

Statistical properties of strongly disordered magnets

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The distribution functions of the local magnetization and susceptibility are calculated in the Bethe-Peierls approximation for a number of problems, and in particular for those cases in which the dispersion of these quantities is large compared with their average values.

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1. INTRODUCTION

In this paper we study the distribution functions of the local magnetization and susceptibility of a disordered Ising magnet in the Bethe-Peierls approximation for two models of disorder; many of the results obtained are also valid for a Heisenberg magnet.

In disordered magnets quantities such as the local magnetization m_i and susceptibility χ_i are, after thermodynamic averaging, random functions in the configurational sense, and their values depend on the site coordinate \mathbf{R}_i . In this case quantities such as

$$\begin{aligned} \langle m_i m_j \rangle &= \langle \langle S_i \rangle_T \langle S_j \rangle_T \rangle_{\text{conf}}, \\ \langle m_i \rangle &= \langle S_i \rangle_T, \end{aligned} \quad (1)$$

and, analogously, $\langle \chi_i \chi_j \rangle$, arise. Here S_i is the spin of the i -th site, m_i is the magnetization and χ_i is the susceptibility, equal to $\chi_i = \partial m_i / \partial H$, where H is the magnetic field. By $\langle \dots \rangle_T$ we mean thermodynamic averaging, and by $\langle \dots \rangle_{\text{conf}}$ configurational averaging. Henceforth, when this cannot cause confusion, we shall omit the symbol "conf" (e.g., when we are talking about configurational averages of such quantities as the magnetization and susceptibility).

Inasmuch as m_i and χ_i are random functions, the problem of the study of their statistical properties arises. It is well known from the theory of random functions^[1] that all their properties can be obtained if their probability measure or characteristic functional is known. However, even in the simplest problems it is impossible to calculate these. On the other hand, in most practical problems it is sufficient to know only the distribution functions $f_1(m_i)$, $f_0(\chi_i)$ and $f(q_i)$ of the local magnetizations, susceptibilities and molecular fields, respectively (q_i is the molecular field; its definition is given in Sec. 2).

We shall discuss in what experiments these quantities can be studied. First of all, there are the Mössbauer spectra. Since the nuclear spins precess much more slowly than the electron spins, they feel the magnetization of their own atom and not the instantaneous value of its spin. In the paramagnetic region, $m_i = \chi_i H$. From the Mössbauer spectra, therefore, it is possible to recover the distribution function of the magnetization in the ferromagnetic region and that of the susceptibility in the paramagnetic region. Such experiments already exist.^[2]

In this work we shall study the distribution function $f_0(\chi)$ in the paramagnetic phase and $f(q)$ in the ferromagnetic phase. It will be shown below that $f_1(m)$ can be expressed in terms of $f(q)$. To calculate these functions it is necessary to have some kind of equation. To obtain this we shall make use of a method developed in the Anderson theory of localization.^[3] The equation obtained, like that in Ref. 3, is exact on a Bethe lattice, and it may be hoped that it will give a qualitatively correct description of the phenomenon in the three-dimensional case too. The present article is devoted to the derivation and analysis of this equation.

2. DESCRIPTION OF THE MODELS. DERIVATION OF THE EQUATIONS FOR q_i AND χ_i

We shall consider two models of disordered ferromagnets. In the first model, which we call the lattice model, the magnetic atoms are situated at the sites of a regular lattice; only nearest neighbors interact, and the exchange integrals J between them are distributed in accordance with a probability law $p(J)$, the values of the exchange integrals for different bonds being uncorrelated. In the second model, which we call the continuum model, magnetic atoms of concentration n are distributed randomly in space and interact with each other through a nonrandom exchange integral $J(r)$. By choosing specific $p(J)$ in the first case and $J(r)$ in the second it is possible to obtain different situations frequently encountered in experiment. The following Hamiltonians correspond to the two models:

$$\begin{aligned} H_1 &= - \sum_{ij} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i, \\ H_2 &= - \sum_{\mathbf{R}_i, \mathbf{R}_j} J(|\mathbf{R}_i - \mathbf{R}_j|) \sigma_i \sigma_j - h \sum_i \sigma_i, \end{aligned} \quad (2)$$

where $h = \mu g H$, μ is the magnetic moment, g is the gyromagnetic ratio, and the σ_i are Ising operators. In H_1 the summation is performed over the sites of a regular lattice, J_{ij} being nonzero for nearest neighbors only, and in H_2 the summation is performed over all the random positions of the magnetic atoms in the given configuration.

We now derive the equation connecting the magnetizations m_i at different lattice sites for the lattice problem. The corresponding equation for the continuum problem is obtained analogously. We consider an arbitrary site

i . Let $Z_{i\pm}$ denote the probability that the i -th spin points up or down. We denote by j the z nearest neighbors of the i -th site, and for these too we introduce quantities $Z_{j\pm}$. We retain in (2) only those terms which connect the site i with the sites j . We then obtain

$$Z_{i\sigma_i} = \exp\left\{\frac{\hbar}{T}\sigma_i\right\} \sum_{\sigma_j} \prod_j \exp\left\{\frac{2J_{ij}}{T}\sigma_i\sigma_j\right\} Z_{j\sigma_j}. \quad (3)$$

If we require that $Z_{j\sigma_j}$ coincide with $Z_{i\sigma_i}$, we obtain a self-consistent equation. The procedure described is analogous to the Bethe-Peierls approximation. The factorization of the density matrix of the nearest neighbors of the i -th site is analogous to the decoupling of the averages in the usual molecular-field approximation. Evidently, the approximation used has the same region of applicability as the ordinary molecular-field approximation, but, unlike the latter, permits us to describe strongly disordered systems right up to the percolation threshold. For those cases for which there is a diagram technique that permits corrections to be calculated, e.g., for the percolation problem or for a magnetic glass, it can be shown that when a long-range parameter is present there is a region (coinciding with the region of applicability of the Landau theory for these problems) in which this approximation is justified. Therefore, it is natural to assume that, in the other cases also, the criterion for applicability of this approximation is the presence of a long-range parameter.

