

Concentration of magnetic transitions in dilute magnetic materials

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Abstract. In this paper the two-sublattice crystalline ferromagnet in the approximation of the Ising model was investigated. In each sub-lattice density of magnetic atoms can vary from 0 to 1. The exchange interactions within each sublattice and between the spins of different sublattices are considered as given. The case of direct exchange was investigated and the conditions for the occurrence of ferromagnetism, antiferromagnetism and ferrimagnetism, depending on the concentration of magnetic atoms in each sublattice were established.

1. Introduction

A large number of magnetic materials both in our country and abroad are currently known, but the experimental and theoretical researches continue in this area, as this problem is quite urgent. The theory of phase transitions has been an active field of research for many decades already. Despite several remarkable achievements on both the conceptual and the applied sides, there still remain open questions galore. As a contribution to the conceptual side, a recent and promising proposal is the random interaction field method to phase transitions [1], connecting the partition function of random fields with the law of interaction and providing an opportunity to evaluate not only the Curie point but also the critical concentration of "ferromagnetic" atoms necessary for the appearance of ferromagnetism.

2. Model of the two-sublattice magnet

If there are two sub-lattices, in accordance with the results of [1], we write the partition function of the random field at an atom of the first sublattice as follows:

$$W(H_1) = \frac{1}{\sqrt{\pi B_1}} \exp \left[\frac{-\{H_1 - M_1 H_{011} - M_2 H_{012}\}^2}{B_1^2} \right], \quad (1)$$

where

$$B_1^2 = 2p_1(1 - M_1^2 p_1) \left(\sum_k \phi_{11k}^2 + \sum_l \phi_{12l}^2 \right),$$

$$H_{011} = p_1 \sum_k \phi_{11k}, H_{012} = p_2 \sum_l \phi_{12l},$$



$$\alpha_1 - \beta_1 = M_1, \alpha_2 - \beta_2 = M_2,$$

index k numbers the atoms of the first type, l numbers the atoms of the second type, φ_k is the exchange "field" created by the atom with the number k on the selected atom placed at the origin, α is the relative number of particles oriented "up", β is the relative number of particles oriented "down" p is the concentration of ferromagnetic particles. Respectively

$$W(H_2) = \frac{1}{\sqrt{\pi}B_2} \exp \left[-\frac{\{H_2 - M_2 H_{022} - M_1 H_{021}\}^2}{B_2^2} \right], \quad (2)$$

where

$$B_2^2 = 2p_2 \left(1 - M_2^2 p_2 \right) \left(\sum_l \varphi_{22l}^2 + \sum_k \varphi_{21k}^2 \right),$$

$$H_{022} = p_2 \sum_l \varphi_{22l}, H_{021} = p_1 \sum_k \varphi_{21k}.$$

In the simplest case $\varphi_{11}, \varphi_{12}, \varphi_{21}, \varphi_{22}$ are constants, $\varphi_{12} = \varphi_{21}$ and summation should be carried out over nearest neighbors. Substantial simplification of the equation can be achieved by replacing the partition function of the rectangle function [1]. Then

$$M_1 = \frac{1}{2B_1} \int_{-B_1}^{B_1} \text{th} \left[\frac{m_1}{kT} (H_1 + M_1 H_{011} + M_2 H_{012}) \right] dH_1, \quad (3)$$

$$M_2 = \frac{1}{2B_2} \int_{-B_2}^{B_2} \text{th} \left[\frac{m_2}{kT} (H_2 + M_2 H_{022} + M_1 H_{021}) \right] dH_2. \quad (4)$$

We introduce the notation: $\frac{m_1}{kT} H_1 = x_1, \frac{m_1}{kT} H_{011} = h_{011}, \frac{m_1}{kT} H_{012} = h_{012}, \frac{m_1 B_1}{kT} = b_1$. Analogous for m_2 , where m_1 and m_2 are magnetic moments of the particles of the first and second sublattices. Then the expression for the magnetization can be expressed as

$$M_1 = \frac{1}{2b_1} \int_{-b_1}^{b_1} \text{th} \left[(x_1 + M_1 h_{011} + M_2 h_{012}) \right] dx_1. \quad (5)$$

