Critical behavior of the Potts model

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The renormalization group method is used to obtain the properties of a phase transition in the continual Potts model with arbitrary number of components s. It is shown that at $s = 3$, in the three-dimensional model, both a first-order and a second-order phase transition are possible, and the critical exponents γ and η are calculated. It is established that the scaling properties of the model at $s = 1$ (the percolation problem) are different in principle than at $s = 3$. At $s > 3$ only a first-order phase transition is possible. The results are compared with the experimental data for physical systems in which the phase transitions are described by the Potts model, as well as with the results of numerical calculations for this model on a lattice.

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INTRODUCTION

In 1952, Potts analyzed the properties of a generalization of the Ising model.[1] In the Potts model (hereafter called the S model), each lattice site can be in one of s states, and the energy of interaction between neighboring sites is equal to ε_0 if their states are identical, and $\varepsilon_1 > \varepsilon_0$ if their states are different.[1)] Obviously, at sufficiently low temperatures, a phase transition takes place in such a system to an ordered state "enriched" with one of the s components. For the S model on a quadratic lattice, it was established in Refs. 1 and 2 that there exists a duality transformation of the partition function, and this made it possible to find T_c of the phase transition at any[2)] value of s:

$$\exp[(\varepsilon_1-\varepsilon_0)/kT_c]=1+\sqrt{s}.$$

The question of the order of this phase transition was solved by Baxter in 1973.[4] He established the connection between the free energy of the S model near T_c and the free energy of the Rys F model for antiferroelectrics,[5] which was previously solved exactly by Lieb,[6] and was able to show rigorously that the phase transition is continuous at $s \leq 4$. The assumption of the continuity of the phase transition in the two-dimensional three-component Potts model was advanced in an earlier paper by Kihara and co-workers[7] on the basis of an analysis of the low-temperature expansions of the partition function, and later by Straley and Fisher,[8] who generalized their results to include the case of an external field. Baxter proved the validity of this assumption and his paper stimulated further investigations of the character of the phase transition in the three-dimensional S model.

Attempts to obtain information on the order of the phase transition by numerical methods led, however, to conflicting results. Thus, Straley[9] and Enting,[10] who investigated the three-component model on cubic and fcc lattices by the method of expansions in series in the temperature and field, concluded that the phase transition is continuous. At the same time, Ditzian and Oitman,[7] who calculated six terms of the series for the susceptibility of a disordered phase in an Ising model with spin $J = 1$ in the presence of a biquadratic interaction, found that the biquadratic exchange parameter at which this model becomes equivalent to the three-component Potts model lies outside the region which they found for continuous transitions, although it does lie close to the boundaries of this region. The conclusion that the phase transition at $s > 2$ will be of first order was reached also by Kim and Joseph, who investigated directly the dependence of the order parameter of the S model on the temperature.[12] The causes of such discrepancies between the conclusions concerning the character of the phase transitions of the three-dimensional S model are apparently the following: First, the inability to determine T_c with sufficient accuracy (the value obtained by reduction of the series for the heat capacity, susceptibility, and order parameter "floats" quite widely for the various series). Second, the expansion coefficients have a rather irregular behavior,[3)] so that when the number of calculated terms is small it is difficult to separate the contribution due to the physical singularity at $T = T_c$ from the background of the unphysical singularities. Thus, the numerical calculations lead to no definite conclusions concerning the order of the phase transition in the three-dimensional S model.

Besides the numerical calculations for the S model on a lattice, field-theory methods were used also to study the critical behavior of the continuous analog of the model. Golner,[14] using Wilson's approximate recursion formulas, performed computer calculations for the three-component model. He observed no stable fixed point for the effective Hamiltonian, and concluded that the phase transition will be of first order. Since the Hamiltonian of the continual S model contains a triple vertex Γ_3, it was stated in a number of papers (see, e.g., Refs. 15 and 16) that the phase transition is continuous only if Γ_3 decreases as $T \to T_c$ more rapidly than the quadruple vertex Γ_4. Calculations of the critical dimensionality near the "Heisenberg" fixed point by the ε-expansion method ($\varepsilon = 4 - d$) have shown, however, that the triple vertex perturbs substantially the critical behavior of the system. None the less, as

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we shall show in detail below (see also Ref. 17), this still does not lead to the unequivocal conclusion that the phase transition must be of first order. Examples of physical systems in which the phase transition is described by a continual S model will be cited at the end of the paper in the discussion of the result.

The S model is of interest also because its analytic properties describe, as $s \to 1$, a continuous phase transition in the problem of the percolation-theory bonds,[18] which has many physical applications (see the review[19]). This analogy makes it possible to construct a microscopic similarity theory for the percolation problem via ε-continuation from six-dimensional space[20] or directly for a three-dimensional space with only one triple vertex taken into account.[21] We do not know, however, how the results obtained in this manner are altered when account is taken of the quadruple vertex, with respect to which a "Gaussian" fixed point in three-dimensional space is also unstable.

