Tricritical Properties of Antiferromagnetic Ising Model on the Square Lattice

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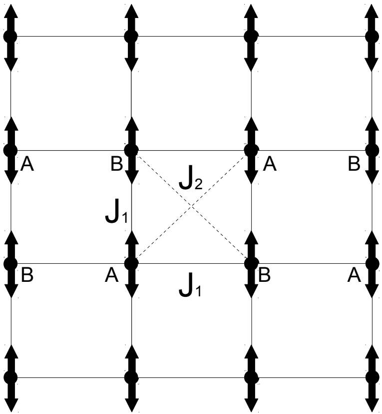
15th **Small Triangle Meeting**

28 October 2013

Hamiltonian of the model

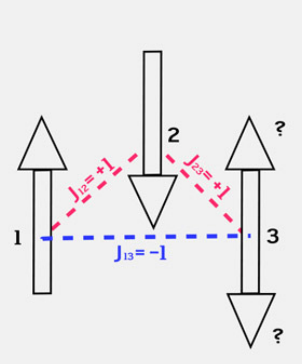
$$\mathcal{H} \;=\; -J_1 \sum_{NN} s_i^A s_j^B - J_2\Big(\sum_{NNN} s_i^A s_k^A + \sum_{NNN} s_j^B s_l^B\Big) - h\Big(\sum_{i \epsilon A} s_i^A + \sum_{j \epsilon B} s_j^B\Big),$$

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



Introduction

- frustration effect for some ratio $J_1/J_2 \to$ non zero entropy at $T = 0$



- enhanced magnetocaloric effect (change of $H \Rightarrow$ change of T)
  O.V.Lounasmaa 1974

- we restrict to the case of zero external field case $H = 0$
- **main goal:** construction of the phase diagram
- study limitations of the exponential (differential) operator technique Taggart,Fittipaldi 1982
- Monte Carlo simulations to confirm our results

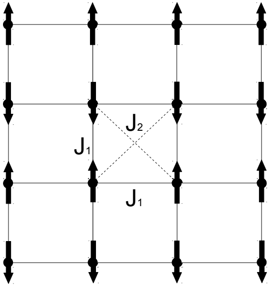
- introduction of dimensionless effective parameters

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

- expected phases are
  a) Antiferromagnetic (AF) phase - small α, low temperatures $t \ll 1$
  b) Paramagnetic phase - high temperatures $t \gg 1$
  c) Superantiferromagnetic (SAF) phase - $|J_2| \gg 1$

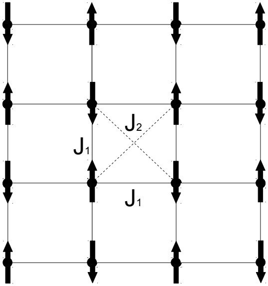
Ground state $T = 0$

SAF phase

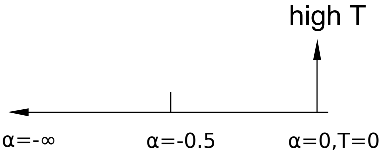


$$\frac{E_{SAF}}{N|J_1|} = 2\alpha$$

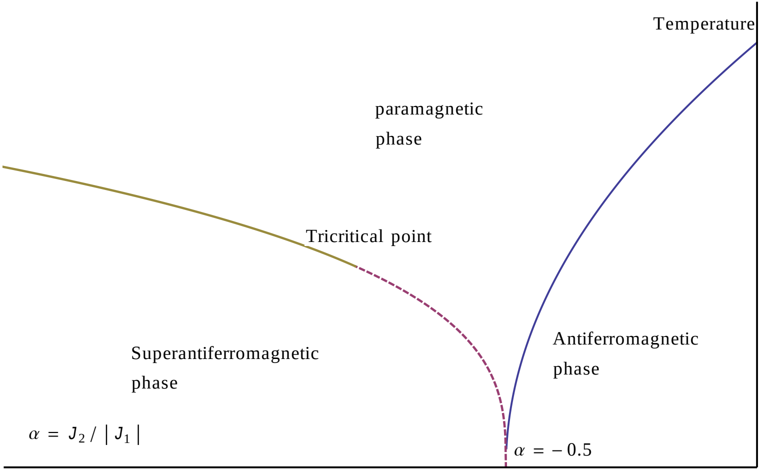
AF phase



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



Phase diagram - general expectation



Effective-field theory with correlations

- improved mean field theory
- use of differential operator technique Honmura & Kaneyoshi 1978

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

- in expressions like

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

  trace over spin variable s_i can be performed

- truncation procedure -
  1) at level of sublattice magnetization $\langle s_i \rangle$
  2) local energy $\langle s_i s_j \rangle$
  3) triple functions $\langle s_i s_j s_k \rangle$, and so on.

Effective-field theory with correlations

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

- coupled equations for sublattice magnetizations $m_\alpha \equiv \langle s_g^i \rangle$ ($i = A$ or B) for AF phase

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

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 of α and t

- heavy use of symbolic calculations - *Mathematica*$^{\text{TM}}$, *Octave*,...

