Research articles

Oguchi's method and random interaction fields' method: Investigation of properties of ferromagnetic materials

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ABSTRACT

The Curie point of a ferromagnetic material is determined in the framework of the Ising model by Oguchi's method and the random interaction fields' method. The heat capacity of the system is also investigated. The jump in the heat capacity is calculated at the Curie point. Comparison with known results is made.

1. Introduction

A well-known, effective (molecular) fields' method has enabled the qualitative understanding of the properties of ferromagnetic materials in the theory of magnetism, although it is far from perfect quantitatively. This method overestimates the Curie point T_c. A noticeable improvement in this method, allowing for local interactions and correlations of spins, is associated with the use of cluster methods [1–5] or by means the random interaction fields' method [6–10].

In contrast to the molecular field method, in Oguchi's and Bethe-Peierls methods, a cluster consisting of two (Oguchi's method or [z + 1] Bethe-Peierls method) interacting magnetic moments, where z is the number of nearest neighbors, is placed in an effective field. Thus, considering the correlation effectively decreases the exchange integral. In particular, in the framework of the Bethe-Peierls method, the exchange integral decreases approximately in $(z-1)/z$ times [8].

In the Ising model framework, the random interaction fields' method allows us to determine the distribution function, with parameters calculated by the spin interaction law (or the magnetic moments of particles, clusters, and grains). This approach has advantages over traditional ones since it allows us to connect possible phase transitions with the concentration of exchange-interacting atoms (ions) and calculate critical concentrations. Simultaneously applying cluster methods and the random interaction fields' method enables a more accurate calculation of the phase transition conditions.

For example, we consider the association of Oguchi's method and the random interaction fields' method to study the properties of ferromagnetic materials.

2. Random interaction fields' method

In a random distribution of exchange-interacting ions in the crystal lattice, the distribution function of the random fields of the exchange interaction has the form [6]:

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

The atom creating a molecular field H (ferromagnetic atoms) is assumed to have a random coordinate for amorphous magnetic material or a random lattice site. A magnetic moment also has a random interaction. Moments of the distribution function are defined as

$$H_0 = p\sum_n \varphi_n, \tag{2}$$

$$B^2 = 2p[1-(\alpha-\beta)^2 p]\sum_n \varphi_n^2, \tag{3}$$

where φ_n describes the law of interaction among particles, α is the relative probability of the spin being up, β is the relative probability of the spin being down, and p is the concentration of the magnetic particles. The mean magnetization is defined as

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$$\langle M \rangle = \int \tanh \left[\frac{mH}{KT} \right] W(H) dH, \tag{4}$$

where $\langle M \rangle = \bar{\alpha} - \bar{\beta}$. Here $\langle ... \rangle$ denotes thermodynamic and configurational averaging, $\bar{..}$ denotes thermodynamic averaging, m is the magnetic moment per ion, k is the Boltzmann constant, and T is the temperature. The angle brackets will be omitted.

After integrating the expression, the magnetization can be determined as

$$M = \frac{1}{2B} \int_{-B}^{B} \tanh \left[\frac{m(H_0 M + H)}{kT} \right] dH. \tag{5}$$

Small M magnetization can be represented in the form

$$M^2 = \frac{3 \left(\frac{H_0}{B} \tanh \left[\frac{mB}{kT} \right] - 1 \right)}{\frac{m^2 H_0^3}{Bk^2 T^2} \left(\tanh \left[\frac{mB}{kT} \right] - \tanh^3 \left[\frac{mB}{kT} \right] \right)}, \tag{6}$$

