The Frustrated Ising Antiferromagnet on the Honeycomb Lattice

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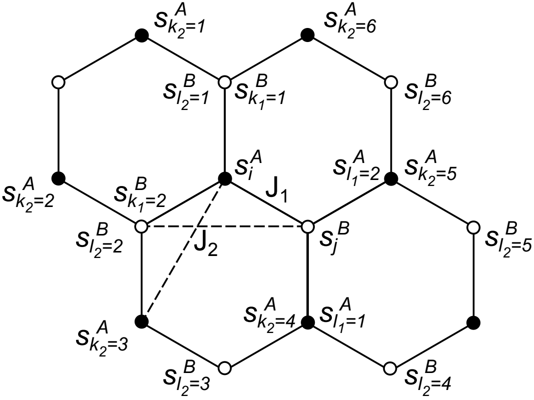
Hamiltonian of the model

$$\mathcal{H} = -J_1 \sum_{\langle i,j \rangle} s_i^A s_j^B - J_2 \Big(\sum_{\langle i,k \rangle} s_i^A s_k^A + \sum_{\langle j,l \rangle} s_j^B s_l^B \Big) - h \Big(\sum_{i \epsilon A} s_i^A + \sum_{j \epsilon B} s_j^B \Big),$$

$$s_i \in \{\pm 1\} \quad \text{and} \quad J_1 < 0, J_2 < 0$$



What we would like to study?

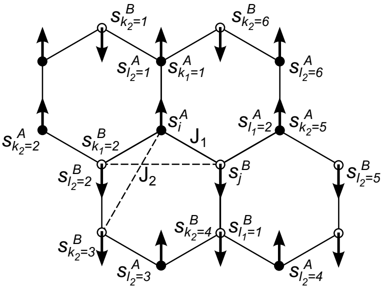
- determine thermodynamic properties of the model
- large negative value of $J_2 \rightarrow$ frustration effect
- identification of the possible phases
- study limitations of the exponential (differential) operator technique
  Taggart,Fittipaldi 1982
- ongoing research

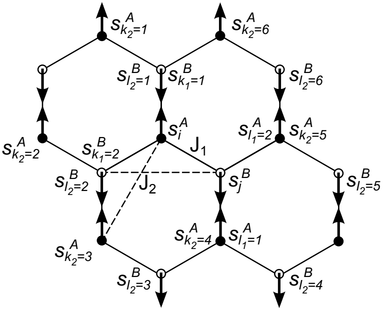
- thermodynamic analysis of the model in zero field $h = 0$
- introduction of dimensionless effective parameters

$$\alpha = \frac{J_2}{|J_1|}, \quad t = \frac{k_B T}{|J_1|}, \quad h = \frac{H}{k_B T}$$

- we expect to observe phases like
  a) Antiferromagnetic (AF) phase - $|J_2| \ll 1$, $t \ll 1$
  b) Paramagnetic phase - $t \gg 1$
  c) Superantiferromagnetic (SAF) - $|J_2| \gg 1$
- 1.step - analysis of Ground State ($T = 0$) - minimization of Hamiltonian

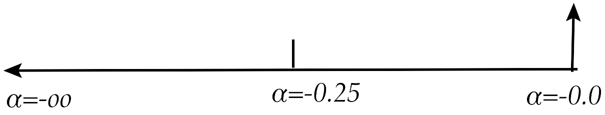
Ground state $T = 0$





$$\frac{E_{SAF}}{N|J_1|} = -\frac{1}{2}(1 - 2\alpha)$$

$$\frac{E_{AF}}{N|J_1|} = -\frac{3}{2}(1 + 2\alpha)$$



Effective-field theory with correlations

- use of differential operator technique Honmura & Kaneyoshi 1978

$$\exp\left(\lambda\frac{\partial}{\partial x}\right)f(x)|_{x=0}=f(\lambda)$$

- expressions like

$$\left\langle \exp\left(\beta J s_i \frac{\partial}{\partial x}\right)\right\rangle \ldots$$

  can be traced out through variable s_i

- two-site cluster approximation

- depending on the phase type $\rightarrow$ set of coupled equations for sublattice magnetizations (or higher correlation functions) can be obtained