In this paper we investigate by the field renormalization group method the critical behavior of the continual S model at arbitrary values of s. We are interested primarily in two questions: 1) What is the order of the phase transition at $s > 2$? 2) Is allowance for one triple vertex sufficient for the construction of a microscopic similarity theory in the percolation problem ($s = 1$)? Zaprduskiĭ[22] has also considered recently, by the field renormalization group, the three-component case, but his paper contains errors that lead both to incorrect numerical results and to a qualitatively incorrect interpretation of the results. The case $s = 3$ is therefore analyzed below anew.

1. CONTINUAL S MODEL. CONDITIONS FOR CONTINUITY OF PHASE TRANSITION

For the continual S model we can introduce a field Hamiltonian in full analogy with Wilson's approach to the Ising model.[16] Namely, the s allowed states of the lattice model must be set in correspondence with a potential that has s minima, and since all these s states are equivalent, the field Hamiltonian $\mathcal{H}$ must be invariant to the symmetry group of a hypertetrahedron with s vertices in $(s-1)$-dimensional space. To take into account this invariance of $\mathcal{H}$ at arbitrary s, as well as to simplify the calculations, it is convenient to introduce s vectors $\mathbf{e}^\alpha (\alpha = 1, \ldots, s)$, directed into the vertices of the hypertetrahedron, such that

$$\sum_{i=1}^{s-1} e_i^\alpha e_i^\beta = s\delta_{\alpha\beta} - 1. \tag{1}$$

Each of these vectors describes one of the s permissible states at the site. Using $\mathbf{e}^\alpha$, we can represent the S-model Hamiltonian in the form[16]

$$\mathcal{H} = \int dx \Big[\frac{1}{2}(\nabla\varphi)^2 + \frac{1}{2} r_0 \varphi^2 + \frac{1}{3!}\lambda_0 \Omega_{ijk}\varphi_i\varphi_j\varphi_k + \frac{1}{4!}(u_0 S_{ijkl} + f_0 F_{ijkl})\varphi_i\varphi_j\varphi_k\varphi_l \Big]. \tag{2}$$

Here

$$\Omega_{ijk} = \sum_\alpha e_i^\alpha e_j^\alpha e_k^\alpha,$$
$$S_{ijkl} = \frac{1}{3}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \quad F_{ijkl} = \sum_\alpha e_i^\alpha e_j^\alpha e_k^\alpha e_l^\alpha \tag{3}$$

are the invariants of third and fourth order of the symmetry group of the hypertetrahadron, φ_i is an $(s-1)$-component real field, $\varphi^2 = \sum_i \varphi_i^2$, and r_0 is a linear function of the temperature.

We discuss now the possibility of the existence of a continuous phase transition in the S model. It is obvious that expansion of the thermodynamic potential in powers of the average order parameter contains odd terms and takes the form

$$\Phi = \sum_{n=2}^{\infty} \frac{1}{n!}\Gamma_n(0)\langle Q\rangle^n = \frac{1}{2!} r\langle Q\rangle^2 + \frac{1}{3!} B\langle Q\rangle^3 + \frac{1}{4!} C\langle Q\rangle^4 + \ldots, \tag{4}$$

where $r(T_0) = 0$, $\Gamma_n(0)$ are irreducible vertex parts at zero momenta, $\langle Q\rangle$ is the equilibrium value of the order parameter in the transition into one of the s ordered phases, and it is assumed that $C > 0$. The potential Φ has, besides the obvious minimum at $\langle Q\rangle = 0$, also a relative minimum at $\langle Q\rangle = Q^* \sim -B/C$. If this minimum "deepens" with decreasing temperature, then a first-order phase transition will take place at a certain temperature $T_c > T_0$. Clearly, this occurs in fact if the fluctuations in the system are small and the phase transition takes place within the region where the Landau theory is valid, when the vertices $\Gamma_n(0)$ at $n > 2$ can be regarded as independent of temperature. The situation changes if the phase transition takes place in the strong-fluctuation region. The vertices $\Gamma_n(0)$ are then strongly renormalized and have a power-law dependence on the reciprocal correlation radius $\varkappa$, and then the dimensionality of $\Gamma_3(0)$, as will be shown below, is such that this vertex does not vanish compared with $\Gamma_4(0)$, and remains essential in the critical region, where

$$\Gamma_3(0, \varkappa) \sim g_3^* \varkappa^{(3-3\eta)/2}, \quad \Gamma_4(0, \varkappa) \sim g_4^* \varkappa^{1-2\eta}. \tag{5}$$

Here g_3^* and g_4^* are the coordinates of the fixed point of the renormalization-group equations for the Hamiltonian (2). Substituting the asymptotic expressions (5) in expression (4) for Φ and recognizing that the reciprocal susceptibility is $r \sim \varkappa^{2-\eta}$, we get

$$\Phi \sim \varkappa^{2-\eta}\langle Q\rangle^2 \Big(\frac{1}{2!} + \frac{1}{3!} g_3^* \varkappa^{-(1+\eta)/2}\langle Q\rangle + \frac{1}{4!} g_4^* \varkappa^{-1-\eta}\langle Q\rangle^2 + \ldots \Big). \tag{6}$$

We see that the phase transition is continuous if it is assumed that $\langle Q\rangle \sim q\varkappa^{(1+\eta)/2}$ and the following condition is satisfied

$$\frac{1}{2!} + \frac{1}{3!} g_3^* q + \frac{1}{4!} g_4^* q^2 + \ldots > 0. \tag{7}$$

In this case the critical fluctuations "smear out" the minimum of Φ at $\langle Q\rangle = Q^*$ so strongly that no phase transition occurs all the way to $\varkappa = 0$.

