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Renormalization of nonlocal degrees of freedom

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Abstract

The renormalization in real space of systems with nonlocal degrees of freedom is discussed and reviewed for the percolation model, for which the degrees of freedom, the clusters, are nonlocal and span all ranges in the system. Previous attempts, including recent ones, are critically examined and shown to lack a theoretical basis; in particular, they do not consider the partition function. It is demonstrated that, in contrast to the case of local degrees of freedom, all ranges of the degrees of freedom must be considered when eliminating nonlocal degrees of freedom at short distances. New couplings are naturally generated, and lead to a mapping between clusters in the original and renormalized systems, and thus to the renormalization-group equations. Remaining questions are discussed.

Keywords: Renormalization-group theory; Nonlocality; Percolation

1. Introduction

The renormalization-group theory of phase transitions was originally developed [1] to solve problems with infinitely many degrees of freedom, which exhibit fluctuations over infinitely many scales. Typical of these problems is that of fluids and magnets at a critical point, at which thermal fluctuations occur over all scales of length. In the case of a magnet, for example, the local degrees of freedom are the spins attached to the sites of a lattice, which interact with each other by typically short-ranged forces.

The strategy of renormalization-group theory is to evaluate the free energy in steps, integrating out the fluctuations step by step, starting with fluctuations on the smallest scale of length (the atomic scale) and successively treating the fluctuations on increasingly larger scales of length, until fluctuations on all scales of length have been dealt with. The problem was originally solved in momentum space for continuous spins, and since then these original methods have been applied to determine the critical behavior of numerous models of phase transitions with local degrees of freedom [2]. For models with local degrees of freedom which are discrete rather than continuous,

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renormalization-group methods were developed in real space and applied successfully to the two-dimensional Ising model of a uniaxial magnet [3a, b].

Probably the simplest system with nonlocal degrees of freedom which displays a critical phase transition is the percolation model. In its site version, the sites of a lattice are, respectively, occupied or empty with probability p or $1 - p$, independently of each other. Occupied sites which are nearest neighbors are grouped into clusters. For small values of p, only finite clusters are present in the infinite lattice; the percolation transition occurs at a critical value of p, p_c, at which an infinite cluster first appears in the system. For $p > p_c$, there is, with certainty, an infinite cluster in the system.

The cluster observables are calculated from a generating function or cluster size distribution, equivalent to the free energy of a magnetic system in the presence of an external magnetic field

$$f(p, h) = \sum_{|\gamma|} \sum_{|\partial\gamma|} 1/|\gamma| A_{|\gamma|,|\partial\gamma|} p^{|\gamma|}(1 - p)^{|\partial\gamma|} e^{-h|\gamma|}, \tag{1}$$

where $A_{|\gamma|,|\partial\gamma|}$ is the number of clusters of size $|\gamma|$ and perimeter $|\partial\gamma|$ containing an arbitrary fixed site, and h is the external field. The external field is represented by an external site independently connected by a bond to each lattice site in a random way, a bond being present with probability $1 - e^{-h}$ and absent with probability e^{-h}. The function $f(p, h)$, according to whether h is zero or not, represents the average number of clusters per site in the absence or presence of the external field h.

From the free energy given by (1), it is seen that the degrees of freedom over which we must sum are by essence nonlocal, being the clusters of size $|\gamma|$ and perimeter $|\partial\gamma|$ containing an arbitrary fixed site.

2. Nonlocal versus local degrees of freedom

To understand the origin of the difficulties associated with the renormalization of nonlocal degrees of freedom, it is useful to recall how one is able to renormalize in real space local degrees of freedom such as those of the Ising model.

The basic relation underlying the method of Niemeijer and van Leeuwen [3a] is

$$e^{H'(s')} = \sum_{\sigma} e^{H(s', \sigma)}, \tag{2}$$

which expresses the mapping of the Hamiltonian of an Ising model to that of a new Ising model in which the spins are grouped into cells and a spin degree of freedom s' is attached to each cell; $H(s', \sigma)$ is the Hamiltonian $H(s)$ of the site system where the site spin variables s are expressed in terms of the new variables s' and σ, and $H'(s')$ is the Hamiltonian of the cell system. It is readily seen by summing both of its sides over s' that relation (2) satisfies the fundamental requirement of renormalization-group theory [4] that the free energy be conserved.

