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COMMENT

Scaling theory for dynamic density profile at criticality

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Abstract. A scaling description for the (dynamic) density profile of kinetic clusters formed by the sites visited during random walks executed on critical percolation clusters is proposed. The analysis is done for both Euclidean and fractal spaces. Various percolative diffusion laws are correctly recovered from this dynamic density profile.

1. Introduction

The subject of percolative diffusion has stimulated much interest recently. Many ramifications of the original 'ant in the labyrinth' problem [1] have been discussed at length both theoretically and 'experimentally' (by Monte Carlo methods) in the literature. In particular, the fractal description of percolation clusters [2] has led to the definition and evaluation of such intrinsic exponents as the fractal dimensionality D , the diffusion exponent d_w (fractal dimensionality of the walk) and the fractal dimensionality d_f (density of states exponent). Most investigations have been done for diffusion at the percolation threshold where an anomalous diffusion exponent is obtained as a result of the fractal nature of critical percolation clusters [3, 4].

The usual procedure involves carrying out random walks on various clusters and measuring the average diffusion length R after time t . One finds that

$$R^{d_w} \propto t \quad (1)$$

where the diffusion exponent d_w depends on the type of average taken for R , e.g. over single clusters containing s sites [3] or over clusters of all sizes [5].

Instead of looking at the diffusion length, one can look at the density profile of the random walk. The density profile of a static s cluster is defined as [6, 7] the probability that a site at position r relative to the cluster centre of mass belongs to that cluster. We may define in a similar way a dynamic density profile (DDP) of the kinetic cluster [8] formed by the sites visited by a random walker on an s cluster as the probability that a site at a distance r from the centre of mass of the kinetic cluster has been visited after time t . These density profiles (static and dynamic) may be defined with respect to either the embedding Euclidean space of dimensionality d or the fractal space of dimensionality D occupied by the clusters themselves.

This comment presents a scaling theory for the DDP of s clusters and the infinite cluster at the percolation threshold and also looks at the behaviour of the DDP when defined with respect to the different spaces. Distances as before are measured as Euclidean lengths.

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2. Scaling theory for static clusters at criticality

Essential to the formulation of a scaling theory for the DDP is the scaling behaviour of the density profile $D_s(\mathbf{r})$ for critical s clusters. The scaling form is given as [9]

$$D_s(\mathbf{r}) \propto s^{-x} D_E(r/R_s) \tag{2}$$

with D_E the scaling function in Euclidean space and R_s the average radius of the s cluster. Integration of (2) over Euclidean space gives the cluster mass s .

Alternatively, we may take the finite fractal space formed by the cluster as the defining space and since only occupied sites constitute this space, we obtain the simple relation

$$D_s(\mathbf{r}) = D_F = 1(\forall s \text{ and } \mathbf{r}) \tag{3}$$

where D_F is the invariant density in the fractal cluster space. Trivially, the product of D_F and the fractal volume of a cluster gives the cluster mass s . The value of the exponent x in (2) was predicted to be δ^{-1} (δ is the usual critical exponent of percolation theory) by Stauffer [9] and this value was confirmed (for large enough s) by Herrmann [10] using Monte Carlo data.

3. Scaling theory for DDP in Euclidean space

3.1. Scaling theory

For random walks executed on critical s clusters we propose the following scaling form for the DDP:

$$D_s(\mathbf{r}, t) \propto t^a f_E(r/R, t/s^u) \tag{4a}$$

or equivalently

$$D_s(\mathbf{r}, t) \propto t^a g_E(r/t^y, t/s^u). \tag{4b}$$

The exponent y in (4b) is simply the reciprocal of d_w as seen from (1). The exponents a and u will be determined from scaling arguments.

As $t \rightarrow \infty$, the DDP reduces to the static density profile $D_s(\mathbf{r})$ since all the cluster sites would have been visited. Therefore the scaling function f_E will have the form

$$f_E(r/R, z) = z^{x/u} D_E(r/R) \quad z \rightarrow \infty \tag{5}$$

where $z = t/s^u$, in order for the correct static density behaviour to be obtained in the limit of large z . (We also have that $R \rightarrow R_s$ after long times.) In addition, in order that the time dependence of the DDP be eliminated, the relation $x/u = -a$ must hold. Furthermore, we note from diffusion length scaling [8, 11] that the time t should scale as the characteristic time for diffusion on an average s cluster. This immediately gives the exponent u as [5]

$$u = d_w/D = 2/d_f. \tag{6}$$

Finally we can rewrite (4a) as

$$D_s(\mathbf{r}, t) \propto t^{-k} f_E(r/R, t/s^u) \tag{7a}$$

and (4b) as

$$D_s(\mathbf{r}, t) \propto t^{-k} g_E(r/t^y, t/s^u) \tag{7b}$$

where $k = D/\delta d_w (= d_r/2\delta)$. The scaling law given by (7) is expected to hold better for large s [10].

We can easily obtain the scaling behaviour of the DDP for walks on the infinite cluster at the threshold. Here, one simply takes the limit $s \rightarrow \infty$ whence we obtain, using (7b),

$$D_\infty(\mathbf{r}, t) \propto t^{-k} g_E(\mathbf{r}/t^y, 0)$$

or

$$D_\infty(\mathbf{r}, t) \propto t^{-k} h_E(\mathbf{r}/t^y) \tag{8}$$

This of course is exactly the behaviour of the DDP for s clusters when $t \ll s^u$ since at these times the presence of the cluster boundary does not affect particle diffusion; self-similarity [12, 13] also precludes s dependence in this regime.