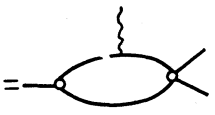
Thus, the phase transition in the S model can be continuous if there exists a gauge-invariant solution (5) for which the condition (7) is satisfied. We note that the condition (7) limits substantially the region of admissible values of g_3^* and g_4^*, so that the statement made in Ref. 22 that the very presence of fixed points of the renormalization-group equations already ensures the existence of a second-order phase transition in the three-component Potts model is incorrect.

2. GAUGE-INVARIANT PROPERTIES OF THE S MODEL

It is easy to show within the framework of the ε-expansion procedure ($\varepsilon = 4 - d \ll 1$) that the triple vertex $\Gamma_3(0)$ greatly influences the critical behavior of the S model. We calculate to this end the gauge dimensionality of $\Gamma_3(0)$ near the fixed point $\Gamma_4(0) = \Gamma_4^*$. It is convenient to illustrate the calculation using as an example the three-component model, where the stable fixed point is isotropic and Γ_4^* is given by

$$\Gamma_4^* \sim \varepsilon \varkappa^\varepsilon + O(\varepsilon^2). \tag{8}$$

The behavior of $\Gamma_3 \equiv \Gamma_3(0)$ at $\Gamma_3^2 \ll \Gamma_4 \varkappa^2$ is described by the normalization-group equation linearized in Γ_3

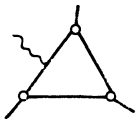
$$\frac{\partial \Gamma_3}{\partial \varkappa^2} =$$  , (9)

where the wavy line means differentiation with respect to $\varkappa^2$ and the vertex $\Gamma_4(0)$ must be replaced by its asymptotic form (8). The solution of (9) is then

$$\Gamma_3 \sim (\varkappa^2)^{\alpha_3}, \quad \alpha_3 = {}^3/_{10}\varepsilon + O(\varepsilon^2). \tag{10}$$

Substituting this solution in (4) we see that the term $\Gamma_3(0)\langle Q\rangle^3$ decreases with temperature more slowly than $\varkappa^{2-\eta}\langle Q\rangle^2$, and consequently the relative contribution of Γ_3 in the critical region increases. It can be similarly verified that at $s > 3$ the fixed points for which $\Gamma_3^* = 0$ are also unstable with respect to Γ_3 (Ref. 16). This instability, however, still does not mean the phase transition must be of first order, since expression (10) is valid only at small values $\Gamma_3^2 \ll \Gamma_4 \varkappa^2$. Therefore, if a fixed point exists such that $(g_3^*)^2 \gg g_4^*$, then the asymptotic form of Γ_3 is (5) and not (10), and if the condition (7) is satisfied a second-order phase transition is possible.

The possible existence of such a phase transition is indirectly indicated by the presence of a fixed point when account is taken of the renormalization of one vertex Γ_3 (without Γ_4). The equation of the renormalization group for the invariant charge $g_3 \sim \varkappa^{(d-6+3\eta)/2}\Gamma_3(0)$ takes in the lowest order in g_3^2 the form

$$\frac{\partial g_3}{\partial t} =$$ 

$$= \frac{6-d-3\eta}{4} g_3 + (s-3) g_3^3, \quad t = -\ln \varkappa^2, \tag{11}$$

where $\eta = \eta(g_3^2)$. It has a nontrivial fixed point:

$$(g_3^*)^2 = (6-d)/(10-3s). \tag{12}$$

Generally speaking, Eq. (11) is correct only at $6 - d = \varepsilon \ll 1$, for in this case the remaining vertices in the critical region are negligible and we can confine ourselves to the lowest-order approximation in the renormalization group, by virtue of the smallness of g_3^*. We note, however, that the fixed point at $s = 3$ is preserved upon continuation into three-dimensional space and in the next order in ε.[23] However, the solution (12) at $s = 3$ is unsatisfactory from the physical point of view, since the condition (7) is obviously not satisfied when Γ_4 is discarded, and the model becomes unstable to precipitation of a condensate. At the same time, as $s \to 1$ (the percolation problem), the solution (12) is perfectly acceptable, for in this case the order parameter $\langle Q\rangle$ has the meaning of the probability of the existence of an infinite cluster, and consequently $\langle Q\rangle \geqslant 0$ and the minimum of Φ corresponds to $\langle Q\rangle^* = 0$, so that condition (7) drops out.

