Inverse renormalization-group transformation in the bond percolation problem

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In the present paper we present a method using the inverse renormalization group transformation of a connected percolation cluster in the bond problem and we investigate the effect of the specific form of the boundary conditions on the properties of the cluster near the percolation threshold.

1. PERCOLATION CLUSTER METHOD

In application to percolation theory, the hypothesis of scale invariance of the properties of a system at a critical point means that an infinite cluster whose unbroken-bond concentration exactly equals the percolation threshold is a geometrically self-similar object or, in the language of the last ten years, a fractal. Different analogs of the renormalization group transformation method have been applied to percolation problems,[1,2] just as in the theory of thermal phase transitions, where this method was first developed on the basis of the idea of scale invariance.

The most successful geometric representation of an infinite cluster—the model of sites, drops (blobs), and loops[3]—can be constructed by applying a scale transformation to an element of a square lattice—the inverse of the procedure of constructing large blocks.[4] In this approach some elements of the geometric structure of an infinite cluster, such as, for example, intersecting bonds[3] in the backbone of the threshold infinite cluster on any scales, as well as its self-similarity, are postulated in the construction of the model.

The geometric properties of clusters on a finite lattice with the concentration of unbroken bonds $p \neq 0$ or 1 are determined by a finite number of realizable configurations. An unphysical choice of an averaging method in the calculation of all possible lattice constants can be avoided by using the procedure of increasing the scale. The point of this procedure is to calculate the effective values of the parameters of a percolation lattice from the values calculated directly only for the initial sample: the effective parameters of the lattice properties are transferred from stage to stage and in the process the characteristics of each bond are replaced by the values calculated at the preceding stage. The iterative increase of the scale by a factor of x per iteration (Fig. 1a) leads to stationary points for the cluster functions. In this manner the size of the lattice is increased to some scale $L_n = l^n$ (where l is the edge length of the initial lattice) that exceeds the correlation length ξ.

Finite rectangular models $\{x,y,z\}$ were investigated in a space of dimension $d=2$ and 3, where x, y, and z are the edge lengths as multiples of the bond lengths (lattice constant); $z=0$ for a two-dimensional lattice. Percolation in the model was flagged by the existence of a cluster of unbroken bonds that connects two opposite faces in the direction of the x-edge, and the density of an infinite cluster $P_\infty(p)$ was defined to be the probability that an unbroken bond belongs to a connecting cluster.

In the case $x,y,z \to \infty$, the density of an infinite cluster satisfies

$$P_\infty(p) = \begin{cases} 0, & p < p_c, \\ 1, & p = 1 \end{cases} \tag{1}$$

and the scaling law

$$P_\infty \propto (p - p_c)^\beta, \quad p > p_c, \tag{2}$$

where p_c is the percolation threshold.

The fractal dimension d_f^{bas} of the main set of bonds (backbone) (Fig. 1a), which is obtained by the inverse renormalization group transformation with $p=1$, can be determined from the dependence of the mass of the backbone (the number of constituent bonds) $M_k^{(n)}$ at the nth stage on the linear size L_n of the lattice (number of bonds along an edge):

$$M_{bas}^{(n)} \sim L_n^{d_f^{bas}}. \tag{3}$$

For example, for a two-dimensional model with $x=y=l$, $z=0$

$$M_{bas}^{(n)} = (2l^2)^n. \tag{4}$$

Since $L_n = l^n$, we obtain

$$M_{bas}^{(n)} = L_n^{2+\ln 2/\ln l}. \tag{5}$$

The dimension of the geometric set on which the renormalization procedure is defined is therefore greater than the topological dimension $d=2$ of the space of the initial model:

$$d_f^{bas} = 2 + \frac{\ln 2}{\ln l}. \tag{6}$$

In the case of an arbitrary dimension d and arbitrary shape of the initial element, the mass of the object obtained by the inverse renormalization group transformation can likewise be determined by factoring out the geometric factor F

