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Microscopic scaling theory in the percolation problem

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By means of field-theoretical methods, the critical indices and correlation functions of percolation theory are calculated and the analog of the equation of state is constructed. For $3 < d < 6$ space dimensions the indices are equal to $\gamma = 8/(2+d)$, $\nu = 4/(2+d)$, $\beta = 2(d-2)/(d+2)$ and $\Delta = \beta + \gamma = 2$. This is in agreement with computer calculations, which for $d = 3$ give the following values of the indices: $\beta = 0.35 \pm 0.05$, $\gamma = 1.69 \pm 0.05$, $\nu = 0.9 \pm 0.05$ and $\Delta = 2.2 \pm 0.3$.

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1. INTRODUCTION

It is well known that the problem of percolation very much resembles the problem of second-order phase transitions (cf., e.g., the reviews[1,2]). In percolation theory, the analog of the order parameter is the "power" of an infinite cluster. This analogy was formulated mathematically rigorously by Kasteleyn and Fortuin,[3] who showed that the percolation problem is the limiting case of the so-called S-model for $S \to 1$. A scaling hypothesis for the percolation problem has been formulated using this analogy.[4–6]

On the other hand, the theory of second-order phase transitions can be formulated from a microscopic point of view (cf., e.g.,[7,8]), using field theory. One can use either the ε-expansion method,[7] or renormalization-group theory directly in three-dimensional space.[9,10] It is therefore natural to attempt to construct, using the field theory for the S-model, a microscopic scaling theory for the percolation problem too. The first attempt in this direction was made by Harris *et al.*,[11] who carried out the ε-continuation from six-dimensional space (since the corresponding field theory is logarithmic in six-dimensional space). In[11], however, the Hamiltonian of the S-model was replaced by another model Hamiltonian, introduced by Golner.[12] This replacement is, generally speaking, not justified, and this is obviously why the Fisher parameter η calculated by Harris *et al.*[11] turned out to be negative, which would be completely incomprehensible.

In the present paper we shall consider the bond problem in percolation theory, using the field theory for the S-model directly in the three-dimensional case, analogously to the way in which this was done earlier[9,10] for the theory of second-order phase transitions. We shall calculate the critical indices, correlation functions and analog of the free energy for the percolation problem, as functions of the concentration q of broken bonds and of the fictitious magnetic field x introduced by Kasteleyn and Fortuin.[3] Using three results, we shall then calculate the thermodynamic functions of a disordered Ising ferromagnet as functions of the temperature and the real magnetic field at low temperatures near the percolation threshold.

2. CONNECTION BETWEEN THE *S*-MODEL AND THE PERCOLATION PROBLEM

Since the analogy between the percolation problem and the partition function of the S-model has been formulated in the language of the mathematical theory of linear finite graphs,[3] we shall briefly derive the principal results of this work in the language of statistical physics. The S-model (the Ashkin-Teller-Potts model[13,14]) is a generalization of the Ising model. Suppose that at each site of the lattice there is a certain object which can be in one of S possible states, while the energy of the interaction between sites depends only on whether the objects at neighboring sites are in the same states or in different states. A solid solution of S components with equal concentrations can serve as one of the realizations of this model (just as one realization of the Ising model is a solution with two components). The S-model with $S=2$ corresponds to the Ising model. We shall write the Hamiltonian of the S-model in two physically equivalent forms:

$$H=-J\sum_{i,k}(\delta_{\sigma_i\sigma_k}-1)-2\omega_0\sum_i(\delta_{\sigma_i 1}-1), \tag{1a}$$

$$H=-J_1\sum_{i,k}P_{\sigma_i\sigma_k}-2\omega_1\sum_i P_{\sigma_i 1}, \tag{1b}$$

$$P_{\sigma_1\sigma_2}=S\delta_{\sigma_1\sigma_2}-1.$$

Here J is the exchange integral, $J_1=JS^{-1}$, $\omega_0=\mu H$, H is the magnetic field, μ is the magnetic moment, $\omega_1=\omega_0 S^{-1}$, S is the number of components, and σ_i is the index labeling the components of the S-model.

Formula (1a) is convenient in that the ground-state energy is equal to zero, but it is more convenient to construct the field theory by starting from formula (1b). We shall consider a simple cubic lattice consisting of N sites and $L = 3N$ bonds between the sites. Then from (1a) it is easy to obtain the following expression for the partition function of the S-model:

$$Z=q^L\sum_{\sigma_i}\Big[\prod_L\Big(1+\frac{p}{q}\delta_{\sigma_i\sigma_k}\Big)\prod_N\exp[x(\delta_{\sigma_i1}-1)]\Big], \tag{2}$$
$$x=2\omega_0/T,\quad q=e^{-2J/T},\quad p=1-q.$$

In the expression (2), Π_L denotes a product over all L bonds and Π_N denotes a product over all N lattice sites.

We shall calculate the partition function (2) by expanding it in p/q and summing the resulting expressions over all possible configurations of the lattice, just as is done for the two-dimensional Ising model.[15] We then obtain, after straightforward calculations,

$$Z=\sum_{\text{conf}}p^Rq^{L-R}\prod_{n=1}^{\infty}[\varkappa(nx)]^{N_n},$$
$$\varkappa(x)=1+(S-1)e^{-x}. \tag{3}$$

In the expression (3) the summation is taken over all possible configurations of the lattice, there being R bonds and $L-R$ broken bonds in each concrete configuration; N_n is the number of connected clusters of size n (concerning the concept of a cluster, see, e.g., [2-6]).