We return now to the formula (3). We introduce the following notation:

$$q_i = \frac{1}{2} \ln \frac{Z_{i+}}{Z_{i-}}, \quad m_i = \frac{Z_{i+} - Z_{i-}}{Z_{i+} + Z_{i-}} = \text{th } q_i. \quad (4)$$

Obviously, in (4) m_i is the dimensionless local magnetization and q_i is the dimensionless molecular field at the site i .

From (3) and (4) we obtain equations connecting q_i with q_j and m_i with m_j :

$$q_i = \frac{\hbar}{T} + \frac{1}{2} \sum_{j=1}^z \ln \frac{1 + \alpha_{ij} \text{th } q_j}{1 - \alpha_{ij} \text{th } q_j}, \quad (5)$$

$$m_i = \text{th} \left\{ \frac{\hbar}{T} + \frac{1}{2} \sum_{j=1}^z \ln \frac{1 + \alpha_{ij} m_j}{1 - \alpha_{ij} m_j} \right\}, \quad \alpha_{ij} = \text{th} \frac{2J_{ij}}{T}.$$

The equations for q_i and m_i are completely equivalent, but the equation for q_i is more convenient and this is the one we shall use. These equations have a simple physical meaning. Let the i -th spin interact with z other spins, the magnetization of which is given and equal to m_j . Then, as a result of the interaction with these spins, the i -th spin is also magnetized, its magnetization m_i being determined by the second formula (5). These formulas are exact on a Bethe lattice,^[4] and it may be hoped that they are a good approximation in the real three-dimensional case, where, for an ordered system, they coincide with the results of the Bethe-Peierls approximation for $z \gg 1$ (cf. formula (16.55) in the book by Huang^[5]).

In the paramagnetic region, $m_i = 0$ and it is necessary to consider the equation for the local susceptibility. From (5) we obtain

$$\chi_i = \rho + \sum_{j=1}^z \alpha_{ij} \chi_j, \quad \chi_i = \mu g \frac{\partial m_i}{\partial H}, \quad \rho = \frac{(\mu g)^2}{T}. \quad (6)$$

Equations (5) and (6) are the basic equations for the subsequent analysis. We recall that α_{ij} are random quantities. We shall consider various particular cases of Eqs. (5). If $\alpha_{ij} \ll 1$, from (5) we obtain the stochastic analog of the molecular-field equation:

$$q_i = \frac{\hbar}{T} + \sum_{j=1}^z \alpha_{ij}^{(0)} \text{th } q_j, \quad (7)$$

$$m_i = \text{th} \left\{ \frac{\hbar}{T} + \sum_{j=1}^z \alpha_{ij}^{(0)} m_j \right\}, \quad \alpha_{ij}^{(0)} = \frac{2J_{ij}}{T}.$$

Near the phase-transition point, $q_i \ll 1$ and we obtain from (5) the stochastic discrete analog of the Landau-Ginzburg equation:

$$q_i = \frac{\hbar}{T} + \sum_{j=1}^z \left\{ \alpha_{ij} q_j - \frac{1}{3} (1 - \alpha_{ij}^2) \alpha_{ij} q_j^3 \right\}. \quad (8)$$

For the continuum problem, in place of (5) and (6) we have

$$q_i = \frac{\hbar}{T} + \frac{1}{2} \sum_{j=1}^N \ln \frac{1 + \alpha_{ij} \text{th } q_j}{1 - \alpha_{ij} \text{th } q_j}, \quad \chi_i = \rho + \sum_{j=1}^N \alpha_{ij} \chi_j, \quad (9)$$

$$q_i = q(\mathbf{R}_i), \quad \chi_i = \chi(\mathbf{R}_i), \quad \alpha_{ij} = \text{th} \frac{2J(|\mathbf{R}_i - \mathbf{R}_j|)}{T},$$

where N is the total number of magnetic atoms in the crystal.

3. CALCULATION OF THE CURIE TEMPERATURE AND ANALYSIS OF THE FLUCTUATIONS OF THE SUSCEPTIBILITY

We consider now the dependence of the Curie temperature T_c and of the fluctuations of the susceptibility on the parameters of the system for different cases. To determine T_c we use the linearized Eq. (5) for q_i , for $\hbar = 0$:

$$q_i = \sum_{j=1}^z \alpha_{ij} q_j. \quad (10)$$

We average (10), assuming that q_i is statistically independent of the α_{ij} and, therefore, $\langle \alpha_{ij} q_j \rangle = \langle \alpha_{ij} \rangle \langle q_j \rangle$. This assumption is completely analogous to the approximation made in the derivation of (3), and we shall use it again in deriving the equation for $f(q)$. These two approximations are basic in the present work. Having made this assumption, we obtain from (10) the following equation for T_c :

$$z \langle \alpha \rangle = 1, \quad \langle \alpha \rangle = \int dJ p(J) \text{th} \frac{2J}{T}. \quad (11)$$

For the continuum problem, in place of (10) and (11) we have from (9)

$$q_i = \sum_{j=1}^n \text{th} \frac{2J(|R_i - R_j|)}{T} q_j, \\ n \int dr \text{th} \frac{2J(r)}{T} = 1, \quad n = \frac{N}{v}. \quad (12)$$

The second formula in (12) is obtained if we take into account that in the continuum problem averaging of $\alpha(r)$ means the integration $v^{-1} \int d\alpha(r)$, where v is the volume of the whole system. In certain cases, e.g., for magnetic glasses, the integrals in (11) and (12) are equal to zero, because $p(J)$ is even in J in the first case or because of the alternating sign of $J(r)$ in the second case. Then, obviously, it is necessary to write equations for q_i^2 , and we obtain for both problems

$$q_i^2 = \sum_{j=1}^n \alpha_{ij}^2 q_j^2, \quad z \langle \alpha^2 \rangle = 1, \\ q_i^2 = \sum_{j=1}^n q_j^2 \text{th}^2 \frac{2J(|R_i - R_j|)}{T}, \quad n \int dr \text{th}^2 \frac{2J(r)}{T} = 1. \quad (13)$$

For simple cases all these formulas lead to simple expressions. For the case of pure percolation (for details about percolation see the review^[6]), for which $p(J)$ in the lattice problem and $J(r)$ is the continuum problem have the form

$$p(J) = (1-p)\delta(J) + p\delta(J - J_0), \\ J(r) = \begin{cases} J_0, & r < R \\ 0, & r > R \end{cases} \quad (14)$$

where p is the concentration of bonds, we have, from (11) and (12),

$$pz \text{th} \frac{2J_0}{T} = 1, \quad v \text{th} \frac{2J_0}{T} = 1, \quad v = \frac{4\pi}{3} nR^3. \quad (15)$$

We see that the equation for T_c is the same for both problems, apart from the replacement of pz by v . Below we shall show that for $z \gg 1$ the equations for $f(q)$ also coincide.