As follows from Eq. (6) a spontaneous magnetic moment can arise only under the condition

$$\frac{H_0}{B} \tanh \left[\frac{mB}{kT} \right] > 1. \tag{7}$$

Accordingly, the Curie point is determined from the equation

$$\frac{H_0}{B} \tanh \left[\frac{mB}{kT_c} \right] = 1. \tag{8}$$

Fields and temperatures are usually measured in energy units $B' = mB$, $H_0' = mH_0$, $T' = kT$. Omitting the primes, we obtain:

$$\frac{H_0}{B} \tanh \left[\frac{B}{T_c} \right] = 1. \tag{9}$$

The theory of the molecular field (TMF) is obtained from the limiting transition $W(H) \to \delta(H - mH_0)$, where $\delta(x)$ is the Dirac delta function. Thus,

$$M = \tanh \left[\frac{M p H_0}{T} \right]. \tag{10}$$

In the direct exchange $\varphi_n = J$, $H_0 = zJ$, J is the exchange integral. At $J = 1$, $T_c = pz$, where z is the number of the nearest neighbors.

Function $W(H)$ can be replaced by "rectangular" function $W(x)$ to simplify the computation:

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

Obviously, $W(x)$ also tends to the Dirac delta function δ at $B \to 0$.

In [6], examples of the numerical solution of the equation for M are given by the exact and approximate functions. Thus, near the phase transition points, where M and B are small, the error in the calculations is negligible. Additional arguments favoring such a possible substitution can be considered as an estimate of the critical density p_c corresponding to the percolation threshold, which is easy to obtain for the direct exchange interaction.

We note immediately that for concentration $p = 1$ and the square lattice in Eq. (8), the Curie point is $T_c = 3.2$, which is closer to the exact solutions than in the conventional TMP. Since $\tanh \left[\frac{B}{T_c} \right] \leqslant 1$, a spontaneous magnetic moment can arise when the condition $\frac{H_0}{B} > 1$ is satisfied. Then for direct exchange, it means (see the definition of H_0 and B^2 under the condition $M \ll 1$):

$$p > p_c = \frac{2}{z}. \tag{11}$$

The values of the critical concentration p_c turned out to be close to the percolation thresholds, so in the direct exchange, naturally, ferromagnetic ordering is possible only when a so-called flowing cluster

appears. Using the critical value $H_0/B = 1$, determining the critical concentrations for other exchange interaction laws is possible, for example, the RKKY.[9].

3. The curie point: Oguchi's method and random interaction fields' method

In Oguchi's method, a pair of exchange-interacting atoms is placed in the effective field H, created by means $(z-1)$ neighbors, the partition function has the form:

$$S = \exp \left[\frac{1 + 2H}{T} \right] + \exp \left[\frac{1 - 2H}{T} \right] + 2 \exp \left[\frac{-1}{T} \right] = 2 \exp \left[\frac{1}{T} \right] \cosh \left[\frac{2H}{T} \right]$$
$$+ 2 \exp \left[\frac{-1}{T} \right], \tag{12}$$

and the magnetic moment is determined as

$$M = \frac{\sinh \left[\frac{2H}{T} \right]}{\cosh \left[\frac{2H}{T} \right] + \exp \left[\frac{-2}{T} \right]}, \tag{13}$$

where $H = (z-1)M$.

The Curie point can be obtained by requiring the derivative of the right-hand side of Eq. (13) to M be equal to one. Thus, $T_c = 3.78$.

Using the random interaction fields' method, the relative magnetic moment can be represented as

$$M = \int \frac{\sinh \left[\frac{2H}{T} \right]}{\cosh \left[\frac{2H}{T} \right] + \exp \left[\frac{-2}{T} \right]} W(H) dH, \tag{14}$$

where $W(H) = \frac{1}{\sqrt{\pi} B} e^{-\frac{(H - MH_0)^2}{B^2}}$, $B = \sqrt{2(z-1)}$.