We note now that, since $p+q=1$ and $q<1$, formula (3) can be given a probability-theory meaning. We introduce the concept of averaging over the configurations of a lattice with broken bonds,[2] with the quantity q playing the role of the probability that a bond is broken. We denote

$$\langle f\rangle_\pi=\sum_{\text{conf}}p^Rq^{L-R}f, \tag{4}$$

where f is a certain physical quantity defined on the lattice (for more detail about the averaging (4), see[2]). Then the formula (3) can be rewritten in the form

$$Z(x)=\Big\langle\prod_{n=1}^{\infty}[\varkappa(nx)]^{N_n}\Big\rangle,$$
$$Z(0)=\langle S^{N_c}\rangle_\pi,\quad N_c=\sum_{n=1}^{\infty}N_n. \tag{5}$$

Precisely such expressions were obtained by Kasteleyn and Fortuin.[3]

We now consider the limit $S\to1$, $N\to\infty$; we shall assume that $(S-1)N\ll1$. We shall calculate the function $K(x)$, which is simply related to the free energy of the S-model:

$$K(x)=\lim_{N\to\infty}\lim_{S\to1}\frac{\ln Z(x)}{N(S-1)}=\sum_n\gamma_ne^{-nx},$$
$$\gamma_n=\lim_{N\to\infty}N^{-1}\langle N_n\rangle_\pi. \tag{6}$$

The function $K(x)$ coincides with the generating function introduced by Essam and Gwilym[4] for the percolation problem. It is then not difficult to show that such quantities as the infinite-cluster power $P(p)$, the analog $S(p)$ of the susceptibility[2] and also the correlation function $g(\mathbf{r})$ can be expressed in the form of averages for the S-model. We note first of all that, for the bond problem[4-6] we are considering,

$$P(p)=1-{\sum_n}'n\gamma_n=1+\lim_{x\to0}K'(x), \tag{7}$$

$$S(p)={\sum_n}'n^2\gamma_n=\lim_{x\to0}K''(x). \tag{8}$$

In the expression (7), and also everywhere in the following, Σ' denotes a sum over finite clusters only.

We shall now define the correlation function[5,6]:

$$g(\mathbf{r}_i-\mathbf{r}_k)=\langle g_{ik}\rangle_\pi, \tag{9}$$

where $g_{ik}=1$ if the sites i and k belong to the same cluster and $g_{ik}=0$ otherwise. It is not difficult to show that for $q<q_c$ (q_c is the critical concentration of bonds), the Fourier transform $g(\mathbf{k})$ has the form

$$g(\mathbf{k})=P^2\delta(\mathbf{k})+g_1(\mathbf{k}), \tag{10}$$

where a sum only over finite clusters appears in g_1. The formula (10) is analogous to the usual formula from the theory of phase transitions.

As in the derivation of (5), it is easy to show that $P(p)$ and $g(\mathbf{r})$ can be represented in the form of averages in the S-model:

$$g(\mathbf{r}_i-\mathbf{r}_k)=\lim_{S\to1}\frac{1}{S-1}\langle(S\delta_{\sigma_i1}-1)(S\delta_{\sigma_k1}-1)\rangle=\lim_{S\to1}\frac{1}{S-1}\langle P_{\sigma_i1}P_{\sigma_k1}\rangle, \tag{11}$$

$$P=\lim_{S\to1}\frac{1}{S-1}\langle S\delta_{\sigma_i1}-1\rangle=\lim_{S\to1}\frac{\langle P_{\sigma_i1}\rangle}{S-1}, \tag{12}$$

where the averaging is performed with the partition function (2) of the S-model. Here it is necessary to remember, as before, that $(S-1)N\ll1$.

We shall also write out the expression for $\langle S\delta_{\sigma_i1}-1\rangle$ for $x\neq0$:

$$\langle S\delta_{\sigma_i1}-1\rangle=(S-1)\varphi_c,\quad \varphi_c=P+{\sum_n}'n\gamma_n(1-e^{-nx}), \tag{13}$$

where φ_c is the complete analog of the magnetization in a magnetic field.

To conclude this section we note that J, H, and T, introduced in this section, are purely formal quantities, while the physical quantities are q and x (we recall that q is the probability that a bond is broken). Therefore, the expansion in J/T, which we shall use in the following, is in fact an expansion in $\ln(1/q)$.

3. THE DIAGRAM TECHNIQUE

We proceed now to construct the diagram technique. For simplicity we shall confine ourselves to the case x

$=0$ and $q > q_c$. The generalization to the case $x \neq 0$ or $q < q_c$ is trivial, and therefore, when we have need of it, we shall simply write out the answer. For $x=0$ and $q > q_c$, obviously, $\varphi_c = 0$, and therefore it is only necessary to consider $g(\mathbf{r})$. In this case we shall use the Hamiltonian (1b) with $\omega_1 = 0$. First of all we note the following. If we attempt to put $S=1$ immediately in (1), absolutely nothing is obtained. Therefore, we shall consider all the quantities of interest to us (the correlators, vertex functions, etc.) for arbitrary values of S, and then take the limit $S=1$ in the final expressions. All quantities containing higher powers of $S-1$ will be discarded. This leads, in particular, to the absence of disconnected graphs in the diagrammatic representation for the free energy.