For the spin-glass model proposed by Edwards and Anderson^[7] the first of Eqs. (13) coincides with the corresponding equation for T_c obtained by Sherrington and Kirkpatrick^[8] for the Ising problem:

$$p(J) = \frac{1}{(2\pi)^{3/2} J_1} \exp\left(-\frac{J^2}{2J_1^2}\right), \\ \frac{z}{(2\pi)^{3/2}} \int dx \exp\left(-\frac{x^2}{2}\right) \left(\text{th} \frac{2J_1 x}{T}\right)^2 = 1. \quad (16)$$

For comparison with the formulas from Ref. 8 it is necessary to note that it is assumed in Ref. 8 that $z \gg 1$; in this case $T_c \gg J_1$, and $\tanh(2J_1 x/T)$ can be expanded in a series and (16) goes over into the corresponding expression from Ref. 8. In this case, $T_c \sim J_1 z^{1/2}$.

We shall consider now two more-interesting examples, namely, ferromagnetism and a magnetic glass for the continuum problem with $v \ll 1$, i.e., for low density.

We shall consider the former case first. We assume that we have a ferromagnet with $J(r) = V_0 e^{-r/R}$, and that v is defined as before by formula (15). Such a ferromagnet is realized, e.g., in the alloy PdFe (for more detail, see Ref. 9). In this case the Curie temperature can be estimated only by various indirect methods,^[9,10] from which it follows that T_c is determined by the interaction over the mean spacing, i.e., in our case, $T_c \sim V_0 \exp(-v^{-1/3})$. We shall show that this follows directly from our formulas.

From (12) we have

$$1 = n \int dr \text{th} \left(\frac{2V_0}{T_c} e^{-r/R} \right) = 3v \int dt \frac{\ln^2 t}{t} \text{th} \frac{2V_0 t}{T_c}. \quad (17)$$

For $v \ll 1$ the principal contribution to (17) is given by the region $t \geq T/2V_0 \ll 1$, whence we obtain

$$\ln^2 \frac{2V_0}{T_c} = \frac{1}{v}, \quad T_c = 2V_0 \exp(-v^{-1/3}). \quad (18)$$

The region $t \leq T/2V_0$ gives

$$v \ln^2 \frac{2V_0}{T_c} \sim v^{1/3} \ll 1,$$

i.e., the contribution from this region is parametrically small.

We consider now a magnetic glass, in which the magnetic atoms interact via the Rudermann-Kittel potential. At large distances this potential has the form

$$J(r) = J_0 \frac{\cos(2p_0 r)}{(p_0 r)^2}, \quad (19)$$

where p_0 is the Fermi momentum. If $n \ll p_0^3$, the interaction $J(r)$ over the mean spacings $r_c \sim n^{-1/3} \gg p_0^{-1}$ varies in its sign. This leads to the formation of a magnetic glass. Because of the alternating sign of $J(r)$ it is necessary to make use of formula (13), from which we have

$$n \int dr \text{th}^2 \left[\frac{2J_0}{T_c} \frac{\cos(p_0 r)}{(p_0 r)^2} \right] = 1. \quad (20)$$

To estimate the integral we can omit $\cos p_0 r$ in (20); then,

$$T_c \sim 2J_0 \frac{n}{p_0^3} \int \frac{dx}{x^2} \text{th}^2 x. \quad (21)$$

Inasmuch as $J_0 n/p_0^3 \sim J_0/(p_0 r_c)^3$ for $r_c \sim n^{-1/3}$, T_c is again determined by the interaction over the mean spacing.

We note that (21) differs sharply from the results of Sherrington and Kirkpatrick.^[8] In Ref. 8 it is assumed that $z \gg 1$ (or, which is the same, $v \gg 1$) and in this case, as we saw in (16), $T_c \sim z^{1/2} \sim v^{1/2} \sim n^{1/2}$. In our case n/p_0^3 and $T_c \sim v \sim n/p_0^3$ play the role of v .

We consider now the fluctuations of the susceptibility. From (6) and (9), decoupling these equations just as in the calculation of T_c , we have

$$\langle \chi \rangle = \rho \left[1 - z \left\langle \operatorname{th} \frac{2J}{T} \right\rangle \right]^{-1}, \quad \langle \chi^2 \rangle = \langle \chi \rangle^2 \left[1 - z \left\langle \left(\operatorname{th} \frac{2J}{T} \right)^2 \right\rangle \right]^{-1}, \quad (22)$$

$$\langle \chi \rangle = \rho \left[1 - n \int dr \operatorname{th} \frac{2J(r)}{T} \right]^{-1}, \quad \langle \chi^2 \rangle = \langle \chi \rangle^2 \left[1 - n \int dr \left(\operatorname{th} \frac{2J(r)}{T} \right)^2 \right]^{-1}$$

The first two formulas pertain to the lattice problem with $z \gg 1$, and the second two to the continuum problem.