When a microscopic similarity theory is constructed for the percolation problem it is important to know whether the solution (12) changes qualitatively on going to $d = 3$, owing to the presence of the vertex Γ_4, which usually determines the critical behavior of the system at $d \leqslant 4$. Whether Γ_4 is significant or not at the critical point determines, for example, the form of the equation of state near the percolation threshold. The role of Γ_4 can be explained by calculating its anomalous dimensionality in the "non-Gaussian" basis (12) at $\varepsilon = 6 - d \ll 1$. This is technically somewhat more complicated than the calculation of Γ_3 near the "Heisenberg" fixed point (8), since it is necessary to renormalize simultaneously four operators A_i having the same dimensionality:

$$A_1 = S_{ijkl}\varphi_i\varphi_j\varphi_k\varphi_l, \quad A_2 = F_{ijkl}\varphi_i\varphi_j\varphi_k\varphi_l,$$
$$A_3 = \varkappa^{-\varepsilon/2}\Omega_{ijk}\varphi_i\varphi_j\nabla^2\varphi_k, \quad A_4 = \varkappa^{-\varepsilon}(\nabla^2\varphi)^2.$$

The renormalization factors A_i for the multiplicatively renormalizable parts are not independent. We must therefore introduce a nondiagonal renormalization matrix A_{ik}:

$$\Gamma_{4,i}^{(R)}(g_3, \varkappa) = \sum_{k=1}^{4} Z_{ik} Z^2 \Gamma_{4,k}(\lambda_0, \varkappa). \tag{13}$$

Here $\Gamma_{4,i}^{(R)}$ and $\Gamma_{4,i}$ are respectively the renormalized and unrenormalized four-point vertices containing as an insert the operator A_i, and z is the renormalization constant of the Green's function. In the critical region, the vertices $\Gamma_{4,i}^{(R)}$ are subject to a matrix (since z_{ik} is not diagonal) renormalization-group equation, so that the power-law asymptotic form is possessed not by the $\Gamma_{4,i}^{(R)}$ themselves, but by their linear combinations (scaling fields) $\tilde{\Gamma}_{4,i}^{(R)}$, which diagonalize the renormalization-group equations:

$$\tilde{\Gamma}_{4,i}^{(R)} \sim \varkappa^{-\lambda_i - 2\eta}. \tag{14}$$

Since the four-point diagram Γ_4 is made up of diagrams that contain only Γ_3^* (12) (without the A_i insert) and is proportional to $\varkappa^{-2+\varepsilon-2\eta}$, the increments of the type $S\varphi^4$ and $F\varphi^4$ to the Hamiltonian do not influence the gauge-invariant behavior that is determined by the triple vertex Γ_3^* alone if

$$2 - \varepsilon - \lambda_i > 0. \tag{15}$$

The scheme for calculating the anomalous dimensionalities λ_i is described in detail in Ref. 24, and we present here only the result: As $s \to 1$, all $\lambda_i < 0$ even as $\varepsilon \to 3$; the condition (15) is satisfied, and consequently the fixed point (12) can actually describe the scale invariant behavior in the phase transition of the percola-

$$\lambda_1=-\varepsilon, \quad \lambda_2=-\varepsilon+\eta,$$

$$\lambda_\pm=\frac{\varepsilon}{3(10-3s)}[(19s-66)\pm(81s^2-348s+1156)^{1/2}]. \tag{16}$$

tion problem. It follows therefore than an equation of state of the "linear model" type is valid near the percolation threshold (at least within the framework of the ε-expansion—for details see Ref. 17). At $s=2$ we have $\lambda_+=0$ and $s>2$ we have $\lambda_+(s)>0$, so that to study the critical behavior of the S model in this case we must consider the evolution, with temperature, of the vertex parts of the operators $\Omega\varphi^3$, $S\varphi^4$, and $F\varphi^4$ jointly.

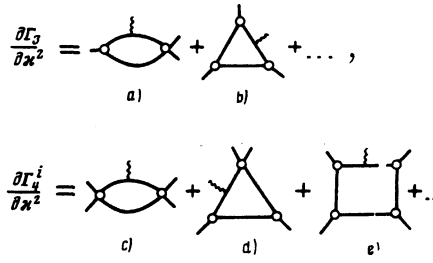
This conclusion, obtained by calculating the dimensionality of Γ_4 in a hypothetical $(6-\varepsilon)$-dimensional space, agrees with the natural physical requirement for the need of taking Γ_4 into account $s>2$ if the stability condition (7) is to be satisfied. We shall present below arguments that are not connected with perturbation theory and confirm that the gauge-invariant properties of the S model are substantially different at $s-1$ and $s>2$.