We shall calculate (11) by expanding in J_1/T. A fact of great importance here is that $P_{\sigma_1\sigma_2}$ is a singular tensor (not possessing an inverse), inasmuch as $\det P = 0$. Furthermore, for P we have

$$(P^2)_{\sigma_1\sigma_2} = SP_{\sigma_1\sigma_2}. \tag{14}$$

In the calculation of (11) it is necessary to choose the zeroth-order Hamiltonian for the calculation of the single-cell averages. It is obvious that for $\omega_1 = 0$ the averaging over the zeroth-order single-cell Hamiltonian has the form

$$\frac{1}{S}\sum_{\sigma_i} f(\sigma_i),$$

e.g.,

$$g_0(r_i - r_k) = \frac{\delta_{ik}}{S-1}\frac{1}{S}\sum_{\sigma_1} P_{1\sigma_1}^2 = \delta_{ik}. \tag{15}$$

It is not difficult to show that a diagram technique for $(S-1)g(r_i - r_k)$ can be formulated in the following way:

1) The diagrams consist of points and lines;

2) to each internal line corresponds a factor $T^{-1}J_{ik}P_{\sigma_i\sigma_k}$, where $J_{ik} = J_1$ if i and k are nearest neighbors and $J_{ik} = 0$ otherwise;

3) tensors $P_{1\sigma_k}$ correspond to end points;

4) a summation is performed over all indices σ_i, with weight $1/S$, and also over all internal coordinates $\mathbf{r}_j$. Obviously, linear-chain summation will give the following expression for the Fourier transform of $g(\mathbf{r})$:

$$g(\mathbf{k}) = \frac{1}{1 - J_1(\mathbf{k})/T}. \tag{16}$$

We shall calculate now the simplest graph that does not appear as a linear chain—that depicted in Fig. 1a. It is not difficult to see that it is equal to

$$g(\mathbf{r}_i - \mathbf{r}_k) = \frac{S-2}{T^4}\sum_{lm} J_{1il}J_{1lm}^2 J_{1mk}. \tag{16'}$$

A very important effect follows from (16'): first, we see that the theory of the S-model for $S \neq 2$ contains three-point vertices, and secondly, the sign of the graph changes as we pass through $S=2$. Thus, the theory is, in a certain sense, an effective $\lambda\varphi^3$-theory. However, as we shall see below, the usual instability for a $\lambda\varphi^3$-theory, associated with the absence of a ground state in this theory, disappears when $S=1$. Naturally, this is associated with the fact that for $S=1$ the physics of the phenomenon turns out to be completely different from that in an ordinary $\lambda\varphi^3$-theory. As usual, in such cases the correlation-function singularities associated with the three-point vertex are stronger than the singularities associated with, e.g., the four-point vertex. In the following, therefore, we shall take into account only the three-point vertex, the bare value of which is equal to $\delta_{\sigma_1\sigma_2}\delta_{\sigma_1\sigma_3}$, where the σ_i are the indices of the operators associated with the vertex. We recall that a summation $S^{-1}\Sigma_\sigma$ is performed at each vertex (we shall assign the tensors $P_{\sigma_i\sigma_k}$ to the correlation function).

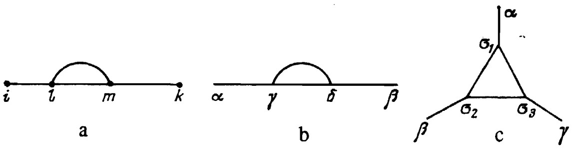

FIG. 1.

As in the theory of phase transitions, in our case the principal role in the internal integrals is played by small momenta. Therefore, we shall renormalize the theory immediately in such a way as to separate out the contribution of the small momenta. As is usual in the site technique,[16,17] we introduce the function

$$V_{\alpha\beta} = V(\mathbf{k})P_{\alpha\beta}, \quad g(\mathbf{k}) = 1 + V(\mathbf{k}),$$
$$V_0(\mathbf{k}) = \frac{J_1(\mathbf{k})}{T}\frac{1}{1 - J_1(\mathbf{k})/T}. \tag{17}$$

A diagram technique is now formulated for the function $V_{\alpha\beta}(\mathbf{k})$,[16,17] and it is natural to choose the function $V_0 P_{\alpha\beta}$ as the zeroth approximation. Here, the fact that $V_{\alpha\beta} \sim P_{\alpha\beta}$ in any order of perturbation theory is extremely important. For example, the tensor part of the graph of Fig. 1b for $V_{\alpha\beta}$ has the form

$$\frac{1}{S^2}\sum_{\gamma\delta} P_{\alpha\gamma}P_{\gamma\delta}^2 P_{\delta\beta} = (S-2)P_{\alpha\beta}, \tag{18}$$

from which we see that the tensor properties of the operator $P_{\alpha\beta}$ lead only to the result that, e.g., a loop gives a factor $S-2$. As we shall see below, an analogous property is possessed by the three-point function.

We now separate out the region of small momenta in $V_0(\mathbf{k})$. We obtain

$$V_0(\mathbf{k}) = r_0^{-2}G_0(\mathbf{k}), \quad J_1(\mathbf{k}) = J_1(0)(1 - k^2r_0^2),$$
$$G_0(\mathbf{k}) = \frac{1}{k^2 + \varkappa_0^2}, \quad \varkappa_0^2 = \frac{T - J_1(0)}{J_1(0)}\frac{1}{r_0^2}, \tag{19}$$
$$\lambda = \Lambda_1^{\varepsilon/2}, \quad \Lambda_1 = a/r_0^2.$$

In the formulas (19), a is the lattice constant, r_0 is defined from the expansion of $J_1(\mathbf{k})$, and λ is the bare three-point vertex obtained as a result of the renormalization. A diagram technique is now constructed for the Green function $G_{\alpha\beta}(\mathbf{k})$, which is simply related to $g(\mathbf{k})$:

$$G_{\alpha\beta}(\mathbf{k})=G(\mathbf{k})P_{\alpha\beta}, \quad g(\mathbf{k})=1+r_0^{-2}G(\mathbf{k}). \tag{20}$$