For the case when $p(J)$ and $J(r)$ are determined by formula (14), we obtain

$$\langle \chi \rangle = \rho \left(1 - pz \operatorname{th} \frac{2J_0}{T} \right)^{-1}, \quad \langle \chi^2 \rangle = \langle \chi \rangle^2 \left[1 - pz \operatorname{th}^2 \frac{2J_0}{T} \right]^{-1}, \quad (23)$$

$$\langle \chi \rangle = \rho \left(1 - \nu \operatorname{th} \frac{2J_0}{T} \right)^{-1}, \quad \langle \chi^2 \rangle = \langle \chi \rangle^2 \left[1 - \nu \operatorname{th}^2 \frac{2J_0}{T} \right]^{-1}$$

Since, near T_c ,

$$\left| pz \operatorname{th} \frac{2J_0}{T} - 1 \right| \ll 1,$$

it can be seen from (23) that near the phase-transition curve the fluctuations of the susceptibility are enhanced as the percolation threshold $pz = \nu = 1$ is approached.

We consider now a low-concentration ferromagnet (for which T_c is determined in (18). From (22), in analogy with the derivation of (17), we have

$$\frac{\langle \chi^2 \rangle}{\langle \chi \rangle^2} = \left\{ 1 - 3\nu \int_0^1 \frac{\ln^2 t}{t} \operatorname{th}^2 \frac{2V_0 t}{T} dt \right\}^{-1} \sim \nu^{-2}. \quad (24)$$

The latter equality in (24) is obtained if we assume that we are very close to T_c , i.e., that (17) is fulfilled in our case.

It can be seen from (23) and (24) that in strongly disordered systems the dispersion of the susceptibility is much greater than the average susceptibility. It can be shown that we have the same situation for the magnetization. It is clear that in this case the average value no longer characterizes anything and it is necessary to study the distribution function.

4. EQUATIONS FOR THE DISTRIBUTION FUNCTIONS OF THE SUSCEPTIBILITY AND MOLECULAR FIELDS

We turn now to the derivation of the equations for the distribution functions $f_0(\chi)$ and $f(q)$ of the susceptibility and molecular fields, respectively. For this we use Eqs. (6) and (9). We first consider (6). From (6) we have

$$f_0(\chi_i) = \int \prod_{j=1}^n p(J_{ij}) f_0(\chi_j) dJ_{ij} d\chi_j \delta \left(\chi_i - \rho - \sum_{j=1}^n \alpha_{ij} \chi_j \right). \quad (25)$$

Here we have again used the assumption, already made in the preceding section, that χ_j is statistically independent of the α_{ij} .

Analogously, for $f(q_i)$ we have, for $h=0$,

$$f(q_i) = \int \prod_{j=1}^n p(J_{ij}) f(q_j) dJ_{ij} d q_j \delta \left\{ q_i - \frac{1}{2} \sum_{j=1}^n \ln \frac{1 + \alpha_{ij} \operatorname{th} q_j}{1 - \alpha_{ij} \operatorname{th} q_j} \right\}. \quad (26)$$

If $p(J) = 0$ for $J < 0$, from (25) and (26) it can be seen that $f(q) \equiv 0$ for $q < 0$ and $f_0(\chi) \equiv 0$ for $\chi < 0$. Therefore, in this case it is possible to define the Laplace transform:

$$F(s) = \int_0^\infty dq f(q) e^{-sq}, \quad F_0(s) = \int_0^\infty d\chi f_0(\chi) e^{-s\chi}. \quad (27)$$

From (25)–(27) we obtain the following equations:

$$F_0(s) = e^{-\rho s} \left[\int_0^\infty dJ p(J) F_0 \left(s \operatorname{th} \frac{2J}{T} \right) \right]^n, \quad (28)$$

$$F(s) = \left\{ \int_0^\infty dJ \int_0^\infty dq p(J) f(q) \exp \left[-\frac{s}{2} \ln \frac{1 + \operatorname{th}(2J/T) \operatorname{th} q}{1 - \operatorname{th}(2J/T) \operatorname{th} q} \right] \right\}^n.$$

We now write out (28) for the important particular case when $p(J)$ is determined by the distribution (14):

$$F_0(s) = e^{-\rho s} \Psi[F(\alpha_0 s)], \quad \alpha_0 = \operatorname{th} \frac{2J_0}{T}, \quad (29)$$

$$F(s) = \Psi \left\{ \int_0^\infty dq f(q) \exp \left[-\frac{s}{2} \ln \frac{1 + \alpha_0 \operatorname{th} q}{1 - \alpha_0 \operatorname{th} q} \right] \right\},$$

$$\Psi(x) = (1 - p + px)^n;$$

for $z \rightarrow \infty$ with $pz = \text{const}$,

$$\Psi(x) \rightarrow \Psi_0(x) = \exp[pz(x-1)].$$

In deriving (29) we have taken into account that $F(0) = 1$. In the expression after (29) we have separated the limiting case $z \gg 1$, $pz = \text{const}$.

We shall derive the corresponding formulas for the continuum problem. From (9), in place of (25) we have

$$f_0(\chi) = \frac{1}{v^n} \int \prod_{j=1}^n d\mathbf{r}_j d\chi_j f_0(\chi_j) \delta \left(\chi_i - \rho - \sum_{j=1}^n \chi_j \operatorname{th} \frac{2J(|\mathbf{r}_i - \mathbf{r}_j|)}{T} \right), \quad (30)$$

where v is the volume of the whole crystal. We also have an analogous formula for $f(q_i)$. From (30) it is easy to obtain an equation for $f_0(\chi)$. We shall write out this equation and the corresponding equation for $f(q_i)$:

$$F_0(s) = \exp \left\{ -\rho s + n \int dr \left[F_0 \left(s \operatorname{th} \frac{2J(r)}{T} \right) - 1 \right] \right\}, \quad (31)$$

$$F(s) = \exp \left\{ n \int dr \int_0^\infty dq f(q) \left[\exp \left(-\frac{s}{2} \ln \frac{1 + \operatorname{th}(2J(r)/T) \operatorname{th} q}{1 - \operatorname{th}(2J(r)/T) \operatorname{th} q} \right) - 1 \right] \right\}.$$

If $J(r)$ is determined by the second of the formulas (14), then from (31) we obtain (29) with $\Psi(x)$ replaced by $\Psi_0(x)$ and pz replaced by ν . Hence it can be seen that the continuum percolation problem is equivalent to the lattice problem for $z \gg 1$.

