Random-field method in the Ising model of a diluted ferromagnet

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The concentration dependence of the Curie temperature $T_c(p)$ and spontaneous magnetization $M(T,p)$ of a diluted crystalline ferromagnet and an amorphous ferromagnet are investigated by averaging over the interaction fields in the framework of the Ising model. It is shown that the function $T_c(p)$ is nonzero in the interval $[p_c, 1]$ $(p_c > 0)$, and the asymptotic behavior of this function at $p \sim p_c$ and $p \sim 1$ is found.

To estimate the spontaneous magnetization and Curie point of a ferromagnet with a random distribution of magnetic atoms over the sites of a crystal lattice (or for amorphous ferromagnets with a random distribution over the volume V of the sample) one can make use of an approach proposed by Chandrasekhar[1] that has been used successfully in the study of the magnetic properties of systems of interacting particles[2–4]—namely, one can calculate the distribution function of the random field H of the exchange interaction from the formula

$$W(H)\,dH = \int \delta\Big[H - \sum_{k=1}^{N} h_k(\mathbf{m}_k, \mathbf{r}_k)\Big] \prod_k \Phi_k(\mathbf{m}_k, \mathbf{r}_k) \times d\mathbf{m}_k\, d\mathbf{r}_k\, dH, \tag{1}$$

where h_k is the exchange-interaction field created at the coordinate origin by atoms that are situated at the points $\mathbf{r}_k$ and possess spin magnetic moments $\mathbf{m}_k$,

$$\delta\Big[H - \sum_k h(\mathbf{m}_k, \mathbf{r}_k)\Big] dH$$

is the probability of finding the field to lie in the interval $(H, H + dH)$ for a given spatial and spin distribution of the atoms, and $\Pi_k \Phi_k d\mathbf{m}_k d\mathbf{r}_k$ is the probability that this distribution is realized. This function can then be used to estimate the mean value of the magnetic moment per atom, and also the Curie point.

In Eq. (1) the choice of the distribution function in the form of a product $\Pi_k \Phi_k d\mathbf{m}_k d\mathbf{r}_k$ presupposes that the orientation of the vector $\mathbf{m}_k$ is independent of the position and orientation of the magnetic moments of the other atoms. In this approximation,

$$\Phi_k = f_k(\mathbf{r}_k)\,\tau_k(\mathbf{m}_k), \tag{2}$$

where $f_k(\mathbf{r}_k) = \delta(\mathbf{r}_k - \mathbf{r}_{k,0})$ if the atoms are positioned at definite sites (e.g., crystal-lattice sites), or $f_k(\mathbf{r}_k) = 1/V$ for amorphous ferromagnets, and

$$\tau_k(\mathbf{m}_k) = \Big[\frac{N-N_0}{N}\delta(m_k) + \frac{N_0}{N}\delta(m_k - m)\Big] \times [\alpha_k \delta(\gamma_k) + \beta_k \delta(\gamma_k - \pi)]\, d\gamma_k \tag{3}$$

for a crystalline ferromagnet and

$$\tau_k(\mathbf{m}_k) = \delta(m_k - m_0)\,[\alpha_k \delta(\gamma_k) + \beta_k \delta(\gamma_k - \pi)]\, d\gamma_k \tag{4}$$

for an amorphous magnet. Here, N_0 is the number of ferromagnetic atoms, N is the number of crystal-lattice sites, m_0 is the magnetic moment of an atom, γ_k is the angle determining the orientation of the vector $\mathbf{m}_k$ with respect to the chosen axis, and α_k and β_k are the probabilities of finding the magnetic moment oriented at an angle $\gamma_k = 0$ or $\gamma_k = \pi$. The next approximation consists in replacing α_k and β_k in Eqs. (3) and (4) by their average values $\bar{\alpha}$ and $\bar{\beta}$, which are given by the relations

$$\bar{\alpha} = \int \frac{\exp(m_0 H/KT)}{2\,\mathrm{ch}(m_0 H/KT)} W(H)\, dH, \qquad \bar{\beta} = 1 - \bar{\alpha}. \tag{5}$$

We note that if we had defined

$$\bar{\alpha} = \frac{\exp(m_0 \bar{H}/KT)}{2\,\mathrm{ch}(m_0 \bar{H})/KT)},$$

where $\bar{H} = \int H W(H)\, dH$, we would have obtained the equations of the molecular-field method. As will become clear below, the method of averaging proposed here makes it possible to give a more exact description of the behavior of a diluted ferromagnet.