3. RENORMALIZATION-GROUP EQUATIONS FOR THIRD AND FOURTH ORDER VERTICES

To analyze the critical behavior of the S model at $s\geq 2$, we write down the system of renormalization group equations for the renormalized vertices

$$\Gamma_3=\Gamma_3(p_i=0, \varkappa), \quad \Gamma_4^i=\Gamma_4^i(q_i=0, \varkappa)=\{u_R, f_R\}.$$

We have



(17)

Usually the solution of the renormalization-group equations provides a qualitatively true picture of the phase transition even in the lowest approximation. Without claiming numerical accuracy of the results, we assume nevertheless that in the S model, too, the phase transitions can be satisfactorily described with only the single-loop diagrams cited in (17). Using the definitions (1)–(3), we obtain for the combinatorial factors of diagrams a to e the values 3/2, 1, 3/2, 6, and 3, and for the corresponding tensor contractions

$$\begin{aligned}
&\text{a)}\ [{}^2/_3 u_R+s(s-2)f_R]\Gamma_3\Omega_{ijk},\\
&\text{b)}\ s^2(s-3)\Gamma_3^2\Omega_{ijk},\\
&\text{c)}\ \left[\frac{(s+7)}{9}u_R^2+\frac{2s(s-1)}{3}u_Rf_R+s^2f_R^2\right]S_{ijkl}\\
&\quad+[{}^4/_3 u_Rf_R+s(s-2)f_R^2]F_{ijkl},\\
&\text{d)}\ \left[\frac{s^2(s-4)}{3}u_R+s^3f_R\right]\Gamma_3^2S_{ijkl}+\left[\frac{2s}{3}u_R+s^2(s-3)f_R\right]\Gamma_3^2F_{ijkl},\\
&\text{e)}\ 2s^4\Gamma_3^4S_{ijkl}+s^3(s-4)\Gamma_3^4F_{ijkl}.
\end{aligned} \tag{18}$$

The derivatives of the integrals $\partial I_k/\partial\varkappa^2$ in the system (17) (k is the number of Green's functions in the diagram prior to differentiation with respect to $\varkappa^2$) are expressed in terms of the Γ function and are equal to

$$\frac{\partial I_k}{\partial\varkappa^2}=-\frac{\Gamma(k+1-d/2)}{2^d\pi^{d/2}\Gamma(k)(\varkappa^2)^{k+1-d/2}}. \tag{19}$$

A change to dimensionless invariant charges

$$g=s^2\frac{\partial I_3}{\partial\varkappa^2}\varkappa^{d-6}\Gamma_3^2, \quad u=\frac{1}{3}\frac{\partial I_2}{\partial\varkappa^2}\varkappa^{d-4}u_R,$$

$$f=\frac{s}{3}\frac{\partial I_2}{\partial\varkappa^2}\varkappa^{d-4}f_R,$$

causes Eqs. (17) to take the form[17]

$$\begin{aligned}
\frac{\partial g}{\partial t}&=\frac{6-d-3\eta}{2}g-3g[2u+3(s-2)f]+2(s-3)g^2,\\
\frac{\partial u}{\partial t}&=\frac{4-d-2\eta}{2}u-\left[\frac{(s+7)}{2}u^2+3(s-1)uf+\frac{9}{2}f^2\right]+2g[u(s-4)+3f]-2Dg^2,\\
\frac{\partial f}{\partial t}&=\frac{4-d-2\eta}{2}f-3\left[2uf+\frac{3}{2}(s-2)f^2\right]+2g[2u+3(s-3)f]-(s-4)Dg^2.
\end{aligned} \tag{20}$$

Here $t=-\ln\varkappa^2$, $D=2(8-d)/3(6-d)$ and the function $\eta(g)$ is given by

$$\eta(g)={}^1/_3(s-2)g. \tag{21}$$

In accord with the conclusion of Sec. 1, the investigation of the character of the phase transition calls for a determination of the fixed points of the system (20) and for checking the condition (7) for these points. This procedure simplifies greatly at $s=2$ and $s=3$, when the symmetry of the model admits of the existence of only one fourth-order invariant. In terms of the contractions of the vectors e^α, this symmetry requirement manifests itself in the fact that we have $S_{ijkl}=2F_{ijkl}$ at $s=2$ and $S_{ijkl}=(9/2)F_{ijkl}$ at $s=3$. Therefore for the case $s=2$ the equation for the only fourth-order coupling constant $\lambda\equiv u+f$ we obtain, adding the last two equations of the system (20),

$$\frac{\partial\lambda}{\partial t}=\frac{4-d}{2}\lambda-\frac{9}{2}\lambda^2. \tag{22}$$

We see that the charge g drops out of Eq. (22), which is the renormalization-group equation for the continual Ising model. It is clear that this property is preserved in the higher orders of perturbation theory, since it is the consequence of symmetry: they hypertetrahedron group degenerates at $s=2$ into the inversion group S_2, which has no odd invariants. From Dyson's equation for the mass operator it follows that the charge g makes no contribution to the renormalization of the Green's function.