All degrees of freedom in both the site and cell systems, namely s, σ and s', are local degrees of freedom attached to a site or to a cell, and the renormalization-group equation (2) is obtained by partially summing over these local degrees of freedom in the original system.

In contrast to this case, due to the nonlocal character of the degrees of freedom of the percolation model, it is not possible to perform, as one does for local degrees of freedom such as those of the Ising model, a summation over degrees of freedom at short distance in the original system and obtain, even in principle, an accurate renormalization-group equation of the type of (2).

If one sums nonlocal degrees of freedom over short ranges, without taking into account the fact that the degrees of freedom span all ranges, one is led to a renormalized cluster probability distribution of a given cluster which contains only partial information about the system and not, as in the case of the Ising model, to the Boltzmann distribution. Such an incorrect procedure will obviously be dependent on the structure of the lattice, and the topological structure of the clusters will not be preserved upon renormalization, so that the free-energy conservation requirement will be violated as well.

It is a fundamental property of renormalization-group theory [1] that new couplings are naturally generated. That additional coupling constants must necessarily be generated in a renormalization-group transformation – in fact infinitely many, at the thermodynamic limit – can be seen from an elementary physical argument. Consider, indeed, two systems which are identical up to their sizes. Clearly, their partition functions will differ and so will their free energies, the later by a factor equal to the size ratio (extensivity). Consequently, the only way the partition functions (free energies) of both systems can be made invariant, i.e., be the same, is by adding new coupling constants. Exceptions to this general rule only occur in very special cases, such as the one-dimensional Ising model with nearest-neighbor couplings, which can be exactly renormalized by modifying a single coupling, without adding new ones [4].

Previous attempts [5] to renormalize the percolation model in real space, together with their numerous applications to scientific and engineering problems exhibiting percolative behavior [6], lack a theoretical basis. This is because instead of considering the partition function and summing over its degrees of freedom [1], and consequently deriving the appropriate renormalization-group equations for the coupling constants, these schemes directly focus on the coupling constants – usually one, sometimes two – in an arbitrary fashion, and rescale them in an ad hoc way. It has even been said by authors of these previous attempts that since one could do well with a single coupling constant, why bother with additional ones, as they only complicate matters!

The same features of earlier schemes characterize the "large-cell' and the recent "cell-to-cell" renormalization-group transformations, which do not consider the partition function, and violate basic principles by postulating a renormalization-group relation involving a single coupling [5h,i].

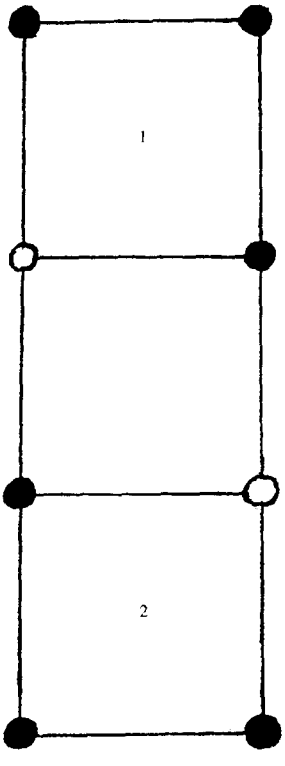

Fig. 1. A disconnected configuration, which does not define a cluster and thus does not contribute as such to the free energy given by Eq. (1), although it apparently "renormalizes" to a cluster, since cells 1 and 2 are occupied and nearest neighbors.

Restricting onself to taking only a single coupling constant into account [5] is tantamount to making Kadanoff's assumption [7] of nearest-neighbor coupling in the Ising model, without reference to Wilson's subsequent discovery [1,2] that additional couplings must be present in the renormalized system.

While the necessity of introducing new couplings when renormalizing the percolation model has recently been briefly mentioned [8a], in particular, to correct inconsistent predictions of renormalization-group transformations based on a single coupling [8b], no method has been developed for constructing appropriate renormalization-group equations.

Heuristic arguments commonly given for the necessity of additional couplings are misleading. For example, Fig. 20(a) of Ref. [9 p. 80], shows a configuration of two clusters in the original system, which "renormalize" to a single cluster. A similar configuration is shown here in Fig. 1 (cell occupancy is defined by a minimum of three sites being occupied). These examples are not appropriate, because such configurations are not clusters and thus do not contribute to the partition function (free energy of Eq. (1)) of the system.

