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Bethe–Peierls Approximation for the Disordered Ising Model

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We study the Ising model for an alloy with an arbitrary number of components. We develop an approximation which reduces to that of Bethe and Peierls when the concentration of one of the components is unity. We investigate within this approximation the dependence of the various thermodynamic quantities, in particular T_c, on the composition of the alloy and the magnetic properties of its constituents. Comparison with the only exact calculation available, that of F. T. Lee *et al.*, for a linear chain, shows extremely satisfactory agreement.

KEY WORDS: Ising model; alloy; disorder; Bethe–Peierls approximation.

1. INTRODUCTION

The role played by the Ising model in the development of our present understanding of phase transitions is well known (see, e.g., Refs. 1). It is one of the simplest models which can be studied in some detail while still containing all the relevant physical ingredients. The purpose of this work is to study the effects of disorder on the Ising model; we will allow different sites to be occupied at random by different kinds of atoms (like an alloy) and investigate how this affects the various thermodynamic quantities, in particular the

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transition temperature T_c. A similar study has already been carried out for the linear chain$^{(2-4)}$; the disadvantage of this, however, is that no phase transition occurs,$^{(5)}$ and so one of the most interesting aspects of the problem is lost.

We define our model and the parameters characterizing disorder in Section 2. The formalism is developed in Section 3, where we also discuss the relation between this work and the Bethe–Peierls approximation for the pure crystal. In Section 4 we derive the various thermodynamic quantities at arbitrary temperature and field, while in Section 5 we study in particular the case of zero field and $T > T_c$. The transition temperature is found as the temperature at which $\chi \equiv (\partial \mathscr{M}/\partial \mathscr{B})_{\mathscr{B}=0}$ diverges. In Section 6 we study in more detail some particular cases, and compare our results with those of Ref. 4. Some final remarks are made in Section 7.

2. DEFINITION OF THE MODEL

We consider the system described by

$$\mathscr{H} = -\sum_{(i,j)} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \tag{1}$$

The symbol (i,j) under the summation sign means that only pairs of nearest neighbors are included. We assume that there are different kinds of atoms $A, B, C,\ldots$ distributed at random on the lattice, with concentrations $c_A, c_B, c_C,\ldots$. The positions of the atoms are "frozen in" forever, and are not affected by temperature. If site i is occupied by an atom of type X ($X = A, B,\ldots$), we set $h_i = \mu_X\mathscr{B}$ ($\mathscr{B}$ is the external field; μ_X is the magnetic moment of species X) and similarly if site i and j are neighbors occupied by an X and a Y atom, we set $J_{ij} = J_{XY}$ in Eq. (1). We assume that σ_i takes only the values ± 1 as in the usual Ising problem. The various species are thus characterized by different magnetic moments and different coupling constants.

To describe the compositional disorder, we introduce an auxiliary random variable X_i for each site, with the probability distribution

$$X_i = \begin{cases} A \text{ with probability } c_A \\ B \text{ with probability } c_B \\ \vdots \end{cases} \tag{2}$$

For simplicity we assume the various X_i uncorrelated, so that the joint probability for several X's factorizes; for example, $\mathrm{Prob}\{X_i = A \text{ and } X_j = B\} = c_A c_B$. A compositional configuration is then specified by the set of variables $\{X_i;\, i = 1, 2,\ldots\} \equiv \mathbf{X}$. The Hamiltonian (1) can now be written in a way which shows explicitly its dependence on configuration

$$\mathscr{H} = \mathscr{H}_{\mathbf{X}} = -\sum_{(i,j)} J(X_i, X_j)\sigma_i\sigma_j - \sum_i h(X_i)\sigma_i \tag{3}$$

A given spin state of the system is specified by the set of numbers $\{\sigma_i\}$, each being either $+1$ or -1. In analogy with the X's, we introduce the notation $\boldsymbol{\sigma} = \{\sigma_i;\, i = 1, 2, 3,\ldots\}$. It should be emphasized, however, that the variables $\mathbf{X}$ and $\boldsymbol{\sigma}$ play quite different roles in the problem: only the σ_i can fluctuate in thermal equilibrium. At temperature T the probability of finding $\mathbf{X}$ and $\boldsymbol{\sigma}$ is equal to the probability of having $\mathbf{X}$ in the first place (determined by the concentrations, independent of temperature), times the probability that a system with Hamiltonian $\mathscr{H}_{\mathbf{X}}$ will be in spin state $\boldsymbol{\sigma}$. From elementary statistical mechanics

$$\operatorname{Prob}\{\mathbf{X}, \boldsymbol{\sigma}\} = \operatorname{Prob}(\mathbf{X}) \frac{\exp[-\beta\mathscr{H}_{\mathbf{X}}(\boldsymbol{\sigma})]}{\operatorname{Tr}_\sigma\{\exp(-\beta\mathscr{H}_{\mathbf{X}})]} \tag{4}$$

At temperature T the thermal energy of the system is

$$U(\beta, \mathscr{B}; \mathrm{X}) = \sum_\sigma \mathscr{H}_{\mathbf{X}} \frac{\exp[-\beta\mathscr{H}_{\mathbf{X}}(\boldsymbol{\sigma})]}{\operatorname{Tr}_\sigma[\exp(-\beta\mathscr{H}_{\mathbf{X}})]} = -\frac{\partial}{\partial\beta} \ln[\operatorname{Tr}_\sigma \exp(-\beta\mathscr{H}_{\mathbf{X}}] \tag{5}$$