The formulas (28), (29) and (31) are the basic formulas of our theory. Inasmuch as $m = \tanh q$, if we know $f(q)$ it is easy to calculate $f_1(m)$. We also write our formula (29) for $T \approx T_c$, where $q \ll 1$, for which we have

$$F(s) = \Psi \left\{ \int_0^{\infty} dq f(q) \exp \left[-s\alpha_0 q \left(1 - \frac{1}{3} (1 - \alpha_0^2) q^2 \right) \right] \right\}. \quad (32)$$

All the formulas of this section are written for the case that $p(J) = 0$ for $J < 0$. If we do not have this condition, the analogous formulas must be written for the Fourier transform

$$F(k) = \int_{-\infty}^{\infty} dq f(q) e^{-ikq} \quad (33)$$

and analogously for $F_0(k)$; in this case it is necessary to make the replacement $s \rightarrow ik$ in all the formulas.

5. SOLUTION OF THE EQUATIONS IN THE HIGH-DENSITY CASE

We shall consider the solution of the second equation (31) in the case $\nu \gg 1$; we shall not assume that $J(r) > 0$, and in this case we shall use formulas (33). If $\nu \gg 1$ it is easy to show that the concrete form of $J(r)$ is unimportant. On the other hand, it can be seen from (13) that in the main region of integration over r we have $J(r) \ll T$ near T_c . Therefore, we can put

$$\text{th} \frac{2J(r)}{T} \approx \frac{2J(r)}{T} \ll 1$$

and expand the logarithm in $J(r)/T$. We then have the following equation for $F(k)$:

$$F(k) = \exp \left\{ n \int_{-\infty}^{\infty} dr \int dq f(q) \left[\exp \left(-2ik \frac{J(r)}{T} \text{th} q \right) - 1 \right] \right\}. \quad (34)$$

For $\nu \gg 1$ the integral in (34) is evaluated by the method of steepest descents. Expanding the expression in square brackets in (34) in k and calculating $f(q)$, we obtain ($J(r) \equiv J(r/R)$)

$$f(q) = \frac{1}{(2\pi\nu Q)^{\nu} \alpha_2} \exp \left[-\frac{(q - \nu\alpha_0 m_0)^2}{2\nu\alpha_2^2 Q} \right], \quad (35)$$

$$\alpha_0 = \frac{3}{4\pi R^2} \int dx \frac{2J(r)}{T}, \quad \alpha_2 = \frac{3}{4\pi R^2} \int dx \left[\frac{2J(r)}{T} \right]^2,$$

$$m_0 = \int_{-\infty}^{\infty} f(q) \text{th} q dq, \quad Q = \int_{-\infty}^{\infty} f(q) \text{th}^2 q dq.$$

The last two formulas are equations for the parameters Q and m_0 . If we substitute the explicit expression for $f(q)$ into these equations we obtain

$$m_0 = \frac{1}{(2\pi)^{\nu}} \int_{-\infty}^{\infty} dx \exp \left(-\frac{x^2}{2} \right) \text{th} [\nu\alpha_0 m_0 + x\alpha_2 (\nu Q)^{\nu}], \quad (36)$$

$$Q = \frac{1}{(2\pi)^{\nu}} \int_{-\infty}^{\infty} dx \exp \left(-\frac{x^2}{2} \right) \text{th}^2 [\nu\alpha_0 m_0 + x\alpha_2 (\nu Q)^{\nu}].$$

The equations (36) coincide with the corresponding equations in the paper by Sherrington and Kirkpatrick.^[8]

Formulas analogous to (35) and (36) can also be obtained for the case of the lattice problem, from Eqs. (28).

6. SOLUTION OF THE EQUATIONS NEAR THE PERCOLATION THRESHOLD

We now consider Eqs. (29) in detail. These equations correspond to a disordered ferromagnet in which some of the exchange integrals are equal to zero and the other exchange integrals form a fraction p . As can be seen from (15), $p = p_c = z^{-1}$ is the critical concentration. For $p < p_c$ there can be no ferromagnetism at all. This critical value is related to the percolation problem.^[9] As we saw in Sec. 3, as the percolation threshold is approached the fluctuations of the susceptibility, and, consequently, of the magnetization, increase. In this section we shall consider $f(q)$ and $f_0(\chi)$ near the percolation threshold in detail.

We consider first the case $T = 0$. Since $\alpha_0(T = 0) = 1$, from (29) we have

$$F_0(s) = e^{-ps} \Psi[F_0(s)], \quad F(s) = \Psi[F(s)]. \quad (37)$$

We consider the second equation first. It can be seen from the explicit expression for $\Psi(x)$ in (29) that the equation $\Psi(x) = x$ with $pz < 1$ has only the one solution $x = 1$, while for $pz > 1$ a second solution appears, which we shall denote by x_0 (of course, $x_0 < 1$). For $|pz - 1| \ll 1$, to calculate x_0 we can expand $\Psi(x)$ in a series about $x = 1$; we then obtain

$$\Psi(x) - x = (pz - 1)(x - 1) + \frac{1}{2}(pz)^2(x - 1)^2, \quad (38)$$

$$x_0 = 1 - 2(pz - 1)/(pz)^2.$$

It can be shown that for $s \neq 0$ the stable solution of the equation $F = \Psi(F)$ is $F(s) = x_0$. On the other hand, by virtue of the normalization condition, $F(s = 0) = 1$. Hence it is not difficult to obtain $f(q)$, and also $f_1(m)$:

$$f(q) = x_0 \delta(q) + (1 - x_0) \delta(q - q_0) |_{q_0 \rightarrow \infty}, \quad (39)$$

$$f_1(m) = x_0 \delta(m) + (1 - x_0) \delta(m - 1).$$

The expression for $f_1(m)$ has a very simple physical meaning. At zero temperature all the magnetic atoms belonging to the infinite cluster have the maximum possible magnetization, while the magnetic atoms belonging to finite clusters give no contribution to the magnetization. Consequently, $1 - x_0$ defines the "power" of the infinite cluster in our approximation.