It thus comes as no surprise that the numerical results [5a–e,h,i] obtained by such procedures are haphazard, although they may be accidentally accurate. These fortuitous numerical successes have unfortunately been taken by most authors as proofs of the validity of such procedures (see, for example, [9, p. 78]), and it appears that this point of view still prevails in much of the current literature.

Further discussion of these previous schemes is made in Section 4.

3. Renormalization-group method

3.1. General method

From the above discussion, it transpires that the only way in which one can deal with the essential nonlocal character of the degrees of freedom is to consider all ranges of the degrees of freedom in the process of elimination of degrees of freedom at short distances. Since the nonlocal degrees of freedom in the percolation model are the cluster degrees of freedom, we must consider the clusters themselves in the process of constructing the renormalization group.

An exact mapping will be defined between clusters in the original and renormalized systems, and for that purpose clusters will be grouped into classes according to their topological structure. Here, the expression "topological structure" refers to the connectedness of the clusters as defined by the various couplings, as will become clear below.

As will be seen below, new couplings of a longer range than the original nearest-neighbor couplings and of a new type are generated by the renormalization-group transformation. These new couplings will provide a most natural way to perform a topological classification of the clusters [10].

To each new coupling generated by the renormalization-group transformation corresponds a topologically distinct class of clusters characterized by the topological property that the connectedness (integrity) of those clusters is lost or ill-defined by removal of that new coupling. In other words, that new coupling is essential to preserve the connectedness (integrity) of these clusters.

In order to define a mapping between the clusters in the original system and those in the renormalized system, new coupling constants must therefore be introduced in the original system. We will thus have to take into account the contribution from different clusters to each type of coupling. To each class of clusters thus defined in the renormalized system there will correspond a class of clusters of the same topological structure in the original system.

Next, consider the probability distribution of each class of clusters and sum over short-ranged degrees of freedom in the original system; this gives the probability distribution of the corresponding class of clusters in the renormalized system, and leads to the implicit renormalization-group equation for the coupling constants.

At each step, one obtains renormalization-group equations of the form

$$\boldsymbol{P}^{(i)}(p_b, r_b, s_b, \dots) = P^{(i)}(p, r, s, \dots), \quad i = 1, 2, 3, \dots, k, \tag{3}$$

where $\boldsymbol{P}^{(i)}$ ($P^{(i)}$) is the probability distribution of the ith class of clusters in the renormalized (original) system, $p, r, s, \dots$ denote the coupling constants in the original system, and p_b, r_b, s_b denote the analogous coupling constants in the renormalized system (b stands for block).

Eqs. (3) are a system of k nonlinear implicit equations in k unknowns, which define the renormalization-group flow in the space of parameters (couplings). The renormalization-group equations (3) are expected to give rise to a single nontrivial fixed point $(p^*, r^*, s^*, \dots)$ defined by

$$p^* = p_b = p\,,$$

$$r^* = r_b = r\,,$$

$$s^* = s_b = s, \text{ etc.},$$

which are solutions of Eqs. (3). Linearization of these equations about this fixed point yields k eigenvalues, of which only one is expected to be larger that one. This eigenvalue, λ_t, determines the thermal exponent y_t

$$y_t = \ln \lambda_t / \ln L\,,$$

where L is the edge length of the cells.

It is readily seen that by summing over i both sides of Eqs. (3), we obtain, up to regular terms, the total free energy of the original and renormalized systems. We return to this important point and to related matters in the discussion of Section 4.

The field exponent (fractal dimension) is obtained by studying the response of the system to a variation of the external field about $h^* = 0$ [3a,10]. One has

$$\delta[\boldsymbol{P}_{\text{tot}}(p_b, r_b, s_b, \dots, h_b)]|_{p^*, r^*, s^*} = \delta[P_{\text{tot}}(p, r, s, \dots, h)]|_{p^*, r^*, s^*}\,, \tag{4}$$

where $\boldsymbol{P}_{\text{tot}}$ and P_{tot} are the sums over the k terms of Eqs. (3), with $h \neq 0$. Linearization of (4) with respect to h about $h^* = 0$ yields the eigenvalue λ_h and thus the field exponent y_h

$$y_h = \ln \lambda_h / \ln L\,.$$

3.2. *Illustration*

The general method described above will be illustrated by the explicit construction of the renormalization-group mapping for the site percolation problem on the square lattice. In the following, the expressions "first order", "second order, ...," are used in the sense of the cluster approximation (expansion) of Niemeijer and van Leeuwen [3a] (the term "cluster" refers here to connected cells, and is not to be confused with the clusters of the percolation model).