Since U is a macroscopic quantity, it should depend on the concentrations $c_A, c_B,\ldots$ but not on the exact positions of the $A, B,\ldots$ atoms. (We assume, of course, that the system is so big that all possible local configurations will occur somewhere in it.) Thus, for almost every $\mathbf{X}$, Eq. (5) must coincide with its average over configurations

$$\begin{aligned} U(\beta, \mathscr{B}; c_A, c_B,\ldots) &= \langle U(\beta, \mathscr{B}; \mathbf{X})\rangle_{\mathbf{X}} \\ &= -\frac{\partial}{\partial\beta}\left\{\sum_{\mathbf{X}} \operatorname{Prob}(\mathbf{X}) \ln[\operatorname{Tr}_\sigma \exp(-\beta\mathscr{H}_{\mathbf{X}})]\right\} \end{aligned} \tag{6}$$

Clearly (6) is the physically relevant quantity, not (5).[2] In any actual experiment only the concentrations, not the exact positions of the atoms of each kind, are known.

A look at (6) suggests that the thermodynamic properties of our alloy can be found by carrying out the following steps: (a) Compute $Z_{\mathbf{X}} = \operatorname{Tr}_\sigma[\exp(-\beta\mathscr{H}_{\mathbf{X}})]$ for each configuration $\mathbf{X}$; (b) average $\ln Z_{\mathbf{X}}$ over configurations to get the mean free energy; and (c) derive all other quantities from $\langle F\rangle$ in the usual way. This is essentially the procedure followed in Ref. 4. We want to propose in the next section an alternative approach, which does not involve the computation of the partition function as an intermediate step.

3. FORMALISM

Consider a pair of nearest-neighbor sites, i, j, and let $P_{ij}^{(2)}(X_i, \sigma_i;\, X_j, \sigma_j)$ be the probability of finding the variables X_i, σ_i, X_j, σ_j when the system is in thermal equilibrium of temperature T. If all these probabilities were known,

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[2] For a clear discussion of the averaging process see Brout.(6)

it would be possible to compute thermodynamic properties, since our Hamiltonian contains only nearest-neighbor interactions. The pair probabilities $P_{ij}^{(2)}$ could in principle be obtained from Eq. (4) by summing out all variables relating to sites other than i, j:

$$P_{ij}^{(2)}(X_i, \sigma_i; X_j, \sigma_j) = \sum_{\substack{X_k, \sigma_k \\ k \neq i; k \neq j}} \mathrm{Prob}\{\mathbf{X}, \boldsymbol{\sigma}\} \tag{7}$$

What we intend to do instead is to write down equations that the $P_{ij}^{(2)}$ must satisfy, in the hope of having enough equations to determine the $P_{ij}^{(2)}$ directly from them, without ever computing the partition functions $Z_{\mathbf{X}}$. To carry out this procedure, we will have to make an approximation, Eq. (14) below, comparable in spirit to the various truncation schemes familiar in the statistical mechanics of dense fluids.

We assume periodic boundary conditions so that the system has no surface and all sites are equivalent.[3] Then $P_{ij}^{(2)}$ will be the same function for all pairs of neighbors i, j and the subindices can be suppressed. It also follows that

$$P^{(2)}(X, \sigma; X', \sigma') = P^{(2)}(X', \sigma'; X, \sigma) \tag{8}$$

Moreover, from the definition of our model we have

$$\sum_{\sigma_i, \sigma_j} P^{(2)}(X_i, \sigma_i; X_i, \sigma_j) = c_{X_i} c_{X_j} \tag{9}$$

because the left-hand side is the probability of finding an X_i and an X_j atom, which is independent of temperature.

In terms of $P^{(2)}$ we can construct single site probabilities

$$P^{(1)}(X, \sigma) \equiv \sum_{X', \sigma'} P^{(2)}(X, \sigma; X', \sigma') \tag{10}$$

as well as the conditional probability that, given a site with X', σ', a neighbor will have X, σ:

$$P^{(c)}(X, \sigma | X', \sigma') \equiv P^{(2)}(X, \sigma; X', \sigma') / P^{(1)}(X', \sigma') \tag{11}$$

Consider now a site (call it 0) and its γ neighbors $1, 2, 3, \ldots, \gamma$ (Fig. 1). The probability of finding simultaneously $X_0, \sigma_0; X_1, \sigma_1; \ldots; X_\gamma, \sigma_\gamma$ is, by definition of conditional probabilities,

$$\begin{aligned} &P^{(\gamma+1)}(X_0, \sigma_0; X_1, \sigma_1; \ldots; X_\gamma, \sigma_\gamma) \\ &\quad = P^{(1)}(X_0, \sigma_0) P^{(c)}(X_1, \sigma_1 | X_0, \sigma_0) \\ &\qquad \times P^{(c)}(X_2, \sigma_2 | X_0, \sigma_0; X_1, \sigma_1) \cdots P^{(c)}(X_\gamma, \sigma_\gamma | X_0, \sigma_0; \ldots; X_{\gamma-1}, \sigma_{\gamma-1}) \end{aligned} \tag{12}$$

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[3] For simplicity we restrict our discussion to ferromagnetic substances from here on. The antiferromagnetic case would require a splitting of our lattice into two sublattices and the separate consideration of two families of $P_{ij}^{(2)}$'s.

