Theory of Disordered Systems

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Lecture 5: Lattice systems: EMA *et al*

Often, especially in the case of very high contrast, it is easier (both from the conceptual and from the numerical point of view) to consider lattice models instead of continuum ones. We concentrate here on the lattice models for conductivity, which are of high experimental relevance in the case of high contrast. In this lecture I follow to a large extent the article by S. Kirkpatrick, Rev. Mod. Phys. **45**, 574-588 (1973).

Let us first consider a lattice model (e.g. on a square lattice, see Fig.1). A large piece of the lattice is switched between the (super)conducting bars kept at a constant voltage. The conductances $g_i = 1/R_i$ of the resistors are taken from some probability distribution. The definition of the characteristic conductivity of the system can be given via the total heat production, or via the connection between the applied voltage and the overall current through the system. The existence of the corresponding variational principles leads to the possibility to obtain the corresponding numerical solution by use of relaxation algorithms which can be formulated and implemented in a very elegant way.

1 EMA for a random resistor model

Let us consider the effective medium approximation for the random resistor lattice model.

Let us consider an ordered medium (a lattice with conductances g_m) with the same overall conductance as our disordered medium. This g_m is essentially exactly what we are looking for. Let V_m be the voltage between the nodes A and B of the lattice in such an ordered medium. Let us consider *one* resistor with conductance g_i switched between the nodes A and B of the lattice. Since this is different from g_m, the voltage V_{AB} differs from V_m by some amount ΔV:

$$\Delta V = V_{AB} - V_m.$$

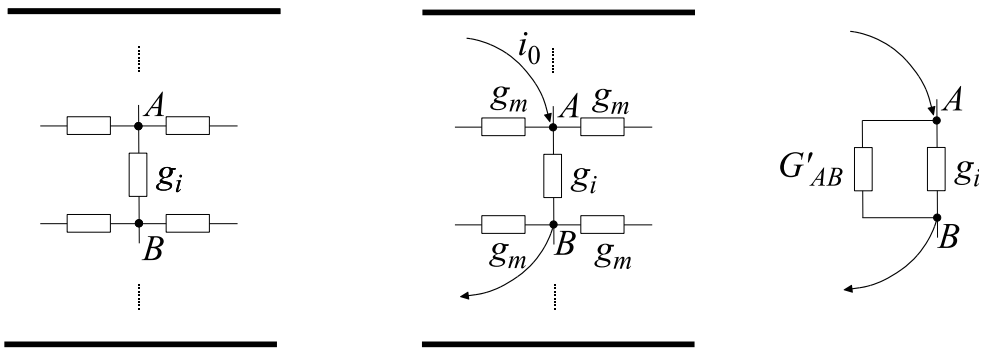

Figure 1: First steps of discussion: the effective circuit of the EMA.

The effective medium is defined (i.e. g_m is chosen) in such a way that $\langle \Delta_V \rangle = 0$.

Finding g_m fulfilling this condition is a task which now will be performed in several elegant steps following from linearity of underlying equations (corresponding to Kirchhoff's laws): The sum of voltages along each closed loop in the system vanishes, the sum of the currents in each node vanishes as well

$$\sum_j i_{ij} = 0$$

(with $i_i j$ being the current flowing from i to j). The current through the resistor between the two nodes i and j is given by

$$i_{ij} = g_{ij} V_{ij} = g_{ij}/(V_i - V_j),$$

where V_{ij} is the voltage between the sites i and j and V_i and V_j are the corresponding potentials. As always, the system has to be considered as placed between the "superconducting" plates of a flat capacitor situated at a macroscopic distance from each other and kept at constant potentials.

One can obtain the solution of the problem without solving them, which is a noble art of theoretical physics.

If g_i under consideration were equal g_m, than we would have $V_{AB} = V_m$, since g_i differs from g_m, there is some deviation of V_{AB} from V_m (the potentials at neighboring nodes will also differ from their values in the ordered system).