Effective-field theory with correlations

- order parameter $m_S = (m_A - m_B)/2$
- magnetization $m = (m_A + m_B)/2 = 0$ (for AF and as well for SAF phase)
- by formal integration the following equation for Landau free energy follows

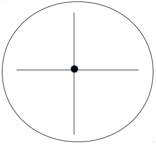
$$f(m_s, t) = f_0(t) + A_2(t) m_s^2 + A_4(t) m_s^4 + A_6(t) m_s^6 + \dots$$

- critical point $A_2 = 0, \quad A_4 > 0$
- tricritical point $A_2 = 0, \quad A_4 = 0$
- for SAF phase different choice of sublattices $\rightarrow$ different equations

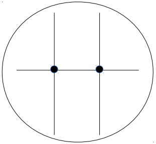
Effective-field theory with correlations

cluster approximation performed for

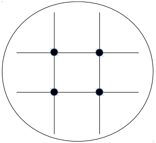
- **1**-site



- **2**-site

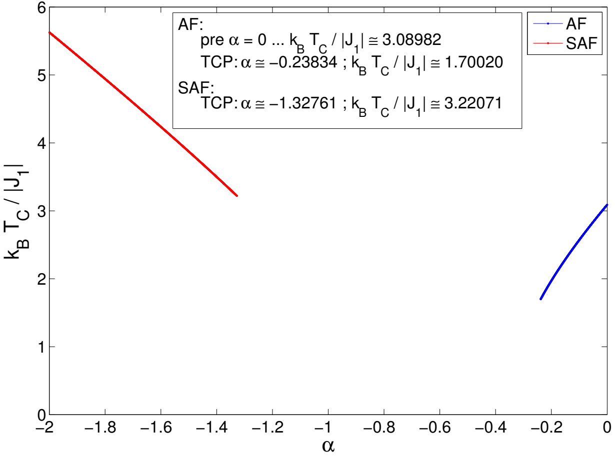


- **4**-site

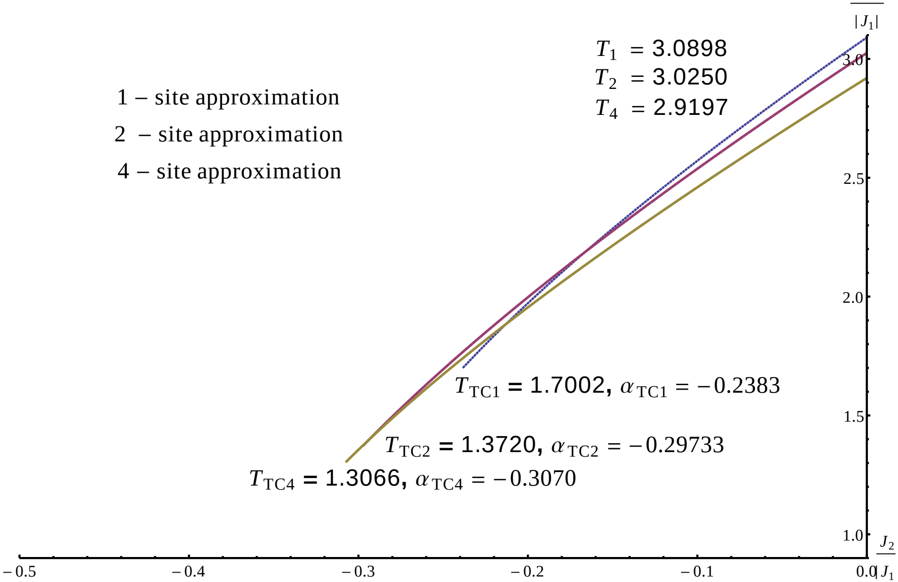


Results - 1 site approximation

appearance of two tricritical points



Results


1 – site approximation
2 – site approximation
4 – site approximation
$T_1 = 3.0898$
$T_2 = 3.0250$
$T_4 = 2.9197$
$T_{TC1} = 1.7002$, $\alpha_{TC1} = -0.2383$
$T_{TC2} = 1.3720$, $\alpha_{TC2} = -0.29733$
$T_{TC4} = 1.3066$, $\alpha_{TC4} = -0.3070$
$\frac{T}{|J_1|}$
$\frac{J_2}{|J_1|}$
−0.5
−0.4
−0.3
−0.2
−0.1
0.0
1.0
1.5
2.0
2.5
3.0

Outline and future work

- Analysis of the 1st order phase transitions $\rightarrow$ need of more sophisticated methods
- Monte Carlo calculations for better quantitative description (troubles with sign problem near $\alpha \approx -0.5$)
- challenging **9**-site cluster approximation be
- AF on honeycomb lattice (which was actually our original goal ☺)
- Take into account higher correlations between spins - $(m_A, m_B, \rho_A, \rho_B, \tau_A, \tau_B)$

Thank you for your attention

For completness ($\beta = 1/\mathrm{k_B}T$ and $h = 0$)

$$f_A = \frac{f_1}{f_0}, \quad f_B = \frac{f_2}{f_0},$$

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

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

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

References

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- M. Borovský, Diploma Thesis, UPJŠ, Košice (2012)
- A. Kalz, A. Honecker, S. Fuchs and T. Pruschke: J. Phys.: Conf. Ser. **145** (2009) 012051; Eur. Phys. J. B **65**, 533-537 (2008)