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**A SIMPLE APPROXIMATION METHOD
FOR DILUTE ISING SYSTEMS¹**

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ABSTRACT

We describe a simple approximate method to analyze dilute Ising systems. The method takes into consideration the fluctuations of the effective field, and is based on a probability distribution of random variables which correctly accounts for all the single site kinematic relations. It is shown that the simplest approximation gives satisfactory results when compared with other methods.

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1 Introduction

During the last decade, various types of approximations dealing with random Ising systems have appeared that employ an effective field theory to study the magnetic properties of such systems [1-12]. However, the various methods used were usually presented in a complicated way. In this paper, we present a simple method which extends the approximation methods developed in [11-12] to dilute systems. It should be stressed, however, that this method is only valid for systems in which randomness can be described by discrete random variables and the geometry of the lattice can be easily taken into account. It is obvious that the effective field acting on a given spin takes different values depending on the occupation and configuration of the neighbouring spins. In particular, in the diluted system, the effective field is a random variable corresponding to the random arrangement of atoms. Thus it is important to take the fluctuation of the effective field into account. We determine the probability distribution of the effective field from the knowledge about the central spin on which the effective field is acting, and to obtain the self consistent equations.

The density matrix of spins is determined by the probability distribution of the effective field acting on the central spin. On the other hand, the probability distribution of the effective field can be obtained from the probability distribution of the configurations of the neighbouring spins. Thus, if it were possible to connect the neighbouring spins with the central one, we could construct a set of the self consistent equations. We present the simplest example of such a treatment in the case of a diluted spin $\frac{1}{2}$ Ising system and as an application of this idea we compute the critical temperature and the critical concentration of the system.

2 The diluted ferromagnet spin $\frac{1}{2}$ Ising model

We consider the diluted ferromagnet spin $\frac{1}{2}$ Ising model on a hypercubic lattice which is described by the hamiltonian

$$H = -J \sum_{(i,j)} c_i c_j S_i S_j \quad (1)$$

where $J > 0$, c_i is the occupation number which takes the values 0 or 1, S_i denotes the z component of quantum spin \vec{S}_i of magnitude $S = \frac{1}{2}$ at site i , and the summation runs over all pairs of nearest neighbours.

In its simplest form the effective field theory is based on a single site cluster theory in which attention is focused on a cluster comprising just a single selected spin, labelled 0, and the neighbouring spins with which it directly interacts.

To this end the hamiltonian is split into two parts $H = H_0 + H'$, where H_0 is that part

of the hamiltonian containing spin 0 namely:

$$H_0 = -Jc_0S_0 \sum_{j=1}^N c_j S_j \quad (2)$$

For classical systems in which H_0 and H' commute, the starting point of the single site cluster theory is a set of formal identities of the type

$$\langle c_0 S_0 \rangle = \langle \frac{\text{trace}_0 [c_0 S_0 \exp(-\beta H_0)]}{\text{trace}_0 [\exp(-\beta H_0)]} \rangle \quad (3)$$

Evaluation of the trace_0 on the right-hand side of this equation leaves one with a transcendental function whose argument contains operators belonging to spins with which the central spin S_0 interacts. For the system under consideration, in the case when the exchange interactions are between nearest neighbour sites only, one finds (for a fixed spatial configuration of the spins)

$$\langle c_0 S_0 \rangle = \frac{1}{2} c \langle F(\sum_{j=1}^N c_j S_j) \rangle \quad (4)$$

where in particular

$$F(x) = \tanh(\frac{1}{2}\beta Jx) \quad (5)$$

with

$$x = \sum_{j=1}^N c_j S_j \quad (6)$$

The sum in Eq. (6) is over the nearest neighbours of the site 0, N being the nearest neighbour coordination number of the lattice. In a mean field approximation one would simply replace these spin operators by their thermal values. However, it is at this point that a substantial improvement to the theory is made by noting that the spin operators and their occupation numbers have a finite set of base states, so that the average over the function F can be expressed as an average over a finite polynomial of spin operators and their occupation numbers belonging to the neighbouring spins. This procedure can be effected by the combinatorial method and correctly accounts for the single site kinematic relations. Up to this point the theory is exact, but the right-hand side of Eq. (4) will contain multiple spin correlation functions. Usually, at this stage a Zernike type decoupling of the multiple spin correlation functions is made that neglects the correlation between quantities pertaining to different sites.

The above thermal averages were for a fixed spatial configuration. In the next step, when computing the average over configurations, the correlations between different sites will be neglected. This is the approximation we shall adopt here.

