THE MAGNETIC ORDERING IN DILUTED CRYSTAL MAGNETS
WITH INDIRECT EXCHANGE INTERACTION

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Abstract

The closed system of equations for a determination of parameters distribution
function for random interaction fields was calculated analytically. The estimations
of critical concentrations for phase transitions in diluted crystal magnets with face
centered cubic (fcc), volume centered cubic (vcc) and simple cubic (sc) lattices with
interaction of Ruderman-Kittel-Kasuya-Yosida between spins were made.

Magnetic properties of disordered systems are investigated for a long time. In this
direction great number of works were made, there are large number of books [1-5] and
reviewed publications [6,7]. The most of approaches to theoretical investigation of mag-
netism of disordered matter use a assumption about random distribution of exchange
integrals in Hamiltonian of spin-spin interaction, at that a parameters of distribution
function must have agreement with experimental data. We have formulated in [8,9] se-
veral different approach, which one help to calculate a distribution function of random
fields of exchange interaction for amorphus magnets. A parameters of such function are
in agree with each other and are calculated with using of law of exchange interaction (or magnetic moments of particles, clusters, grains etc.). In this article the proposed approach was extend for investigation of magnetic properties of crystal materials.

1. DENSITY OF FIELD DISTRIBUTION

In [8] the density of distribution of random field exchange interaction have been calculated for amorphous ferromagnetic material. In this case the probability of the hit of particle in element with volume \( dV \) can be determinate as \( \frac{dV}{V} \), and density of distribution of particles over magnetic moment \( S \)

\[
\tau(S)dS = \frac{1}{2\pi S^2 \sin^2 \vartheta} \delta(S - S_0)[\alpha \delta(\vartheta) + \beta \delta(\vartheta - \pi)]dS \tag{1}
\]

For crystal lattices difference is in that the density of distribution of interacting particles, which ones have same magnetic moment \( S_0 \), over \( S_k \) in the model of Ising is

\[
\tau_k(S_k)dS_k = \frac{1}{2\pi S^2 \sin^2 \vartheta_k}[\alpha_k \delta(\vartheta_k) + \beta_k \delta(\vartheta_k - \pi)] \left[ \frac{N - N_0}{N} \delta(S_k) + \frac{N_0}{N} \delta(S_k - S_0) \right] dS \tag{2}
\]

Here \( \alpha_k \) — a relative number of particles, which ones have orientation in "positive" direction, \( \beta_k \) — "negative", \( \alpha_k + \beta_k = 1 \), \( \delta(\vartheta_k) \) — delta-function of Dirac, \( N \) — number of sizes of crystal lattice, \( N_0 \) — number of interacting particles. The characteristic function in this case is

\[
A(\rho) = \prod_k [1 - p] + p \left[ \alpha \exp \{i\rho \varphi_k(S_0, r_{k,0})\} + \beta \exp \{-i\rho \varphi_k(S_0, r_{k,0})\}] \right] \exp \{i\rho \varphi_k(S_0, r_{k,0})\}, \tag{3}
\]

where \( p = \frac{N_0}{N} \), \( \varphi_k(S_0, r_{k,0}) \) — field, which one was created in origin of coordinates by particle in cite \( r_{k,0} \). If to leave only three terms of expansion of exponent then

\[
\ln A(\rho) \approx i(\alpha - \beta)pp \sum_k \varphi_k - \frac{1}{2!}p \left[ 1 + (\alpha - \beta)^2 p \right] \rho^2 \sum_k \varphi_k \approx
\]
\[ \approx i(\alpha - \beta)p\rho \sum_k \varphi_k - \frac{1}{2!}pp'^2 \sum_k \varphi_k. \]  

(4)

The distribution function for random field exchange interaction \( W(H) \) (it is same as in case of amorphus magnet) is "extended" \( \delta \)-function with view

\[
W(H) = \frac{1}{\sqrt{\pi B}} \exp \left( \frac{[H - H_0(\alpha - \beta)]^2}{B^2} \right),
\]

(5)

\[ H_0 = p \sum_k \varphi_k, \quad B^2 \approx 2p \sum_k \varphi_k^2. \]

Remind that for amorphus magnets

\[ H_0 = n \int_V \varphi dV, \quad B_0^2 \approx 2n \int_V \varphi^2 dV, \]

where \( n \) — volume concentration.

After thermodynamical averaging of characteristics of field "origin" in cite

\[ \overline{\alpha} = \exp \left\{ \frac{S_0H}{kT} \right\}, \quad \overline{\beta} = \exp \left\{ -\frac{S_0H}{kT} \right\}, \]

(6)

\[ |\overline{S}| = S_0 \left| \tanh \left\{ \frac{S_0H}{kT} \right\} \right|, \]

(7)

and after configuration averaging for relative magnetization \( M \) per one cite, for \( < H_0 > \) and \( < B^2 > \) easy to receive a system of selfconsistented equations

\[
\begin{cases}
< M > = \int \tanh \left\{ \frac{S_0H}{kT} \right\} W(H) dH \\
< H_0 > = p \sum_k \varphi_k \int \left| \tanh \left\{ \frac{S_0H}{kT} \right\} \right| W(H) dH \\
< B^2 > = 2p \sum_k \varphi_k^2 \int \tanh^2 \left\{ \frac{S_0H}{kT} \right\} W(H) dH.
\end{cases}
\]

(8)

This system is analog of Sherrington-Kirkpatrick’s system of equations, see for example [10,11]. Here \( B \) — parameter of order (similar to \( q \)), and in case of \( M = 0 \) it describes a spin glass state. The advantage of system (8) is in that the basic parameters of distribution function (\( < H_0 >, < B^2 > \)) are connected with each other and depend of law of interaction.
of particles. Here and future for $<H_0>$ and $<B^2>$ we shall have left out a sign of averaging.