Thus, at $s=2$ the triple vertex has no effect whatever on the behavior of real physical quantities, and this behavior is determined only by the stability of the finite point of Eq. (22). It is obvious from (22) that $\Gamma_4^*\sim\varkappa^{4-d}$ at $s=2$, and consequently [cf. (16)] the result that $\lambda_+(2)=0$, obtained in Sec. 2 by perturbation theory in hypothetical $(6-\varepsilon)$-dimensional space, is in fact not connected with perturbation and is exact. A discussion of the generally trivial case $s=2$ was useful to us for a comparison of the scaling properties of the S model as $s-1$ and at $s>2$. As will be shown below, at $s=3$ the renormalization group equation have fixed points with $\Gamma_3^*\neq 0$ and $\Gamma_4^*\neq 0$, therefore the conclusion in Sec. 2 that

$\lambda_+(3) > 0$ is confirmed. It is natural to assume that on the segment [1, 3] the function $\lambda_+(s)$ is monotonic.[4)] Then $\lambda_+(s)$ reverses sign at $s=2$ and is negative as $s \to 1$. The condition (15) is then satisfied, and consequently the similarity properties of the percolation problem are determined only by the triple vertex.

In the case $s=3$, the system (20) again reduces to two equations for g and $L \equiv u + (3/2)f$ (L is the invariant charge of the only (isotropic) fourth-order vertex):

$$\frac{\partial g}{\partial t} = \frac{6-d}{2} g - 6gL - \frac{g^2}{2},$$
$$\frac{\partial L}{\partial t} = \frac{4-d}{2} L - 5L^2 + \frac{11}{3} gL - \frac{1}{2} Dg^2. \qquad (23)$$

Renormalization-group equations at $s=3$ were derived also by Zaprudskiĭ.[22] Unfortunately, the values of the combinatorial factors indicated by him for diagrams d and e [see (17)] are smaller than the true ones by factors 2 and 6, respectively, and this affects the numerical results in the determination of the fixed points and the critical exponent γ of the susceptibility. An additional difference between the system (23) and the renormalization group equations of Zaprudskiĭ is that in (23) account is taken of the contribution due to the renormalization of the Green's function, neglected in Ref. 22. The system (23) has besides the stable "Gaussian" (see Ref. 10) and "Heisenberg" fixed points with $g^*=0$ also two other fixed points, A_+ and A_-, whose coordinates are real at $d < d_c \approx 4.00$:

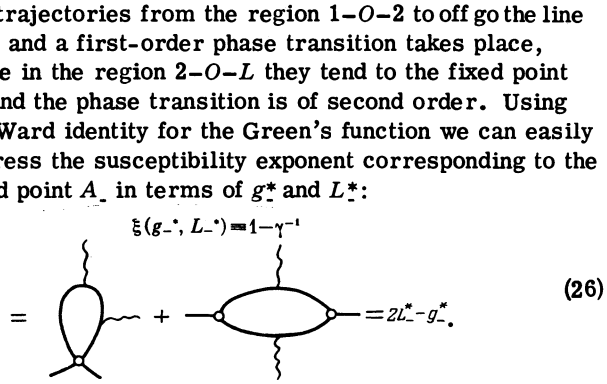
$$L_\pm^* = \frac{6-d-g_\pm^*}{12},$$
$$g_\pm^* = \frac{6-d}{678-97d}\{6(25-4d) \pm (673d^2 - 7296d + 18432)^{1/2}\}. \qquad (24)$$

The fixed point A_+ turns out to be a saddle, and A_- a stable focus. In our first-order approximation in the renormalization group, the condition (7) reduces to the absence of real roots of the quadratic equation and takes the form

$$g^* < 27/2 L^*, \qquad (25)$$

Both fixed points A_+ and A_- land in this case in a region of values of g and L which is free of the appearance of a condensate.

The phase trajectories of the system (23) (at $d=3$) is shown in the figure. The line $1-O$ corresponds to the condition (25), and in our approximate a first-order phase transition into the ordered phase takes place on it. The phase trajectory $2-O$, which passes through the fixed point A_+, divides the phase plane into two parts; the trajectories from the region $1-O-2$ to off go the line $1-O$ and a first-order phase transition takes place, while in the region $2-O-L$ they tend to the fixed point A_- and the phase transition is of second order. Using the Ward identity for the Green's function we can easily express the susceptibility exponent corresponding to the fixed point A_- in terms of g_-^* and L_-^*:



(26)

In three-dimensional space we get $\xi = 0.25$ and $\gamma = 1.33$. Substituting $g = g_-^*$ in (21), we get $\eta = 0.07$.

We discuss now the connection between the foregoing results for the continual three-component model and its initial lattice version. The lattice model can be represented with the aid of functional integration in the form of a field theory with a nonpolynomial interaction potential in which all the nonrenormalized constants are rigorously connected with one another.[5)] We do not know whether we can confine ourselves in the description of a phase transition in the lattice model to the expansion terms written out in (2), but if the Hamiltonian (2) can be used for this purpose, then it will correspond to the lattice model only at a definite relation between the values of λ_0, u_0, and f_0. Therefore the kinetic behavior of the lattice model will be described by some single phase trajectory of the system (23).

