Solid State Theory[1]

Prof. Vadim Geshkenbein, FS 2021
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Summary Room at HIT, me writing on the whiteboard numerous pens of different color were offered. Examiner and co-examiner are sitting in the back row of the room (Corona). Language: English.

Description of the content: Lecture 3, 6, 13, 19, 22

Ablauf Entered the room, the professor and the co-examiner were asking about the origin of my name and where my ancestors were from. We spent quite some time doing small talk before the exam.

Prof: Can you derive conductivity from the Boltzmann equation?

Me: Let me start by saying a few words about the Boltzmann equation. We looked at a particle density $f(\mathbf{k}, \mathbf{r}, t)$ in the phase space Γ, where the particle density describes the number of particles found within an infinitesimal small volume

$$f(\mathbf{k}, \mathbf{r}, t) d^3r \frac{d^3k}{(2\pi\hbar)^3}. \tag{1}$$

There are three possibilities resulting in a change of particles number: One of which is a simple flow through the small volume which can written as

$$f(\mathbf{k}, \mathbf{r}, t) = f(\mathbf{k}, \mathbf{r} - t\mathbf{v}, 0), \tag{2}$$

where we assumed that Liouvilles theorem holds. By taking a Taylor expansion this equation leads to the term $\mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}}$. Another possibility is by applying a field where we can then use the same arguments as above leading to the term $\mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{k}}$ which indeed describes the change in number of particles by application of an external field. The last possibility includes the collision integral which is due to collision of particles inside the infinitesimal small phase space volume. Adding all the terms we find the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{k}} = I(f), \tag{3}$$

where we used semi-classical dynamics. For isotropic problems and elastic scattering the collision

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integral can be approximated by

$$I(f) = -\frac{f - f_0}{\tau} \tag{4}$$

where τ corresponds to the average time between the collisions of particles. This ansatz is known as the relaxation time approximation.

Prof: What is f_0?

Me: It is simply given by the Fermi-Dirac distribution where the notation $f = f_0 + f_1$ is introduced. *I totally forgot to mention that we assumed $f_1 \ll f_0$, see below.*

So for a uniform and time independent electric field we can drop two terms in the Boltzmann equation leading to

$$e\mathbf{E} \cdot \frac{\partial f}{\partial \mathbf{k}} = \frac{f_0}{\tau}. \tag{5}$$

Solving for f_1 leads to

$$f_1 = \tau v \mathbf{E} \frac{\partial f}{\partial \mathbf{k}}. \tag{6}$$

The current density is given by

$$\mathbf{j} = -2e \int \frac{d^3k}{(2\pi\hbar)^3} f(k) \frac{\partial \varepsilon}{\partial \mathbf{k}} \tag{7}$$

where we can use that f_0 would not contribute to the current density just by the fact that it is symmetric with respect to $\mathbf{k} \to -\mathbf{k}$ as well as that the energy dispersion is symmetric hence the current density vanishes. In the next step we again use semi-classics where we finally arrive at the expression

$$\mathbf{j} = e^2 \tau \int N(\varepsilon) \frac{\partial f}{\partial \varepsilon} v = \underbrace{\frac{1}{3} N(\varepsilon_F) e^2 \tau v_F^2}_{\sigma} \mathbf{E}. \tag{8}$$

Prof: Why did you write $\partial f / \partial \varepsilon$ and not $\partial f_1 / \partial \varepsilon$?

Me: *Absolutely no clue why and trying to dodge the question.* Well we need that $\partial f / \partial \varepsilon \sim -\delta(\varepsilon - \varepsilon_F)$.

Prof: *Not impressed and definitely not satisfied with my answer.*

Me: *After some discussion about which term scales like which I found out that the answer he was looking for is that within relaxation time approximation we had to assume that $f_1 \ll f_0$.*

The derived result can be re-written into the form of Drude

$$\sigma = \frac{ne^2\tau}{m^*}, \tag{9}$$

which however hides the important part that the electrons at the Fermi surface contribute to conductivity which can be seen more nicely in the form of Equation 8. So overall we started with the Boltzmann equation and arrived at the Drude result.

Prof: Can you find the result for AC conductivity?

