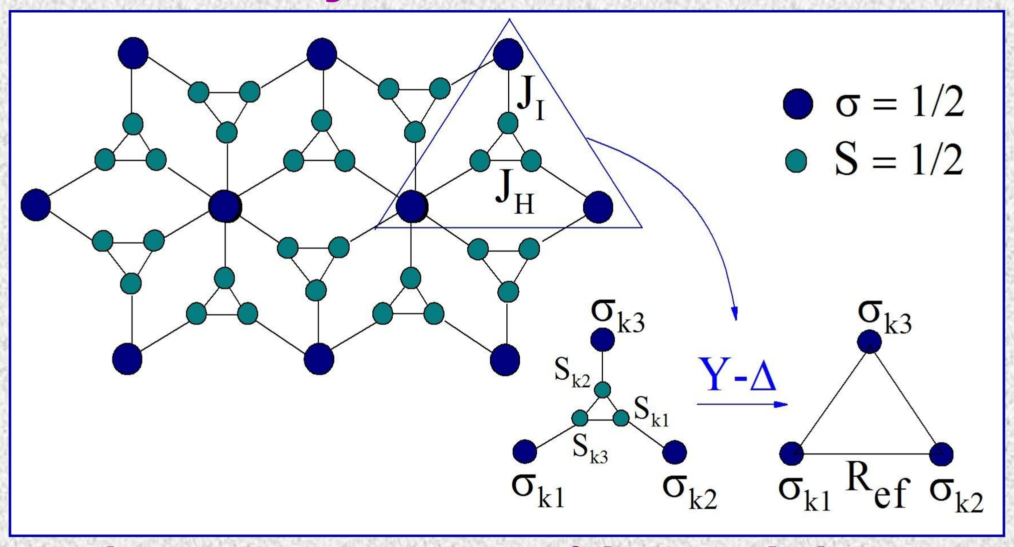
Introduction

Theoretical study of geometrically frustrated quantum spin models attracts a great deal of research interest [1-6], because the intriguing physical phenomena such as an existence of reentrant phase transitions [1], macroscopically degenerate spin-liquid ground states [2], the existence of quantum plateaus [3,4], quantum "order-from-disorder effect" [5,6], or enhanced magneto-caloric effect [3] can be observed in these systems. Recently, geometrically frustrated „triangles-in-triangles" structures described within the framework of classical Potts and Ising models have been studied from a percolation viewpoint as well as from the viewpoint of their critical behaviour [8-12].

Model system



Schematic representation of the triangle-hexagon lattice described by the Ising-Heisenberg model

Motivation

The present study is devoted to a theoretical investigation of geometrically frustrated spin-1/2 Ising-Heisenberg model on a triangle-hexagon planar lattice, which is schematically depicted in the above figure. The considered magnetic structure of consists of smaller triangular-shaped entities embedded in elementary unit cells of a simple triangular lattice. The main goal of this study is to investigate magnetic and thermodynamic properties of the model under consideration.