We shall formulate the rules for constructing diagrams for $G_{\alpha\beta}(\mathbf{k})$: 1) The diagrams consist of points and lines; 2) corresponding to each line is a $G_{0\alpha\beta}(\mathbf{k})$; 3) corresponding to each point is a factor λ; 4) at each point there is a summation over all internal indices, with weight $1/S$, and there is also integration over the internal momenta. For example, the graph of Fig. 1b is equal to

$$\begin{aligned}\Delta G_{\alpha\beta}(\mathbf{k})&=\frac{\lambda^2}{S^2}\sum_{\gamma\delta}G_{0\alpha\gamma}(\mathbf{k})G_{0\delta\beta}(\mathbf{k})\int\frac{d^3p}{(2\pi)^3}G_{0\gamma\delta}(\mathbf{p})G_{0\gamma\delta}(\mathbf{p}+\mathbf{k})\\&=\lambda^2(S-2)P_{\alpha\beta}G_0^2(\mathbf{k})\int\frac{d^3p}{(2\pi)^3}G_0(\mathbf{p})G_0(\mathbf{p}+\mathbf{k}).\end{aligned} \tag{21}$$

In any order of perturbation theory, $G_{\alpha\beta}\sim P_{\alpha\beta}$.

Inasmuch as $P_{\alpha\beta}$ is a singular tensor, the self-energy part cannot be defined in a tensor form. Therefore, we shall put

$$G^{-1}(k)=G_0^{-1}(\mathbf{k})-\Sigma(\mathbf{k}). \tag{22}$$

We now determine the renormalized vertex. We shall consider the simplest diagram (Fig. 1c; $\Delta K_{\alpha\beta\gamma}$) for the three-point function. A simple calculation gives the following expression for the tensor part of this graph:

$$\frac{1}{S^3}\sum_{\sigma_1\sigma_2\sigma_3}P_{\alpha\sigma_1}P_{\beta\sigma_2}P_{\gamma\sigma_3}P_{\sigma_1\sigma_3}P_{\sigma_2\sigma_3}P_{\sigma_2\sigma_1}=(S-3)\frac{1}{S}\sum_{\sigma}P_{\alpha\sigma}P_{\beta\sigma}P_{\gamma\sigma}. \tag{23}$$

We see that summation over all the σ_i has led to a summation over one variable σ and to the appearance of the factor $S-3$. It is easy to show that the same thing will also happen for an arbitrary diagram. Thus, the diagram of Fig. 1c gives the following expression for $\Delta K_{\alpha\beta\gamma}$:

$$\begin{gathered}\Delta K_{\alpha\beta\gamma}=\Delta\Gamma_3\frac{1}{S}\sum_{\sigma}G_{0\alpha\sigma}G_{0\beta\sigma}G_{0\gamma\sigma},\\\Delta\Gamma_3=(S-3)\int\frac{d^3p}{(2\pi)^3}G_0(\mathbf{p})G_0(\mathbf{p}+\mathbf{k}_1)G_0(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2).\end{gathered} \tag{24}$$

Completely analogously, in arbitrary order of perturbation theory we obtain

$$K_{\alpha\beta\gamma}=\Gamma_3\frac{1}{S}\sum_{\sigma}G_{\alpha\sigma}G_{\beta\sigma}G_{\gamma\sigma}, \tag{25}$$

where $G_{\alpha\beta}$ are exact Green functions and $K_{\alpha\beta\gamma}$ is the exact three-point function.

4. EQUATIONS FOR THE VERTEX AND GREEN FUNCTION

The theory is constructed below in analogy with the theory of second-order phase transitions. We shall follow our previous paper.[9] The renormalization of the theory is carried out fairly easily, and we shall not dwell on it here. Near the phase-transition point, $G(\mathbf{k})$ has the form

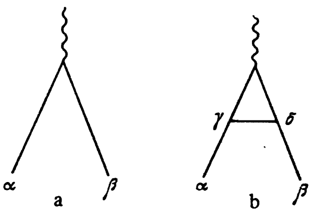

FIG. 2.

$$G(\mathbf{k})=\frac{z}{k^2+\varkappa^2-\Sigma_R}, \tag{26}$$

where $\varkappa^2$ is defined by the condition that G has a pole at $k^2=-\varkappa^2$. As was shown in[9], in the region $k^2\sim\varkappa^2$ we have $\Sigma_R\sim\eta$. Inasmuch as $\eta\ll 1$, we shall disregard Σ_R; the quantity z is also determined by η, and, therefore, we shall assume for simplicity that $z=1$; at the end of this section we shall calculate η from simple considerations.

After these simplifications for the calculation of the Green function, only $\varkappa^2$ remains to be calculated. This can be done with the aid of a Ward identity, using the formula

$$dr/d\tau=t_R, \quad r=\varkappa^2, \tag{27}$$

where t_R is a vertex whose definition is clear from Fig. 2a, in which we have denoted the differentiation with respect to τ by a wavy line. In its turn, t_R is also determined by a Ward identity. This Ward identity is conveniently written in a form with a derivative not with respect to τ but with respect to r directly. For example, differentiation of the graph of Fig. 2b with respect to r will give the expression

$$(S-2)\lambda^2\frac{\partial K}{\partial r}, \quad K(r)=\int\frac{d^3p}{(2\pi)^3}G^3(\mathbf{p}). \tag{28}$$

We now replace λ by the renormalized vertex Γ_3 taken at zero momenta, and replace the point at which the wavy line enters by t_R; we then obtain for t_R the equation

$$\frac{\partial t_R}{\partial r}=(S-2)t_Ru_R^2\frac{\partial K}{\partial r}, \quad u_R=\Gamma_3(\mathbf{p}_i=0). \tag{29}$$

It is convenient to separate out the scaling part from u_R. We put

$$u_R=\alpha g r^{3/4}, \quad \alpha^2=-\left(r^{3/2}\frac{\partial K}{\partial r}\right)^{-1}. \tag{30}$$

Then from (29) we obtain

$$\frac{\partial\ln t_R}{\partial t}=\xi_0(g)=(2-S)g^2, \quad t=\ln r. \tag{31}$$

It is also easy to show that, as previously,[9] allowance for the more complicated graphs will give the equation

$$\frac{\partial\ln t_R}{\partial t}=\xi(g), \tag{32}$$

$\xi_0(g)$ being the first term of the expansion of ξ in g.