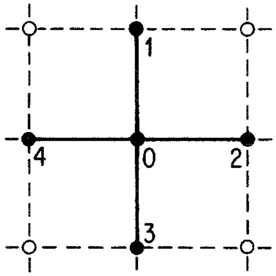

Fig. 1. A site and its γ nearest neighbors (in this case $\gamma = 4$).

It is not true that, for example

$$P^{(c)}(X_2, \sigma_2 | X_0, \sigma_0; X_1, \sigma_1) = P^{(c)}(X_2, \sigma_2 | X_0, \sigma_0) \tag{13}$$

among other reasons because there will be many paths other than $1 \to 0 \to 2$ along which the spin at site 1 can influence the spin at site 2. We will nevertheless assume that (13) and its generalization

$$P^{(c)}(X_i, \sigma_i | X_0, \sigma_0; X_1, \sigma_1; \ldots; X_{i-1}, \sigma_{i-1}) = P^{(c)}(X_i, \sigma_i | X_0, \sigma_0) \tag{14}$$

are approximately valid, in order to get a closed system of equations for the $P^{(2)}$'s. We will show that 14 leads to the well-known Bethe–Peierls approximation when applied to a pure crystal. The procedure to be followed here is therefore a generalization of the Bethe–Peierls approach to the case of a compositionally disordered system.

Let us now write down, assuming (14), the probability that site 0 has $(X_0, \sigma_0) = (A, \uparrow)$ surrounded by n_A sites with $(A, \uparrow)$; m_A sites with $(A, \downarrow)$; n_B sites with $(B, \uparrow)$; etc:

$$\begin{aligned} \text{Prob}\{A, \uparrow, n_A, m_A, n_B, \ldots\} &= \frac{\gamma!}{n_A!\, m_A!\, n_B! \cdots} P^{(1)}(A, \uparrow)[P^{(c)}(A, \uparrow | A, \uparrow)]^{n_A} \\ &\quad \times [P^{(c)}(A, \downarrow | A, \uparrow)]^{m_A}[P^{(c)}(B, \uparrow | A, \uparrow)]^{n_B} \cdots \end{aligned} \tag{15}$$

Suppose now that the central spin is flipped, everything else remaining the same. We have in analogy with (15)

$$\begin{aligned} \text{Prob}\{A, \downarrow, n_A, m_A, n_B, \ldots\} &= \frac{\gamma!}{n_A!\, m_A!\, m_B! \cdots} P^{(1)}(A, \downarrow) \\ &\quad \times [P^{(c)}(A, \uparrow | A, \downarrow)]^{n_A}[P^{(c)}(A, \downarrow | A \downarrow)]^{m_A}[P^{(c)}(B, \uparrow | A, \downarrow)]^{n_B} \cdots \end{aligned} \tag{16}$$

The state of Eq. (16) has the energy of the state Eq. (15) increased by an amount

$$\Delta E = 2\mu_A \mathscr{B} + 2J_{AA}(n_A - m_A) + 2J_{AB}(n_B - m_B) + \cdots \tag{17}$$

It now follows for elementary statistical mechanics that

$$\frac{\text{Prob}\{A,\ \uparrow,\ n_A,\ m_A,\ n_B,\ldots\}}{\text{Prob}\{A,\ \downarrow,\ n_A,\ m_A,\ n_B,\ldots\}} = e^{\beta\Delta E} \tag{18}$$

Combining Eqs. (15)–(18) and using the definition of conditional probability (11), we get

$$\left[\frac{P^{(1)}(A,\ \downarrow)}{P^{(1)}(A,\ \uparrow)}\right]^{\gamma-1} \prod_{Q=A,B,\ldots} \left[\frac{P^{(2)}(Q,\ \uparrow;\ A,\ \uparrow)}{P^{(2)}(Q,\ \uparrow;\ A,\ \downarrow)}\right]^{n_Q} \left[\frac{P^{(2)}(Q,\ \downarrow;\ A,\ \uparrow)}{P^{(2)}(Q,\ \downarrow;\ A,\ \downarrow)}\right]^{m_Q} = \prod_{Q=A,B,\ldots} \exp[2\beta J_{AQ}(n_Q - m_Q) + 2\mu_A\mathscr{B}] \tag{19}$$