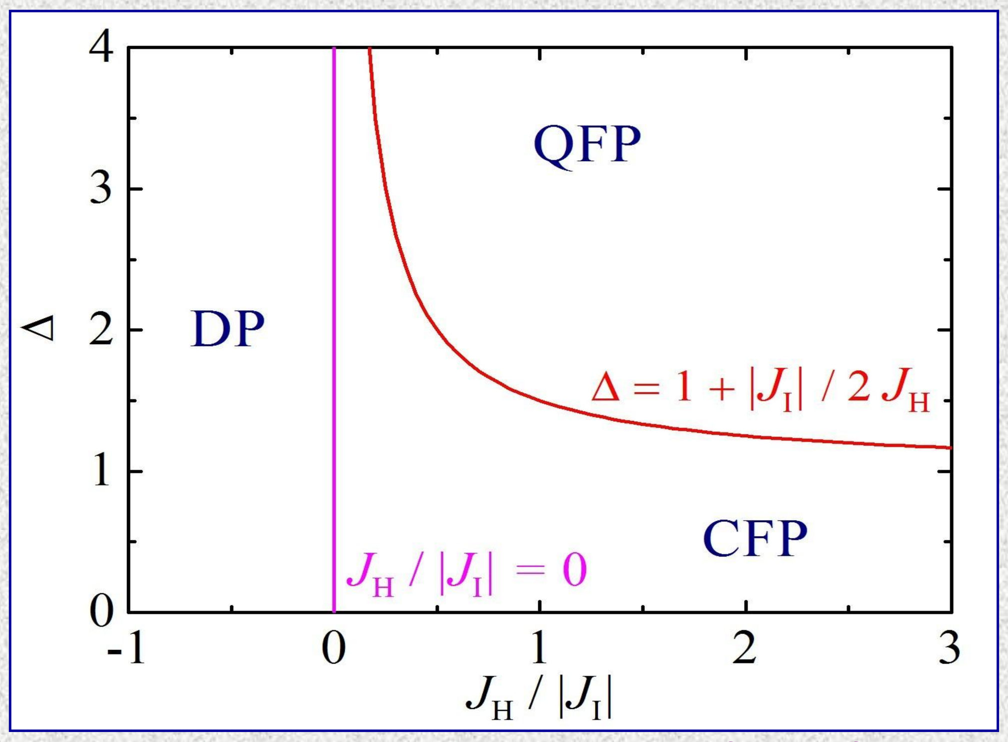
Model system and its Hamiltonian

The Hamiltonian of the spin-1/2 Ising-Heisenberg model on a triangle-hexagon lattice can be written as a sum of cluster Hamiltonians, where each cluster Hamiltonian contains all the interaction terms associated with k-th Heisenberg trimer

$$\hat{H} = \sum_{k=1}^{N} \hat{H}_k \qquad \hat{H}_k = -J_H \sum_{i=1}^{3} [\Delta(\hat{S}_{k,i}^x \hat{S}_{k,i+1}^x + \hat{S}_{k,i}^y \hat{S}_{k,i+1}^y) + \hat{S}_{k,i}^z \hat{S}_{k,i+1}^z] - J_I \sum_{i=1}^{3} \hat{S}_{k,i}^z \hat{\sigma}_{k,i}^z$$

Above, $\hat{S}_{ki}^{\alpha}$ and $\hat{\sigma}_{ki}^{\alpha}$ (α = x,y,z; i = 1,2,3) label spatial components of the spin-1/2 operator, the parameter J_I represents the Ising-type interaction between the nearest-neighbour Ising and Heisenberg spins and the parameter J_H labels the XXZ Heisenberg interaction bewteen the nearest-neighbour Heisenberg spins in the inner triangles, Δ is an exchange anisotropy and relations $\hat{S}_{k4}^{\alpha} = \hat{S}_{k1}^{\alpha}$ and $\hat{\sigma}_{k4}^{\alpha} = \hat{\sigma}_{k1}^{\alpha}$ are implied for convenience.

Ground-state phase diagram



Ground-state phase diagram in the form of the frustration ratio vs. the exchange anisotropy

The star-triangle transformation

Exact analytical solutions of the Ising-Heisenberg model under investigation can be obtained using the generalized star-triangle mapping transformation [13,14], which enables one to derive all the basic thermodynamic properties from the known exact results for the corresponding spin-1/2 Ising model on a triangular lattice [15,16]. The physical meaning of this algebraic transformation [13,14] lies in removing all interactions associated with the Heisenberg spins from the k-th inner triangle and replacing them with new effective interactions between the outer Ising spins σ.

$$Z_k(\hat{\sigma}_{k1}^z, \hat{\sigma}_{k2}^z, \hat{\sigma}_{k3}^z) = A \exp[\beta R_{ef}(\hat{\sigma}_{k1}^z \hat{\sigma}_{k2}^z + \hat{\sigma}_{k2}^z \hat{\sigma}_{k3}^z + \hat{\sigma}_{k3}^z \hat{\sigma}_{k1}^z)] \longrightarrow Z_{IHM}(\beta, J_H, J_I, \Delta) = A^N Z_{IM}(\beta, R_{ef})$$

Ground-state phases

Disordered spin-liquid phase (DP): $[\langle \hat{\sigma}_k^z \rangle; \langle \hat{S}_k^z \rangle] = [0;0]$