Let us now connect an additional current source (a battery) to the nodes A and B and tune its voltage until the potential difference between A and B gets equal to V_m. This means that after introducing such a battery the potentials of all nodes are restored, and all currents through other resistors are the same as in the case when g_i were equal to g_m. Let i_0 be the current flowing into node A and from node B under such situation, see Fig.1. Since restoring V_m between the nodes A and B restores all other potentials, all currents in such a system with the additional current are the same as they were if g_i were equal to g_m. This means that the whole additional current flows through g_i and does not redistribute over other resistors. Therefore the current i_0 is connected with g_i via $i_0 = (g_m - g_i)V_m$. Let us now consider what happens if we switch off this current (i.e. add a current of strength i_0 flowing in the opposite direction). Since the equivalent circuit consist of the two conductances, g_i of the resistor considered and G'_{AB} of the rest of the system, switched parallel, the voltage will change by

$$\Delta V = \frac{i_0}{g_i + G'_{AB}}$$

i.e. by

$$\Delta V = V_m \frac{g_m - g_i}{g_i + G'_{AB}}.$$

The self-consistency requirement of the EMA then suggests that this ΔV has to vanish on the average if g_m is chosen correctly, i.e. gives the following equation for g_m:

$$\left\langle \frac{g_m - g}{g + G'_{AB}} \right\rangle_g = \int \frac{g_m - g}{g + G'_{AB}} p(g) dg = 0 \tag{1}$$

where $p(g_0)$ is the probability density of the distribution of g.

Our next task will be to find G'_{AB}. To do so we consider our ordered system (all resistors have the conductance g_m) as placed into a superconducting box (of spherical shape) of a very large (infinite) size, and compare three situations depicted on Fig.2 (from the left to the right): (a) the external current of magnitude i is entering the system at site A and leaving the system through the outer border, (b) the current, same in the magnitude, is entering the system through the outer border and leaves it through a wire connected to site B, and (c) the current of magnitude i enters the system in A and leaves it via B.

In the first case, since the border is very far away, the entering current is equally distributed among all z branches connected to A, so that the current through the particular resistor between the terminals A and B is exactly i/z. The same is true in the case (b). In the case (c), due to linearity, the current through the resistor is the sum of those in cases (a) and (b) (no current leaves the system via the external boundary, all currents are the sums of those in cases (a) and (b)), i.e. is equal to $i_{AB} = 2i/z$.

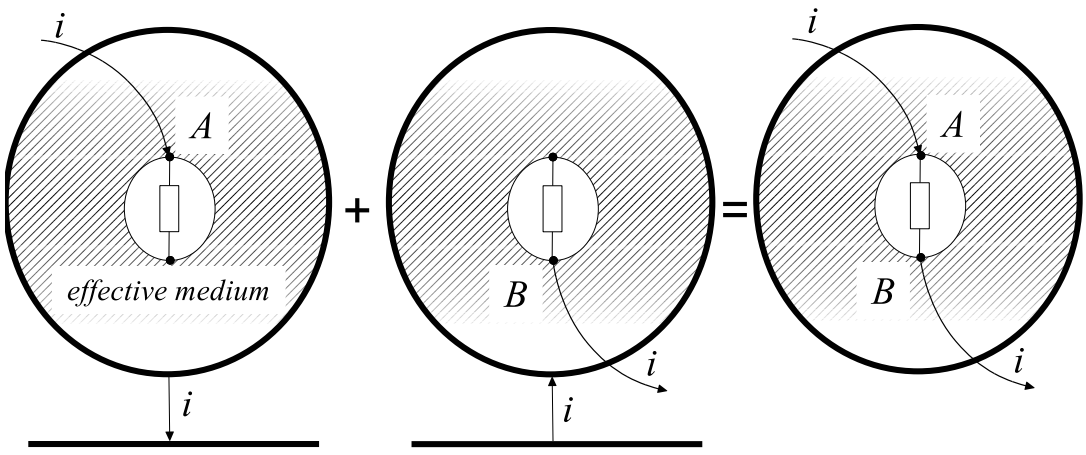

Figure 2: The constructions corresponding to cases (a), (b) and (c) discussed in the text