At high temperatures

$$M_1 = \frac{\text{th} b_1}{b_1} (h_{011} M_1 + h_{012} M_2) - \frac{1}{3} \frac{\text{th} b_1}{b_1 \text{ch}^2 b_1} (h_{011} M_1 + h_{012} M_2)^3. \quad (6)$$

Analogous,

$$M_2 = \frac{\text{th} b_2}{b_2} (h_{022} M_2 + h_{021} M_1) - \frac{1}{3} \frac{\text{th} b_2}{b_2 \text{ch}^2 b_2} (h_{022} M_2 + h_{021} M_1)^3. \quad (7)$$

The conditions under which different types of magnetic ordering are observed, can be determined by solving the system of equations (6, 7) for any values $h_{011}, h_{012}, h_{022}, h_{021}$. In general, the solution is rather complicated, but it is possible to consider some simple options.

If $h_{022} = 0$ then

$$M_2 \approx \frac{\text{th} b_2}{b_2} h_{021} M_1. \quad (8)$$

According to (8) and (6)

$$M_1^2 = \frac{\frac{\text{th}b_1}{b_1} \left(h_{011} + h_{012} \frac{\text{th}b_2}{b_2} h_{021} \right) - 1}{\frac{1}{3} \frac{\text{th}b_1}{b_1 \text{ch}^2 b_1} \left(h_{011} + h_{012} \frac{\text{th}b_2}{b_2} h_{021} \right)^3}. \quad (9)$$

Thus, the condition of a non-zero magnetisation M_1 :

$$\frac{\text{th}b_1}{b_1} \left(h_{011} + h_{012} \frac{\text{th}b_2}{b_2} h_{021} \right) > 1. \quad (10)$$

In the case of a direct exchange at $T \rightarrow 0$ the values $\text{th}b_1$ and $\text{th}b_2$ cannot be greater than one, so from the definition of H_{011} , H_{012} , B_1 and B_2 , the condition of appearance of the concentration of the phase transition can be determined as:

$$\frac{p_1 z_1}{\sqrt{2p_1 z_1}} + \frac{p_1 z_1 p_2 z_2}{\sqrt{2p_1 z_1} \sqrt{2p_2 z_2}} > 1. \quad (11)$$

If $H_{011} = 0$, then this relation simplifies

$$\frac{p_1 z_1 p_2 z_2}{\sqrt{2p_1 z_1} \sqrt{2p_2 z_2}} > 1. \quad (12)$$

And finally, in the case of equivalent sublattices $p_1 = p_2, z_1 = z_2$ and condition for the occurrence of antiferromagnetic ordering is determined as:

$$p > \frac{2}{z}. \quad (13)$$

At $h_{012} = 0$ two separate sublattices are considered for each of which there is a different transition condition. Fulfillment of conditions (10) and (12) is substantially depends on the concentration of "ferromagnetic" atoms in sublattices so there are critical concentrations of such atoms below which ones ordering cannot occur.

The above-mentioned fundamental relationships determine the possibility of a corresponding ordering. To determine the Curie point T_c , use the relation (10):

$$\frac{\text{th} \left[\frac{m_1 \sqrt{2p_1 z_1}}{kT_c} \right]}{\frac{m_1 \sqrt{2p_1 z_1}}{kT_c}} \left(\frac{m_1}{kT_c} p_1 z_1 + \frac{m_1}{kT_c} p_2 z_2 - \frac{\text{th} \left[\frac{m_2 \sqrt{2p_2 z_2}}{kT_c} \right]}{\frac{m_2 \sqrt{2p_2 z_2}}{kT_c}} \frac{m_2}{kT_c} p_1 z_1 \right) > 1. \quad (14)$$

3. Monte Carlo simulations of two-sublattice magnets

In model of two-sublattice ultrathin magnetic film with competing ferromagnetic-antiferromagnetic direct exchange interactions was obtained spin-glass properties. It was shown that the Ising model on a 2D lattice with $z = 8$ nearest neighbors takes place divergence between the ZFC and FC magnetization curves, Fig. 1. A weak antiferromagnetic interaction between ferromagnetically ordered sublattices and approximately the same values of the magnetic moments in the sites could lead to very complex magnetic properties. Theoretical magnetic phase diagram for the plain structures with random dilution was built.