3 Probability distribution

We begin with a discussion of a function $F(c_i S_i)$ with $S_i = -\frac{1}{2}, \frac{1}{2}$ and $c_i = 0, 1$ involving the variables of a single spin with its occupation number. Because the spin and its occupation number have a finite set of base states, one can expand the function as follows

$$F(c_i S_i) = a_0 + a_1 c_i + a_2 S_i + a_3 c_i S_i \quad (7)$$

By considering the possible values of c_i and S_i in turn the following equations are then generated

$$F\left(\frac{1}{2}\right) = a_0 + a_1 + \frac{1}{2}a_2 + \frac{1}{2}a_3 \quad (8)$$

$$F\left(-\frac{1}{2}\right) = a_0 + a_1 - \frac{1}{2}a_2 - \frac{1}{2}a_3 \quad (9)$$

$$F(0) = a_0 + \frac{1}{2}a_2 \quad (10)$$

$$F(0) = a_0 - \frac{1}{2}a_2 \quad (11)$$

On substituting the quantities a_i , as extracted from these equations, into Eq. (7) the following result is obtained

$$F(c_i S_i) = (1 - c_i)F(0) + \frac{1}{2}c_i[(1 + 2S_i)F\left(\frac{1}{2}\right) + (1 - 2S_i)F\left(-\frac{1}{2}\right)] \quad (12)$$

It may be noted that in the special case when $F(c_i S_i)$ is just $\exp(ac_i S_i)$ this equation reduces to

$$\exp(ac_i S_i) = 1 - [1 - \cosh\left(\frac{1}{2}a\right)]c_i + 2\sinh\left(\frac{1}{2}a\right)c_i S_i \quad (13)$$

which is the Van der Waerden identity for the dilute spin $\frac{1}{2}$ Ising model. One may therefore regard Eq. (12) as a generalised Van der Waerden identity for a general function $F(c_i S_i)$. If one now takes the thermal and configurational averages on both sides of Eq. (12) the following result is obtained

$$\langle\langle F(c_i S_i) \rangle\rangle = \sum_{c_i=0}^1 \sum_{S_i=-\frac{1}{2}}^{\frac{1}{2}} P(c_i, S_i) F(c_i S_i) \quad (14)$$

where the distribution function $P(c_i, S_i)$ is given by

$$\begin{aligned} P(c_i, S_i) = & \frac{1}{2}(1 - c)\delta(c_i)[\delta(S_i + \frac{1}{2}) + \delta(S_i - \frac{1}{2})] \\ & + \frac{1}{2}\delta(c_i - 1)[(c - 2m)\delta(S_i + \frac{1}{2}) + (c + 2m)\delta(S_i - \frac{1}{2})] \end{aligned} \quad (15)$$

with

$$c = \langle\langle c_i \rangle\rangle \quad (16)$$

and

$$m = \langle\langle c_i S_i \rangle\rangle = \langle\langle S_i \rangle\rangle \quad (17)$$

It is important to stress that Eq. (14) is exact and thus it correctly accounts for the kinematic relations of the spin operators. We now generalise this result to the situation in which the function F contains spin operators pertaining to several sites. In particular, in effective field theories for a dilute spin $\frac{1}{2}$ Ising system one is interested in functions of the type

$$F(x) = F\left(\sum_{j=1}^N c_j S_j\right) \quad (18)$$

Let us introduce Dirac's delta function

$$\begin{aligned} \delta(y - x) &= \delta\left(y - \sum_{j=1}^N c_j S_j\right) \\ &= \int \frac{d\lambda}{2\pi} \exp\left[i\lambda\left(y - \sum_{j=1}^N c_j S_j\right)\right] \\ &= \int \frac{d\lambda}{2\pi} \prod_{j=1}^N \exp(-i\lambda c_j S_j) \exp(i\lambda y) \end{aligned} \quad (19)$$

Therefore Eq. (18) can be written in the form

$$\begin{aligned} F(x) &= \int dy \delta(y - x) F(y) \\ &= \int dy \int \frac{d\lambda}{2\pi} \prod_{j=1}^N \exp(-i\lambda c_j S_j) \exp(i\lambda y) F(y) \end{aligned} \quad (20)$$

