Frustrations and phase transitions in the Ising model on square lattice

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The problem of frustrations and phase transitions in Ising model on 2D square lattice is explored in a great many works, but the overwhelming majority of investigations [1,2] consider one particular case.

In this work, we studied the problem of frustration origination and of phase transition suppression in Ising model on 2D square lattice with account of interactions between the nearest and the second neighbors in an external magnetic field. We considered more general cases, when the interactions between the nearest and the second neighbors change both in a value and in a sign.

The Hamiltonian of antiferromagnetic Ising model on the square lattice can be written as

$$\mathrm{H} = -J_{NN}\sum_{\langle i,j\rangle}(S_i \cdot S_j) - J_{NNN}\sum_{\langle i,j\rangle}(S_i \cdot S_j) - h\sum_i s_i \,, \qquad (1)$$

where $S_{i,j}$=±1 is the Ising spin. The first term in the Equation (1) accounts for the exchange interaction of nearest neighbors by the value of $J_{NN}<0$, and the second term considers second nearest neighbors by $J_{NNN}<0$, h is the external magnetic field.

We used highly effective replete exchange algorithm of the Monte-Carlo method. A detail description of the replete exchange algorithm was reported in previous work [3].

The points and lines of frustrations, at which the phase transitions disappeared, were detected depending on signs and relative values of interactions and magnetic fields. The heat capacity, at that, lost a lambda-wise feature. The dependences of phase transition points on the relative values of interactions and magnetic field were obtained.

A new effect – the heat capacity splitting near the frustration points – was found. Also we found new magnetic structures and a new type of ordering, namely, the ordering in one direction and lack of ordering in other direction [4].

It was shown that passage through any frustration point (both with magnetic field and without it) causes a fundamental change in the structure.

The lack of interaction between nearest neighbors produced a frustrated field, and the presence of these interactions split this field on two; when increasing the external magnetic field the magnetic structure underwent a transformation twice and, except initial Neel and finite ferromagnetic structure, here appeared an intermediate structure.

Since the external magnetic field tended to order the spins ferromagnetically, it competed with antiferromagnetic interactions, which resulted appearance of new points frustrated depended on the value of exchange parameters and magnetic field.

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1. A. Kalz, A. Honecker, S. Fuchs and T. Pruschke. Phase diagram of the Ising square lattice with competing interactions. Eur. Phys. J. B, Vol. 145, 012051, (2009).
2. H.J.W. Zandvliet and C. Hoede. Spontaneous magnetization of the square 2D Ising lattice with nearest- and weak next-nearest-neighbour interactions, Phase Transitions, Vol. 82, pp. 191—196 (2009).
3. A.K. Murtazaev, M.K. Ramazanov: Phys. Rev. B, Vol. 76, (2007), p. 174421.
4. F.A. Kassan-Ogly, B.N. Filippov, A.K. Murtazaev, M.K. Ramazanov, M.K. Badiev, JMMM. 324, 3418 (2012).