Theory of Disordered Systems

Prof. Dr. Igor Sokolov

Lecture 1: Continuous inhomogneous media

In this lecture we discuss the simplest question on how e.g. the effective conductivity of a disordered mixture of materials with different conductances can be defined and obtain the (simple and optimal) boundaries for this conductivity.

1 Mean conductivity

In what follows we discuss the mean conductivity of a disordered system between the two conducting plates as measured by an ohm-meter. We assume that localy the medium is characterized by the coordinate-dependent conductivity $\sigma(\mathbf{r})$, for example it can be a binary mixture of two conductors with conductances σ_1 and σ_2.

Let us consider our system as placed between the two conducting plates kept at constant potentials. Locally the Ohm's law applies:

$$\mathbf{j} = \sigma(\mathbf{r})\mathbf{E}(\mathbf{r}) \tag{1}$$

The current field is divergency-free, and (in the absence of time-dependent magnetic field) the electric field is irrotational, so that Eq.(1) gives us a linear realtion between a divergency-free and an irrotational field, and we have first to understand what the corresponding mean σ^* really means.

There are many mathematically equivalent problems of evaluating the mean coefficient connecting an irrotational and a divergency free field; some of them are summarized in the table below.

	Conductivity	Thermal conduct.	Diffusion	Dielectric const.	Magnetic permeab.
coeff.	$\sigma(\mathbf{r})$	$\lambda(\mathbf{r})$	$D(\mathbf{r})$	$\epsilon(\mathbf{r})$	$\mu(\mathbf{r})$
div.-free	$\mathbf{j}$	$\mathbf{q}$	$\mathbf{j}$	$\mathbf{D}$	$\mathbf{B}$
irrotat.	$\mathbf{E}$	∇T	∇n	$\mathbf{E}$	$\mathbf{H}$

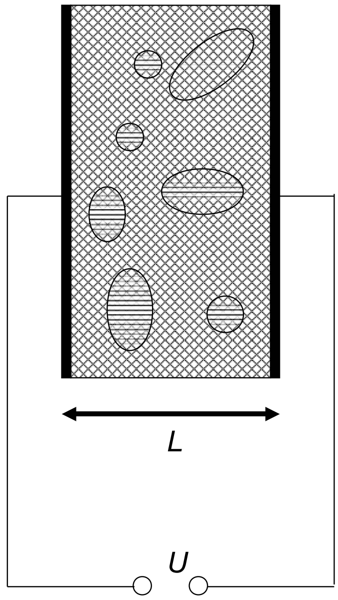

Figure 1: A sketch of a binary mixture of two conductors with conductances σ_1 and σ_2 placed between the plates of a flat capacitor. This setup will be used for the discussion of the conductance of a disordered medium during the whole first three lectures.

(it is assumed that the medium is free of charges and other sources of the corresponding fieleds, and, in the magnetic case, free of external currents). There are several related (but more complex) situations, like calculating the elastic properties of an inhomogeneous media (mean coefficients characterizing the linear dependence between the two tensors, e.g. stain and stress) which follow the same lines. We do not consider this situations in the present course.

To be concrete, in the first few lectures we concentrate on the electric conductivity, keeping in mind that other situations listed in the table are equivalent.

What is the mean conductivity of the medium? We know that the mean is easily defind for the additive quantities, so that we have to look for an additive thermodynamical quantity whose mean is per definition the arithmetic mean, and then translate the properties of this additive quantity into the properties of the coefficient of interest. In the case of electric conductivity such additive quantity is a Joule heat.

Let us consider our medium as put between the two parallel plates (of a flat capacitor, see fig.1) at distance L from each other and kept at a constant potential difference U. The heat production per unit time (Joule heat) is defined by U and by the total current I: $Q = UI$. The total current is the integral over the whatever plane (parallel to the plates) of the local current densities: $I = \int_S \mathbf{j}(\mathbf{r})d\mathbf{s}$. Since I over a whatever plane is constant (here it is where the divergency-free nature of the current plays the role), one can write $Q = (U/L)\int_V \mathbf{j}(\mathbf{r})d\mathbf{r}$ where $V^{-1}\int_V \mathbf{j}(\mathbf{r})d\mathbf{r} = \mathbf{J}$ defines the mean current density over the volume of our system and $U/L = |\mathbf{E}_0|$ is the mean absolute value of the electric field. Therefore $Q = VE_0J$, which relation holds also in general (in a vector form) $Q = V\mathbf{E_0}\mathbf{J}$.