We shall show from other considerations that the equation for x_0 determines the power of the infinite cluster in an approximation which we shall call the molecular-field approximation in the percolation problem. Let $p(p)$ be the power of the infinite cluster, and $R = 1 - P$. We shall consider any particular site, surrounded by z nearest neighbors. Then the probability R that our site belongs to a finite cluster is equal to G^z , where G is the probability that, on moving along a given selected bond, we do not go away to infinity. In its turn, $G = 1 - p + pR$, since our bond may, with probability $1 - p$, be broken, and if it is not broken (probability p) the neighboring site should belong to a finite cluster. Hence we immediately obtain for R

$$\Psi(R) = R, \quad R = x_0, \quad P = 1 - R = 1 - x_0. \quad (40)$$

This argument is very similar to the corresponding arguments of the usual molecular-field approximation in the theory of ferromagnetism; this is why we call it the molecular-field approximation in the percolation problem. From (38) and (40) it can be seen that the percolation threshold $p_c = z^{-1}$, and near p_c we have $p(p) \sim p - p_c$, i.e., the index $\beta = 1$. From (22) it can be seen that at $T=0$ the susceptibility $\chi \sim (p_c - p)^{-1}$ and, thus, the index $\gamma = 1$. As is well known (see, e.g., Ref. 11), these indices correspond to the analog of the Landau theory for the percolation problem, and, thus, Eq. (40) does indeed correspond to the molecular-field approximation. From the results of a previous paper^[11] it can be seen that when a long-range parameter is present there is a region of applicability of the Landau theory for the percolation problem. It is precisely for this region that our theory is valid.

We consider now the first of Eqs. (37). We rewrite it in the form

$$F_0(x) = x \Psi[F_0(x)], \quad x = e^{-\rho x}. \quad (41)$$

Equation (41) is a functional equation for $F_0(x)$ and can be solved exactly. Expanding $F_0(x)$ in a series in x , we obtain

$$F_0(x) = \sum_{m=0}^{\infty} q_m x^m, \quad q_m = \frac{1}{2\pi i} \oint \frac{F_0(x)}{x^{m+1}} dx, \quad (42)$$

where the contour integral in (42) goes round the coordinate origin. Making the change of variable $x = F_0[\Psi(F_0)]^{-1}$ in (42) and, for simplicity, using the function $\Psi_0(x)$ from (29) in place of $\Psi(x)$, we obtain after straightforward calculations

$$q_m = e^{-\rho m} \frac{(pz m)^{m-1}}{m!}, \quad (43)$$

$$F_0(s) = \sum_{m=0}^{\infty} q_m e^{-\rho m s}, \quad f_0(\chi) = \sum_{m=0}^{\infty} q_m \delta(\chi - \rho m),$$

$$q_m \xrightarrow{m \gg 1} m^{-3} \exp[-1/2(pz-1)^2 m].$$

The distribution for q_m is called the Borel-Tanner distribution. From (43) it can be seen that the susceptibility takes only integer values (in units of ρ). This should be the case at $T=0$, inasmuch as each finite cluster acts at $T=0$ as a single spin, and q_m gives the distribution over the cluster sizes. We shall calculate $\langle \chi \rangle$ and $\langle \chi^2 \rangle$. For this we make use of the asymptotic form of q_m for $m \gg 1$; we then obtain

$$\langle \chi \rangle \sim \frac{1}{1-pz}, \quad \langle \chi^2 \rangle \sim \frac{1}{(1-pz)^2}. \quad (44)$$

Comparing (23) and (44) we see that (23) goes over into (44) at $T=0$. From (44) it can also be seen that the dispersion of $f_0(\chi)$ is large compared with $\langle \chi \rangle$.

We consider now the case of finite temperatures. Near the curve $T_c(p)$ we can use Eq. (32). We represent the argument of the exponential in (32) in the form

$$-s \{ q/pz + (\alpha_0 - 1/pz) q - 1/3 \alpha_0 (1 - \alpha_0^2) q^2 \}. \quad (45)$$

In (45) all the terms are small except the first; there-

fore, we expand the exponential in (32) in these small terms:

$$F(s) = \Psi \left\{ F \left(\frac{s}{pz} \right) + \int_0^{\infty} dq f(q) \exp \left(-\frac{sq}{pz} \right) \times \left[\left(\alpha_0 - \frac{1}{pz} \right) q - \frac{\alpha_0}{3} (1 - \alpha_0^2) q^2 \right] \right\}. \quad (46)$$

We shall solve (46) in the following way. Let $\Phi_0(s)$ be the solution of the equation

$$\Phi(s) = \Psi[\Phi(s/pz)], \quad (47)$$

for which $\Phi'(0) = -1$. This implies that for the corresponding distribution function $f(q)$ we have $\langle q \rangle = 1$. Thus, in $\Phi_0(s)$ the scale is not fixed. We can fix this scale if we require that the integral in (46) vanish for $s=0$. Thus, we represent $F(s)$ in the form of a sum $\Phi(s) + F_1(s)$, where $\Phi(s)$ is the solution of Eq. (47) with the supplementary condition

$$\int_0^{\infty} dq \varphi(q) \left[\left(\alpha_0 - \frac{1}{pz} \right) q - \frac{\alpha_0}{3} (1 - \alpha_0^2) q^2 \right] = 0, \quad (48)$$

where $\Phi(s)$ is the Laplace transform of $\phi(q)$.