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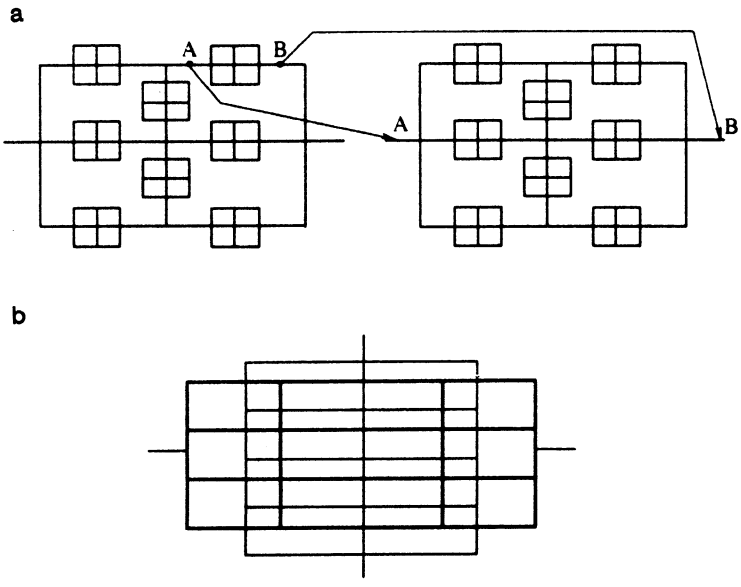

FIG. 1. Renormalizable models: a—illustration of a stage of the transformation for the case $x=y=l=2$, $z=0(p=1)$; b—relatively dual model, $x=y=l=3$, $z=0$ and $x=4$, $y=2$, $z=0$.

$$M_{bas}^{(n)}=(Fl^d)^n=F^nL_n^d. \tag{7}$$

Then Eq. (6) assumes the form

$$d_f^{bas}=d+\frac{\ln F}{\ln l}. \tag{8}$$

It follows from Eq. (8) that the dimension of the main set of bonds equals the Euclidean dimension only in the limit of an infinite renormalized block:

$$\lim_{l\to\infty} d_f^{bas}=d, \tag{9}$$

which is obviously valid for any model.

The correlation length of the percolation lattice delimits the region of so-called intermediate asymptotic behavior in the lattice. Expressed in units of the lattice constants, this range of scales L is determined by the two-sided inequality

$$1\ll L<\xi. \tag{10}$$

Over this range, the structure of the percolation cluster is geometrically similar to the structure of an infinite cluster with $p=p_c$, where $\xi\to\infty$:

$$\xi\sim|p-p_c|^{-\nu}. \tag{11}$$

One characteristic of self-similarity of an infinite cluster with $p=p_c$ is its fractal dimension d_f. The mass $M_{PC}^{(n)}$ of the fractal, which the percolation cluster is in the scale interval (10), depends on L_n as

$$M_{PC}^{(n)}\sim L_n^{d_f}. \tag{12}$$

The density of the percolation cluster is

$$\rho_{PC}^{(n)}=\frac{M_{PC}^{(n)}}{M_{bas}^{(n)}}\sim L_n^{d_f-d_f^{bas}}. \tag{13}$$

We introduce the notation

$$Y_\rho=d_f-d_f^{bas}=-\alpha-\frac{\ln F}{\ln l}, \tag{14}$$

where $\alpha=d-d_f$. Since $Y_\rho<0$, we find that the density of the percolation cluster with $p=p_c$ approaches zero as the number n of the stage of the renormalization-group transformation increases, i.e., with increasing L_n:

$$\lim_{L_n\to\infty} \rho_{PC}(L_n)=0. \tag{15}$$

For $p>p_c$ on scales greater than $\xi(L_n>\xi)$, the percolation cluster becomes uniform with constant density, and Eq. (15) assumes the form

$$\lim_{L_n\to\infty} \rho_{PC}(L_n)=\rho_0>0. \tag{16}$$

The exponent β is related, via the dimension d_f of the percolation cluster, to the critical exponent ν by a hyperscaling relation:

$$d_f=d-\beta/\nu, \tag{17}$$

as a result of which, and using Eq. (14), we obtain $\alpha=\beta/\nu$.

The percolation probability R of the initial model for fixed concentration of unbroken bonds depends only on the geometry, the size of the lattice, and the method used to determine percolation (for example, only in one direction or in both directions simultaneously). This quantity was calculated as the ratio of the number of percolating configurations to the number of all scattering events. The value of R, being a polynomial of degree N—the number of all bonds in the sample ($N=2l^2$ in a two-dimensional space with $x=y=l$)—can be determined as accurately as desired for arbitrary p. This is also true for the density $P_\infty(p;x,y,z)$ of a cluster connecting two opposite faces of the lattice.