Thus, we see that the problem has been reduced to the calculation of the renormalized dimensionless coupling constant g. To calculate g we shall write the Ward identity for u_R. The simplest graph for u_R is represented by Fig. 1c with all the outgoing momenta equal to zero. Arguing in exactly the same way as in the derivation of Eq. (29) for t_R, we obtain the following equation for u_R and g:

$$\frac{\partial u_R}{\partial r}=(S-3)u_R^3\frac{\partial K}{\partial r},$$
$$\frac{\partial g}{\partial t}=\psi_0(g)=-\frac{3}{4}g+(3-S)g^3. \tag{33}$$

Just as before,[9] it is easy to show that allowance for the more complicated graphs gives the equation

$$\partial g/\partial t=\psi(g). \tag{34}$$

Equation (34) is the Gell-Mann–Low equation for g, and $\psi(g)$ is the Gell-Mann–Low function. The zeros of $\psi(g)$ are the fixed points of Eq. (34). If g_0 is a zero of $\psi(g)$, the susceptibility index γ is determined by the formula[9]

$$\gamma=\frac{1}{1-\xi(g_0)}. \tag{35}$$

In the present article we shall confine ourselves to treating $\xi(g)$ and $\psi(g)$ in only the lowest orders of perturbation theory, i.e., we shall consider only $\xi=\xi_0$ and $\psi=\psi_0$. First of all we note that, in $\psi_0(g)$ and $\xi_0(g)$, only the term in $\psi_0(g)$ linear in g depends on the dimensionality of space. This is connected with the fact that for arbitrary dimensionality d of space (we shall consider only the case $3\leqslant d\leqslant 6$), $u_R\sim r^{(6-d)/4}$ and, therefore, (30) is replaced by

$$u_R=\alpha_d g r^{(6-d)/4},\qquad \alpha_d^2=-\left(r^{(8-d)/2}\frac{\partial K_d}{\partial r}\right)^{-1}, \tag{36}$$

and $K_d(r)$ is defined analogously to (28), but with arbitrary dimensionality d. Then ξ_0 preserves its form, and for ψ_0 we obtain

$$\psi_0(g)=-{}^1/_4(6-d)g+(3-S)g^3, \tag{37}$$

from which, in particular, it can be seen that we have a logarithmic situation for $d=6$. For arbitrary d there is a fixed point at

$$g^2={}^1/_8(6-d)\qquad (S=1), \tag{38}$$

which leads to the following expression for γ:

$$\gamma=8/(2+d). \tag{39}$$

If we neglect the Fisher parameter η, we obtain from the scaling laws the following expressions for the "large" indices:

$$\gamma=\frac{4}{2+d},\quad \beta=\frac{2(d-2)}{d+2},\quad \alpha=-\frac{2(d-2)}{d+2},\quad \Delta=\gamma+\beta=2. \tag{40}$$

Computer calculations for the three-dimensional case give[4,6]

$$\gamma=1.69\pm0.05;\quad \beta=0.35\pm0.05;\quad \nu=0.9\pm0.05;\quad \Delta=2.2\pm0.3, \tag{41}$$

which agree fairly well with our results. Even for the two-dimensional case, for which our theory should be rather poorly applicable inasmuch as the dimensions of all vertices differ only by the quantity η when $d=2$, the values of γ and Δ differ only by 15–20% from the computer-calculated values[4] $\gamma=2.37\pm0.03$, $\Delta=2.4\pm0.2$. This suggests that the approximation used in the present paper is fairly good. (Inasmuch as the index $\beta\sim\eta$ for $d=2$, it is natural that, as follows from (40), $\beta(d=2)=0$.)

We now write out explicit expressions for g, u_R and t_R in the three-dimensional case:

$$g=g_0\left(1+\frac{64\pi}{3}g_0^2\frac{r^{3/2}}{\Lambda_1^3}\right)^{-1/2},$$
$$u_R=\Lambda_1^{3/2}\left(1+\frac{3}{64\pi g_0^2}\frac{\Lambda_1^3}{r^{3/2}}\right)^{-1/2}, \tag{42}$$
$$t_R=\left(1+\frac{3}{64\pi g_0^2}\frac{\Lambda_1^3}{r^{3/2}}\right)^{-1/4}.$$

The expressions (42) are obtained from the conditions $t_R(r\gg\Lambda_1)=1$ and $u_R(r\gg\Lambda_1)=\Lambda_1^{3/2}$; we have taken into account that $\alpha^2=64\pi/3$.

