

Oct 1st - Class 1, Ph 135, Gil Refael

I. INTRODUCTION

This class is called Introduction to Condensed Matter physics. For many years I wanted to teach this class, but had to compromise on teaching 12b, or 127, or the occasional EM. But I really wanted to teach this class, since it is about my favorite particle - the electron. I know some of you are big fans if other particles - quarks, maybe some gauge bosons - maybe the Higgs? Maybe even particles that have not yet been discovered, like supersymmetric partners - the neutralino? Or of strings. But let me extoll the electron: It lives forever! It is point like, but most importantly, it is the particle on which our technology depends. Starting with magnets, going through incandescent bulbs, semiconductors and computers, our communication system (also through if you are using smoke signals, btw) and next - superconductors and quantum computers.

Our class will concentrate on what electrons are up to in metals and in semiconductors. We will start by thinking about how they move, discuss their band structure, talk about how electronics works, and then get to more exotic modes of behavior. Spin orbit coupling and last but not least, talk about topological insulators. You will quickly see that our class will require your knowledge in quantum mechanics as well as in statistical mechanics. And also, as is befitting any advanced class, a good chunk of fourier transforms and complex analysis. Brush up on these a bit. BTW, electrons are also the particle of choice for chemists, I believe, which makes all condensed matter practitioners have a bit of a chemistry envy. So if you're looking for places to show your superiority over me - brush up on some chemistry as well.

The class specifics. We will start off with a loose connection to Ashcroft and Mermin. I recommend having the book though. It is a good compendium of good old solid-state physics, and is the first stop for any question about electrons. Some of the later chapters are not covered in it, and I'll provide references as we go. I'll also give you notes as we go. There will be a weekly problem set, and a weekly section, which I encourage you to go to.

II. ELECTRONS IN METALS: A REVIEW FROM PH127A

The best place to start our discussion of electrons in metals is to just pretend that the electrons are like free particles, with a hamiltonain:

$$H = \frac{\vec{p}^2}{2m} + V(\vec{r}) \quad (1)$$

with $V(\vec{r})$ the potential energy they are subject too, which, not in the least, keeps them confined in the metal (think particle in a box). This model of metals is fondly called the 'Jellium model'. If you need to visualize why, it is because it is assumed that the electrons are swimming in a jelly of nuclei that pose no periodic structure, or any structure otherwise for that matter, and only provide a background positive charge to hold the electrons in place. In a couple of weeks we will do better than that.

For now, let's derive the density of states that such a metal jellyum has, recall the Fermi distribution and fermi surface, and do a bit of gymnastics with the Sommerfeld expansion.

A. Electronic states

The electrons in this class are quantum, and something we'll constantly need is the one-particle quantum states. We assume that the electrons are in a translationally invariant box, and further, we make the leap of faith that the box has periodic boundary conditions. So that:

$$\psi(\vec{x}) = \psi(\vec{x} + L_i \hat{x}_i) \quad (2)$$

This allows us some computational ease and doesn't change the physics of the bulk electrons.

The fact that the system is translationally invariant means that the wave function, is necessarily given by a plane wave solution:

$$\psi(\vec{x}) = \frac{1}{(L_1 L_2 \dots L_d)^{1/2}} e^{i\vec{k} \cdot \vec{x}} \quad (3)$$

The boundary conditions impose periodicity in the size of the box:

$$e^{ik_j(x_j+L_j)} = e^{ik_jx_j} \quad (4)$$

which immediately implies:

$$k_iL_i = 2\pi n_i \quad (5)$$

For all dimensions. The numbers n_i determine the quantum state, (n_1, n_2, \dots, n_d) . Note that I didn't use the Hamiltonian at all yet. Just translational invariance.

In this treatment we used a rather ambiguous way of numbering our quantum states, we use the set (n_1, n_2, \dots, n_d) , but also the vector

$$\vec{k} = \left(\frac{2\pi n_1}{L_1}, \dots, \frac{2\pi n_d}{L_d} \right) \quad (6)$$

B. State counting

Ultimately, we would like to sum over states:

$$\sum_{n_1, n_2, \dots, n_d = -\infty}^{\infty} \quad (7)$$

We can describe this by drawing the n -space. Each integer value of the n 's is a quantum state. Actually, it would be much easier to sum over the k 's - but that's no problem. We just draw the same diagram, but now for k . The side of each box in dimension i is:

$$dk_i = \frac{2\pi}{L_i} dn_i = \frac{2\pi}{L_i} \quad (8)$$

So the number of states in k -space, is the k -space volume, K , over the product of the box sizes for all dimensions:

$$g = \frac{K}{\prod_{i=1}^d (2\pi/L_i)} = V \frac{K}{(2\pi)^d} = V \frac{d^d k}{(2\pi)^d} \quad (9)$$

Now that we know how to count states, we no longer need the crutch of the n 's. Also, we can notice here another benefit: the connection with the classical energy counting schemes. Since:

$$k = p/\hbar \quad (10)$$

the above counting scheme is just:

$$g = V \frac{d^d p}{(2\pi\hbar)^d} = V \frac{d^d p}{h^d}. \quad (11)$$

And you recall that in statmech, we always divide $dx dp$ by h - this is why.

C. Density of states

This brings us to the Density of states, $\rho(\epsilon)$. Above we carried out the sums with respect to wave number k . But what if we want to carry it out in terms of energy? How many states do we have in a given energy range $[\epsilon, \epsilon + d\epsilon]$ per volume?