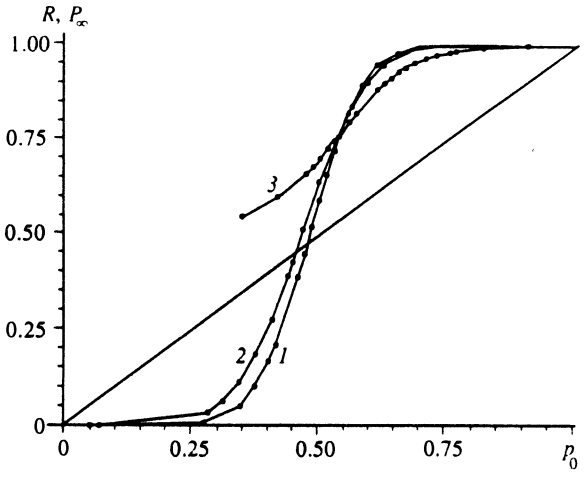

FIG. 2. Plots of the functions $R(p_0;x,y,z)$ and $P_\infty(p_0;x,y,z)$ with the initial concentration of unbroken bonds p_0: *1*—$R(p_0;5,4,0)$; *2*—$R(p_0;5,5,0)$; *3*—$P_\infty(p_0;5,4,0)$.

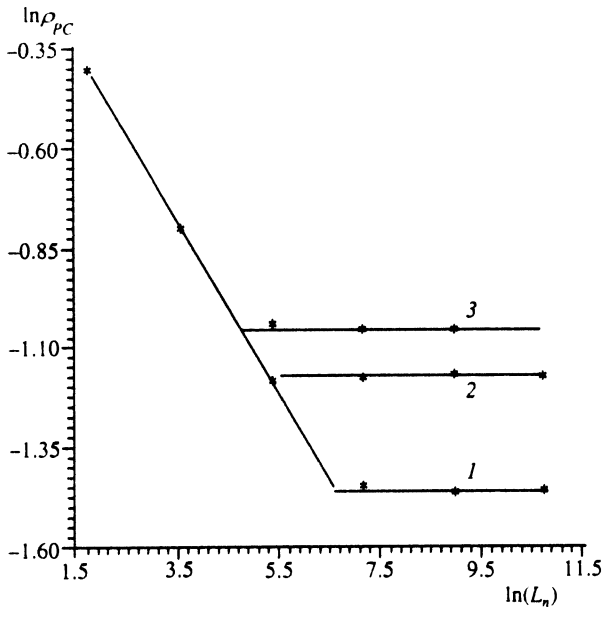

FIG. 3. Density of a percolation cluster as a function of its scale L_n for three values of $p_0(\Delta p \equiv p_0 - p_*)$: *1*—$\Delta p = 5\cdot 10^{-4}$; *2*—$1.5\cdot 10^{-3}$; *3*—$2.5\cdot 10^{-3}$.

We now introduce the model-dependent percolation probability $R(p_0;x,y,z)$ (first stage) on a lattice, where p_0 is the initial density of unbroken bonds. At the second stage of the transformation the percolation probability $p_2 = R(p_1;x,y,z)$ corresponds to a lattice with an effective length of x^2 bonds along an edge and with renormalized probability of a bond being unbroken on it $p_1 = R(p_0;x,y,z)$; for the third and n-th stages we have

$$p_3 = R(p_2;x,y,z),$$
$$\vdots$$
$$p_n = R(p_{n-1};x,y,z). \tag{18}$$

We determine the unstable stationary point $p_*(x,y,z) = R(p_*;x,y,z)$—the limit of the iteration sequence (18)—from a plot of the function $R(p_0;x,y,z)$ (curves *1* and *2* in Fig. 2). We term this point the percolation threshold of the model $\{x,y,z\}$. The trajectory of the inverse renormalization-group transformation terminates at the n-th stage at the stationary point 0 or 1:

$$R_n = \begin{cases} 1, & R(p_0;x,y,z) > p_*, \\ 0, & R(p_0;x,y,z) < p_*. \end{cases} \tag{19}$$

The results for the percolation thresholds of the models are presented in Table I, where the indicated error limits are of a statistical origin.