Effective-field theory with correlations for AF phase

- coupled equations for sublattice magnetizations $m_\alpha \equiv \langle s_g^\alpha \rangle$ ($\alpha = A$ or B) (normalized per site)

$$
\begin{aligned}
m_\alpha \quad = \quad & \Big[A_x(1)A_y(2) + B_x(1)B_y(2) + m_B\Big(A_x(1)B_y(2) + A_y(2)B_x(1)\Big)\Big]^2 \times \\
& \Big[A_y(1)A_x(2) + B_y(1)B_x(2) + m_A\Big(A_x(2)B_y(1) + A_y(1)B_x(2)\Big)\Big]^2 \times \\
& \Big[\Big(A_x(2) + m_A B_x(2)\Big)\Big(A_y(2) + m_B B_y(2)\Big)\Big]^4 f_\alpha(x,y)\Big|_{x=0,y=0},
\end{aligned}
$$

  where , $A_\mu(\nu) = \cosh(J_\nu D_\mu)$, $B_\mu(\nu) = \sinh(J_\nu D_\mu)$, ($\nu = 1, 2$), $D_\mu = \partial/\partial\mu$ ($\mu = x, y$) and f_α is a given function

- order parameter $m_S = (m_A - m_B)/2$

- magnetization $m = (m_A + m_B)/2$

Effective-field theory with correlations for SAF phase

- different choice of sublattices than for AF

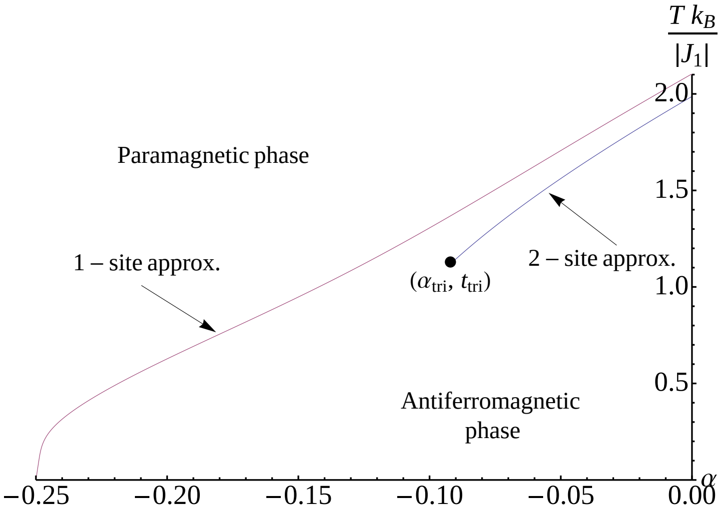
- effective equations

$$
\begin{aligned}
m_\alpha \quad = \quad & \Big[A_x(1)A_y(2) + B_x(1)B_y(2) + m_A\Big(A_x(1)B_y(2) + A_y(2)B_x(1)\Big)\Big] \times \\
& \Big[A_x(1)A_y(2) + B_x(1)B_y(2) + m_B\Big(A_x(1)B_y(2) + A_y(2)B_x(1)\Big)\Big] \times \\
& \Big[A_y(1)A_x(2) + B_y(1)B_x(2) + m_A\Big(A_x(2)B_y(1) + A_y(1)B_x(2)\Big)\Big] \times \\
& \Big[A_y(1)A_x(2) + B_y(1)B_x(2) + m_B\Big(A_x(2)B_y(1) + A_y(1)B_x(2)\Big)\Big] \times \\
& \Big[\Big(A_x(2) + m_A B_x(2)\Big)\Big(A_y(2) + m_B B_y(2)\Big)\Big] \times \\
& \Big[\Big(A_y(2) + m_A B_y(2)\Big)\Big(A_x(2) + m_B B_x(2)\Big)\Big]^3 f_\alpha(x,y)\Big|_{x=0,y=0},
\end{aligned}
$$

- resulting equations are amenable to based on the heavy use of symbolic calculations - *Mathematica*™, *Octave*,...