In the approximation of a Zernike decoupling of the multiple correlation functions, one has in the place of Eq. (14)

$$\langle\langle F(x) \rangle\rangle = \int dy \int \frac{d\lambda}{2\pi} [\langle\langle \exp(-i\lambda c_j S_j) \rangle\rangle]^N \exp(i\lambda y) F(y) \quad (21)$$

where

$$\begin{aligned} [\langle\langle \exp(-i\lambda c_j S_j) \rangle\rangle]^N &= \left[\sum_{c_j=0}^1 \sum_{S_j=-\frac{1}{2}}^{\frac{1}{2}} P(c_j, S_j) \exp(-i\lambda c_j S_j) \right]^N \\ &= 2^{-N} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} 2^\mu C_\mu^N C_\nu^{N-\mu} (1-c)^\mu (c-2m)^\nu (c+2m)^{N-(\mu+\nu)} \\ &\quad \exp\left(-i\frac{\lambda}{2}[N - (\mu + 2\nu)]\right) \end{aligned} \quad (22)$$

Taking into account the above relation (Eq. (22)) in Eq. (21), we get the following relation

$$\begin{aligned} \langle\langle F(x) \rangle\rangle &= 2^{-N} \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} 2^\mu C_\mu^N C_\nu^{N-\mu} (1-c)^\mu (c-2m)^\nu (c+2m)^{N-(\mu+\nu)} \\ &\quad F\left[\frac{1}{2}(N - (\mu + 2\nu))\right] \end{aligned} \quad (23)$$

The relation Eq. (23) derived above will now be used to investigate the magnetization for the dilute spin $\frac{1}{2}$ Ising model. Using Eq. (23) it follows from Eq. (4), that the magnetization is given by

$$m = 2^{-N+1} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} 2^{\mu} C_{\mu}^N C_{\nu}^{N-\mu} (1-c)^{\mu} (c-2m)^{\nu} (c+2m)^{N-(\mu+\nu)} F\left[\frac{1}{2}(N-(\mu+2\nu))\right] \quad (24)$$

We have thus obtained the self consistent equation Eq. (24) for the magnetization m , that can be solved directly by numerical iteration. No further algebraic manipulation is necessary. This is the advantage of introducing the probability distribution technique. The same equations hold for an arbitrary lattice structure with a coordination number, N , and therefore results for different structures can be obtained without carrying out the detailed algebra encountered when employing other techniques.

4 Critical temperature and critical concentration of the dilute spin $\frac{1}{2}$ Ising system

As an application of the method, we calculate the critical temperature and the critical concentration of this system. The Curie temperature T_c/J is determined as the lowest temperature at which Eq. (24) has a non trivial solution $m \neq 0$. In other words, when Eq. (24) is expanded into power series of m , the coefficient of the linear term of m on the right-hand side is equal to unity at $T/J = T_c/J$. Thus the equation for T_c/J becomes

$$1 = 2^{-N+1} c \sum_{\mu=0}^N \sum_{\nu=0}^{N-\mu} \sum_{j_1=0}^{\nu} \sum_{j_2=0}^{N-(\mu+\nu)} (-1)^{j_1} 2^{\mu+j_1+j_2} C_{\mu}^N C_{\nu}^{N-\mu} C_{j_1}^{\nu} C_{j_2}^{N-(\mu+\nu)} (1-c)^{\mu} c^{N-(\mu+j_1+j_2)} \delta(j_1+j_2-1) F\left[\frac{1}{2}(N-(\mu+2\nu))\right] \quad (25)$$

The critical concentration c_{crit} is the concentration at which the Curie temperature T_c/J becomes zero.

The numerical values of T_c/J and c_{crit} for various lattices are shown in the tables together with those obtained by other methods.

Table 1: The numerical values of T_c/J for various lattices.

	Linear chain N=2	Square lattice N=4	Simple cubic N=6	b.c.c. N=8	f.c.c. N=12
<i>Weiss</i>					
<i>Approximation</i> ^[11]	0.5	1.0	1.5	2.0	3.0
<i>Present</i>	0.0000	0.7724	1.2683	1.7651	2.7611

Table 2: The numerical values of c_{crit} for various lattices.

	Linear chain N=2	Square lattice N=4	Simple cubic N=6	b.c.c. N=8	f.c.c. N=12
<i>C - V</i> ^[11]	-	-	-	0.25	0.17
<i>C - B</i> ^[11]	-	-	-	0.17	0.11
<i>R - M</i> ^[11]	-	0.48	0.28	0.22	0.18
<i>Abe</i> ^[11]	-	-	-	0.21	0.17
<i>Present</i>	0.0000	0.4284	0.2928	0.2224	0.1502

One sees that the various methods give similar values, and it may be concluded that the various approximations are qualitatively equivalent. This method has a favourable point because of the simplicity of the calculation.

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