Similar equations hold of course with A replaced by B, C, etc., since any of the species could have been called A. The above equation must be satisfied for all acceptable values of the n's and m's [by acceptable we mean that the n's and m's are nonnegative integers and that $\sum(n_Q + m_Q) = \gamma$]. We prove in the appendix that the set of equations (9) and (19) is sufficient to determine all the $P^{(2)}$'s. If new variables ω_Q are defined by

$$e^{4\omega_Q} \equiv P^{(2)}(Q,\ \uparrow;\ Q,\ \uparrow)/P^{(2)}(Q,\ \downarrow;\ Q,\ \downarrow) \tag{20}$$

we also prove there that for any two species X, Y (possibly the same, $X = Y$)

$$P^{(2)}(X,\ \uparrow;\ Y,\ \uparrow) = c_X c_Y[\exp(\omega_X + \omega_Y)]/D_{XY} \tag{21a}$$

$$P^{(2)}(X,\ \uparrow;\ Y,\ \downarrow) = c_X c_Y[\exp(\omega_X - \omega_Y - 2\beta J_{XY})]/D_{XY} \tag{21b}$$

$$P^{(2)}(X,\ \downarrow;\ Y,\ \downarrow) = c_X c_Y[\exp(-\omega_X - \omega_Y)]/D_{XY} \tag{21c}$$

with

$$D_{XY} \equiv 2[\cosh(\omega_X + \omega_Y) + \exp(-2\beta J_{XY})\cosh(\omega_X - \omega_Y)] \tag{22}$$

The ω's in turn are determined by the set of equations

$$\omega_X = \frac{\mu_X\beta}{\gamma} + \frac{\gamma - 1}{2\gamma} \ln \frac{\sum_Q c_Q\{[\exp(\omega_X + \omega_Q) + \exp(\omega_X - \omega_Q - 2\beta J_{XQ})]/D_{XQ}\}}{\sum_Q c_Q\{[\exp(\omega_X - \omega_Q) + \exp(\omega_Q - \omega_X - 2\beta J_{XQ})]/D_{XQ}\}} \tag{23}$$

The knowledge of the $P^{(2)}$'s permits the computation of all thermodynamic properties (this will be shown in the next section) and therefore our problem is completely solved.

4. THERMODYNAMIC PROPERTIES

Neglecting boundary effects, the Hamiltonian can be written as a sum of contributions from bonds:

$$\mathscr{H} = -\sum_{(i,j)} J(X_i, X_j)\sigma_i\sigma_j + \tfrac{1}{2}[h(X_i)\sigma_i + h(X_j)\sigma_j] \tag{24}$$

The mean energy per bond is therefore

$$
\begin{aligned}
U &\equiv \langle \mathscr{H} \rangle / N_{\text{bonds}} \\
&= - \sum_{X, X', \sigma, \sigma'} P^{(2)}(X, \sigma; X', \sigma') \{ J(X, X') \sigma \sigma' + \tfrac{1}{2} [h(X) \sigma + h(X') \sigma'] \} \qquad (25)
\end{aligned}
$$

and after the use of (21) and some algebra we obtain

$$
\begin{aligned}
U = &- \sum_{X,Y} (c_X c_Y / D_{XY}) \\
&\times \{ 2 J_{XY} [\cosh(\omega_X + \omega_Y) - \exp(-2\beta J_{XY}) \cosh(\omega_X - \omega_Y)] \} - \mathscr{B} \mathscr{M} \qquad (26)
\end{aligned}
$$

where $\mathscr{M}$, the mean magnetization *per bond*, is

$$
\begin{aligned}
\mathscr{M} = &\sum_{X,Y} (c_X c_Y / D_{XY}) [(\mu_X + \mu_Y) \sin(\omega_X + \omega_Y) \\
&+ \exp(-2\beta J_{XY}) (\mu_X - \mu_Y) \sinh(\omega_X - \omega_Y)] \qquad (27)
\end{aligned}
$$

Once U and $\mathscr{M}$ are known, all other properties can be obtained from the well-known rules of thermodynamics.

5. ZERO FIELD

The case $\mathscr{B} = 0$ is particularly simple to study. A look at (23) shows that $\omega_Q = 0$, all Q, is always a solution of (23) provided $\mathscr{B} = 0$. This solution corresponds to the absence of spontaneous magnetization [see Eq. (27)]. We also know from general principles that this must be the only solution for large T. Inserting $\omega_Q = 0$ in (26) and (27), we find

$$
U = - \sum_{X,Y} c_X c_Y J_{XY} \tanh(\beta J_{XY}) \qquad (28)
$$

$$
\mathscr{M} = 0 \qquad (29)
$$

and by differentiation of (28) we get the specific heat

$$
C = k \sum_{X,Y} c_X c_Y [\beta J_{XY} / \cosh(\beta J_{XY})]^2 \qquad (30)
$$

These equations hold for $T > T_c$, the transition temperature, which has yet to be found. It is interesting to remark that for $\mathscr{B} = 0$ and a one-dimensional chain they are exact. The reader can verify that (30) reproduces exactly the curves presented as Fig. 1 in Ref. 4.

Returning to the case of arbitrary dimension, we can also calculate the magnetic susceptibility at high T,

$$
\begin{aligned}
\chi \equiv \left. \frac{\partial \mathscr{M}}{\partial \mathscr{B}} \right|_{\mathscr{B} = 0} = &\sum_{X,Y} c_X c_Y \left\{ \mu_X \frac{\partial \omega_X}{\partial \mathscr{B}} + \mu_Y \frac{\partial \omega_Y}{\partial \mathscr{B}} + \tanh(\beta J_{XY}) \right. \\
&\left. \times \left[\mu_X \frac{\partial \omega_Y}{\partial \mathscr{B}} + \mu_Y \frac{\partial \omega_X}{\partial \mathscr{B}} \right] \right\} \qquad (31)
\end{aligned}
$$