Our value $\gamma = 1.33$ is much larger than the $\gamma = 0.9 - 1.0$ obtained from numerical calculations for the lattice model.[6)] [9,13,25] of course, it is perfectly possible that this discrepancy is due to the excessively low accuracy of our lower-bound renormalization-group approximation. However, a study of the phase diagram of the solutions of (23) (see the figure) shows that the discrepancy can be due to special properties of the model itself.

We note first that the fixed point A_- is a focus, and therefore oscillating additions to the scaling appear. Although they decrease as $T \to T_c$, they can hinder the reduction of the temperature-field expansions by, say, the Padé method. Second, the phase trajectory corresponding to the lattice model can pass in the region $1-O-2$, but somehow close to the fixed point A_+. Then, even if a first-order phase transition takes place, the behavior of the thermodynamic quantities near T_c will be describd by the effective critical exponents corresponding to this fixed point. Calculation yields $\gamma = 0.6$ for the fixed point A_+. This, too, is quite far from the values (given in Refs. 9, 13, and 25); nevertheless, both cited causes of the discrepancy seem worthy of attention.

We note that the phase diagram given in Ref. 22 has a separatrix that passes through a "Heisenberg" fixed point and a fixed point of type A_+, so that as a result there exists a region of small values of the coupling constant of the quadrupole vertex, for which the phase transition is of first order no matter how small coupling constant of the triple vertex. This led in Ref. 22 to the conclusion that the results of Golner's computer calculations,[14] which revealed a first-order phase transition, can be attributed to the choice of too small a value of the coupling constant for the first-order term in the nonrenormalized Hamiltonian. In fact, however, there is no such separatrix (even for the renormalization-group equations used in Ref. 22), and the phase diagram is of first-order for the values of the nonrenormalized coupling constants in the region $1-O-2$ (see the figure), and the transition to the disordered phase, in our renormalization-group approximation, follows the line $1-O$ and not $L-0$ as indicated in Ref. 22. Therefore Golner's result can be due either to the insufficiently small triple coupling constant at the chosen quadruple

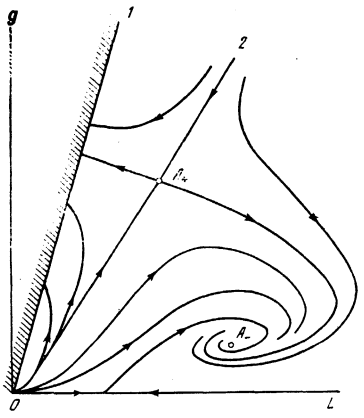


FIG. 1. Phase diagram of the system of renormalization-group equations (23). In the shaded area the symmetrical (degenerate) state is thermodynamically unprofitable.

one, or to the fact that the approximate integral formula which he used does not describe well enough the critical behavior of the S model.

We consider now the properties of the phase transition in the S model at $s>3$. Since the fixed points of the system (20) with $g^*=0$ are unstable relative to small g,[16] the second-order phase transition can be due only to the presence of a fixed point with $g^*\neq 0$. At $s>3$ the fourth-order invariants in the S model are independent, and therefore the search for such fixed points by making two substitutions in (20) reduces to solution of a fourth-order equation for the value of f^* at the sought fixed point. Inasmuch as this equation is very cumbersome for arbitrary $s>3$, we write down first the equation for $s=4$, and also put immediately $d=3$:

$$2525f^{*4}+1556f^{*3}+504.5f^{*2}-86.44f^*+3.28=0. \quad (27)$$

This equation has no real roots,[7)] and consequently there are no fixed points with $g^*\neq 0$ for $s=4$. By virtue of the instability of the remaining fixed points (with $g^*=0$) this means that in the three-dimensional four-component S model only a first-order phase transition is possible. We have ascertained in similar fashion that at $s=5$ and 6 there are likewise no real fixed points with $g^*\neq 0$. At large values of s the results of the average-field theory are valid (it predicts a first-order phase transition[26]), so that it is natural to assume that the phase transition will be of first order also at $s>6$.

The fact that fixed points with $g^*\neq 0$ exist in the case $s=3$ but not at $s>3$, while obtained by solving the renormalization group equations in the lowest approximation, does not seem fortuitous to us. It is apparently connected with the various symmetry properties of the S model at $s=3$ and $s>3$. In fact, it is easy to verify that even at $s=3$ there are *no* real values of u^*, f^*, and $g^*\neq 0$ such that the right hand sides of all *three* equations in (20) vanish, i.e., in the space of the three variables u, f, and g there are no fixed points with $g^*\neq 0$ either at $s>3$ or at $s=3$. At $s=3$, however, the group C_3 admits of a smaller number invariants than the permutation group at $s>3$, and this leads to degeneracy of the system (20) into the system (23) and makes the space of the renormalization-group variables two-dimensional. We see that it is not simply the parametric dependence of the coefficients in the renormalization group equations on s, but certain distinct symmetry properties of the three component model which cause the character of the phase transitions in this model to be different than in models with $s>3$.

