Theory of Disordered Systems

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Lecture 8: Conductivity and diffusion on fractal structures.

We now come back to the question, how does the conductivity or the resistivity of the lattice percolation system depend on the concentration. Here we use our already existing knowledge on the geometric structure of the infinite cluster. Moreover, the nontrivial dependence of the conductivity on size in the fractal domain is reflected in the anomalous nature of diffusion in such systems.

1 Conductivity exponent

As already discussed, close to p_c the conductivity σ of a percolation system behaves as

$$\sigma(p) \propto (p - p_c)^{\mu}$$

with $\mu > 1$ (at variance with the EMA prediction $\mu = 1$).

As we have seen previously, the percolation cluster slightly above the threshold can be considered as a homogeneous structure on scales larger than the correlation length ξ. This structure is built of fractal blocks of size ξ. Therefore, if the corresponding effective resistance R_ξ of one block is known, the overall conductivity as a function of the system's size L follows from the parallel switching of $(L/\xi)^{d-1}$ columns of blocks, in each of which L/ξ blocks are switched in a sequence. Therefore

$$R_{\rm tot} = R_\xi \frac{L}{\xi} \left(\frac{L}{\xi}\right)^{-(d-1)} = L^{-d+2} R_\xi \xi^{d-2}.$$

Thus, if the dependence of R_ξ on ξ in a fractal regime is given by a power law

$$R_\xi \propto \xi^{\zeta}$$

the overall ξ-dependence of the resistance is given by

$$R_{\rm tot}(\xi) \propto L^{-d+2} \xi^{\zeta+d-2}.$$

To see that the dependence of the resistivity of the fractal object can indeed be given by a power-law one can again consider the Sierpinsky gasket example. Taking the resistance between the two terminals of the gasket of a lower generation to be r we can easily calculate the resistance between the corresponding terminals of a gasket of the next generation by performing the triangle-star transformation (see Fig. 1) to get

$$R = 2\frac{r}{2} + \frac{1}{1/r + 1/2r} = (5/3)r$$

so that

$$\zeta = \frac{\ln(5/3)}{\ln 2} \approx 0.737....$$

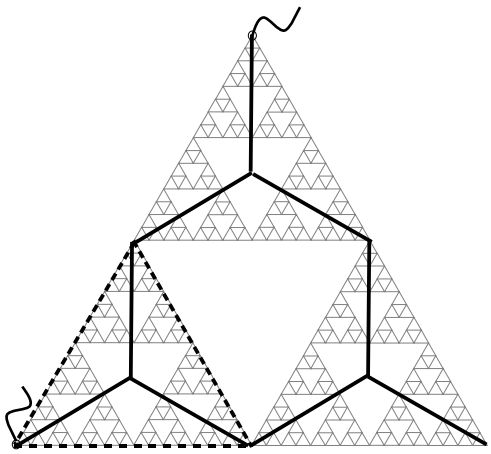

Figure 1: Triangle-star transformation for a Sierpinsky gasket

Taking now $\xi \propto (p - p_c)^{-\nu}$ and using the definition $R \propto (p - p_c)^{\mu}$ we get

$$R(p) \propto L^{-d+2}[(p - p_c)^{-\nu}]^{\zeta+d-2}.$$

Translating this into the conductivity of the system ($\sigma = R/L^{2-d}$) we get

$$\mu = \nu(d + \zeta - 2).$$

One often introduces the reduced exponent $\tilde{\mu} = \mu/\nu$. This one is given by

$$\tilde{\mu} = d + \zeta - 2.$$

Calculating $\tilde{\mu}$ from the known values of μ and ν gives $\tilde{\mu} \approx 0.97$ in $d = 2$ and $\tilde{\mu} \approx 2.2$ in $d = 3$, i.e. in this cases $\tilde{\mu}$ is not too far from $d-1$ and thus ζ is not too far from unity (although it is not equal to unity and can be both larger and smaller). The value $\zeta = 1$ would correspond to simple sequential switching of "elementary resistors", i.e. to a simply wired regular network at the lower scales. The values $\zeta < 1$ (slower growth) show that considerable part of the "wires" are shunted by parallely switched parts of the network ("blobs"), as we have seen in the example of Sierpinsky gasket. The values $\zeta > 1$ correspond to the cases when the predominant effects stem from the tortuosity of the corresponding paths, so that the wires whose ends are at a typical distance ξ are effectively much longer than ξ.