1. CRYSTALLINE DILUTED FERROMAGNETS

The characteristic function $A(\rho) = \int W(H) \times \exp(i\rho H)\, dH$ for a crystalline ferromagnet has the form

$$A(\rho) = \prod_k \int (1-p)\exp[i\rho h_k(0, \mathbf{r}_{k,0})] + p\exp[i\rho h_k(\mathbf{m}_0, \mathbf{r}_{k,0})] \times [\bar{\alpha}(\gamma_k) + \bar{\beta}(\gamma_k - \pi)]\, d\gamma_k,$$

where $p = N_0/N$ is the concentration of magnetic atoms. We shall confine ourselves to the case of nearest-neighbor interaction, when $h_k = m_0 J \cos\gamma_k$. Then

$$A(\rho) = [(1-p) + p(\bar{\alpha}\exp(i\rho m_0 J) + \bar{\beta}\exp(-i\rho m_0 J))]^{z}.$$

Here, J is the exchange integral and Z is the number of nearest neighbors. Hence,

$$W(H) = \sum_{k=0}^{z} \sum_{l=0}^{k} C_z^k p^k (1-p)^{z-k} C_k^l \bar{\alpha}^l (1-\bar{\alpha})^{k-1} \times \delta[H - (2l-k) m_0 J], \tag{6}$$

where C_Z^k and C_k^l are binomial coefficients.

From (5), for the spontaneous magnetization μ per magnetic atom we obtain

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$$\sum_{i=0}^{\left[\frac{Z-1}{2}\right]} \left[\sum_{k=1}^{Z} A_Z^i(t)\, C_Z^k p^k (1-p)^{Z-k}\right] \nu^i = 1, \qquad (7)$$

$$A_k^i(t) = \begin{cases} 0, & i > \left[\dfrac{k-1}{2}\right], \\ \dfrac{1}{2^{k-1}} \displaystyle\sum_{m=0}^{i} (-1)^m \sum_{l=m}^{\frac{k-1}{2}-(i-m)} C_l^m C_k^l C_{k+2l}^{2(i-m)+1} \operatorname{th}\left(\dfrac{k-2l}{t}\right), & i \le \left[\dfrac{k-1}{2}\right], \end{cases}$$

$$t = \frac{KT}{m_0^2 J}, \quad \nu = (\bar\alpha - \bar\beta)^2 = \mu^2.$$

Equation (7) has a nonzero solution only for $Z \geqslant 3$. For a fixed concentration p this solution is non-negative in the interval of T from zero to $T_c(p)$. For $T > T_c(p)$ we have $\mu = 0$. The equation for $T_c(p)$ has the form

$$\sum_{k=1}^{Z} A_k^0(T_c) C_Z^k p^k (1-p)^{Z-k} = 1.$$

This function is equal to zero for $0 \leqslant p \leqslant p_c$, and, for $p > p_c$, increases monotonically to a value $T_c(1)$ equal to the Curie temperature of the undiluted magnet. For $p \sim p_c$,

$$T_c(p) \sim -\frac{2Jm_0^2}{k \ln(p-p_c)}, \qquad (8)$$

while for $p \sim 1$,

$$\frac{T_c(p)}{T_c(1)} - p = -\lambda(Z)\bar p + O(\bar p^2), \qquad (9)$$

$$\bar p = 1-p, \quad \lambda(Z) \approx \frac{Z - {}^1/_3}{Z^2 - Z + {}^2/_3}.$$

The quantity p_c depends only on the coordination number and is determined from the equation

$$\sum_{m=1}^{Z} C_Z^m d(m) p_c^m (1-p_c)^{Z-m} = 1, \qquad (10)$$

$$d(m) = \begin{cases} \displaystyle\prod_{p=1}^{\left[\frac{m-1}{2}\right]} \left(1 + \frac{1}{2p}\right), & m > 2 \\ 1, & m \le 2 \end{cases}.$$

For $Z = 3, 4, 6, 8$, and 12 the values of p_c are 0.56, 0.43, 0.29, 0.22, and 0.15, respectively. It is interesting to compare the quantities $p_c(Z)$ with the values of the site-percolation thresholds p_c^s and bond-percolation thresholds p_c^b for lattices with the corresponding coordination numbers Z. For three-dimensional lattices it is found that the values of $p_c(Z)$ lie between p_c^s and p_c^b, the deviation of $p_c(Z)$ from the arithmetic mean $(p_c^s + p_c^b)/2$ being no more than a few percent. Of couse, the question of the extent to which this coincidence is accidental remains open.

Thus, in the proposed model there exists a concentration phase transition at $p = p_c$. This transition and the dependence of the Curie temperature T_c on the concentration of magnetic atoms in diluted ferromagnets have been investigated by many authors, using various approaches. For example, in Ref. 5 the technique of high-temperature expansions was employed, and in Ref. 6 the concentration dependence of the Curie temperature near the percolation threshold p_c^p was obtained in the framework of scaling theory. The author of Ref. 7 used an approach in which a factor (important for the phase transtion) correponding to the partition function of an amorphous alloy of Ising spins with fluctuating exchange integral and coordination number was separated out from the partition function of an infinite cluster.