We now calculate the Fisher parameter. For this we express $\Sigma_1(\mathbf{k})=\Sigma(\mathbf{k})-\Sigma(0)$ in terms of the renormalized vertex Γ_3:

$$\Sigma_1(\mathbf{k})=-\int\frac{d^3p}{(2\pi)^3}\Gamma_3^2(\mathbf{p})G(\mathbf{p})[G(\mathbf{p}+\mathbf{k})-G(\mathbf{p})]. \tag{43}$$

The minus sign has arisen from the factor $S-2$, just as in formula (18). For large p the vertex $\Gamma_3(\mathbf{p})=bp^{3/2}$ and the integral in (43) diverges logarithmically:

$$\Sigma_1(\mathbf{k})\approx-b^2\int\frac{d^3p}{(2\pi)^3}p^3G(\mathbf{p})[G(\mathbf{p}+\mathbf{k})-G(\mathbf{p})]\approx-\frac{b^2}{6\pi^2}k^2\ln\frac{\Delta}{k}, \tag{44}$$

where Λ is the momentum cutoff. Comparing (44) with the expansion of $G(k)$ for $\eta\ln(\Lambda/k)\ll1$, we obtain

$$\eta=b^2/6\pi^2. \tag{45}$$

Thus, to calculate η we need to know the coefficient b. It does not, of course, coincide with the coefficient αg_0 in u_R. In order to calculate b, it is necessary to take the derivative of the graph of Fig. 1c with respect to the external momentum k, rather than with respect to r. As a result we obtain

$$\frac{d\Gamma_3}{dk}=\frac{3}{\pi^2k^4}\Gamma_3^3. \tag{46}$$

Substituting $\Gamma_3=bk^{3/2}$ into (46), we obtain

$$b^2=\pi^2/2,\qquad \eta={}^1/_{12}. \tag{47}$$

To conclude the present section we shall return to the formula (26). From (26) we have the following asymptotic forms of G in the coordinate representation:

$$G\sim r^{-1-\eta},\qquad r\ll1/\varkappa;$$
$$G\sim r^{-1}e^{-\varkappa r},\qquad r\gg1/\varkappa. \tag{48}$$

These formulas, which have been known for a long time in the theory of second-order phase transitions, give very important information about the arrangement of finite clusters in the percolation problem.

5. ANALOG OF THE EQUATION OF STATE FOR THE PERCOLATION PROBLEM

For the calculation of the order parameter P it is necessary to write the equation of state, in which the magnetic field x must necessarily appear, since (as is well-known[8]) for $x=0$ we cannot pass through the point $\tau=0$. Therefore, it is not P that should appear in the equation, but the quantity φ_c defined in (13), which is the analog of the magnetization in a magnetic field, together with $\chi(x)$, which is the analog of the susceptibility. We shall write out both these quantities:

$$\begin{aligned}\varphi_c(x)&=1+\frac{\partial K}{\partial x}=1-\sum_n{}' n\gamma_n e^{-nx},\\ \chi(x)&=\frac{\partial^2 K}{\partial x^2}=\sum_n{}' n^2\gamma_n e^{-nx}.\end{aligned}\tag{49}$$

It can be seen from (49) that for $x\gg 1$ the quantity $\varphi_c=1$, i.e., we have, as it were, complete magnetization, while for $x\to 0$ we have $\varphi_c(x)=P+S(p)$ where $S(p)$ is defined in (8) ($S=\chi(x=0)$). For $x\to 0$ this expression coincides with the usual expression for the magnetization in weak fields.

Before writing the equation of state for the quantities of percolation theory we shall write it for a one-component system in ordinary $\lambda\varphi^4$-theory.[9] The renormalized Hamiltonian of this problem has the form

$$\frac{H}{T}=\int d\mathbf{r}\left\{\frac{1}{2}(\nabla\varphi_0)^2+\frac{1}{2}r_0\varphi_0^2+\frac{1}{4!}\Gamma_{40}\varphi_0^4-H\varphi_0\right\},\tag{50}$$

where H is the magnetic field. We introduce the average φ_c:

$$\varphi(\mathbf{r})=\varphi_0(\mathbf{r})-\varphi_c,\quad \langle\varphi_0(\mathbf{r})\rangle=\varphi_c.\tag{51}$$

We then obtain

$$\begin{gathered}H=H_0+H_1+FV,\\ \frac{H_0}{T}=\int d\mathbf{r}\left(\frac{1}{2}r_0+\frac{1}{4}\Gamma_{40}\varphi_c^2\right)\varphi^2,\\ \frac{H_1}{T}=\int d\mathbf{r}\left(\frac{1}{3!}\Gamma_{40}\varphi_c\varphi^3+\frac{1}{4!}\Gamma_{40}\varphi^4+\left(r_0\varphi_c+\frac{1}{3!}\varphi_c^3\Gamma_{40}-H\right)\varphi,\right.\\ \frac{F}{T}=\frac{1}{2!}r_0\varphi_c^2+\frac{1}{4!}\Gamma_{40}\varphi_c^4,\end{gathered}\tag{52}$$

where V is the volume of the whole space and F is the free energy.

The equation of state is obtained from the conditions

$$\begin{aligned}\frac{\partial F}{\partial\varphi_c}&=H=r_0\varphi_c+\frac{1}{6}\Gamma_{40}\varphi_c^3,\\ \frac{\partial^2 F}{\partial\varphi_c^2}&=\frac{1}{\chi}=r_0+\frac{1}{2}\Gamma_{40}\varphi_c^2.\end{aligned}\tag{53}$$

Fulfilment of the first Eq. (53) causes the term linear in φ in H_1/T to vanish. From (53) we have

$$H=\frac{1}{\chi}\varphi_c-\frac{1}{3}\Gamma_{40}\varphi_c^3,\quad \chi=\frac{\partial\varphi_c}{\partial H}.\tag{54}$$

The second equation is obtained from the definition of χ and φ_c.