TABLE I. Effective percolation thresholds of the models.

d	x	y	p_*
2	2	2	0.3670 ± 0.0001
	3	3	0.4266 ± 0.0005
	4	4	0.4536 ± 0.0005
	5	4	0.5
	5	5	0.468 ± 0.001
	6	6	0.4765 ± 0.0005
	9	8	0.5
	9	9	0.488 ± 0.002
3	3	3	0.211 ± 0.001

Simultaneously with the percolation probability $R(p_0;x,y,z)$ we investigated on the initial block the quantity $P_\infty(p_0;x,y,z)$—the relative number of bonds belonging to a connecting cluster (curve *3* in Fig. 2). By analogy with Eq. (18), after n iterations of the inverse renormalization group transformation the density of the percolation cluster on the grid with an effective scale l^n can be determined from the formula

$$P_\infty^{(n)}(p_0,l) = \prod_{i=0}^{n} P_\infty^{(n)}(p_i,l), \tag{20}$$

where $P_\infty^{(0)}(p_0,l) \equiv p_\infty(p_0,l)$ is the density of the connecting cluster at the zeroth stage and p_0 is the initial concentration of unbroken bonds. The equality (20) is a formal expression of the fact that an unbroken bond belongs to an infinite cluster only if it participates in connecting the two faces at all stages of the transformation.

It follows from Fig. 2 that for any l

$$\lim_{n\to\infty} P_\infty^{(n)}(p_0,l) = \begin{cases} P^{(\infty)}(p_0,l) > 0, & p_0 > p_*, \\ 0, & p_0 \leqslant p_*. \end{cases} \tag{21}$$

For $p_0 \neq p_*$ the limit of the product (20) for a finite number of steps is Eq. (21), since sooner or later the next factor becomes 0 ($p_0 < p_*$) or 1 ($p_0 > p_*$). An infinite product of quantities different from zero or 1 is possible only if $p = p_*$, and in this case a fractal with zero density P_∞ and nonzero mass is obtained.

The correlation length ξ can be estimated by changing the power-law decay of the density of the connected cluster on scales determined for each $p > p_c$: in Fig. 3 the logarithm of ξ corresponds to the ordinate of the point of intersection of the horizontal and sloping sections of the plot. Calculating ξ gives values which are many times greater than the dimen-

TABLE II. Results of the inverse renormalization group transformation on different models.

d	x	y	Δp	P_∞	$\ln M_{bas}^{(n)}$	$\ln \rho_{PC}^{(n)}$	ξ
2	3	3	$5\cdot10^{-4}$	0.2440	7.243	−4.880	94.27
			$1.5\cdot10^{-3}$	0.2628	6.594	−4.511	66.69
			$2.5\cdot10^{-3}$	0.2959	6.269	−4.259	52.63
	5	4	$5\cdot10^{-4}$	0.3128	11.29	−3.954	739.1
			$1.5\cdot10^{-3}$	0.3838	9.806	−3.408	294.1
			$2.5\cdot10^{-3}$	0.4058	8.888	−3.112	178.8
2	6	6	$5\cdot10^{-4}$	0.2034	12.72	−4.539	1382
			$1.5\cdot10^{-3}$	0.2909	10.57	−3.731	377.7
			$2.5\cdot10^{-3}$	0.3122	9.548	−3.398	221.3
2	9	8	$5\cdot10^{-4}$	0.2986	14.23	−3.640	2666
			$1.5\cdot10^{-3}$	0.3548	12.11	−3.111	829.2
			$2.5\cdot10^{-3}$	0.4089	10.80	−2.771	391.5
	9	9	$5\cdot10^{-4}$	0.1283	20.47	−5.653	$7.934\cdot10^4$
			$1.5\cdot10^{-3}$	0.1719	18.81	−5.131	$2.766\cdot10^4$
			$2.5\cdot10^{-3}$	0.1953	16.97	−4.670	$1.091\cdot10^4$
3	3	3	$5\cdot10^{-4}$	0.0170	9.046	−11.52	198.2
			$1.5\cdot10^{-3}$	0.0353	7.465	−9.462	76.88
			$2.5\cdot10^{-3}$	0.0521	6.800	−8.463	48.55

sions of the initial block $\{x,y,z\}$, and this is a good prerequisite for modeling the properties of an infinite cluster over the corresponding range of lengths.