Now we solve the equation for the Ohm's law under the condition div$\mathbf{j} = 0$, find actual values $\mathbf{E}(\mathbf{r})$ and the one of the mean field

$$\mathbf{E}_0 = \frac{1}{V}\int \mathbf{E}(\mathbf{r})d\mathbf{r},$$

the mean Joule heat per unit volume

$$q = \frac{1}{V}\int \sigma(\mathbf{r})\mathbf{E}^2(\mathbf{r})d\mathbf{r}$$

and finally determine *define* σ^* comparing this q with the one obtained from the averaged field:

$$\sigma^*\mathbf{E}_0^2 = q, \tag{2}$$

so that

$$\sigma^* = \frac{V\int \sigma(\mathbf{r})\mathbf{E}^2(\mathbf{r})d\mathbf{r}}{\left(\int \mathbf{E}(\mathbf{r})d\mathbf{r}\right)^2} = \frac{V\int \sigma(\mathbf{r})\left(\nabla\phi(\mathbf{r})\right)^2 d\mathbf{r}}{\left(\int \nabla\phi(\mathbf{r})d\mathbf{r}\right)^2}.$$

Note that the integral in denominator $\int \nabla\phi(\mathbf{r})d\mathbf{r} = -V\mathbf{E}_0 = \oint \phi(\mathbf{r})d\mathbf{s}$ depends only on the boundary conditions (prescribed potentials of plates) but not on the internal structure of the system and that it is a true *volume mean* of the electric field in the system.

Equivalently, the effective conductivity can be defined via the heat production and the mean current:

$$\frac{\mathbf{J}^2}{\sigma^*} = q. \tag{3}$$

2 Variational principle

Now we formulate a simple variational principle which allows us to find the bounds on the possible conductivities of an inhomogeneous medium (later we dwewrive much more involved ones). The simplest one is:

- *The Joule heat prodiced in a body under given boudary conditions is extremel (minimal).* (VP1)

Let us prove this statement. Thus, the Joule heat is

$$q(\mathbf{r}) = \mathbf{jE} = \frac{\mathbf{j}^2(\mathbf{r})}{\sigma(\mathbf{r})}$$

under additional constraint

$$\text{div}\, \mathbf{j}(\mathbf{r}) = 0.$$

We look for the condition under which $\delta Q = 0$ with

$$Q = \int q d\mathbf{r}.$$

Using the Lagrange multiplier method we thus write

$$\delta Q = \delta \int \left(\frac{\mathbf{j}^2}{\sigma} - 2\phi \text{div}\, \mathbf{j} \right) d\mathbf{r} = 0$$

(where the Lagrage multiplier is denoted by 2ϕ and may be position-dependent: $\phi = \phi(\mathbf{r})$). Now

$$\delta Q = \int \left(2\frac{\mathbf{j}\delta\mathbf{j}}{\sigma} - 2\phi \text{div}\, \delta\mathbf{j} \right) d\mathbf{r}.$$

Performing partial integration in the second term $\int \phi \text{div}\, \delta\mathbf{j} d\mathbf{r} = \int \phi \delta\mathbf{j} d\mathbf{s} - \int \delta\mathbf{j} \text{grad}\, \phi d\mathbf{r}$ and noting that the surface integral vanishes since $\delta\mathbf{j} = 0$ outside of the system we get

$$\int \left(\frac{\mathbf{j}}{\sigma} + \text{grad}\, \phi \right) \delta\mathbf{j} d\mathbf{r} = 0$$

so that (due to the arbitrariness of $\delta\mathbf{j}$) $\mathbf{j}/\sigma + \text{grad}\, \phi = 0$ or

$$\mathbf{j}(\mathbf{r}) = -\sigma(\mathbf{r}) \text{grad}\, \phi(\mathbf{r}).$$

Associating now $\phi(\mathbf{r})$ with the electric potential we obtain

$$\mathbf{j}(\mathbf{r}) = \sigma(\mathbf{r})\mathbf{E}(\mathbf{r})$$

i.e. the Ohm's law. Thus, the Ohm's law follows from the continuity equation under the assumption of the extermal propery of the heat production. If the Ohm's law holds, the heat production is extremal.

Notes:

- Calculating the second variation of Q we can prove that the extremum is the (absolute) minimum.
- The existence of the variational pronciple is the basis for relaxation methods for calculating the conductivity, which (calculation) is otherwise numerically complex.

We can give another form of the same principle. Let us assume that the Ohm's law holds, and show that if the heat production is extremal, the divergency of the current must vanish. To do this we restart from

$$Q = \int \sigma(\mathbf{r})\mathbf{E}^2(\mathbf{r})d\mathbf{r}$$

with $E_i = \partial\phi/\partial x_i$, so that

$$Q = \int \sigma(\mathbf{r})\frac{\partial\phi}{\partial x_i}\frac{\partial\phi}{\partial x_i}d\mathbf{r}$$

(summation over repeated indices!) and

$$\delta Q = 2\int \sigma(\mathbf{r})\frac{\partial\phi}{\partial x_i}\delta\frac{\partial\phi}{\partial x_i}d\mathbf{r} = -2\int \frac{\partial}{\partial x_i}\left[\sigma(\mathbf{r})\frac{\partial\phi}{\partial x_i}\right]\delta\phi d\mathbf{r}.$$

From the extremality then follows:

$$\frac{\partial}{\partial x_i}\left[\sigma(\mathbf{r})\frac{\partial\phi}{\partial x_i}\right] = 0$$

i.e. $\mathrm{div}\sigma\mathbf{E} \equiv \mathrm{div}\mathbf{j} = 0$: the continuity equation follows from the Ohm's law under the extremality of heat production, or, in other words, if both, the continuity and the Ohm's law are fulfilled, the heat production is extremal.