In all these papers it was established that the dependence $T_c(p)$ near $p \sim p_c^p$ has the form

$$T_c(p) \sim -\frac{2J}{\ln(p-p_c^p)},$$

i.e., coincides with (8), if p_c^p is replaced by p_c. In addition, it is well known[8] that the spin polarization in the Ising model of a diluted ferromagnet coincides at $T = 0$ with the probability $P(p)$ that a randomly chosen magnetic atom belongs to an infinite cluster of connected sites. The functions $P(p)$ calculated for different lattices[8] have the following common features: $P(p) = 0$ for $p < p_c^p$, $P(p) \sim (p - p_c^p)^\theta$ for $p \geqslant p_c^p (\theta < 1)$, and $P'(p)|_{p=1} = 0$.

In the model that we have proposed, the spin polarization $\mu(T,p)|_{T=0}$ can be obtained from (7):

$$\mu(0,p) = \left[\frac{3p(1-p)^2 + 3p^2(1-p) + {}^3/_2 p^3 - 1}{{}^1/_2 p^3}\right]^{1/2}.$$

The behavior of this function [and also of $\mu(0,p)$ for other values of Z] has all the distinctive features that are characteristic for the probability $P(p)$.

Thus, the distinctive features of the concentration phase transition that occurs in this model are analogous to those of the percolation transition in the Ising model of a diluted ferromagnet.

2. AMORPHOUS FERROMAGNETS

For an amorphous ferromagnet,

$$A(\rho) = \left[\int \exp(i\rho h(\mathbf{m},\mathbf{r}))\,\tau(\mathbf{m}) \frac{dV}{V}\right]^N$$

$$= \left[1 - \frac{1}{V}\int (1 - \exp(i\rho h(\mathbf{m},\mathbf{r}))\,\tau(\mathbf{m})\, d\mathbf{m}\right]^N \exp(-ca),$$

$$a = \int [1 - \exp(i\rho h(\mathbf{m}, r)]\,\tau(\mathbf{m})\, d\mathbf{m}, \qquad c = \frac{N}{V}.$$

Taking $h = m_0 J \cos\gamma$ for $|\mathbf{r}| \leqslant |\mathbf{r}_0|$ and $h = 0$ for $|\mathbf{r}| > |\mathbf{r}_0|$, we obtain

$$a = v_0[1 - \bar\alpha \exp(i\rho m_0 J) - \bar\beta \exp(-i\rho m_0 J)], \quad v_0 = {}^4/_3 \pi r_0^3.$$

Correspondingly,

$$W(H) = \exp(-cv_0) \sum_{k=-\infty}^{\infty} C_k \delta(H - km_0 J),$$

$$C_k = \begin{cases} \displaystyle\sum_{n=k}^{\infty} \frac{\bar\alpha^n \bar\beta^{n-k} (cv_0)^{2n-k}}{n!\,(n-k)!}, & k > 0 \\ \displaystyle\sum_{n=|k|}^{\infty} \frac{\bar\beta^n \bar\alpha^{n-|k|} (cv_0)^{2n-|k|}}{n!\,(n-|k|)!}, & k < 0 \end{cases}$$

$$\mu = \exp(-cv_0) \sum_{n}^{\infty} B_n \operatorname{th}\left(\frac{nm_0J}{KT}\right),$$

$$B_n = \sum_{n=k}^{\infty} \frac{(cv_0)^{2n-k}(\bar{\alpha}\bar{\beta})^{n-k}}{n!\,(n-k)!}(\alpha^n-\beta^n). \qquad (11)$$

From (11) we can obtain an equation describing the dependence of the Curie temperature T_c on the quantity $y = cv_0$:

$$e^{-y} \sum_{n=0}^{\infty} \frac{y^n}{n!} \sum_{l=0}^{\frac{n-1}{2}} \frac{C_n^{\,l}}{2^{n-1}} (n-2l) \operatorname{th}\left(\frac{n-2l}{t}\right) = 1.$$

The quantity $T_c(y) = 0$ for $y \leqslant y_k$ and increases monotonically for $y > y_k$. The value of y_k is determined from the equation

$$e^{-y} \sum_{n=1}^{\infty} \frac{y^n}{n!} d(n) = 1$$

and is found to be equal to $y_k \approx 1.85$ (y_k has the meaining of the limit of the product $p_c Z$ as $Z \to \infty$).

Thus, the method proposed gives a more adequate reflection of the concentration dependence of the Curie temperature and spontaneous magnetization than does the molecular-field method, and can be generalized to the case of magnetic systems more complicated than a simple ferromagnet with nearest-neighbor interaction.

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