We assume now that Γ_{40} is a function only of χ and is defined in the same way for $\tau>0$ and $\tau<0$. Then, using the results of the previous paper[9] in the quadratic approximation and taking into account that $\Gamma_{40}=3u_R$ (u_R was determined in[9]), we obtain (since $\chi=r^{-1}$)

$$\varphi_c/\chi-{}^{16}/{}_9\pi\varphi_c^3\chi^{-1/2}=H.\tag{55}$$

Equation (55) is easily reduced to the linear parametric equation of state that was discussed by Migdal[18] (cf. also[8]). First of all we note that in the quadratic approximation it follows from our previous work[9] that for a one-component field $\gamma=1.2$, $\beta=0.3$ and $\gamma+\beta=\frac{3}{2}$. The condition $\gamma+\beta=\frac{3}{2}$ is necessary[8,18] to make Eq. (55) self-consistent. If we put

$$m=\varphi_c\chi^{\beta/\gamma},\quad h=H\chi^{(\beta+\gamma)/\gamma},\tag{56}$$

then Eq. (55) is brought to the form

$$h=\varphi(m)=m-{}^{16}/{}_9\pi m^3.\tag{57}$$

Equation (57) is the simplest equation of state in parametric form.

Repeating almost verbatim the calculations carried out above, using the expression (30) for u_R and taking into account that $\Gamma_{30}(\chi)=u_R(r=\chi^{-1})$, we obtain the following equation of state for the percolation problem:

$$\varphi_c/\chi-2\sqrt{\pi}\varphi_c^2/\chi^{3/4}=x,\quad \chi=\partial\varphi_c/\partial x.\tag{58}$$

Like (55), Eq. (58) can be written in the following form:

$$\begin{gathered}h=\varphi(m)=m-2\sqrt{\pi}m^2,\\ m=\varphi_c\chi^{\beta/\gamma},\quad h=x\chi^{(\beta+\gamma)/\gamma}.\end{gathered}\tag{59}$$

From (40) it can be seen that we have $\gamma=1.6$, $\beta=0.4$ and $\beta+\gamma=2$, the latter being necessary for the self-consistency of (59). We note that (59) differs from (57) in that an m^2 term appears in (59) in place of m^3 in (57). This is connected, naturally, with the fact that the order parameter is our case is an essentially positive quantity, and there is no invariance with respect to replacement of m by $-m$. For space dimensionalities $d>6$ Eq. (58) (for $x=0$) is replaced by the following equation:

$$\tau\varphi_c+g\varphi_c^2=0,\tag{60}$$

which is the exact analog of the Landau theory of phase transitions for the percolation problem. In this case the indices are equal to $\beta=1$, $\gamma=1$, $\nu=\frac{1}{2}$ and $\eta=0$.

We turn now to the solution of (59). The self-consistency condition for the solution of (59) is the condition $\beta+\gamma=2$, which is fulfilled in our approximation. Solving (59) as in[8,18], we obtain the following expression for χ:

$$\chi(m,\tau)=C\left(\frac{1-4\sqrt{\pi}\,m/\gamma}{\tau}\right)^{\gamma},\tag{61}$$

where C is a constant. If we put

$$\theta=2\pi^{1/2}m, \quad \rho=(C/\chi)^{1/\gamma}, \tag{62}$$

we obtain from (59), (61) and (62)

$$x=A\theta(1-\theta)\rho^{\beta+\gamma}, \quad \varphi_c=B\theta\rho^{\beta}, \quad \tau=\rho(1-2\theta/\gamma), \tag{63}$$

where A and B are constants. The expressions (61)–(63) determine the equations of state in parametric form.

The fact that $\beta+\gamma=2$ gives us the possibility of solving these equations in explicit form. As a result, we obtain

$$\chi=\frac{C_1}{x^{\gamma/2}}\left[\frac{(y^2+1)^{1/2}+{}^3/{}_2y}{{}^8/{}_5y^2+{}^5/{}_2}\right]^{\gamma}, \tag{64}$$

$$\varphi_c=B_1x^{\beta/2}\frac{y^2+{}^5/{}_2-y(y^2+1)^{1/2}}{2y^2+{}^{25}/{}_8}\left[\frac{{}^8/{}_5y^2+{}^5/{}_2}{{}^3/{}_5y+(y^2+1)^{1/2}}\right]^{\beta} \qquad y=\tau(A/x)^{1/2}. \tag{65}$$

It can be seen from (64) that $\varphi_c\to 0$ for $\tau\gg x^{1/2}$ and $\tau>0$, and $\varphi_c\sim(-\tau)^{\beta}$ for $|\tau|\gg x^{1/2}$ and $\tau<0$. Also, $\chi\sim|\tau|^{-\gamma}$ for $|\tau|\gg x^{1/2}$, the coefficients of $|\tau|^{-\gamma}$ being different for $\tau>0$ and $\tau<0$. At $\tau=0$ we have $\chi\sim x^{-\gamma/2}$, and $\varphi_c\sim x^{\beta/2}$.

Inasmuch as χ and φ_c are related to the cluster-size distribution γ_n, we can determine the asymptotic forms of γ_n from (64). For this it is most convenient to use formula (49). Since the principal contribution to the sum (49) is given by values $n\gg 1$, γ_n can be calculated by replacing the sum in (49) by a Laplace integral and inverting the latter. As a result, we obtain for $\tau>0$

$$\begin{gathered}\gamma_n\sim n^{-g}, \quad n\ll 1/A\tau^2,\\ \gamma_n\sim\exp\{-A_1\tau^2n\}, \quad n\gg 1/A\tau^2,\\ g=3-\gamma/2=2.2.\end{gathered} \tag{66}$$

We have omitted the pre-exponential factor in the second of the formulas (66). In the paper[4] of Essam and Gwilym the following expression for g, calculated on a computer, is given: $g=2.2\pm0.2$, which agrees with (66).