This is obtained by differentiation of (27). The derivatives $\partial\omega_Q/\partial\mathscr{B}$ are found from (23); with some rearranging of terms we have

$$\frac{\partial\omega_X}{\partial\mathscr{B}} - (\gamma - 1)\sum_Q c_Q \frac{\partial\omega_Q}{\partial\mathscr{B}} \tanh(\beta J_{XQ}) = \mu_X\mathscr{B} \tag{32}$$

From here we can determine the transition temperature. The derivatives $\partial\omega_Q/\partial\mathscr{B}$, which determine χ, come from solving the linear inhomogeneous system of equations (32) with determinant

$$\mathrm{Det}\|c_Y \tanh(\beta J_{XY}) - [\delta_{XY}/(\gamma - 1)]\| \tag{33}$$

The susceptibility χ therefore diverges when

$$\mathrm{Det}\|c_Y \tanh(\beta J_{XY}) - [\delta_{XY}/(\gamma - 1)]\| = 0 \tag{34}$$

A closer look at the problem reveals that the condition (34) actually determines the critical temperature T_c; our problem is not one of the pathological cases considered, for example, in Stanley's book.(1) The set of equations (23) is of the form

$$f_X(\omega_A, \omega_B, \ldots) = 0 \tag{35}$$

and (34) tells us precisely that

$$\left.\frac{\partial(f_A, f_B, \ldots)}{\partial(\omega_A, \omega_B, \ldots)}\right|_{\omega_Q = 0} = 0 \tag{36}$$

This means that the map $\omega_X' = f_X(\omega_A, \omega_B, \ldots)$ is no longer one-to-one in the

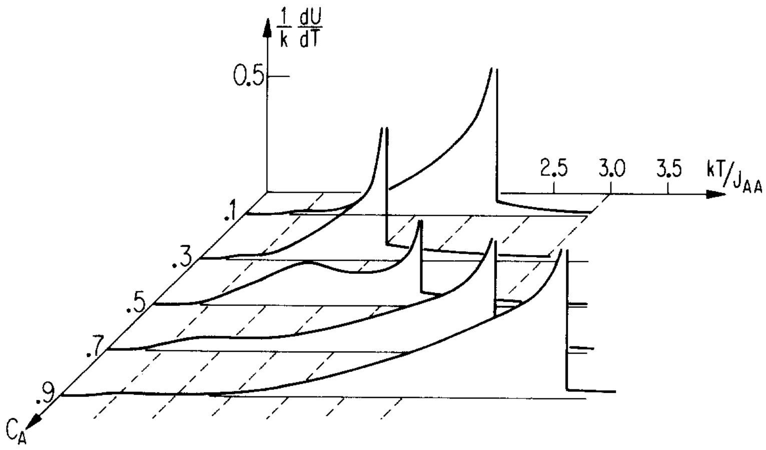

Fig. 2. Specific heat of a binary alloy as a function of temperature for various compositions. The arbitrarily chosen parameters are: coordination number $\gamma = 6$, $J_{AB} = 0.05 J_{AA}$, $J_{BB} = 0.5 J_{AA}$, and zero field. The specific heat does not diverge but becomes quite large at $T = T_c^-$.

neighborhood of the origin when $T = T_c$. As T crosses T_c from above, a second root of (23) appears for $T = T_c$ and moves continuously away from $\omega_Q = 0$. The system exhibits a second-order phase transition in complete analogy with the usual Bethe–Peierls approximation.

We have so far bound analytic expression for the thermodynamic quantities at zero field and $T > T_c$, as well as the condition (34) determining T_c. The cases $\mathscr{B} \neq 0$ and/or $T < T_c$ have to be treated numerically. The system (23) can easily be solved on a computer, and once this is done everything else can be calculated from Eqs. (26) and (27). As an example of the results obtained, we have computed the specific heat of a binary alloy with arbitrarily chosen values $\gamma = 6$, $J_{BB} = 0.5J_{AA}$, $J_{AB} = 0.1J_{AA}$, and $\mathscr{B} = 0$ of the parameters for several concentrations. The results are shown in Fig. 2.

6. SOME PARTICULAR CASES

6.1. One Component

In the absence of disorder, Eq. (34) reduces to

$$(\gamma - 1)\tanh(J/kT_c) = 1 \tag{37}$$

or

$$T_c = \frac{2J}{k\ln[\gamma/(\gamma - 2)]} \tag{38}$$

This is precisely the Bethe–Peierls result (see, e.g., Ref. 7), as we had anticipated in Section 3.

6.2. Dilute Ferromagnet

We consider a binary alloy, but assume that only one component is magnetic. We set $J_{AA} = J$; $J_{AB} = J_{BB} = 0$; $c_A = c$; $c_B = 1 - c$. Equation (34) then becomes

$$\begin{vmatrix} 1 - c(\gamma - 1)\tanh(J/kT_c) & 0 \\ 0 & 1 \end{vmatrix} = 0 \tag{39}$$

or solving for T_c,

$$T_c = \frac{2J}{k\ln\{[c(\gamma - 1) + 1]/[c(\gamma - 1) - 1]\}} \tag{40}$$

This result has been derived by Sato *et al.*,$^{(8)}$ and we recapture it here as a particular case of our formalism. As a function of concentration T_c looks as shown in Fig. 3. Notice that no transition is possible for $c \leqslant c_{\text{crit}} = 1/(\gamma - 1)$.