Technological features of multicomponent compounds containing ferromagnetic atoms make them attractive for a wide variety of modern electronic devices, such as materials for storage devices. Therefore, in recent years, these materials are the subject of intense experimental and theoretical research [2].

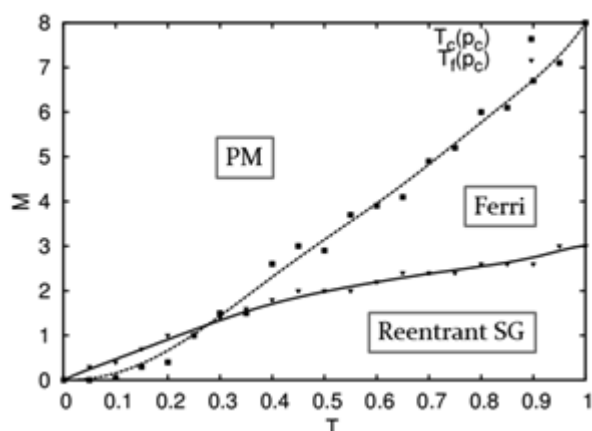


Figure 1: Temperature dependence of the average FC and ZFC magnetization, the external magnetic field $H=0.4$, $p_c=0.9$.

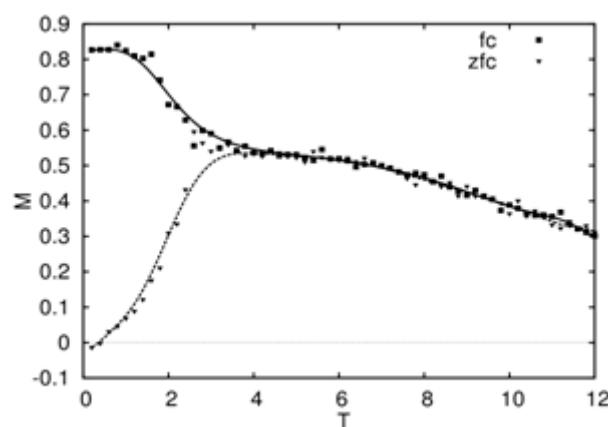


Figure 2: Theoretical magnetic phase diagram for a two-sublattice magnet

The presence of the divergence between the ZFC and FC magnetization curves are usually associated with the appearance of the spin-glass phase. If to use point of divergence between the ZFC and FC curves - T_f and the temperature of occurrence of the ferromagnetic ordering in the sublattices - T_c , it is possible to construct a theoretical magnetic phase diagram of a two-sublattice 2D Ising magnet for a given exchange integrals: $J_{AA} = 1$, $J_{BB} = 2$, $J_{AB} = -0.5$, Fig. 2. The presence of divergence in ZFC and FC temperature dependence could be caused by the ordering in the sublattices, accompanied by compensation of magnetization and an increase in frustrations in the system as a whole.

The weak antiferromagnetic direct interaction between ferromagnetically ordered sublattices was shown to complex behavior of the average magnetization of the system of spins.

Was calculated the theoretical magnetic phase diagram for the two-sublattice magnet.

4. Conclusions

Thus, the random interaction field method is a tool for the study of phase transitions and critical phenomena. It allows exploring the complex model systems, the study of which by other methods is facing great difficulties. A specific example is a two-sublattice magnetic material, which is composed of both magnetic and non-magnetic atoms are considered the results of the study of the critical properties, determined the critical concentration of "ferromagnetic" of atoms necessary for the existence of ferro-, ferri-and antiferromagnetism.

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References

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