Me: In this case we can not drop the time dependent term leading to[2]

$$\frac{\delta f}{dt} - e\mathbf{E} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{\delta f}{\tau} \tag{10}$$

which in Fourier space is given by

$$-i\omega\delta f - e\mathbf{E} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{\delta f}{\tau} \tag{11}$$

and hence

$$\delta f(\frac{1}{\tau} - i\omega) = e\mathbf{E} \cdot \frac{\partial f}{\partial \mathbf{k}}. \tag{12}$$

This term is exactly equivalent to the previous derivation of the conductivity in the constant field.

Prof: Please show it.

Me: If we define $g = (\frac{1}{\tau} - i\omega)$ and insert it into Equation 7 we find the result

$$\sigma = \frac{\sigma_0}{1 - i\omega\tau}. \tag{13}$$

I don't know why but he was simply not satisfied with this answer as he insisted on me doing the whole derivation so I actually inserted it into the current density and then found the result after three more lines of calculation.

[2]Different definition as above: $f = f_0 + \delta f$.

Prof: Can you derive conductivity for a lattice with cubic symmetry?

Me: First of all we used the relaxation time approximation which only holds for isotropic problem and hence is not applicable if we have cubic symmetry.

Prof: But can you say something about the directions? Which has increased conductivity?

Me: *Drew a cube just to get some time to think and while drawing the cube I realized that for problems in 2D this questions sounded familiar.* We know that resistivity is a symmetric rank 2 tensor which defines a quadratic form

$$q(\mathbf{x}) = \mathbf{x}^T \rho \mathbf{x}. \tag{14}$$

However from the symmetry of the lattice we have to impose the same symmetry on the resistivity leading to

$$U^{-1} \rho U = \rho \tag{15}$$

where U is a unitary transformation and hence

$$q(\mathbf{x}) = \mathbf{x}^T \rho \mathbf{x} = (U\mathbf{x})^T \rho (U\mathbf{x}). \tag{16}$$

Just for fun we can then set this equation equal unity where we know from linear algebra that this will define an ellipse for positive definite ρ. *I sketched an ellipsoid and drew the reflection symmetry planes.* On the other hand, we know that U defines a further symmetry which has the representation of a rotation of the ellipse. As this problem has to be invariant with respect to U the only way to satisfy the conditions is if $\rho \propto I_n$ (the identity) and the ellipse is a circle. From this we can deduce that the resistivity is isotropic for a sample with a cubic lattice.

Prof: How can we distinguish insulators from metals without measuring the resistivity?

Me: This can be done by measuring the specific heat as we derived in the lecture that

$$C_v \sim \gamma T + BT^3, \tag{17}$$

where γ is the Sommerfeld coefficient (*denoted as A in Figure 1*). The linear term describes the electron contribution which is characteristic for metals as this term is not present in insulators. The cubic term describes the phonon contribution. Given that

$$\int \frac{d^3k}{(2\pi\hbar)^3} \sim T^3 \tag{18}$$

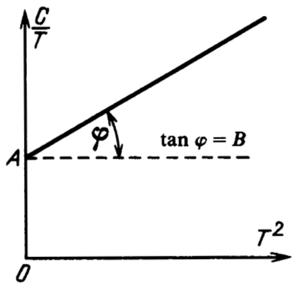

Figure 1: Specific heat as a function of temperature in metals. Figure taken from Abrikosov - Fundamentals of the theory of metals.

and that each phonon contributes an energy of $\sim T$ the specific heat scales as T^3. In the case of electron contribution...

Prof: You do not have to derive this.

Me: *I sketched Figure 1.* For an insulator there is no y-axis intercept which enables us to distinguish an insulator from a metal.

Prof: What happens in the case of an Anderson insulator?

Me: I honestly do not know the answer to this question. But I assume that as we have localization of the electrons, we do not get any contribution to the specific heat from the electrons.

Prof: No, there is still contribution to the specific heat as the electrons can be thermally excited to higher states. (*I can not fully remember the arguments he used for this statement*). Okay, good.

Final Remarks Prof. Geshkenbein did not interrupt me when I said a few more words about the theory and derivations of a given question before actually answering it (see for example my introduction to the Boltzman equation). Hence I think it is certainly not disadvantageous to say a bit more about what one knows than just simply answering the question. What is of utmost importance are the exercise sheets as he likes to ask them during exams. I mostly used the books: Abrikosov - Fundamentals of the Theory of Metals, Ziman - Principles of the Theory of Solids, Landau Lifshitz Vol. 5 and Vol. 9 and Ashcroft Mermin - Solid State Physics. Please do not take the derived results for granted, as I might have done some mistakes. Good luck!

Expected mark: 5.5
Received mark: 5.75