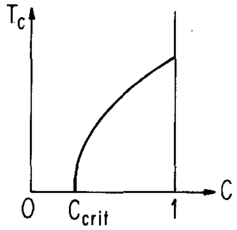

Fig. 3. Transition temperature vs. concentration for a dilute ferromagnet.

It is well known that the Bethe–Peierls approximation amounts to replacing the lattice by a Cayley tree(9); it is therefore not too surprising that c_{crit} coincides with the percolation threshold on this pseudolattice.(10) Of course a necessary condition for a phase transition is that infinite clusters of magnetic atoms should exist; we have shown that, at least within our approximation, this condition is also sufficient.

6.3. General Case

The transition temperature is the solution of

$$\begin{vmatrix} c_A \tanh\left(\frac{J_{AA}}{kT_c}\right) - \frac{1}{\gamma - 1} & c_B \tanh \frac{J_{AB}}{kT_c} & c_C \tanh \frac{J_{AC}}{kT_c} & \cdots \\ c_A \tanh \frac{J_{AB}}{kT_c} & c_B \tanh\left(\frac{J_{BB}}{kT_c}\right) - \frac{1}{\gamma - 1} & \vdots & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{vmatrix} = 0 \quad (41)$$

For given c_A, c_B,... the equation can only be solved numerically for T_c. But if T_c and all except two of the concentrations are considered as independent variables, it becomes trivial to solve for the remaining concentrations. Suppose, for instance, c_C, c_D, etc., as well as T_c are given; setting $c_B = 1 - c_A - c_C - c_D \cdots$ in (41) gives a second-order algebraic equation which can then be solved for c_A. In this way a phase diagram can be constructed. To exemplify this procedure we have done so for the case of a binary alloy, choosing arbitrarily $\gamma = 6$, $J_{BB} = 0.5 J_{AA}$, and various values of J_{AB}. The results are presented in Fig. 4.

6.4. One Dimension

In order to check our approximation, we have recalculated with the present formalism several of the one-dimensional results given in Ref. 4. As already mentioned in the preceding section, our approximation becomes exact for the linear chain in zero field, so only the situation $\mathscr{B} \neq 0$ has yet to be considered, Lee *et al.*(4) give plots of the magnetization $\mathscr{M}$ and a reduced

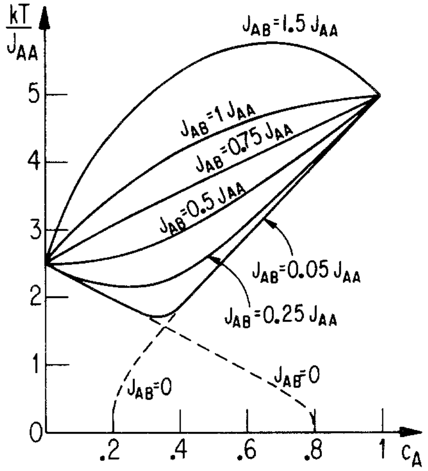

Fig. 4. Transition temperature vs. composition for a binary alloy; the parameters were arbitrarily chosen:

$$\gamma = 6, J_{BB} = 0.5J_{AA}.$$

susceptibility defined as $kT(\partial\mathscr{M}/\partial\mathscr{B})/\mu_A{}^2$ in Figs. 4 and 5 of their paper, choosing $J_{AB} = -0.05J_{AA}$, $J_{BB} = 0$, $\mu_A = \mu_B$, and $\mu_A\mathscr{B}/J_{AA} = 0.1$. We have calculated the same quantities; our results are given in Figs. 5 and 6.

For $kT/J_{AA} > 0.5$ the curves we obtain coincide with theirs almost exactly. If there is any difference, it would not be visible in the figures. For $kT/J_{AA} < 0.5$ there are some discrepancies; in particular the reduced suscep-

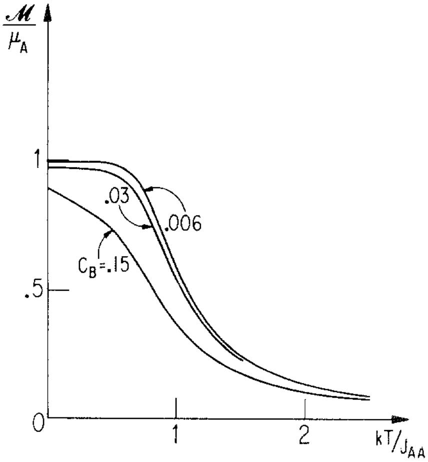

Fig. 5. Magnetization of a linear chain at finite field. Parameters chosen:

$$J_{AB} = -0.05J_{AA}, \quad J_{BB} = 0, \; \mu_A = \mu_B,$$

and

$$\mu_B\mathscr{B} = 0.1J_{AA}.$$

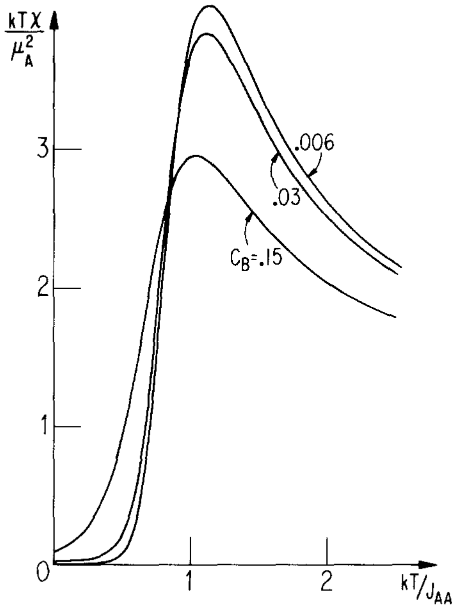

Fig. 6. Reduced susceptibility $kT(\partial\mathcal{M}/\partial\mathcal{B})\ \mu_A^2$ of a linear chain at finite field. Same parameters as in Fig. 5.

tibility remains finite as $T \to 0$ in our data,[4] while it seems to vanish in theirs. We believe that this is due to an error in Ref. 4; probably their Fig. 5 was constructed by extrapolating without due care their finite-temperature curves to $T = 0$. The analytic expressions in Ref. 4 would yield a nonvanishing reduced susceptibility in very good agreement with ours.

7. CONCLUDING REMARKS

We have presented an approximation formalism for the study of a disordered Ising model, the disorder consisting in the presence of several different kinds of atoms randomly distributed on the lattice. The approximation made, Eq. (14), is an extension to the disordered case of the Bethe–Peierls approximation. We would therefore expect our results to have an accuracy comparable to that of the Bethe–Peierls result in the pure crystal problem: poor in two dimensions and low coordination number, fairly good in three dimensions with high coordination number. Critical exponents will of course be

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[4] This finite reduced susceptibility is accidental, due to the particular condition $2J_{AB} + \mu_B\mathcal{B} = 0$ satisfied by the parameters. With this choice the ground state of an isolated B atom in a completely magnetized chain of A's is degenerate: the magnetic energy $\mu_B\mathcal{B}$ and the interaction with neighbors $2J_{AB}$ cancel exactly. As a consequence isolated B's make a Curie contribution $\chi \propto T^{-1}$ to the susceptibility.

given incorrectly, as is always the case with mean field theories.

But where the present work should be most useful is in providing some preliminary insight into the effects of *disorder* on the magnetic properties of a material. One could, for example, have imagined that disorder would smear out or broaden the magnetic phase transition; it is instructive to see that, at least within our approximation, T_c is shifted but the transition remains sharp. The dependence of T_c on concentration obtained here makes good sense (the Gaussian model, for instance, would predict unphysical results on this point), and the case of the dilute ferromagnet also seems to be well described; plain mean field theory would instead predict a transition even for arbitrarily small c. In view of all this, we believe that the present treatment constitutes a reasonable approximation for the problem under consideration.

APPENDIX

We consider Eq. (19),

$$\left[\frac{P^{(1)}(A,\downarrow)}{P^{(1)}(A,\uparrow)}\right]^{\gamma-1}\prod_{Q=A,B,\dots}\left[\frac{P^{(2)}(Q,\uparrow;A,\uparrow)}{P^{(2)}(Q,\uparrow;A,\downarrow)}\right]^{n_Q}\left[\frac{P^{(2)}(Q,\downarrow;A,\uparrow)}{P^{(2)}(Q,\downarrow;A,\downarrow)}\right]^{m_Q}$$
$$= e^{2\mu_A\beta\mathscr{B}}\prod_Q e^{2\beta J_{AQ}(n_Q-m_Q)} \tag{A.1}$$

which must hold for all acceptable values of n_Q and m_Q. Suppose we change n_A into n_A+1 and n_X into n_X-1. In the process the right-hand side of (A.1) gets multiplied by $\exp[2\beta(J_{AA}-J_{AX})]$ while the left-hand side gets multiplied by another factor involving four of the $P^{(2)}$'s. Since we want the equality in (A.1) to hold both before and after the substitution on the n's, it is clear that the two factors must be equal:

$$\frac{P^{(2)}(A,\uparrow;A,\uparrow)\,P^{(2)}(X,\uparrow;A,\downarrow)}{P^{(2)}(A,\uparrow;A,\downarrow)\,P^{(2)}(X,\uparrow;A,\uparrow)} = e^{2\beta(J_{AA}-J_{AX})} \tag{A.2}$$

A similar argument based on the substitution $n_A \to n_A+1$, $m_X \to m_X-1$ yields

$$\frac{P^{(2)}(A,\uparrow;A,\uparrow)\,P^{(2)}(X,\downarrow;A,\downarrow)}{P^{(2)}(A,\uparrow;A,\downarrow)\,P^{(2)}(X,\downarrow;A,\uparrow)} = e^{2\beta(J_{AA}+J_{AX})} \tag{A.3}$$

Let us now define

$$e^{4\omega_Q} \equiv P^{(2)}(Q,\uparrow;Q,\uparrow)/P^{(2)}(Q,\downarrow;Q,\downarrow), \qquad Q = A, B,\dots \tag{A.4}$$