Replacing $W(H)$ by the "rectangular" function [6] and passing to the new coordinates $H = H + MH_0$, we obtain

$$M = \frac{1}{2B} \int_{-B}^{B} \frac{\sinh \left[\frac{2(H + MH_0)}{T} \right]}{\cosh \left[\frac{2(H + H_0)}{T} \right] + \exp \left[-\frac{2}{T} \right]} dH. \tag{15}$$

Considering Eq. (15) near T_c for small M, we have

$$M^2 = \frac{\left(\frac{H_0}{B} \frac{\sinh \left[\frac{2B}{T} \right]}{\cosh \left[\frac{2B}{T} \right] + \exp \left[-\frac{2}{T} \right]} - 1 \right) \left(\cosh \left[\frac{2B}{T} \right] + \exp \left[-\frac{2}{T} \right] \right)^3}{\frac{2}{3} \frac{H_0}{B} \left(\frac{H_0}{T} \right)^2 \sinh \left[\frac{2B}{T} \right] \left(2 + \cosh \left[\frac{2B}{T} \right] \exp \left[-\frac{2}{T} \right] - \exp \left[-\frac{4}{T} \right] \right)}. \tag{16}$$

The Curie point is found from the equation

$$\frac{H_0}{B} \frac{\sinh \left[\frac{2B}{T} \right]}{\cosh \left[\frac{2B}{T} \right] + \exp \left[-\frac{2}{T} \right]} = 1. \tag{17}$$

At $z = 4$, the Curie point is $T_c = 2.75$. If we do not use the approximations adopted above and determine the distribution function as the exact binomial function for $z = 4$ (in our case, $z - 1 = 3$)

$$W(H) = \sum_{k=0}^{3} C_k^3 \frac{(1 + M)^k (1 - M)^{(3-k)}}{2^3} \delta \left(H - \left(2k - 3 \right) \right), \tag{18}$$

where C is the binomial coefficient, then the Curie point is determined from Equation:

$$M = \sum_{k=0}^{3} C_k^3 \frac{(1 + M)^k (1 - M)^{(3-k)}}{2^3} \frac{\sinh \left[\frac{2(2k-3)}{T} \right]}{\cosh \left[\frac{2(2k-3)}{T} \right] + \exp \left[-\frac{2}{T} \right]}, \tag{19}$$

whose solution is $T_c = 2.74$. The use of the binomial function, even for such a small value as $z = 3$, does not give a noticeable improvement in the result

This result provides a more accurate value of the Curie temperature than in the Bethe-Peierls method, wherein the Curie point is

$T_c = 2.89$. The exact Curie temperature obtained by Onsager is $Tc = 2.28$.

4. Heat capacity: Oguchi's method and random interaction fields' method

In the theory of random interaction fields, the mean value of the square of the magnetic moment is defined as

$$\langle M^2 \rangle = \frac{1}{2B} \int_{-B}^{B} \tanh^2 \left[\frac{H + MH_0}{T} \right] dH$$
$$= 1 - \frac{T}{2B} \left(\tanh \left[\frac{B}{T} + \frac{MH_0}{T} \right] + \tanh \left[\frac{B}{T} - \frac{MH_0}{T} \right] \right). \quad (20)$$

If $T > T_c$ then $M = 0$; if $T < T_c$ then $M \neq 0$; and near the Curie point T_c the magnitude of M is determined from Eq. (6).

Because of the expansion in a series of a value $\tanh \left[\frac{B}{T} \pm \frac{MH_0}{T} \right]$, we obtain

$$\tanh \left[\frac{B}{T} \pm \frac{MH_0}{T} \right] = \tanh \left[\frac{B}{T} \right] \pm \left(1 - \tanh^2 \left[\frac{B}{T} \right] \right) \frac{MH_0}{T}$$
$$+ \left(-\tanh \left[\frac{B}{T} \right] + \tanh^3 \left[\frac{B}{T} \right] \right) \left(\frac{MH_0}{T} \right)^2. \quad (21)$$

When Eq. (21) is substituted into Eq. (20), the second term drops out during summation. Thus the average value of the square of the magnetic moment is defined as

$$\langle M^2 \rangle = 1 - \frac{T}{2B} \left(2 \tanh \left[\frac{B}{T} \right] + 2 \left(-\tanh \left[\frac{B}{T} \right] + \tanh^3 \left[\frac{B}{T} \right] \right) \left(\frac{MH_0}{T} \right)^2 \right). \quad (22)$$

The energy per atom is $U = -zM^2/2$.

