Computer Modeling of Phase Transitions of Semibounded Antiferromagnets

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Abstract. The article gives a machine modeling of surface and bulk phase transitions in semibounded antiferromagnetic Ising model. Distinct values of exchange integrals proportion were considered. Dependency of temperature of phase transitions from surface energy value was calculated. System phase diagram was constructed. Availability of tetracritical point was shown. Conditions of surface phase transition were obtained. Temperature and properties of tetracritical point was determined.

1. Introduction
The phenomenon of surface magnetism consists of distinction between ordering temperature of the surface spins and ordering temperature of other system spins. The reason for this phenomenon is difference between values of exchange integral on surface and exchange integral in depth of sample. Surface ordering for antiferromagnetic systems was observed in a series of contributions [1, 2, 3]. In the abstract, within the framework of the mean-field theory surface magnetism was reported in paper [4], in which it was shown that the phase transition temperature on the surface may vary from the corresponding Néel temperature. System phase diagram was obtained in this and in other papers [5, 6, 7]. It consist of three phases: disordered phase (SD/BD), surface-ordered bulk-disordered phase (SO/BD), surface-ordered bulk-ordered phase (SO/BO) Figure 1.

In addition, three transition lines crossing at a tetracritical point are observed on phase diagram. SD/BD to SO/BD transition is referred to surface phase transition, SO/BD to SO/BO transition is referred to extraordinary phase transition, SD/BD to SO/BO transition is referred to ordinary or bulk phase transition. Crossing of these three transition lines form a multicritical point. Phase transition in this point named special phase transition. Transition names was first introduced in the paper [8]. Critical behavior of semibounded Ising model was considered in the papers [9, 10] as part of field-theoretical approach.

The purpose of our article is research of phase transitions in semibounded antiferromagnetic Ising model by machine modeling at distinct values of surface energy and construction of phase diagram.
2. Description of the system

Hamiltonian of semibounded antiferromagnetic Ising model may be written as:

\[ H = -J_B \sum_b S_i S_j - J_S \sum_s S_i S_j, \]  

(1)

where \( S_i \) is value of spin \( i \) point (+ \( \frac{1}{2} \) or \( -\frac{1}{2} \)). Addition is carried out over nearest neighbours. The second sum include surface spins only, the first sum include the others. Surface \( (J_S) \) and bulk \( (J_B) \) exchange integrals have different values in most real systems. Besides \( J_S \) may have values bigger then \( J_B \) as well as smaller then \( J_B \).

In this paper machine modeling of 3D systems was carried out with cubical lattice having linear dimensions \( L \times L \times 2L \) by Monte Carlo using the Metropolis algorithm. Free boundary plane was given by equation \( z = 0 \). System was found semi-space \( z \geq 0 \). Periodic boundary conditions were used. Spins from plane \( z = L \) were considered neighbours for spins from plane \( z = 2L \). Theory of finite-dimensional scaling was used for determination phase transition temperature.

Let us introduce two order parameter \( -m \) and \( m_S \) to describe the antiferromagnetic ordering. Order parameter \( m \) is calculated as staggered magnetization of all system. It is equal to difference between magnetic moments of two sublattice. Surface order parameter \( m_S \) was calculated as staggered magnetization of free-surface located spins.

Fluctuation relations were used to monitor the behaviour of heat capacity and susceptibility in bulk of system and on its surface:

\[ C = NK^2 \left( \langle E^2 \rangle - \langle E \rangle^2 \right) \]  

(2)
\[
\chi = NK\left(\langle m^2 \rangle - \langle m \rangle^2 \right)
\]
(3)
\[
C_s = SK^2\left(\langle E_s^2 \rangle - \langle E_s \rangle^2 \right)
\]
(4)
\[
\chi_s = SK\left(\langle m_s^2 \rangle - \langle n_s \rangle^2 \right)
\]
(5)
\[
K = |J_s|/k_B T,
\]
(6)
\[
N = 2L^2,
\]
(7)
\[
S = L^2.
\]
(8)

(7) – number of system points, (8) – number of surface points, \(E\) – internal energy, \(E_s\) – surface energy. Angle brackets signify thermodynamic averaging.

Critical temperature of transition was defined by bulk and surface Binder’s quartic cumulants:

\[
U = 1 - \frac{\langle m^4 \rangle}{3\langle m^2 \rangle^2}, \quad U_s = 1 - \frac{\langle m_s^4 \rangle}{3\langle m_s^2 \rangle^2}.
\]
(9)

Temperature of phase transition can be defined by the position of the intersection point of cumulants for systems with different sizes of \(L\). Temperature of bulk phase transition \(T_N\) was defined by intersection point of bulk cumulants \(U\), temperature of surface phase transition \(T_S\) was defined by intersection point of surface cumulants \(U_s\).

### 3. Results of computer modeling

Computer experiment was carried out for systems with linear sizes from \(L = 12\) to \(L = 32\) in increments of \(L = 4\). The number of steps of Monte Carlo for the spin was equal to 100 000. The number of steps of Monte Carlo for the spin was equal to 100 000. The value of the ratio of the exchange integrals \(R = J_s / J_B\) ran from \(R = 1.0\) to \(R = 2.0\) in increments of \(\Delta R = 0.1\). The modeling was carried out in the interval from \(R = 1.30\) to \(R = 1.45\) with step \(\Delta R = 0.01\). The critical temperature of the phase transition on the surface of the system and in the bulk of the system was determined for each value of \(R\). Phase diagram of the system shown in figure 2.
Figure 2. Phase diagram of the system.
The temperature of bulk phase transition $T_n$ dependence on relations of exchange integrals $R$ shown as a solid graph. The temperature of surface phase transition $T_s$ dependence on $R$ shown as a dotted graph.

One can see from the phase diagram, the presence of the surface-disordered bulk-ordered phase (SD/BO) was observed in the system. The possible existence of this condition was experimentally detected for $Fe_3BO_6$ [11, 12] and $FeBO_3$ [13]. Surface energy lower than bulk energy is a criterion for the persistence of this phase.

Also it is worth noting that tetracritical point is present on the phase diagram of antiferromagnets that observed at $R = 1.38$, in contrast to the theoretical predictions, and similar results for the ferromagnetic systems.

The distribution of magnetization in the layers close to the surface is significantly different on the left and right of tetracritical point. Figure 3 shows the magnetization dependence on the layer number with the Neel temperature $T_n = 4.51$ at $R = 1.00$ for the system with linear size $L = 32$. It is seen from the figure the magnetization increases deep into the sample.
Figure 3. The dependence of the magnetization on the distance to the free surface \( d \) at \( R = 1.00 \).

Figure 4 shows the magnetization dependence on the layer number with the Neel temperature \( T_n = 4.51 \) at \( R = 1.50 \) for the system with linear size \( L = 32 \).

Figure 4. The dependence of the magnetization on the distance to the free surface \( d \) at \( R = 1.50 \).

Figure 5 shows the magnetization dependence on the layer number with the Neel temperature \( T_n = 4.51 \) at \( R = 1.38 \) for the system with linear size \( L = 32 \).
Figure 5. The dependence of the magnetization on the distance to the free surface $d$ at $R = 1.38$.

From the comparison of the last three figures it is evident that the character of distribution of magnetization changes with distance from the surface of the system when passing through tetracritical point.

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