Formally, we write:

$$V\rho(\epsilon)d\epsilon = V \int \frac{d^d k}{(2\pi)^d} \delta(\epsilon - \epsilon_{\vec{k}})d\epsilon \quad (12)$$

The volumes cancel, and the last part of the equation is just one, as the dirac delta function is just one over the energy differential in the desired range. This is a formal expression that can usually be much simpler. For instance, for a d-dimensional gas with a free particle hamiltonian, we have:

$$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} \quad (13)$$

Therefore we can also write:

$$V\rho(\epsilon)d\epsilon = V \frac{\Omega_d k^{d-1} dk}{(2\pi)^d} \quad (14)$$

Where Ω_d is the ratio of a the surface area of a d-dimensional sphere to the radius to the power of $d - 1$. Therefore the differential in the RHS, is just the volume of a spherical shell in k -space. Dividing by $d\epsilon$:

$$V\rho(\epsilon) = V(2s + 1) \frac{\Omega_d k^{d-1} d|k|}{(2\pi)^d d\epsilon} \quad (15)$$

This could also be formally obtained using the manipulation of the delta-function:

$$\delta(\epsilon - \epsilon_{\vec{k}})d\epsilon = \delta(k - k_\epsilon)dk \quad (16)$$

and dividing by $d\epsilon$ to get the inverse dispersion relation. And by putting it up in Eq. 12 , we get the last result.

For a free particle:

$$\frac{d\epsilon_{\vec{k}}}{dk} = \frac{\hbar^2}{m}k \quad (17)$$

so:

$$\rho(\epsilon) = (2s + 1) \frac{\Omega_d k^{d-1}}{(2\pi)^d} \frac{m}{\hbar^2 k} = V(2s + 1) \Omega_d \left(\frac{\sqrt{2m}}{2\pi\hbar} \right)^d \epsilon^{d/2-1} \quad (18)$$

So instead of integrating over the k 's, we can integrate over the energies with the density of states function:

$$g = V \int d\epsilon \rho(\epsilon). \quad (19)$$

Notice that $\rho(\epsilon)$ is very dimensional dependent. At $d=2$ it is a constant, and for $d=1$ it diverges like $1/\sqrt{\epsilon}$, marking the aggregation of states near the bottom of the dispersion.

D. Fermi-Dirac distribution

How are these states get occupied? That depends on the temperature and chemical potential of the electrons. For each state \vec{k} , with a given spin state $\sigma^z = \pm 1$ for electrons, there is a grand-canonical partition function:

$$\mathcal{Z}_{\vec{k}} = \sum_{N_{\vec{k}}=0}^{N_{max}} e^{-(\epsilon_{\vec{k}} - \mu)\beta} = 1 + e^{-(\epsilon_{\vec{k}} - \mu)/T} \quad (20)$$

since for Fermions, each state can be either occupied or empty.

The occupation follows very quickly. For every state we have:

$$n_{\epsilon_{\vec{k}}} = \frac{e^{-(\epsilon_{\vec{k}} - \mu)/T}}{1 + e^{-(\epsilon_{\vec{k}} - \mu)/T}} \quad (21)$$

and the total number:

$$N = V \int d\epsilon \rho(\epsilon) n_{\epsilon_{\vec{k}}} = V(2s + 1) \int \frac{d^d k}{(2\pi)^d} \frac{1}{e^{(\epsilon_{\vec{k}} - \mu)\beta} + 1} \quad (22)$$

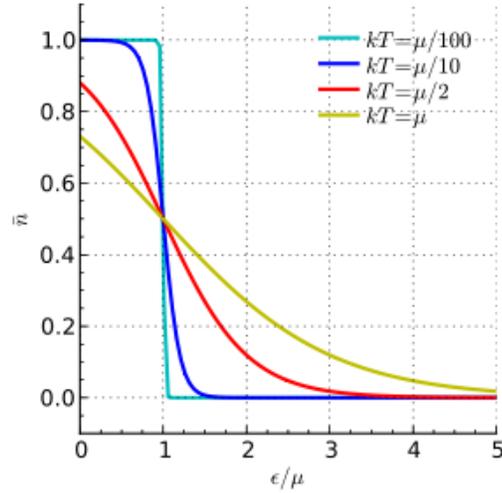


FIG. 1. The Fermi-Dirac distribution as a function of energy. Taken from wikipedia.

This is a very important result. Let's interpret it. Everything in front of the fraction is simply an enumeration of the states - $d^d k / (2\pi)^d$, $(2s + 1)V$, it's all counting stuff. The integrand, $n_{\epsilon_{\vec{k}}} = f(\epsilon_{\vec{k}})$, is called the Fermi-function, or the Fermi-Dirac distribution.

The Fermi-Dirac distributions for the theory of metals is what the cosine function is to the theory of triangles. with it, you can calculate everything. And like the cosine, you can get away with a lot just knowing how it behaves for a small angle, i.e., at a low temperature.

What does this function look like at zero temperature? Assuming that our energy spectrum stretches from zero up, (which we can always do by setting the lowest energy eigenvalue in the problem to zero), if $\mu < 0$ then:

$$f(\epsilon_{\vec{k}}) = \frac{1}{e^{(\epsilon_{\vec{k}} - \mu)/T} + 1} \rightarrow 0 \quad (23)$$

since the exponent is large. For positive μ it becomes:

$$f(\epsilon_{\vec{k}}) = \frac{1}{e^{(\epsilon_{\vec{k}} - \mu)/T} + 1} = \begin{cases} 1 & \epsilon_{\vec{k}} < \mu \\ 0 & \epsilon_{\vec{k}} > \mu \end{cases} \quad (24)$$

It is a step like function. Only states below the chemical potential are occupied, we call the chemical potential in this case - the Fermi energy.