3.2. Some properties of $D_s(\mathbf{r}, t)$

In addition to those mentioned at the end of the last section, some other properties are worth mentioning. Firstly, from the definition of the DDP, it is clear that at $t = 0$ (diffusing particle at origin), $D_s(\mathbf{r}, t)$ is simply a delta function, i.e.

$$D_s(\mathbf{r}, 0) = \delta(\mathbf{r}). \tag{9}$$

Thus $D_s(\mathbf{r}, t)$ evolves from a delta function at $t = 0$ to the static density profiles $D_s(\mathbf{r})$ in the limit of long times.

Secondly, the number of distinct sites visited as a function of time, $S(t)$, is given by the integral of $D_s(\mathbf{r}, t)$ over (Euclidean) space. Stauffer [8] has given the scaling form of $S(t)$ as

$$S(t) = t^{1/u} V(t/s^u) \tag{10}$$

where V is a scaling function and the exponent u was previously given in (6). As stated above,

$$S(t) = \int D_s(\mathbf{r}, t) d^d r. \tag{11}$$

Substituting the proposed form for $D_s(\mathbf{r}, t)$ given by (7b) in (11) we get (neglecting constant factors)

$$\begin{aligned} S(t) &= t^{-k} \int g_E(\mathbf{r}/t^y, t/s^u) r^{d-1} d\mathbf{r} \\ &= t^{-k+dy} \int g_E(\mathbf{q}, t/s^u) q^{d-1} d\mathbf{q} \\ &= t^{(d-D/\delta)/d_w} \int g_E(\mathbf{q}, t/s^u) q^{d-1} d\mathbf{q} \end{aligned} \tag{12}$$

in d -dimensional Euclidean space. Now, from cluster radius scaling and hyperscaling [9],

$$D = (\sigma\nu)^{-1} = d - \beta/\nu \tag{13}$$

where σ , β and ν are critical exponents of percolation theory [9]. Using (13) along with the scaling law $\sigma = 1/\beta\delta$ [9], (12) becomes

$$S(t) = t^{D/d_w} V(t/s^u) \quad (14)$$

where

$$V(t/s^u) = \int g_E(q, t/s^u) q^{d-1} dq. \quad (15)$$

Clearly, (14) reduces to (10) by using (6).

Of course, for the infinite cluster the scaling function V is a constant and we obtain, using (6)

$$S(t) \propto t^{d/2} \quad (16)$$

which is the familiar percolative diffusion law [14].

The average 'radial extension' $\lambda(t)$ [15] of the kinetic cluster is defined by

$$\lambda(t) = \frac{1}{S(t)} \int D_s(\mathbf{r}, t) r d^d r. \quad (17)$$

This integration is easily performed and we obtain for the infinite cluster or in the $t \ll s^u$ regime

$$\lambda(t) \propto t^{1/d_w} \quad (18)$$

as expected (see (1)).

In concluding this section we note that, so far, the DDP has been defined with respect to the centre of mass of the kinetic cluster. If the centre of mass is replaced in the definition by the origin of the walk, the basic form of the DDP (i.e. scaling function and time-dependent prefactor) will not change. In fact, the prefactor is identical in both cases since the correct time dependences of such quantities as $S(t)$ and $\lambda(t)$ must be recovered with space integration. The scaling function will however change its functional form, so that if ρ is the position relative to the origin of the walk, the DDP can be written as

$$D_s(\rho, t) \propto t^{-k} F_E(\rho/R, t/s^u) \quad (19)$$

where F_E is a different function of the two scaled variables than the one given in (7a). (If the origin is chosen randomly, it is expected that the scaling functions F_E and f_E will have the same form apart from constants.)

4. Scaling theory in the fractal space

It is interesting to look at the scaling form of the DDP when it is defined with respect to the intrinsic fractal space occupied by critical clusters. We assume a similar form to the Euclidean counterpart:

$$D_s^F(\mathbf{r}, t) \propto t^\omega g_F(r/t^y, t/s^u) \quad (20)$$

where the designator F refers to the fractal space and ω is an exponent to be determined. Applying the same scaling arguments as before and noting that in the long time limit (20) must reduce to (3), it is found that $\omega = 0$ and (20) becomes

$$D_s^F(\mathbf{r}, t) = g_F(r/t^y, t/s^u) = f_F(r/R, t/s^u). \quad (21)$$

Equation (21) shows that the DDP at $r = R$ is a constant for the infinite cluster or in the $t \ll s^u$ regime, i.e.

$$D_s^F(R) = \text{constant} \quad (s \rightarrow \infty \text{ or } t \ll s^u). \quad (22)$$

This equation of course holds for diffusion in a cartesian continuum (cf [16, p 229]). Furthermore, the DDP in fractal space must exhibit the same properties as its Euclidean counterpart, as discussed in the previous section. In particular, by integrating the proposed form of the DDP given by (21) over the fractal space we regain the time dependence of the number of distinct sites visited by the random walker $S(t)$:

$$S(t) = \int D_s^F(\mathbf{r}, t) d^D r. \quad (23)$$

If ρ (distance from the origin of the walk) is used instead of r in the definition of the DDP, (23) becomes

$$S(t) = \int D_s^F(\rho, t) d^D \rho. \quad (24)$$

Now, the probability $P(\rho, t)$ that the random walker is at position ρ at time t is assumed for the infinite cluster to have the form [15, 17]

$$P(\rho, t) \propto R^{-D} f(\rho/R). \quad (25)$$

It is easily seen from (1), (16) and (24) that $P(\rho, t)$ is the properly normalised DDP in the fractal space.

Summarising, we have proposed a scaling theory for the density profile of kinetic clusters at criticality in Euclidean and fractal spaces. It was then shown how this proposed dynamic density profile correctly reproduces the various well known percolative diffusion laws.

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