The system (8) can be essentially simplified, if to make a substitute of distribution function

$$W(x) = \frac{1}{\sqrt{\pi B}} \exp \left\{ -\frac{x^2}{B^2} \right\}$$

(9)

by rectangular

$$\tilde{W}(x) = \begin{cases} 0, & -B > x, \quad B < x \\ \frac{1}{2B}, & -B \leq x \leq B. \end{cases}$$

(10)

There are example of numerical solving of equation for $M$ with exact and approximated functions [9]. Near of points of phase transition (small $M$ and $B$) error in calculations is negligible. The available estimations of critical density $p_c$ are addition argument in favour of this substitution. $p_c$ corresponds to percolation threshold. It can be received if to consider of system (8) for case of direct exchange.

So, from equation

$$M = \frac{1}{2B} \int_{-B}^{B} \tanh \left\{ \frac{S_0 (H + H_0)}{kT} \right\} \, dH$$

(11)

it follows that a Curie point can be determined from relation

$$\frac{H_0}{B} \tanh \left\{ \frac{S_0 B}{kT} \right\} = 1.$$  

(12)

It is obviously that condition $\frac{H_0}{B} = 1$ defines a maximal concentration $p_c$, below of which a ordering does not exist even at $T = 0$. For direct exchange $\varphi_k = f_0$, and summation must goes over nearest neighbors.

$$\gamma = \frac{H_0}{B_0} = \frac{p_c f_0}{\sqrt{2p_c z f_0}} = 1,$$  

(13)

where $z$ — number of nearest neighbors.

The critical concentrations $p_c$, calculated by help of formula (13), have good agreement with knowing results in theory of percolation [12-15].
2. RKKY Interaction

For RKKY interaction the "strength of exchange field" is

$$\varphi = AF(x),$$  \hspace{1cm} (14)

where \( x = 2k_F R, k_F \) — impulse of free electron on Fermi surface,

$$F(x) = \frac{x \cos x - \sin x}{x^4},$$  \hspace{1cm} (15)

and \( A \) has dimension of magnetic field and defines of intensity of exchange interaction.

Since for "standard" metal \( k_F^3 = 3\pi^2 n_s \), where \( n_s \) — concentration of free electrons, Fermi-impulse is comparable with parameter of lattice \( (k_F \sim a) \). The results of summation in formulas for \( H_0 \) and \( B^2 \) can have significant dependence from mutual disposition of interacting atoms, i.e. from type of crystal lattice. It is known that distance between atoms for different lattices can be calculated as

1) SC

$$R_{n_1,n_2,n_3} = a \sqrt{n_1^2 + n_2^2 + n_3^2},$$  \hspace{1cm} (16)

2) FCC

$$R_{n_1,n_2,n_3} = \frac{a}{2} \sqrt{(n_1 + n_2)^2 + (n_1 + n_3)^2 + (n_2 + n_3)^2},$$  \hspace{1cm} (17)

2) VCC

$$R_{n_1,n_2,n_3} = \frac{a}{2} \sqrt{(n_1 + n_2 - n_3)^2 + (n_1 + n_3 - n_2)^2 + (n_2 + n_3 - n_1)^2},$$  \hspace{1cm} (18)

where \( n_1, n_2 \) and \( n_3 \) — whole numbers. The number of atoms, which ones have same distances, equals to number of integer roots of equations (16-18).

The parameters of distribution function \( H_0 \) and \( B^2 \) for crystal magnetic alloys, which ones have given type of lattice, can be calculated by summation:

$$H_0 = pA \sum_{n_1,n_2,n_3} F(2k_F R_{n_1,n_2,n_3}),$$  \hspace{1cm} (19)
\[ B^2 = 2pA^2 \sum_{n_1, n_2, n_3} F^2(2k_FR_{n_1, n_2, n_3}). \]  

(20)

At the calculation of \( H_0 \) and \( B^2 \) it is necessary to have in view, that concentration of free electrons \( n_s = \frac{4}{a^3} \) for FCC lattice, for VCC \( n_s = \frac{2}{a^3} \) and for SC lattice \( n_s = \frac{1}{a^3} \).

The numerical estimations of parameters of distribution function \( W(H) \), which ones have been made with taking in account a first 20 roots of equations (16-18), when sums (19-20) go to saturation, for FCC, VCC and SC lattice, correspondingly, are:

- **FCC**: \( H_0 = 0.037 pA, \quad B = 0.012 \sqrt{p}A, \quad \frac{H_0}{B} = 3.14 \sqrt{p}; \)

- **VCC**: \( H_0 = 0.032 pA, \quad B = 0.011 \sqrt{p}A, \quad \frac{H_0}{B} = 2.83 \sqrt{p}; \)

- **SC**: \( H_0 = 0.011 pA, \quad B = 0.016 \sqrt{p}A, \quad \frac{H_0}{B} = 0.69 \sqrt{p}. \)

From this data it follows that for FCC lattice in case of RKKY exchange in standard metal the ferromagnetic state is possible at \( p > p_c \cong 0.32 \), and the spin glass ordering takes place at \( p < p_c \). For VCC the ferromagnetism is possible only at \( p > p_c \cong 0.35 \). And for SC it is possible only the spin glass state at low temperature and the paramagnetism at high one.

Thus, the method of random field exchange interaction allows to make a estimations of critical concentrations of phase transitions in diluted magnets in dependence of crystal structure and of type of exchange interaction.

This work was made at financial support of Ministry of Education and Science of Russian Federation, and at mutual grant of Ministry of Education and Science of Russian Federation and DAAD, program M. Lomonosov (ref: 325-A/05/05416).

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