3.2.1. First and second orders

In these cases, no new couplings are generated by the renormalization-group mappings, and there is thus only one class of topologically distinct clusters, namely, those with nearest-neighbor couplings. These mappings, respectively, lead to the renormalization-group equations

$$\boldsymbol{P}(p_b) = p_b, \qquad P(p) = p^4 + 4p^3(1-p) \tag{5}$$

and

$$\boldsymbol{P}(p_b) = p_b^2, \qquad P(p) = p^8 + 8p^7(1-p) + 14p^6(1-p)^2 . \tag{6}$$

The nontrivial fixed points are, respectively,

$$p^* = 0.768 \text{ and } 0.789 .$$

The eigenvalues of the linearized equations (5) and (6) lead, respectively, to the correlation length exponents ($\nu = y_t^{-1}$)

$$\nu = 1.40 \text{ and } 1.42 .$$

The presumed exact value is 1.33 (4/3).

Note that the first-order approximation coincides with the block-cluster approach previously developed by one of us [5f]. But in contrast to this earlier approach which, in spite of its numerical success up to the upper critical dimension of 6 [5g], retained a heuristic character, the present approximation is the lowest-order of a well-defined approximation (expansion).

3.2.2. Third order

Two new couplings are generated at this order of the approximation, as shown in Fig. 2. Fig. 2(a) illustrates a cluster in which cell 2, while not occupied, contains an occupied site which establishes a connection between next-nearest-neighbor occupied cells 1 and 3. This corresponds to the generation of a next-nearest-neighbor coupling between cells 1 and 3.

Consequently, in order to preserve the topological properties of the clusters of the original system upon renormalization, a new coupling, that is, a diagonal coupling, is introduced in the original system.

Fig. 2(b) illustrates a cluster, where cell 1 is occupied, but is not connected to its nearest-neighbor occupied cell 2. This corresponds to the generation of a bond coupling between nearest-neighbor occupied cells 1 and 2 in the renormalized system. In the case of Fig. 2(b), the bond coupling must be specified to be absent as shown by the hatched line. Consequently, a new coupling must again be introduced, namely, a bond coupling between nearest-neighbor sites.

Therefore, the addition of new couplings leads to a precise mapping between the clusters in the original and renormalized systems. In the present case of the