We shall not write out the equation for $F_1(s)$, since it is rather unwieldy. It turns out that $F_1(s) \ll \Phi(s)$ in the parameters $pz - 1$ and $pz\alpha_0 - 1$. We now solve (47). Since we have $|pz - 1| \ll 1$, (47) can be represented in the form

$$(pz-1)s \frac{d\Phi}{ds} = \Psi[\Phi(s)] - \Phi(s). \quad (49)$$

The solution of (49) satisfying the boundary conditions $\Phi(0) = 1$ and $\Phi'(0) = -1$ has the form

$$s = (1 - \Phi) \exp \left\{ \int_1^{\Phi} dx \left[\frac{pz-1}{\Psi(x)-x} + \frac{1}{1-x} \right] \right\}. \quad (50)$$

Since it is clear that $x_0 < \Phi < 1$ we can use the expansion (38) for $\Psi(x)$. We then obtain

$$\Phi_0(s) = x_0 + \frac{(1-x_0)^2}{s+1-x_0}, \quad (51)$$

$$\phi_0(q) = x_0 \delta(q) + (1-x_0)^2 e^{-(1-x_0)q}.$$

In deriving (51) we used the condition $|pz - 1| \ll 1$.

From (48) and (51) we have, finally,

$$\Phi(s) = x_0 + \frac{(1-x_0)^2}{q_0 s + 1 - x_0},$$

$$\phi(q) = x_0 \delta(q) + \frac{(1-x_0)^2}{q_0} \exp \left(-\frac{1-x_0}{q_0} q \right), \quad (52)$$

$$q_0 = \left(\frac{pz\alpha_0 - 1}{pz - 1} \right)^{1/2} (1-x_0),$$

$$\langle q \rangle = q_0 \sim [(pz-1)(pz\alpha_0-1)]^{1/2},$$

$$\langle q^2 \rangle / \langle q \rangle^2 \sim 1/(pz-1).$$

From the formulas (52) it can be seen that the spins (fraction x_0) belonging to finite clusters make no contribution to the magnetization. From (52) we can also see how the index β changes from $\beta = 1$ for pure perco-

lation to $\beta = \frac{1}{2}$ for the disordered ferromagnet. The dispersion of $\phi(q)$ is large compared with q_0 . Thus, $f(q) = \phi(q)$ gives the solution of the problem of the distribution function of the molecular fields near the percolation threshold.

We consider now the equation for the distribution function of the susceptibilities in the paramagnetic region, i.e., the first of Eqs. (29). Near the phase-transition curve and percolation threshold, $|\alpha_0 - 1| \ll 1$ and $|pz - 1| \ll 1$. Below we shall be interested in the region of small s . Taking all this into account we obtain the following equation for $F_0(s)$:

$$as \frac{dQ}{ds} + \frac{1}{2} Q^2 - bQ - \rho s = 0: \quad (53)$$

$$Q = 1 - F_0, \quad a = \frac{1}{\alpha_0} - 1, \quad b = pz - 1, \quad \rho s \ll a^2.$$

Equation (53) is the complete Riccati equation. The solution of this equation, satisfying the necessary asymptotic conditions, has the form

$$Q = b + (2\rho s)^{1/2} I_{-b/a} \left(\frac{2\rho s}{a^2} \right)^{1/2} / I_{-b/a} \left(\frac{2\rho s}{a^2} \right)^{1/2}. \quad (54)$$

Inasmuch as we derived Eq. (53) under the assumption that $\rho s \ll a^2$, we can only use the asymptotic form of (54) for $\rho s \ll a^2$. Then, finally, we have

$$F_0 = 1 - 2a + \frac{4a^2(a-b)}{sp + 2a(a-b)},$$

$$f_0(\chi) = \frac{4}{\rho} a^2(a-b) \exp \left[-\frac{2\chi}{\rho} a(a-b) \right], \quad (55)$$

$$a - b = \frac{1}{\alpha_0} (1 - pz\alpha_0) \approx 1 - pz\alpha_0.$$

In (55) we have written out only the asymptotic form of $f_0(\chi)$ for $\chi \sim [a(a-b)]^{-1}$. The term $1 - 2a$ restoring the normalization of $F_0(s)$ and $f_0(q)$ corresponds to the region $\chi \ll a(a-b)$, which is not of interest to us. We shall assume that we are closer to the phase-transition curve than to the percolation threshold; then, $|a - b| \ll a \sim b \ll 1$ and $sp \sim a(a-b) \ll a^2$, i.e., our assumption that $sp \ll a^2$ is correct. Taking into account that $a - b \ll a \sim b$, we obtain from (55)

$$f(\chi) = \frac{4}{\rho} (pz - 1)^2 (1 - pz\alpha_0) \exp \left\{ -\frac{2}{\rho} \chi (pz - 1) (1 - pz\alpha_0) \right\},$$

$$\langle \chi \rangle = \rho (1 - pz\alpha_0)^{-1}, \quad \langle \chi^2 \rangle = \langle \chi \rangle^2 (pz - 1)^{-1},$$

$$|1 - pz\alpha_0| \ll |pz - 1|. \quad (56)$$

The formula (56) solves the problem of the susceptibility fluctuations. The expressions for $\langle \chi \rangle$ and $\langle \chi^2 \rangle$ coincide with (23) if we assume there that $|1 - pz\alpha_0| \ll |pz - 1|$, as we assumed in the derivation of (56).

7. SOLUTION OF THE EQUATIONS FOR THE LOW-DENSITY CONTINUUM PROBLEM

We consider now the continuum problem with

$$J(r) = V_0 e^{-r/R} \quad (57)$$

with the condition $\nu = 4\pi n R^3/3 \ll 1$. As we have already

said, such a ferromagnet is realized in alloys of the PdFe type. After a change of variables, Eq. (31) for $f(q)$ takes the form

$$F(s) = \exp \left\{ 3\nu \int_0^1 \ln^2 t \frac{dt}{t} \int_0^{\infty} dq f(q) \right. \\ \left. \times \left[\exp \left(-\frac{s}{2} \ln \frac{1 + \text{th } q \text{ th}(2V_0 t/T)}{1 - \text{th } q \text{ th}(2V_0 t/T)} \right) - 1 \right] \right\}. \quad (58)$$

Exactly as in the derivation of (18) from (17), we can show that the principal contribution to the integral in (58) is given by the region $t \geq T/2V_0 \ll 1$, while the region $t \leq T/2V_0$ gives a small contribution $\sim \nu^{1/3} \ll 1$. Therefore, we first take into account the contribution to (58) from the region $t \geq T/2V_0$. In this region, $\tanh(2V_0 t/T) \approx 1$, and we obtain

$$F(s) = \exp \left\{ \nu \left(\ln \frac{2V_0}{T} \right)^2 [F(s) - 1] \right\}. \quad (59)$$