The voltage between A and B in this case is equal to $V_{AB} = i_{AB}/g_m$, and the overall conductivity measured between A and B is

$$G_{AB} = \frac{i_{AB}}{V_{AB}} = g_m \frac{z}{2}.$$

Since G_{AB} is the conductivity of the system corresponding to parallel switching of G'_{AB} and g_m we get

$$G'_{AB} = G_{AB} - g_m,$$

and Eq.(1) gives us

$$\left\langle \frac{g_m - g}{g_m(z/2-1)+g} \right\rangle_g = 0. \tag{2}$$

In the case of a binary mixture with $g = g_1$ with probability p and $g = g_2$ with probability $1 - p$ we get

$$\frac{g_m - g_1}{g_m(z/2-1) + g_1} p + \frac{g_m - g_2}{g_m(z/2-1) + g_2}(1-p) = 0$$

leading to a quadratic equation for g_m. In the percolation limit (infinite contrast) $g_2 = 0$, this solution is

$$g_m = g_1 \frac{(z/2)x - 1}{z/2 - 1}$$

for $p > 2/z$ and

$$g_m = 0$$

for $p < 2/z$ which defines the critical concentration for the percolation transition $p_c = 2/z$. For hypercubical lattices with $z = 2d$ (d being the dimension of space) we get $p_c = 1/d$.

2 Numerics

Most of the theoretical information we have on the actual dependence of conductivity of lattice systems (especially in the percolation setup) on the distribution of the resistor strength is obtained from numerical simulations. It is in general not to be advised to solve the (extremely large and extremely rarefied) system of the Kirchhoff's equations by use of matrix algebra, since its implementation is time- and even more memory intensive. The existence of the corresponding variational principles leads to the possibility to obtain the numerical solutions by use of relaxation algorithms which can be formulated and implemented in a very elegant way.

The relaxation algorithm to solve a system of equation for the site potentials V_i consists in fixing $V_i = 0$ and $V_i = V$ at the boundaries, and then iteratively solving the linear system of equations for V_i in the bulk of the system. Starting from

$$i_{ij} = (V_i - V_j) g_{ij}$$

and

$$\sum_j i_{ij} = 0$$

for internal sites we get $V_i \sum_j g_{ij} - \sum_j V_j g_{ij} = 0$ or

$$V_i - \sum_j V_j g_{ij} \Big/ \sum_j g_{ij} = 0. \tag{3}$$

The naive way to perform iteration is to formally solve numerically the differential equations

$$\frac{d}{dt} V_i = -\alpha \left(V_i - \sum_j V_j g_{ij} \Big/ \sum_j g_{ij} \right)$$

for the vector of potentials $\{V_i\}$ whose solution will converge (in course of the time t) to the vector leading to vanishing right hand side, i.e. to the solution of Eq.(3). This is done explicitly by considering a difference approximation

$$V_i^{(n)} = V_i^{(n-1)} - \alpha \left(V_i - \sum_j V_j g_{ij} \Big/ \sum_j g_{ij} \right)$$

(n is a number of the iteration). The parameter $\alpha > 0$ is chosen in a way that guarantees the convergence. The corresponding implicit schemes for better convergence can be used as well.

The less naive way corresponds to putting Eq.(3) into a form

$$V_i = \sum_j V_j g_{ij} \Big/ \sum_j g_{ij}.$$

We first chose all resistors to be of equal conductance, say $g = 1$, and initiate V_i with the values they would have in such an ordered system. Then those g_{ij} which will be zero in the percolation case are put to $g_{ij} = 1/2$ and the potentials are iterated several times according to

$$V_i^{(n)} = \sum_j V_j^{(n-1)} g_{ij} \Big/ \sum_j g_{ij},$$

after which the corresponding g_{ij} are put to 1/4, 1/8, *etc* until the whole converges.

In two dimensions there exists an *exact* method of calculation the conductivity for a given configuration of the system based on the *bond propagation*

algorithm, see D.J. Frank and C.J. Lobb, Phys. Rev. B **37** 302-307 (1988), which has to be preferred in situations when very high accuracy is desired. The example of implementation of this algorithm is discussed in Homework 3.

Numerical investigations have shown that percolation concentrations often differ from the predictions of EMA (the square lattice in $2d$ being a seldom exclusion), and that close to p_c the effective conductivity does not vanish linearly in $p - p_c$ as predicted by EMA, but in a "softer" way, i.e. together with its derivative, so that $g^* \propto (p - p_c)^\mu$ with $\mu \approx 1.3$ in $2d$, $\mu \approx 2$ in $3d$ and approaching $\mu = 3$ in dimensions 6 and more.