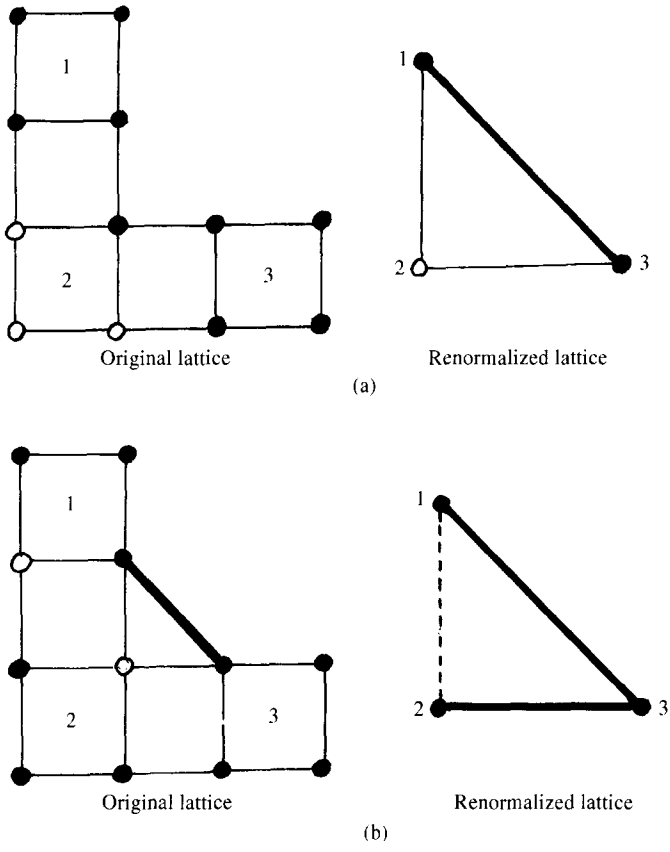

Fig. 2. Illustration of generation of new couplings by the renormalization-group transformation corresponding to Eqs. (7)–(9). ● (○) denotes occupied (empty) site or cell. (a) Cluster showing necessity of introducing next-nearest-neighbor coupling: cells 1 and 3 are occupied and connected via cell 2, which is empty. (b) Cluster in original system showing necessity of introducing nearest-neighbor bond coupling: two nearest-neighbor cells 1 and 2 are occupied, but are not connected. Empty bond coupling is shown by broken line.

third-order approximation, there are three classes of topologically distinct clusters. The first class contains those clusters in which all nearest-neighbor cells that are occupied are connected by the nearest-neighbor couplings of the original site model. In the second class, diagonal couplings are generated, while the third class contains all clusters in which nearest-neighbor bond couplings are generated.

Each cluster in the renormalized system belongs to one and only one of these classes. To each of these three classes, corresponds a class of clusters of the same topological structure in the original system. Any subset of one of these three classes of clusters in the original system maps into one and only one cluster in the renormalized system. This mapping is surjective ("onto") and defines the renormalization-group equation for the probability distributions of the corresponding classes of

clusters, which read

$$\begin{aligned} \boldsymbol{P}_{\mathrm{nn}}(p_{\mathrm{b}}, r_{\mathrm{b}}, d_{\mathrm{b}}) &= p_{\mathrm{b}}^3 r_{\mathrm{b}}^2 d_{\mathrm{b}} + p_{\mathrm{b}}^3 r_{\mathrm{b}}^2 (1 - d_{\mathrm{b}}) + 2p_{\mathrm{b}}^2 r_{\mathrm{b}} [r_{\mathrm{b}}(1 - p_{\mathrm{b}})(1 - d_{\mathrm{b}}) \\ &\quad + r_{\mathrm{b}} d_{\mathrm{b}}(1 - p_{\mathrm{b}}) + (1 - r_{\mathrm{b}}) d_{\mathrm{b}}(1 - p_{\mathrm{b}}) + (1 - d_{\mathrm{b}})(1 - r_{\mathrm{b}}) \\ &= P_{\mathrm{nn}}(p, r, d)\,, \end{aligned} \tag{7}$$

$$\begin{aligned} \boldsymbol{P}_{\mathrm{bond}}(p_{\mathrm{b}}, r_{\mathrm{b}}, d_{\mathrm{b}}) &= p_{\mathrm{b}}^2 d_{\mathrm{b}} [r_{\mathrm{b}}^2 (1 - p_{\mathrm{b}}) + 2r_{\mathrm{b}}(1 - r_{\mathrm{b}})(1 - p_{\mathrm{b}}) + (1 - r_{\mathrm{b}})^2] \\ &= P_{\mathrm{bond}}(p, r, d)\,, \end{aligned} \tag{8}$$

$$\begin{aligned} \boldsymbol{P}_{\mathrm{nnn}}(p_{\mathrm{b}}, r_{\mathrm{b}}, d_{\mathrm{b}}) &= 2p_{\mathrm{b}}^3 r_{\mathrm{b}}(1 - r_{\mathrm{b}}) d_{\mathrm{b}} \\ &= P_{\mathrm{nnn}}(p, r, d)\,. \end{aligned} \tag{9}$$

The subscripts nn and nnn stand for nearest-neighbor and next-nearest-neighbor, respectively; $p(p_{\mathrm{b}})$ is the probability that a site (cell) is occupied, $r(r_{\mathrm{b}})$ is the probability that a nearest-neighbor bond is present between two sites (cells), and $d(d_{\mathrm{b}})$ is the probability that two next-nearest-neighbor sites (cells) are connected by a diagonal bond. The left-hand sides of Eqs. (7)–(9) are most conveniently derived by referring to Fig. 3.