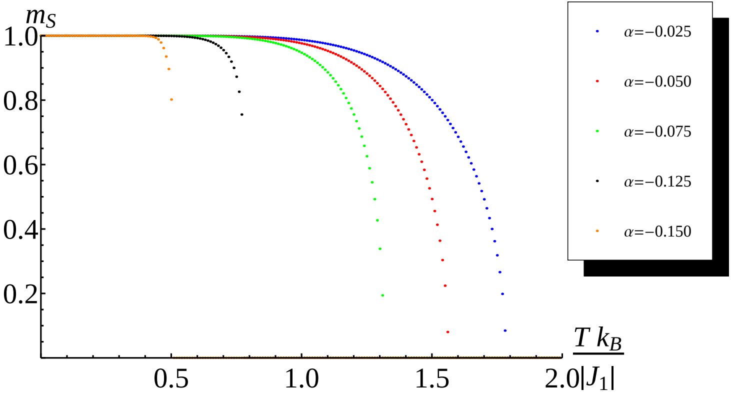
Results - Phase diagram

appearance of tricritical point : $(t_{tri} = 1.1360, \alpha_{tri} = -0.0907)$
quite different qualitative behaviour in comparison with square lattice

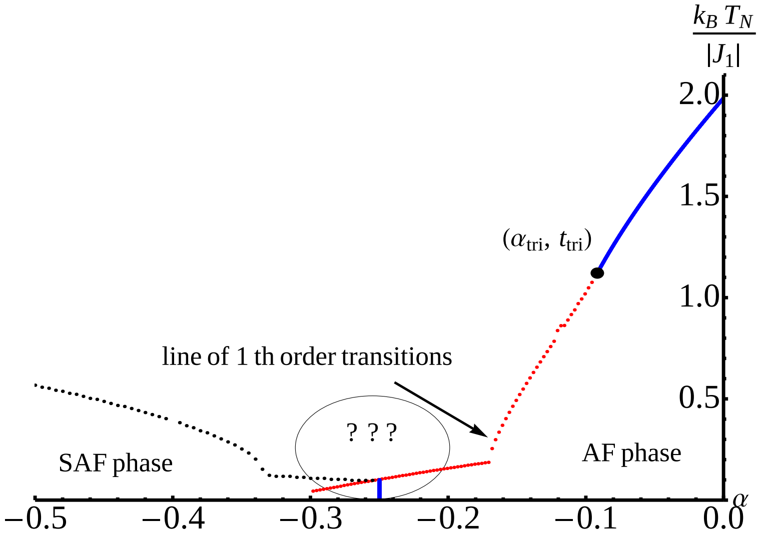


Results

Magnetization process



Qualitative picture of phase diagram



For completness ($\beta = 1/\mathrm{k_B}T$)

$$f_A = \frac{f_1(x,y)}{f_0(x,y)}, \quad f_B = \frac{f_2(x,y)}{f_0(x,y)},$$

$$f_1(x,y) = \sinh\beta(x+y+2h) + e^{-2\beta J_1}\sinh\beta(x-y),$$

$$f_2(x,y) = \sinh\beta(x+y+2h) - e^{-2\beta J_1}\sinh\beta(x-y),$$

$$f_0(x,y) = \cosh\beta(x+y+2h) + e^{-2\beta J_1}\cosh\beta(x-y).$$

References

- G. Bruce Taggart and I. P. Fittipaldi, Phys. Rev. B, **25**, 7026 (1982)
- R. honmura and T. Kaneyoshi, Prog. Theor. Phys. **60**, 635 (1978).
- M. Borovský, Diploma Thesis, UPJŠ, Košice (2012)

Outline and future work

- Take into account higher correlations between spins - $(m_A, m_B, \rho_A, \rho_B, \tau_A, \tau_B)$
- Analysis of the 1st order phase transitions $\rightarrow$ need of more sophisticated methods
- Monte Carlo calculations for better quantitative description
- Heisenbeg generalization of the two-site cluster approximation

Thank you for your attention!