Average (over all iterations) critical exponents of the percolation theory (Table III) were determined by calculating the characteristics of a percolation cluster which were obtained by the inverse renormalization group transformation (Table II): the average value $\langle\nu\rangle_r$ was calculated from Eq. (17) and $\langle\nu\rangle_d$ was calculated from the definition of the exponent (11).

Comparing the published values of the computed critical exponents, in which we also include the fractal dimension d_f of an infinite cluster, shows that small initial lattices $(x,y,z\leqslant10)$ are suitable for studying both qualitatively and quantitatively threshold phenomena in spaces of dimension $d=2$ and 3.

2. SMALL MODELS IN THE METHOD OF FINITE-DIMENSIONAL SCALING

It follows from the results obtained above that the regularities in the statistical properties of a percolation cluster can be studied even on length intervals of the order of the lattice constant. For this reason we shall analyze in greater detail the method of finite scales,[5] which was implemented on the smallest models. To this end, we separate the set of all possible initial cells in two-dimensional space into classes according to the following criterion: a model belongs to class $C(n)$ if the difference $x-y$ for the model equals n, where $n\in Z$.

We choose a finite-dimensional representation for the density of an infinite cluster in the form

$$P_\infty^{-1}=l^{\beta/\nu}-[a_1+a_2g_P(l)], \tag{22}$$

where the function $g_p(l)$ is a correction to the scaling and l characterizes the size of the square model $\{x,y,0\}$ in the sense that the number of bonds in the class increase as a power-law function (7) with exponent d.

A computer calculation performed on small lattices $(x<10)$ in two-dimensional space suggests that $G\equiv\ln[P_\infty^{-1}(p_*(l))]/\ln l$ is a linear function of $1/\ln l$ (Fig. 4):

$$\frac{\beta}{\nu}+\frac{\ln[a_1+a_2g_p(l)]}{\ln l}=\frac{\beta}{\nu}+f(n)+\frac{B}{\ln l}, \tag{23}$$

where $f(n)$—the difference of the coordinates of the point of intersection of the experimental straight line for a given class $C(n)$ and the G axis—and the ratio β/ν are singled out on the right-hand side for purposes of generalization. Then the assumption of linearity determines the form of the function $g_p(l)$ in Eq. (22):

$$a_1+a_2g_P(l)=l^{f(n)}\exp B. \tag{24}$$

TABLE III. Critical indices of a percolation cluster.

d	x	y	$\langle\beta\rangle$	$\langle\alpha\rangle$	$\langle\nu\rangle_d$	$\langle\nu\rangle_r$	d_f
2	3	3	0.11	0.31	0.33	0.36	1.62
	5	4	0.15	0.17	0.88	0.92	1.73
	6	6	0.25	0.21	1.16	1.22	1.79
	9	8	0.18	0.12	1.17	1.29	1.83
	9	9	0.22	0.16	1.19	1.27	1.84
3	3	3	0.68	0.76	0.87	0.90	1.79

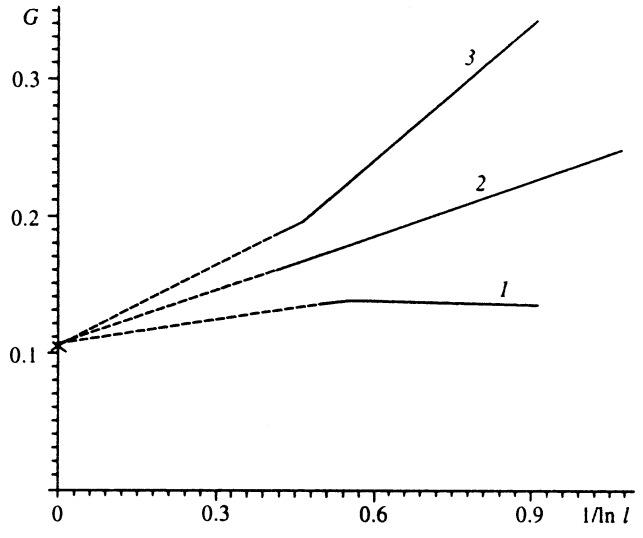

FIG. 4. $G=\ln(P_\infty^{-1})/\ln l$ versus $1/\ln l$ for the model classes *1*—C(2), *2*—$C(1)$, and *3*—$C(0)$.