Using (A.3) with $X = A$, and (A.4), we have

$$P^{(2)}(A,\uparrow;A,\downarrow) = e^{-2\omega_A}e^{-2\beta J_{AA}}P(A,\uparrow;A,\uparrow) \tag{A.5}$$

and combining (A.4) and (A.5) with

$$\sum_{\sigma,\sigma'} P^{(2)}(A,\sigma;A,\sigma') = c_A{}^2 \tag{A.6}$$

we finally express all $P^{(2)}(A, \sigma; A, \sigma')$ in terms of ω_A:

$$P^{(2)}(A, \uparrow; A, \uparrow) = c_A{}^2 e^{2\omega_A}/D_{AA} \tag{A.7}$$

$$P^{(2)}(A, \uparrow; A, \downarrow) = c_A{}^2 e^{-2\beta J_{AA}}/D_{AA} \tag{A.8}$$

$$P^{(2)}(A, \downarrow; A, \downarrow) = c_A{}^2 e^{-2\omega_A}/D_{AA} \tag{A.9}$$

with

$$D_{AA} \equiv 2(\cosh 2\omega_A + e^{-2\beta J_{AA}}) \tag{A.10}$$

Our next step will be to eliminate $P^{(2)}(A, \uparrow; A, \uparrow)/P^{(2)}(A, \uparrow; A, \downarrow)$ from (A.2) and (A.3) using (A.7) and (A.8):

$$P^{(2)}(X, \uparrow; A, \downarrow)/P^{(2)}(X, \uparrow; A, \uparrow) = e^{-2\beta J_{AX}} e^{-2\omega_A} \tag{A.2$'$}$$

$$P^{(2)}(X, \downarrow; A, \downarrow)/P^{(2)}(X, \downarrow; A, \uparrow) = e^{2\beta J_{AX}} e^{-2\omega_A} \tag{A.3$'$}$$

Of course similar equations with X and A interchanged must also hold. We can therefore write

$$P^{(2)}(X, \uparrow; A, \downarrow) = e^{-2\beta J_{AX}} e^{-2\omega_A} P^{(2)}(X, \uparrow; A, \uparrow) \tag{A.11}$$

$$P^{(2)}(X, \downarrow; A, \uparrow) = e^{-2\beta J_{AX}} e^{-2\omega_Q} P^{(2)}(X, \uparrow; A, \uparrow) \tag{A.12}$$

$$P^{(2)}(X, \downarrow; A, \downarrow) = e^{-2(\omega_X + \omega_A)} P^{(2)}(X, \uparrow; A, \uparrow) \tag{A.13}$$

Substituting the last three in

$$\sum_{\sigma,\sigma'} P^{(2)}(X, \sigma; A, \sigma') = c_A c_X \tag{A.14}$$

we get

$$P^{(2)}(A, \uparrow; X, \uparrow) = c_A c_X e^{(\omega_A + \omega_X)}/D_{AX} \tag{A.15}$$

$$P^{(2)}(A, \downarrow; X, \uparrow) = c_A c_X e^{-2\beta J_{AX}} e^{\omega_X - \omega_A}/D_{AX} \tag{A.16}$$

$$P^{(2)}(A, \downarrow; X, \downarrow) = c_A c_X e^{-(\omega_A + \omega_X)}/D_{AX} \tag{A.17}$$

$$D_{AX} \equiv 2[\cosh(\omega_A + \omega_X) + e^{-2\beta J_{AX}}(\omega_A - \omega_X)] \tag{A.18}$$

We have succeeded in expressing all $P^{(2)}$'s in terms of the ω's in Eqs. (A.15)–(A.18); in particular our earlier equations (A.7)–(A.9) are obtained from these by putting $X = A$. What we have not determined up to this point are the ω's. Notice that we have only required so far that both sides of (A.1) *change* in the same way when the n's and m's change, but we must still impose that (A.1) is an equality for some particular set $\{n_Q\}$, $\{m_Q\}$. Let us pick, for instance, $n_A = \gamma$; all other n's and m's zero. Then (A.1) reads

$$\left[\frac{P^{(1)}(A, \downarrow)}{P^{(1)}(A, \uparrow)}\right]^{\gamma-1} e^{2\gamma(\beta J_{AA} + \omega_A)} = e^{2\mu_A \beta \mathscr{B}} e^{2\gamma\beta J_{AA}} \tag{A.19}$$

or

$$\omega_A = \frac{\mu_A \beta \mathscr{B}}{\gamma} + \frac{\gamma - 1}{2\gamma} \ln \frac{P^{(1)}(A, \uparrow)}{P^{(1)}(A, \downarrow)} \tag{A.20}$$

Both $P^{(1)}(A, \uparrow)$ and $P^{(1)}(A, \downarrow)$ are defined [Eq. (10)] in terms of $P^{(2)}$, and with the help of (A.15)–(A.17) we write

$$\omega_A = \frac{\mu_A \beta \mathscr{B}}{\gamma} + \frac{\gamma - 1}{2\gamma} \ln \frac{\sum_Q c_Q[(e^{\omega_A + \omega_Q} + e^{-2\beta J_{AQ}} e^{\omega_A - \omega_Q})/D_{AQ}]}{\sum_Q c_Q[(e^{-\omega_A - \omega_Q} + e^{-2\beta J_{AQ}} e^{\omega_Q - \omega_A})/D_{AQ}]} \tag{A.21}$$

as the equations determining the ω's.

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