CONCLUSION

A large class of systems for which the magnetic and structural phase transitions are described by the continual three-component S model is made up of crystals with cubic sy-metry and three easy axes. In particular, this model is applicable to a number of compounds having a general structure A-15, such as Nb_3Sn, Nb_3Al, V_3Si, V_2Si, and others, in which a martensitic phase transition from the cubic to the tetragonal phase takes place.[8)] Experiment has revealed in the properties of these crystals, near the phase transition, strong temperature anomalies that point to a proximity of the phase transition to a continuous one.[27] The predictions of the Landau theory can then be reconciled with the experimental temperature dependences only by assigning to the coefficient of the cubic term of the free-energy expansion a value much lower than obtained from estimates based on microscopic considerations. Using the results obtained by us above, that continuous or near-continuous phase transition in systems having the symmetry of the three-component S model are possible, it is natural to assume that the smallness of γ_3, which is common to the different compounds, is due to strong interaction of the fluctuations that lead, by virtue of the special symmetry properties of the three-component S model, to an effective decrease of γ_3 in the critical region.[9)]

Arguments have been advanced[28] that the phase transition in cubic ferromagnets (Fe, $PrAl_2$, $NdAl_2$, and others) to which a small magnetic field (of the order of the anisotropy field) is applied along the [111] diagonal, is also described by the three-component S model. The question of the order of the phase transition in this model is of great interest and therefore, in view of the indication[28] that this model is physically realizable in cubic crystals, an attempt was made[29] to determine a number of phase transitions experimentally. To this end, the EPR method was used to investigate the properties of the structural phase transition from the trigonal ($R\bar{3}c$) phase into the tetragonal ($I4/mcm$) in $SrTiO_3$ under pressure applied in the [111] direction. It was found that the phase transition is of first order, but owing to the strong fluctuations the exponent of the discontinuity of the order parameter differs from the Landau value and is in fair agreement with the prediction of the renormalization-group method. Thus, the existence of a region of the type 1–O–2 in the three-component S model can be regarded as experimentally proved. Unfortunately, as is clear from Ref. 29 itself, this method cannot be used to study the critical behavior of the S model at very small values of the triple coupling constant, for in this case the phase transition occurs in the vicinity of a bicritical point on the phase diagram, where the effective Hamiltonian is of "Heisenberg" rather than S-model form. The question whether the phase transition becomes continuous at small unrenormalized values of the triple vertex remains open and should

be experimentally investigated.

In addition to those mentioned, there are also other physical systems in which the phase transition is described by the S model, for example the phase transition in HoSb.[30] A common feature of these phase transitions is that they are close to continuous. We have shown in this paper that this behavior can be explained within the framework of the renormalization-group method. We have also verified that a microscopic similarity theory can be constructed for the percolation problem by taking into account only one triple vertex. Inasmuch as in this case we have in the first-order renormalization-group approximation $\Delta \equiv \beta + \gamma = 2$, the equation of state for dilute ferromagnets at low temperatures near the percolation threshold can be expressed in a form similar to the "linear model." This form of the equation of state makes it possible to obtain expressions for the susceptibility and the heat capacity as functions of the magnetic field and the concentration, so that these formulas can be verified experimentally. We emphasize in conclusion that while it is, of course, difficult to assess the reliability of numerical results of the solution of the renormalization-group equations in first-order approximation, the qualitative features of the solution, such as the appearance of fixed points with $\Gamma_3^* \neq 0$ at $s=3$ and their absence at $s>3$, as well as the fundamental difference between the scaling properties of similarity theory for the percolation problem from the properties of the three-component model, are apparently valid by virtue of their symmetry origin.

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[1)] A model with four states per site, including the case $s=4$ of the Potts model, was investigated even earlier by Ashkin and Teller.[2]

[2)] T_c was later obtained also for triangular and hexagonal lattices.[3]

[3)] See, e.g., the results of the calculation of the critical isotherm in Ref. 13.

[4)] In fact, tensor contractions for any diagram of the S model are monotonic functions of s, and we think it most unlikely that the exact function $\lambda_+(s)$ would have a minimum at $s=2$. Formula (16) obtained by perturbation theory agrees with this point of view.

[5)] In analogy with the well known representation for the Ising model.

[6)] It was found in Ref. 22 by the renormalization-group model that $\gamma \approx 1.1$, and good agreement with the numerical calculations was noted. Actually, however, there is no such agreement, and the reasons are explained in the text following Eqs. (23).

[7)] We have verified that there are none not only at $d=3$ but also at all $d<6$. The expressions for the coefficients as functions of d are not given in the text, again because they are too cumbersome.

[8)] The temperature of this phase transition is somewhat lower than the temperature of the superconducting phase transition.

[9)] It is interesting to note that a value $\gamma \approx 0.86$ was obtained experimentally for Nb_3Sn; this is quite close to the numerical value for the lattice model.

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