Note: The situation gets more involved when the continuum percolation models are considered (B.I. Halperin, S. Feng and P.N. Sen, Phys.Rev. Lett. **54**, 2391 (1985); see S. Havlin and D. ben Avraham, Adv. in Physics, **36** 695-798 (1987) for a review). As an example let us discuss the so-called Swiss cheese model (where the percolation takes place over the cheese, and the "holes", all of the same radius r, do not conduct) or in the inverse swiss cheese model, where the holes conduct and the cheese does not. For the cheese model close to its percolation transition the conductivities g_i of the (weakest) existing bonds are distributed according to a power law

$$p(g) \sim g^{-\alpha}$$

(for small g) with

$$\alpha = \frac{2d-5}{2d-3}$$

(a nice electrotechnical problem!). The distribution is nonsingular in $d = 2$ ($\alpha = -1$) but strongly singular in $d = 3$ ($\alpha = 1/3$), many extremely small conductivities) in $d = 3$. The existence of very weak bonds changes the critical exponent of conductivity from its value μ to some other value μ' for the continuous model.

We can now make an estimate on how does this singularity affect the critical exponent when assuming the simply-wired network (the one with $\zeta = 1$, i.e. neglecting the tortuosity and the blobs) on the lowest scale.

Eq.(1) corresponds to the following distribution of the resistivity $R = 1/g$ of the bonds,

$$p(R) \simeq p(g(R))\frac{dg}{dR} \sim R^{\alpha-2}.$$

For $0 < \alpha < 1$ the sum of N such random variables tends in distribution to a Lévy stable law of index $\gamma = 1 - \alpha$ and its typical value depends on N as

$$R(N) \simeq N^{1/\gamma} N^{\frac{1}{1-\alpha}}. \tag{1}$$

Since the number of resistors in our simply wired model is proportional to the size of the fractal cell, this corresponds to the value of $\zeta' = \frac{1}{1-\alpha}$ and to

$$\mu' \approx \nu\left(d - 2 + \frac{1}{1-\alpha}\right).$$

A more detailed argumentation lead to an inequality

$$\nu(d-2) + \frac{1}{1-\alpha} \leq \mu' \leq \mu + \frac{\alpha}{1-\alpha}.$$

Those not acquainted with Lévy laws may rationalize Eq.(1) by noting that for strongly singular distributions the overall resistance R of the chain is practically dominated by the largest resistance R_L, i.e. $R \sim R_L$. This maximal resistance can be evaluated from

$$N\int_{R_L}^{\infty} p(R)dR \simeq NR_L^{\alpha-1} \sim 1$$

so that $R \sim R_L \sim N^{\frac{1}{1-\alpha}}$.

2 Percolative conduction and anomalous diffusion

The problem of calculating the conductivity of a random sample is mathematically equivalent to the problem of calculating the diffusion coefficient of the particles in the corresponding percolation structure. In this case a typical model is the one allowing the transition between each connected pair of lattice sites i and j in the bond model, or a transition from an intact site i to any of its intact neighbors in the site model of percolation theory. The

typical waiting time on a site is taken to be τ, the value $D_0 = a^2/d\tau$ defines the diffusion coefficient for the non-diluted network (i.e. the one with $p = 1$).

The random walks of particles on a network can be described by a master equation (which is perfectly valid for the exponential waiting time distribution on a site and asymptotically valid in case of all other waiting time distributions with finite mean waiting time τ): Let $\mathbf{p}(t)$ be the vector with elements $p_i(t)$ being the probabilities to find a particle at node i at time t. The master equation that gives then the temporal changes in this probability (remember the *Kinetics* lecture) reads

$$\frac{d}{dt}\mathbf{p} = \mathbf{i} + \mathbf{W}\mathbf{p} \tag{2}$$

where $\mathbf{i} = \{i_i\}$ is the vector comprising the probability currents to (from) site i in the case the particles are introduced to this site from the outside. A similar equation with the temporal derivative changed to d/dn describes the n-dependence for the probabilities $p_{i,n}$ in a random walk as a function of the number of steps, provided n is large enough to be considered as a continuous variable. The matrix $\mathbf{W}$ describes the transition probabilities between the nodes of the lattice or network. The non-diagonal elements of the corresponding matrix are w_{ij}, the transition probabilities from site i to site j per unit time or in one step. The diagonal elements are the sums of all non-diagonal elements in the corresponding lines taken with the opposite site: $w_{ii} = -\sum_j w_{ji}$, which represents the probability conservation law. The situation of unbiased random walks corresponds to a symmetric matrix $\mathbf{W}$: $w_{ij} = w_{ji}$. Considering homogeneous networks and putting all nonzero w_{ij} to unity, one sees that each the difference operator represented by a line of the matrix is a symmetric difference approximation to a Laplacian. The master equation (2) is pertinent to the situations corresponding to the initial value problems, and also to situations when some $p_i(t)$ are given (e.g. kept constant on the boundaries), and the other ones have to be calculated.