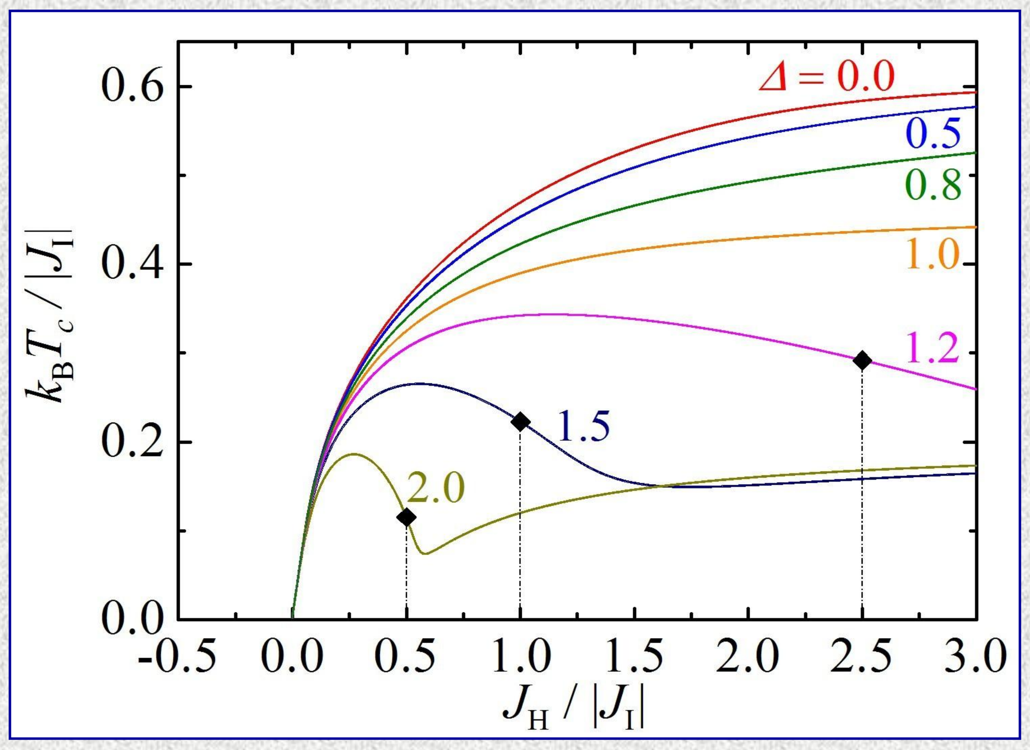
Classical ferromagnetic phase (CFP): $[\langle \hat{\sigma}_k^z \rangle; \langle \hat{S}_k^z \rangle] = [1/2;1/2]$

Quantum ferromagnetic phase (QFP): $[\langle \hat{\sigma}_k^z \rangle; \langle \hat{S}_k^z \rangle] = [1/2;1/6]$

Limiting case (Δ<1):

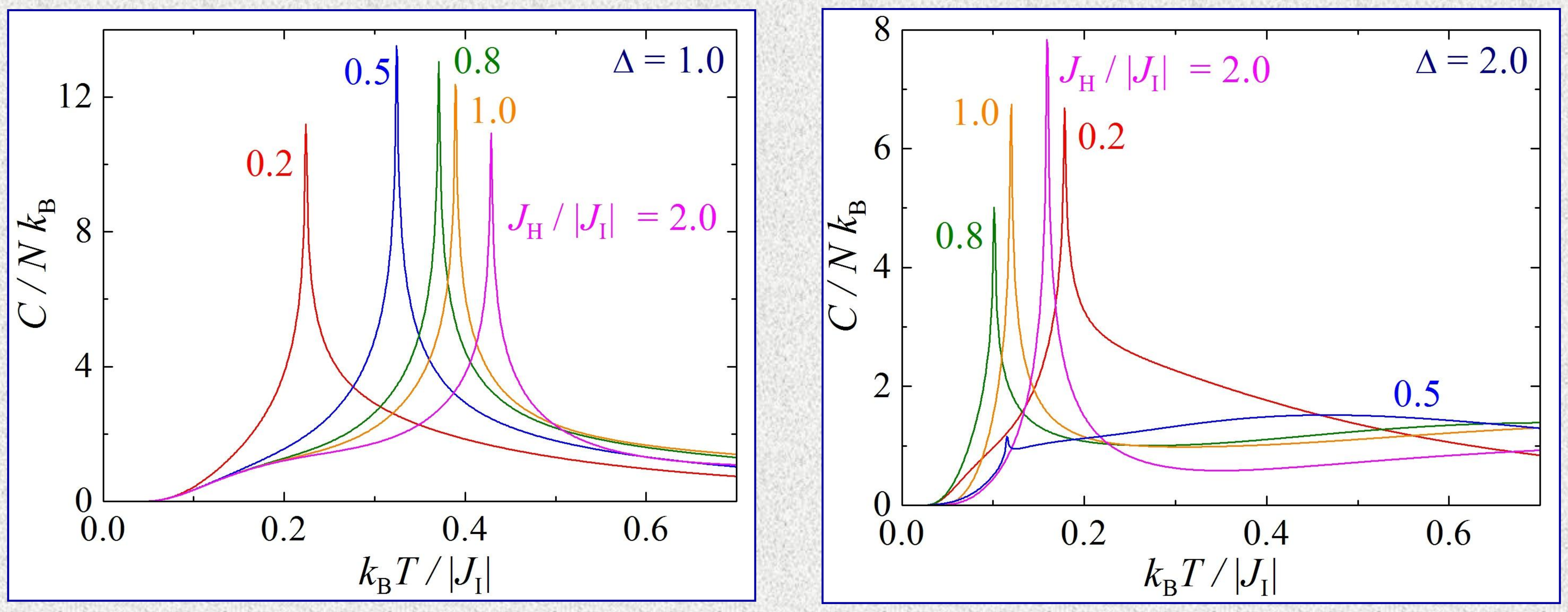
$$\lim_{\frac{J_H}{|J_I|} \to \infty} \frac{k_B T_C}{|J_I|} = \frac{1}{2 \ln\left[\left(1+\sqrt{3}+\sqrt{2}\sqrt[4]{3}\right)/2\right]}$$