Equation (59) coincides with the second equation (37) for the continuum problem (we recall that for this problem it is necessary to replace $\Psi(x)$ by $\Psi_0(x)$ and pz by ν). In this case the parameter ν in (37) is replaced by $\nu \ln^2(2V_0/T)$. The corresponding equation for $f_0(\chi)$ coincides with the first of Eqs. (37). This means that in the lowest approximation in ν the phase transition with respect to the temperature reduces to an effective percolation problem and, in particular, the critical indices are "percolation indices." This statement has a simple physical meaning. Inasmuch as $\nu \ll 1$ and $T \ll 2V_0$, all the spins situated at distances less than the mean distance are, by virtue of the exponential dependence of $J(r)$, very tightly bound to the infinite cluster, while spins situated at distances greater than the mean distance are not magnetized; the infinite cluster appears at $T = T_c$. Such a picture has been discussed earlier, starting from physical considerations,^[10] but no formulas confirming it had been obtained. We note that from (59) the expression (18) for T_c follows. It is obvious that all the formulas following from (37) are also valid for (59).

We now calculate the next approximation for $F(s)$. For this we take the first of Eqs. (39) as the solution of (59) and substitute it into (58); then, changing from the variable t to r , we obtain

$$F(s) = \exp \left\{ nP \int dr [e^{-2sJ(r)/T} - 1] \right\}, \quad (60)$$

where P is the power of the infinite cluster. This formula is the Holtzmark formula, with concentration nP . The contribution to the integral from the region where $2J(r) \geq T$, i.e., $r \leq R \ln(2V_0/T)$, is equal to $-\nu P \ln^3(2V_0/T)$, and taking this contribution into account gives Eq. (59) exactly, inasmuch as it can be seen from (37) and (40) that $F(s) = 1 - P$. The contribution from the region $r \geq R \ln(2V_0/T)$ is small in the parameter $\nu^{1/3}$ and gives the magnetization, by the infinite cluster, of the spins that are unmagnetized in the zeroth approximation.

If in (60) we change back to the variable t , integrate by parts and take into account that for $s \gg T/2V_0$ we can

replace the upper limit in the integral over t by infinity, we obtain

$$\begin{aligned}
 F(s) &= \exp\left\{\frac{2\nu PV_0 s}{T} \int_0^{\infty} \ln^2 t \exp\left(-\frac{2V_0 t s}{T}\right) dt\right\} \\
 &\approx \exp\left\{\frac{2\nu PV_0 s}{T} \int_0^{\infty} \ln^2 t \exp\left(-\frac{2V_0 t s}{T}\right) dt\right\} \quad (61) \\
 &= \exp\left\{-\nu P \left[\left(C + \ln \frac{2V_0 s}{T}\right)^2 + \frac{\pi^2}{2} \left(C + \ln \frac{2V_0 s}{T}\right) - \Psi''(1) \right] \right\},
 \end{aligned}$$

where C is Euler's constant and $\Psi(z) = d \ln \Gamma(z) / dz$. The formula (61) gives an explicit expression for the distribution function. From (61) it can be seen that if $|\ln s| \ll \ln(2V_0/T) \approx \nu^{-1/3}$, then, in the lowest approximation in $\nu^{1/3}$, we again obtain (59). We can also calculate $f_0(\chi)$ in exactly the same way. In the zeroth approximation we obtain an expression of the type (43). We shall not calculate the corrections.

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Influence of spatial dispersion and of a surface layer on the phase of light reflected from a CdS crystal

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Measurements were made of the change in the phase of light as a result of reflection from a CdS crystal in the region of the A absorption band at $T = 4.2$ and 77°K . The experimental results did not agree with a theory ignoring spatial dispersion but were in satisfactory agreement with a theory allowing for the dispersion subject to boundary conditions giving rise to an exciton-free layer on the surface of the crystal. However, when the reflection spectrum was calculated using the layer thickness and the exciton damping parameter which agreed best with the experimental data on the change in the phase of light at 4.2°K , the results differed from the spectrum determined experimentally at 4.2°K . It was concluded that the boundary conditions should be refined within the framework of the spatial dispersion theory so that the reflection spectrum and the spectrum of the change in the phase would be described by the same set of parameters.

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Pekar^[1] demonstrated theoretically the importance of the spatial dispersion effects in interpreting the low-temperature exciton spectra of crystals. The most convincing argument in support of the need to allow for the spatial dispersion effect in CdS crystals at 4.2°K is the ability to describe the optical properties measured in transmitted and reflected light by a single complex refractive index $n^* = n + i\kappa$, where n is the real refractive index and κ is the absorption coefficient.^[2,3] It should be noted that the spatial dispersion theory makes it possible to find the effective quantities $n^{\text{eff}}(\lambda)$ and $\kappa^{\text{eff}}(\lambda)$ representing the reflection (amplitude and phase) of light from a crystal and, at the same time, find the parameters describing the transmission experiments.^[3]

The spectral dependence of the change in the phase of

the reflected light $\Delta\varphi(\lambda)$ is a characteristic which supplements the reflection coefficient $R(\lambda)$. According to the spatial dispersion theory, the peak-to-peak amplitude of $\Delta\varphi(\lambda)$ should be considerably greater than that predicted by classical crystal optics when use is made of the values $n^{\text{eff}}(\lambda)$ and $\kappa^{\text{eff}}(\lambda)$, deduced from light transmitted by a crystal. However, there have been practically no experimental studies of the reflection of light in the exciton absorption region of crystals, including measurements of $\Delta\varphi(\lambda)$.

Hopfield and Thomas^[4] described the results of their measurements of $R(\lambda)$ by introducing boundary conditions leading to the idea of an exciton-free "dead" layer on the surface of a crystal. It follows from crystal optics that the presence of a dead layer may also affect