In course of the time the stationary situation establishes, the one with

$$\mathbf{W}\mathbf{p} = -\mathbf{i} \tag{3}$$

giving the stationary concentration distribution. For this stationary distribution the diffusion (random walk) problem is absolutely equivalent to the electrical one of calculating the conductivity for given potentials or currents at some nodes. Calculating concentrations formally corresponds to calculating the voltages on the nodes of the resistor network of the same geometry

using the Kirchhoff's laws. The fact that the probability current between nodes i and j is proportional to the difference $p_i - p_j$ is replaced by the Ohm's law. The conductivities of resistors connecting nodes i and j have to be taken 1 if the nodes are connected and zero otherwise. The total probability conservation corresponds then to the second Kirchhoff's law representing the fact that the sum of all currents to/from the node i is zero, and the first Kirchhoff's law follows from the uniqueness of the solution.

Therefore the diffusion coefficient of the particles through a percolation system behaves as

$$D(p) \propto (p - p_c)^t$$

vanishing exactly at the percolation threshold. Close to this threshold the diffusivity in the fractal regime (i.e. for length scales $L < \xi$) is a function of the size of the system and goes as a power law

$$D(L) \propto L^{-\zeta}$$

This power-law explicit dependence of the diffusion coefficient on the size means that the diffusion close to the percolation threshold is anomalous and *does not* follow the normal Fickian pattern according to which

$$\langle x^2(t) \rangle \propto t.$$

Numerical simulations of random walks on percolation clusters (the *ant in the labyrinth* model) show indeed that

$$\langle x^2(t) \rangle \propto t^\alpha \tag{4}$$

with $\alpha < 1$ (subdiffusion) as long as $\langle x^2(t) \rangle < \xi$, i.e. for quite a time for p close to p_c and at all times exactly at p_c. Assuming this power law, we can find the connection between the exponent of anomalous diffusion α and ζ and therefore t, i.e. establish the connection between the short time behavior in diffusion and the concentration dependence of conductivity in the percolation system.

Here we use the qualitative scaling arguments which are strongly backed by the results of numerical simulations.

First, we note that one can reverse Eq.(4) and use it e.g. for the mean first passage time $\langle T \rangle$ from the origin to the boundary at the distance R from the point where the particle is introduced into the system

$$\langle T \rangle \propto R^{2/\alpha}. \tag{5}$$

Here another notation can be used. The number of steps, or the time necessary to make the walk can be considered as a measure of the "mass" of the trajectory of the random walk, and R is its size in the Euclidean space. Therefore Eq.(5) can be interpreted as the one of the type $M \propto R^{d_f}$ with d_f being the fractal dimension of the walk's trajectory (which is typically denoted as d_w and called the *walk dimension*), and therefore

$$d_w = \frac{2}{\alpha}.$$

We now find the connection of d_w (and thus of α) with already known critical exponents d_f and ζ characterizing the infinite cluster.

The mean first passage time to the boundary (or mean sojourn time of particles inside the boundary) can be calculated using the *flow over population* approach (see the *Kinetic* course, or remember the introductory lecture to *Complex systems and macromolecules*).

Let us consider particles as inserted at some site with a system, on the average I per unit time. Using the flow-over-population method we then get $\langle T \rangle \propto N/I$, where I is the probability current through the system (the number of particles entering A per unit time), N is the overall stationary number of particles within the system. Here $\langle T \rangle$ is essentially the mean time a particle spends inside the system, which coincides with the mean first passage time from A to B.

The mean number of particles inside the system is proportional to a typical concentration of particles, which, in its turn is proportional to their concentration at some given place (and thus, say, to the probability p_A to find a particle at site A for the given current I), *and* to the number of sites. The concentration (being a counterpart of the voltage) for a given current scales as the system's resistivity, $p_A \propto R \propto L^{\zeta}$, and the number of sites scales as L^{d_f} where L is the system's size, so that $\langle t \rangle \propto L^{d_f+\zeta}$. Comparing this with Eq.(5) we thus get

$$d_w = d_f + \zeta.$$

Considering the d-dimensional generalizations of Sierpinski gaskets and using analogous considerations we get $\zeta = \log[(d+3)/(d+1)]/\log 2$. Combining this with the fractal dimension $d_f = \log(d+1)/\log 2$ of a gasket this gives us for the dimension of the walks $d_w = \log(d+3)/\log 2$.