Critical behaviour



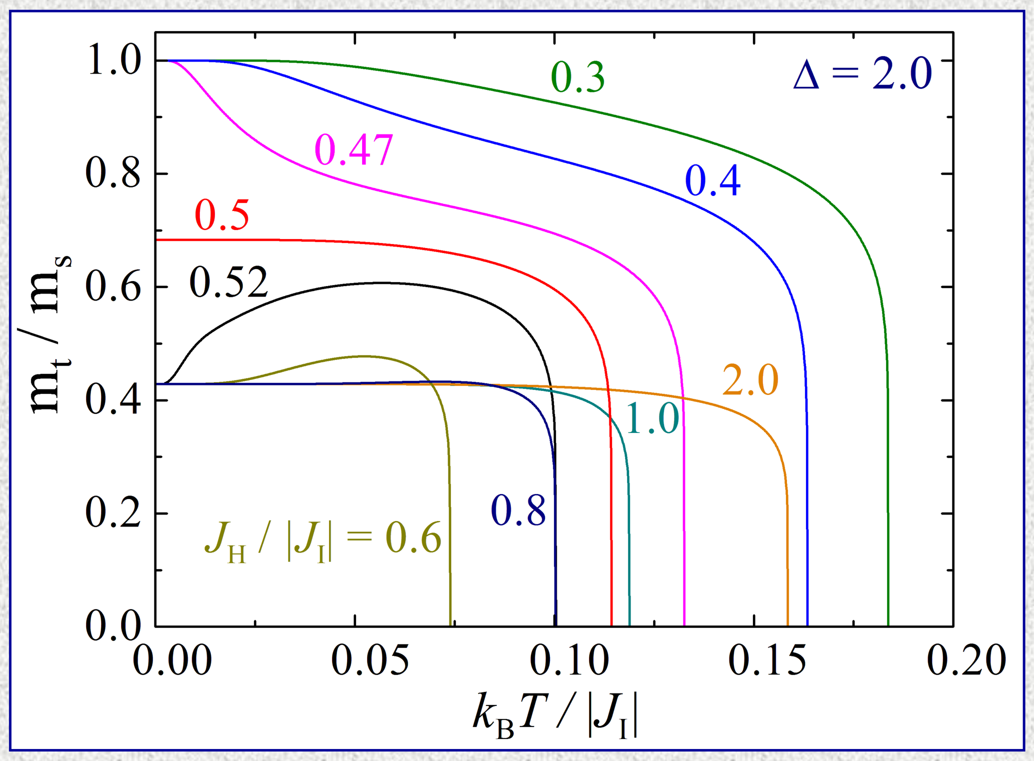
Finite-temperature phase diagram in the form of critical temperature vs. frustration ratio dependence.

Temperature dependence of specific heat



Typical temperature dependences of the specific heat for two different values of the exchange anisotropy Δ and various values of the frustration ratio $J_H / |J_I|$

Spontaneous magnetization



Thermal dependence of the total magnetization normalized with respect to its saturation value for Δ=2.0.

References: [1] H.T.Diep, Magnetic Systems with Competing Interaction, World Scientific, Singapore, 2004. [2] C. Lhuillier and G. Misguich, Lecture Notes in Physics 595 (2002) 161. [3] J.Richter, J.Schulenburg, A. Honecker, Lecture Notes in Physics 645 (2004) 85-155. [4] A. Honecker, J.Schulenburg and J.Richter, J.Phys.: Condens. Matter. 16 (2004) S749. [5] J. Strečka, L.Čanová, M.Jaščur, M.Hagiwara, Phys. Rev. B 78 (2008) 024427. [6] D.X. Yao, Z.L.Loh, E.W.Carlson, M.Ma, Phys. Rev. B 78 (2008) 024428. [7] J.S. Miller and M. Drillon, Magnetism: Molecules to Materials, Wiley-VCH, Weinheim, 2001. [8] A.H.Akbari, R.M.Ziff, Phys. Rev. E (2009) 021118. [9] Ch.R. Scullard, R.M. Ziff, J. Stat. Mech. (2010) P03021. [10] J. C. Wierman, R. M. Ziff, arXiv:0903.3135. [11] F. Y. Wu, Phys. Rev. E 81 (2010) 061110. [12] Ch. Ding, Z.Fu, W.Guo, F.Y.Wu, Phys. Rev. E 81 (2010) 061111. [13] M.E. Fisher, Phys. Rev. 113 (1959) 969. [14] O. Rojas, J.S. Valverde, S.M. de Souza, Physica A 388 (2009) 1419. [15] R.M.F. Houtappel, Physica 16 (1950) 425. [16] H.N.V. Temperley, Proc. Roy. Soc. A 203 (1950) 202.