The heat capacity "from the left" of the Curie point has the form:

$$C_1 = \left(\frac{3}{T_c} \frac{1}{\cosh^2 \left[\frac{B}{T_c} \right]} - \left(\frac{1}{T_c} \sec^2 \left[\frac{B}{T_c} \right] - \frac{1}{H_0} \right) \right) \frac{z}{2}. \quad (23)$$

Given that $\tanh^2 \left[\frac{B}{T_c} \right] = 1 - \frac{1}{\cosh^2 \left[\frac{B}{T_c} \right]} = \left(\frac{B}{H_0} \right)^2$ then $\frac{1}{\cosh^2 \left[\frac{B}{T_c} \right]} = 1 - \left(\frac{B}{H_0} \right)^2$.

After this the heat capacity can be defined as:

$$C_1 = \left(\frac{3}{T_c} \left(1 - \left(\frac{B}{H_0} \right)^2 \right) - \left(\frac{1}{T_c} \left(1 - \left(\frac{B}{H_0} \right)^2 \right) - \frac{1}{H_0} \right) \right) \frac{z}{2}. \quad (24)$$

In the direct exchange $B^2 = 2pz$, $H_0^2 = p^2 z^2$ near $T = T_c$. At $p = 1$, $z = 4$, and $T_c = 3.2$, the heat capacity at the Curie point is $C_1 = 1.2$.

The heat capacity "to the right" from the Curie point is determined by the right-hand term of Eq. (24)

$$C_2 = -\left(\frac{1}{T_c} \left(1 - \left(\frac{B}{H_0} \right)^2 \right) - \frac{1}{H_0} \right) \frac{z}{2}. \quad (25)$$

In the direct exchange at the Curie point, the heat capacity is $C_2 = 0.2$.

Thus, at a point $T = T_c$, the heat capacity experiences a jump relatively smaller than in the Bragg-Williams approximation, but a nonzero heat capacity is associated with random fluctuations of the effective field of the exchange interaction.

In Oguchi's method, the thermodynamically averaged internal energy $\overline{U}$ per atom is determined by the formula

$$\overline{U} = \left(\frac{1}{2} - \frac{H \sinh \left[\frac{2H}{T} \right] - \cosh \left[\frac{2H}{T} \right]}{\left(\cosh \left[\frac{2H}{T} \right] + \exp \left[-\frac{2}{T} \right] \right)} \right) \frac{z}{2}. \quad (26)$$

The configuration averaging by the function $W(H)$ allows us to calculate U by the formula

$$U = \frac{z}{4B} \int_{-B}^{B} \left(\frac{1}{2} - \frac{H \sinh \left[\frac{2(H + MH_0)}{T} \right] - \cosh \left[\frac{2(H + MH_0)}{T} \right]}{\left(\cosh \left[\frac{2(H + MH_0)}{T} \right] + \exp \left[-\frac{2}{T} \right] \right)} \right) dH. \quad (27)$$

Determining the heat capacity "from the left" of the Curie point, differentiating the expression for U with respect to temperature, and using Eq. (17) are necessary. At $T = 2.75$, the heat capacity "to the left" of the Curie point is $C_1 = 3.98$. For $M = 0$, the heat capacity "to the right" of the Curie point is $C_2 = 0.24$.? Thus, the heat capacity experiences a stronger jump at $T = T_c$ than in the random interaction field approximation applied to an isolated atom.

5. Conclusion

Preserving the relative simplicity of the molecular field theory, the random interaction fields' method combined with Oguchi's correlations provides a closer estimate of the Curie point and specific heat discontinuity than the Bethe-Peierls and Bragg-Williams methods.

Acknowledgement

Appendix A. Supplementary data

Supplementary data associated with this article can be found, in the online version, at https://doi.org/10.1016/j.jmmm.2018.09.065.

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