6. THERMODYNAMICS OF A DISORDERED ISING FERROMAGNET NEAR THE PERCOLATION THRESHOLD

In this section we shall consider the thermodynamic functions of a disordered Ising ferromagnet at low temperatures $T\ll J_0$ and with $\mu H\sim T\tau^{\Delta}$, where J_0 is the exchange integral, T is the temperature and H is the magnetic field (of course, J_0, T and H have no relation to the formal J_0, T and H in the S-model that we introduced in Sec. 2). We consider first of all the ground-state energy E. Inasmuch as

$$E=\sum_{ik}J_{ik}\langle S_i^zS_k^z\rangle_{\pi}, \tag{67}$$

it is easy to show also (as is done in the usual theory of phase transitions[6]) that the singular part of E is equal to

$$E_{\text{sing}}\sim\tau^{1-\alpha}, \tag{68}$$

where α is the analog in the percolation problem of the specific-heat index. It can be seen from (40) that only the second derivative $\partial^2E/\partial q^2$ goes to infinity.

In order to calculate the magnetization and susceptibility we shall calculate the free energy. Following Dunn *et al.*,[5] we shall assume that for $T\ll J_0$ the dependence on the exchange integral drops out, inasmuch as all the spins are ordered within the finite clusters. Then the free energy f per lattice site is equal to

$$f=-T\sum_n{}'\gamma_n\ln[1+e^{-2n\mu H/T}]. \tag{69}$$

The magnetization M and susceptibility χ_R per site are respectively equal to

$$M=\mu\left[1-2\sum_n{}'\frac{n\gamma_n}{1+e^{nx}}\right], \tag{70}$$

$$\chi_R=\frac{4\mu^2}{T}\sum_n{}'n^2\gamma_n\frac{e^{nx}}{(1+e^{nx})^2}, \tag{71}$$

where $x=2\mu H/T$. The connection between the real thermodynamic functions and the percolation functions can be seen immediately from the expressions (70) and (71). For example, from (6) and (70) we have

$$f=-T\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m}K(mx), \tag{72}$$

while M is analogously related to φ_c, and χ_R to χ.

From the expressions (49) and (71) we obtain the relationship between the asymptotic forms of M and χ_R and the asymptotic forms of φ_c and χ:

$$\begin{gathered}M=\mu\varphi_c, \quad \chi_R=\mu^2\chi/T, \quad x\ll\tau^{\Delta};\\ M=\mu\left[1-2\sum_n{}'n\gamma_ne^{-nx}\right], \quad \chi_R=4\mu^2\chi/T, \quad x\gg\tau^{\Delta}.\end{gathered} \tag{73}$$

Using the asymptotic form of χ, we obtain for χ_R the following expressions:

$$\begin{gathered}\chi_R\sim 1/T\tau^{\gamma}, \quad \mu H\ll T\tau^{\Delta},\\ \chi_R\sim 1/T^{1-\gamma/2}H^{\gamma/2}, \quad \mu H\gg T\tau^{\Delta},\end{gathered} \tag{74}$$

and, since $1-\gamma/2=0.2$, $\chi_R\sim T^{-0.2}$ in the second case. We note that, by using the explicit expressions (64) and (65) for χ and φ_c, we can also write corresponding expressions for M and χ_R; however, we shall not do this here.

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Carrier statistics and thermal relaxations in inhomogeneous semiconductors

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The statistics of electrons in an inhomogeneous semiconductor in which the energy bands are modulated by a Gaussian random potential are considered. It is assumed that only one type of partially compensated donor level is present in the semiconductor. The position of the chemical-potential level, the degeneracy criterion, the features of the temperature dependences of the free carrier density, and conductivity are investigated, as is also the kinetics of the establishment of the stationary conductivity following an abrupt variation of the sample temperature. It is shown that in an inhomogeneous and weakly compensated semiconductor the process is characterized by anomalously high relaxation times that have an activation dependence on the temperature.

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1. INTRODUCTION

It is well known that statistical fluctuations or technological inhomogeneities of the impurity ion concentration can produce in semiconductors an inhomogeneous electrostatic potential that modulates the energy bands. In some cases (for example in strongly compensated or irradiated semiconductors) the amplitude of this potential can become appreciable. This leads to a number of singularities in the kinetic properties of the semiconductors, such as a residual photoconductivity, an anomalous temperature dependence of the Hall mobility, etc.[1] These phenomena are observed in experiment quite frequently, as is evidenced by the significant inhomogeneity of many real semiconductors. A consistent theoretical study of the properties of inhomogeneous semiconductors is therefore useful.

This paper deals with the statistics of the carriers and, in particular, with the question of the temperature dependences of the equilibrium concentration and conductivity in inhomogeneous semiconductors. The kinetics of the establishment of the indicated equilibrium values following an abrupt change of temperature is also investigated.

2. CHEMICAL-POTENTIAL LEVEL AND DEGENERACY CRITERION

We consider a semiconductor with a modulating random potential $V(\mathbf{r})$ described by a distribution function $F(V)$. Assume that the sample contains uniformly distributed donor levels with concentration N_D and binding energy ε_i. The random potential is due to the inhomogeneous distribution of the acceptors having an average concentration N_A.[1)] If the correlation length of $V(\mathbf{r})$ exceeds the radius of the donor states, then the energy of the latter can be described by the same distribution function F.

We assume that the electron density n in the band is quite small, $n \ll N_A$. We can then neglect the dependence of the random potential on n, and determine the chemical-potential level ζ from the expression

$$\int_{-\infty}^{\infty} dV F(V) f(V-\varepsilon_i) = (N_D - N_A)/N_D \qquad (1)$$

where $f(\varepsilon)$ is the Fermi function. There being no alternate assumptions, we take the random potential to be Gaussian