The exact determination of the functions $P_{\mathrm{nn}}(p, r, d)$, $P_{\mathrm{nnn}}(p, r, d)$, and $P_{\mathrm{bond}}(p, r, d)$ in Eqs. (7)–(9) requires a large number of clusters to be counted. The calculation is conveniently performed on a computer, in which all clusters are enumerated and classified as described above. Here, we present the results of a slightly approximate calculation in which a small fraction of the clusters in the original system is overcounted.

The renormalization-group equations (7)–(9) give rise to a single nontrivial fixed point (p^*, r^*, d^*) given by

$$p^* = 0.794, \qquad r^* = 0.632, \qquad d^* = 0.487\,.$$

Linearizing both sides of Eqs. (7)–(9) about the fixed point (p^*, r^*, d^*) enables us to obtain the thermal exponent by determining the eigenvalues of the 3×3 matrix

$$\begin{pmatrix} \dfrac{\partial \boldsymbol{P}_{\mathrm{nn}}}{\partial p_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{nn}}}{\partial r_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{nn}}}{\partial d_{\mathrm{b}}} \\ \dfrac{\partial \boldsymbol{P}_{\mathrm{bond}}}{\partial p_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{bond}}}{\partial r_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{bond}}}{\partial d_{\mathrm{b}}} \\ \dfrac{\partial \boldsymbol{P}_{\mathrm{nnn}}}{\partial p_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{nnn}}}{\partial r_{\mathrm{b}}} & \dfrac{\partial \boldsymbol{P}_{\mathrm{nnn}}}{\partial d_{\mathrm{b}}} \end{pmatrix}^{-1}_{p^*, r^*, d^*} \cdot \begin{pmatrix} \dfrac{\partial P_{\mathrm{nn}}}{\partial p} & \dfrac{\partial P_{\mathrm{nn}}}{\partial r} & \dfrac{\partial P_{\mathrm{nn}}}{\partial d} \\ \dfrac{\partial P_{\mathrm{bond}}}{\partial p} & \dfrac{\partial P_{\mathrm{bond}}}{\partial r} & \dfrac{\partial P_{\mathrm{bond}}}{\partial d} \\ \dfrac{\partial P_{\mathrm{nnn}}}{\partial p} & \dfrac{\partial P_{\mathrm{nnn}}}{\partial r} & \dfrac{\partial P}{\partial d} \end{pmatrix}_{p^*, r^*, d^*} .$$

The eigenvalues of this matrix are

$$\lambda_1 = 1.646, \qquad \lambda_2 = 0.594, \qquad \lambda_3 = 0.387\,,$$

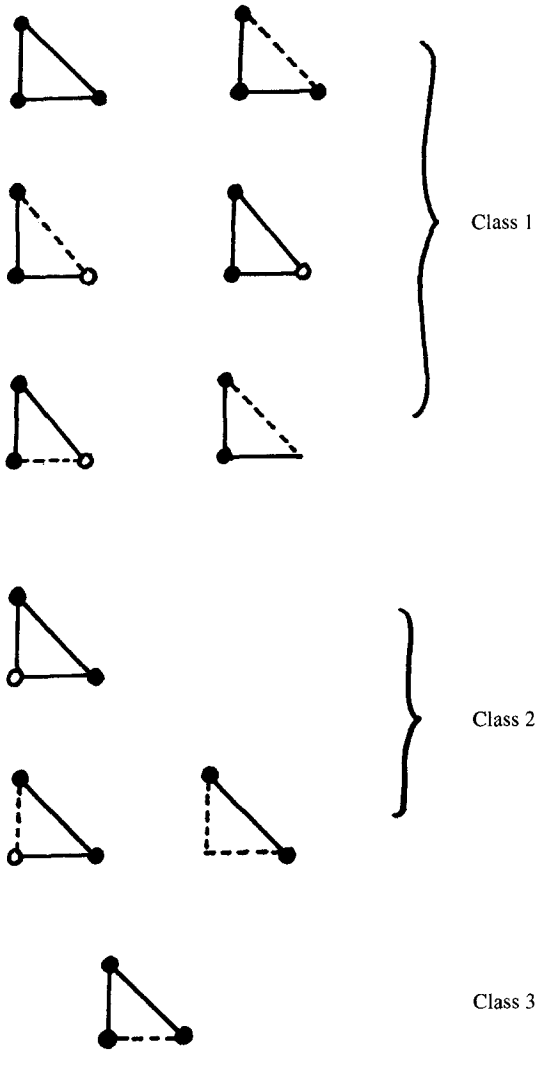

Fig. 3. Classes of clusters in renormalized system, up to symmetry operations, corresponding to Eqs. (7)–(9).