The relation between the scaling exponent of the conductivity and the dimension of a random walk on a fractal system can be used in the opposite

way, since d_w can easily be obtained numerically for a whatever structure. On the other hand, the solutions of the Kirchhoff's equations on the complex structure (i.e. the solution of a large system of algebraic equations) in a dimension higher than 2, which is typically achieved using relaxation algorithms, is numerically much more involved.

A different discussion of the same problem based on the Einstein's relation between diffusion coefficient and conductivity an on crossover arguments can be found in in the Havlin and ben Avraham's review.

2.1 The spectral dimension

In the case of random walks on regular lattices, the probability to find the walker at the origin behaves as

$$p(0,t) \propto \frac{1}{(Dt)^{d/2}}$$

i.e. follows the power-law decay governed by the spatial dimension of the system. In a fractal system the power-law decay is also observed, and the long-time asymptotics of this decay

$$p(0,t) \propto \frac{1}{t^{d_s/2}} \tag{6}$$

defines a new characteristics of a fractal system, its spectral dimension d_s. In the case of Euclidean lattices $d_s = d_f = d$, but for fractals d_s and d_f are rather independent characteristics (although it is known the $d_s < d_f$).

Let us return to our means squared displacement, Eq.(4). This equation can be interpreted in the sense that most of sites visited by the random walker during time t are situated within a ball with radius of around $R \propto t^{\alpha/2}$ centered at the walker's initial position, and the overall number of the visited sites (i.e. the ones within the ball) is given by $N(t) \propto [R(t)]^{d_f} \propto t^{\alpha d_f/2}$. Assuming that all these sites can be visited with a comparable probability and that the origin is just one of these more or less equivalent sites, we conclude that $P(0,t) \propto \frac{1}{t^{\alpha d_f/2}}$. Comparing this with Eq.(6) we get

$$d_s = \alpha d_f = \frac{2d_f}{d_w},$$

connecting the properties of walks with geometric properties of the fractal substrate.

For percolation clusters in any dimension d_s is very close to 4/3. Although the initial assumption that it is exactly 4/3 [S. Alexander and R. Orbach, Journal de Physique Lett. **43**, L625 (1982)] was proven wrong, with the largest deviation of around 2% observed in two dimensions [P. Grassberger, Physica A **262**, 251 (1999)], the Alexander-Orbach conjecture $d_s = 4/3$ can still be considered as exact for a whatever practical purpose.

A few words about the history of the name "spectral dimension". From the spectral (Laplace) representation of the solution of the master equation we can easily find the probability $P(0,t)$ that the walker starting at site 0 at $t = 0$ is found at the same site at time t. This one reads

$$P(0,t) = \sum_{i=1}^{\infty} a_i \exp(-\epsilon_i t)$$

where ϵ_i is the i-th eigenvalue of the matrix $\mathbf{W}$ and a_i is the amplitude of its i-th eigenvector at site 0. Considering the lattice as infinite we can pass from discrete eigenvalue decomposition to a continuum

$$P(0,t) = \int_0^{\infty} \mathcal{N}(\epsilon) a(\epsilon) \exp(-\epsilon t) d\epsilon.$$

For long times, the behavior of $P(0,t)$ is dominated by the behavior of $\mathcal{N}(\epsilon)$ for small values of ϵ. Here $\mathcal{N}(\epsilon)$ is the density of states of a system described by the matrix $\mathbf{W}$. The forms of such densities are well known for many Euclidean lattices, since the problem is equivalent to the calculating of spectrum in tight-binding approximation used in the solid state physics: for all Euclidean lattices $\mathcal{N}(\epsilon) \propto \epsilon^{d/2-1}$, which gives us the forms of famous van Hove singularities of the spectrum. Assuming $a(\epsilon)$ to be nonsingular at $\epsilon \to 0$ we get $P(0,t) \propto t^{-d/2}$. The exponent d_s replacing the Euclidean dimension d in the expression for the probability of being at the origin and therefore also in the one for the density of states (spectrum) of the corresponding disordered system is then reasonably called the **spectral dimension** of a fractal lattice. It describes the properties of spectrum of fractal analog of a Laplace operator. In the early days it was also often called **fracton dimension** of the structure, since the corresponding eigenvectors of the matrix (corresponding to eigenstates in tight-binding model) are called **fractons**.

The spectral dimension of the network governs the behavior of the mean number of different sites visited by the random walk. A random walk of n steps having a property of compact visitation typically visits all sites within

the radius of the order of its typical displacement $R_n \propto n^{1/d_w}$. The number of these sites is $S_n \propto R_n^{d_f}$ where d_f is the fractal dimension of the network, so that $S_n \propto n^{d_s/2}$ (provided $d_s \leq 2$, i.e. provided the random walk is recurrent and shows compact visitation).