Calculation of the second variation then proves again the minimality of this production.

Therefore for whatever test functions $\mathbf{j}_T(\mathbf{r})$ or $\mathbf{E}_T(\mathbf{r})$

$$Q \leq \int \frac{\mathbf{j}_T^2(\mathbf{r})}{\sigma(\mathbf{r})} d\mathbf{r}$$

and

$$Q \leq \int \sigma(\mathbf{r}) \mathbf{E}_T^2(\mathbf{r}) d\mathbf{r}.$$

Dividing these expressions by V we obtain the inequalities for mean specific heat production q.

Now let us note that $\mathbf{E}_0$ depends only on the boundary conditions and not on the internal structure of the system and teake it as a test function. According to the definition of σ^* we get:

$$q = \sigma^* \mathbf{E}_0^2 \leq \frac{1}{V} \int \sigma(\mathbf{r}) \mathbf{E}_0^2(\mathbf{r}) d\mathbf{r} = \mathbf{E}_0^2 \frac{1}{V} \int \sigma(\mathbf{r}) d\mathbf{r},$$

i.e.

$$\sigma^* \leq \frac{1}{V} \int \sigma(\mathbf{r}) d\mathbf{r} = \langle \sigma(\mathbf{r}) \rangle \,,$$

where the mean value has to be understood as a simple mean over the volume of the system. Analog, taking a test function for the current $\mathbf{j}_T(\mathbf{r}) = \mathbf{J} = const$ (which automatically fulfills the continuity equation) we get

$$q \leq \frac{1}{V} \int \frac{\mathrm{J}^2}{\sigma(\mathbf{r})} d\mathbf{r} = \mathrm{J}^2 \frac{1}{V} \int \sigma^{-1}(\mathbf{r}) d\mathbf{r},$$

so that, according to Eq.(3) we have

$$\frac{\mathrm{J}^2}{\sigma^*} \leq \mathrm{J}^2 \frac{1}{V} \int \sigma^{-1}(\mathbf{r}) d\mathbf{r}$$

and

$$\frac{1}{V} \int \sigma^{-1}(\mathbf{r}) d\mathbf{r} \geq \frac{1}{\sigma^*} \qquad \text{i.e.} \qquad \left\langle \sigma^{-1}(\mathbf{r}) \right\rangle^{-1} \leq \sigma^*,$$

where the mean value is again the volume mean. Combining both boundaries we obtain

$$\left\langle \sigma^{-1}(\mathbf{r}) \right\rangle^{-1} \leq \sigma^* \leq \langle \sigma(\mathbf{r}) \rangle \tag{4}$$

which shows that the actual mean conductivity of the system always lies between the geometric and the arithmetic volume means of the local conductivities.

3 Optimality

The boundaries given by application of our simple variational principle to the system are *optimal* which means that it is always possible to construct a system for which both are realizable. Let us consider for example a medium which consists of n different materials with specific conductivities σ_i. The lower boundary is then realized in a layered medium in which the layers of different materials are parallel to the plates of the capacitor, which corresponds to the sequential switching of the corresponding resitances. The upper bound is realized e.g. in the case when the layers of different paterials are perpendicular to the plates and their resistances are switched in parallel.

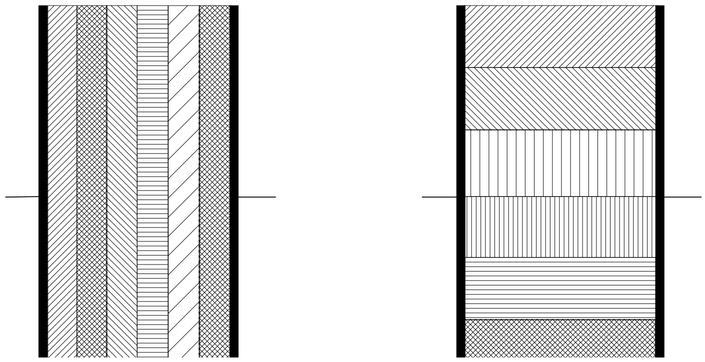

Figure 2: A sketch of the situations which realize the boundaries of the conductivity of a mixture of different conductors, Eq.(4). Note that none of them corresponds to what we could call "disordered".

None of these constructions can be considered "disordered", and indeed, the probability that each of them would be realized without an external (or internal) driving force is vanishingly small. Thus, we learned something about conductivity but very little about disorder.

The situations are not disordered since they lack rotational symmetry. Before turning to situations with rotational symmetry we will consider some other cases, not pretending to build a consequent theory but following the historical direction of the development of the theory of disordered systems.