of which only one, λ_1, is relevant, i.e., larger than unity. The thermal exponent is given by

$$y_t = \ln \lambda_t / \ln 2 = 0.72 ,$$

which yields the correlation length exponent $\nu = 1.39$.

The field exponent (fractal dimension) is calculated as described above at the end of Section 3.1, and found to be, respectively, equal to 1.79, 1.81 and 1.84 in the first-, second- and third-order approximations [10]. The presumed exact value is 1.89.

4. Discussion

The renormalization in real space of systems with nonlocal degrees of freedom has been reviewed and discussed for the percolation model, and previous attempts have been critically examined. The latter were shown to lack of theoretical basis. A recent renormalization-group transformation was described which appears to have the required properties a renormalization-group transformation should have. It was shown that it is necessary to consider all ranges of the degrees of freedom when eliminating nonlocal degrees of freedom at short distances. It was then seen that new coupling constants are naturally generated, as they should be in any renormalization-group transformation [1].

The renormalization-group equations derived above possess a nontrivial fixed point and the predicted values of the critical exponents appear to converge to the presumed exact values as higher orders are considered. However, this renormalization-group method raises several questions which deserve further study.

First, one is unable to assess the effect of the higher-order couplings which are generated by the renormalization-group transformation as the system size increases. This is like in the real-space cluster-approximation renormalization-group method [3a], but is in contrast to the momentum–space renormalization-group method [1]. The present results indicate that the nearest-neighbor coupling is the strongest one, as found in earlier studies of the two-dimensional Ising model [3a,11].

It is desirable to verify this property at higher orders and for other lattice structures, such as the triangular lattice. We do not believe that the definition of cell occupancy will affect the results at the higher orders of the approximation. Also, the numerical results obtained for the third- and fourth-order [10] approximations should be tested with more refined computer algorithms.

Unfortunately, for the fourth and higher orders, such a verification may require prohibitive computational capabilities. The same difficulty characterizes the cluster-expansion method applied to the two-dimensional Ising model [3a], which becomes very laborious for large clusters. It would clearly be desirable to be able to build into the renormalization-group transformation, like in Kadanoff's decimation transformation, an arbitrary parameter which can be optimized by internal consistency considerations.

It is well known [2] that with any renormalization-group transformation, be it in momentum or real space, there is no guarantee that it will exhibit fixed points. There is not only no guarantee that the renormalization-group equations for larger systems will admit a nontrivial fixed point but also, there is no certainty that, at the limit of an infinite system, the infinite system of renormalization-group equations for the infinitely many couplings (one for each coupling, as seen above in Section 3), will remain analytic. Analyticity is of course not in question for finite systems.

The form of the renormalization-group equations (3) shows that, at the thermodynamic limit, the singular part of the free energy is split into infinitely many terms, each

term involving infinitely many couplings. It is hoped that each such term remains analytic at the thermodynamic limit. The same situation prevails in earlier studies [3a].

This is in contrast to the case of previous schemes such as those involving large cells [5d], where the singular part of the free energy is equated to the rescaled coupling p'. Apart from lacking a theoretical basis (as seen above), such schemes clearly violate the renormalization-group requirement of analyticity of the renormalization-group equations at the thermodynamic limit, since the corresponding free energy is singular at the critical point. The inappropriateness of such procedures has been emphasized by Wilson [1], who urged never to renormalize the free energy itself, because it is singular at a critical point. Large-cell renormalization schemes with a single coupling, which are commonly used to analyze computer data [8b], also lead to other basic inconsistencies and incorrect predictions, as recently pointed out [8a].

Finally, we note that the recent mathematical proofs of possible pathologies of real-space renormalization-group transformations, including lack of analyticity at the thermodynamic limit [12], are irrelevant, in particular, as they apply away from the critical point.

Acknowledgements

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