During self-similar growth of the model, the similarity dimension of the statistically homogeneous fraction arising in this case can be estimated right at the percolation threshold by the quantity

$$D(l)=d+\frac{\ln[P_\infty(p_*(l))]}{\ln l}+\frac{\ln[Fp_*(l)]}{\ln l}, \tag{25}$$

which, generally speaking, takes on different values for different models. Using Eqs. (22) and (25) we obtain

$$D(l)-d+\frac{\beta}{\nu}=-f(n)-\frac{B}{\ln l}+\frac{\ln[Fp_*(l)]}{\ln l}. \tag{26}$$

The fractal dimension d_f of an infinite cluster (limiting value of $D(l)$ in the limit $l\to\infty$) satisfies Eq. (16), which determines the asymptotic behavior of the function $p_*(l)$:

$$\lim_{l\to\infty}\frac{\ln[p_*(l)]}{\ln l}=f(n). \tag{27}$$

It is evident from Eq. (26) that the decrease, recorded during numerical modeling, of the nonzero quantity $\delta(l)=|p_*(l)-p_c|$ [power-law decrease with exponent $-1/\nu$ as $l\to\infty$ (Ref. 6)] satisfies Eq. (27) only if $f(n)=0$ [we note that in this case $a_2=0$ in Eq. (24)]. Then the curves *1* and *3* in Fig. 4 are convex and concave sections, respectively, with respect to the horizontal axis, since for the classes $C(0)$ and $C(2)$ the linearity assumption leads to $f(2)$, $f(0)\neq 0$. Thus the assumption (23) can be expressed in the most general case as follows: there exists a value of F such that the curves $G[\ln^{-1}(l)]$ for classes $C(n)$ and $C(2-n)$, where $n\in Z$, are symmetric with respect to one another relative to the x axis. The x axis itself in this case will be the plot for the class $C(1)$, which is distinguished among the other classes by the property

$$p_*(x,y,0)|_{C(1)}=0.5. \tag{28}$$

To prove Eq. (28) we drop from the geometric centers of the interstitial squares of the model $\{x,y\}$, which we call the initial model, perpendiculars to all its bonds. We continue the perpendiculars to the outer edges of the model and connect them as in Fig. 1b, forming in this manner a dual square model, whose bonds are in one-two-one correspondence with the bonds of the initial model (the intersection of bonds in Fig. 1b indicates this correspondence). The new model $\{x,y\}_d\equiv\{y+1,x-1\}$ has the property that

$$R_d(p;x,y)=R(p,y+1,x-1)=1-R(1-p;x,y), \tag{29}$$

i.e., the percolation probabilities of mutually dual models are symmetric relative to the point (0.5, 0.5).

A general argument in proof of the property (28) is as follows. We form with the dual model a configuration starting from a connected (unconnected) configuration on the initial model according to the following principle: an unbroken bond in the initial model transforms into an broken bond corresponding to it and vice versa. Then, the resulting "symmetric" configuration will be disconnected (connected). The formal proof is constructed for the corresponding models of sites which are subsets of the so-called covering lattice.[7]

Since self-dual models are of class $C(1)$, the property (28) is proved (the exact equality $p_c=0.5$ is proved simultaneously for the problem of bonds on a square lattice). It is obvious that the inverse assertion will also be true: Any model for which $p_*=0.5$ will belong to class $C(1)$.

The result that $P_\infty=\text{const}\cdot l^{-\beta/\nu}$ for class $C(1)$ is confirmed by the fact that the result $\beta/\nu=0.1041\pm0.0013$ [the average value over the data obtained using the four models with $x=3$, 4, 5, and 9 from $C(1)$] agrees with the exact value 5/48.[8] Therefore small experimental models, together with models in which the number of sites is $\sim 10^6$ or larger, are suitable for calculating the finite-dimensional scaling ratios of the critical exponents (it can be inferred that β/ν is only one such ratio).

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