

(Instructor: James Analytis)

# Physics 141A: Solid State Physics notes

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These are some notes taken from UC Berkeley's Physics 141A during the Fall '24 session, taught by James Analytis.

This template is based heavily off of the one produced by [Kevin Zhou](#).

## Contents

<b>1 August 28: Introduction</b>	<b>2</b>
1.1 What is condensed Matter / Soild State Physics? . . . . .	2
1.2 Heat Capacity . . . . .	2
<b>2 August 30: Missed lecture. Ask in Office Hours.</b>	<b>6</b>
<b>3 September 2: Labor Day! No class</b>	<b>7</b>
<b>4 September 4: Debye Model</b>	<b>8</b>
4.1 1D case . . . . .	8
4.2 3D case . . . . .	8
4.3 Debye's Calculation following Planck . . . . .	9
<b>5 September 6:</b>	<b>12</b>
<b>6 September 9: Drude Model Continued, Hall Effect</b>	<b>15</b>
6.1 Conducting Wire, Drude Conductivity . . . . .	15
<b>7 September 11:</b>	<b>19</b>
7.1 Thermal Conductivity . . . . .	19
7.2 Wiedemann-Franz Law . . . . .	21
<b>8 September 13: Sommerfeld Model</b>	<b>23</b>

## 1 August 28: Introduction

### 1.1 What is condensed Matter / Solid State Physics?

(Write afterwards)

### 1.2 Heat Capacity

What is the Heat Capacity of a solid?

Essentially, it quantifies how the average energy of a solid changes with increases in temperature.

$$C_{P(V)} = \left. \frac{dQ}{dT} \right|_{P(V)}$$

But then, one might ask, what exactly *is* Temperature? We all know what it is intuitively, but can we give it a more rigorous definition?

## Kinetic Theory of Gases

In statistical mechanics, we define the temperature by connecting it to the number of possible microstates a system can occupy. From here, we state that the probability of occupying a specific state  $r$  is given by the **Boltzmann Factor**

$$P(\epsilon_r) \propto e^{\epsilon_r/k_B T}$$

where  $\epsilon_r$  is the energy of state  $r$  and  $T$  is the temperature.

(Give analogy with number of flips of dice thrown slow vs fast)

To get the probability itself, we normalize by the sum of *all* the boltzmann factors corresponding to the different energy states.

$$P(\epsilon_r) = \frac{e^{\epsilon_r/k_B T}}{\sum_i e^{\epsilon_i/k_B T}}$$

Consider a two-state system

$$\epsilon \longrightarrow P(\epsilon) = \frac{e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}}$$

$$0 \longrightarrow P(0) = \frac{e^{-\beta \cdot 0}}{1+e^{-\beta \cdot 0}} = \frac{1}{1+P(\epsilon)} = \frac{e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}}$$

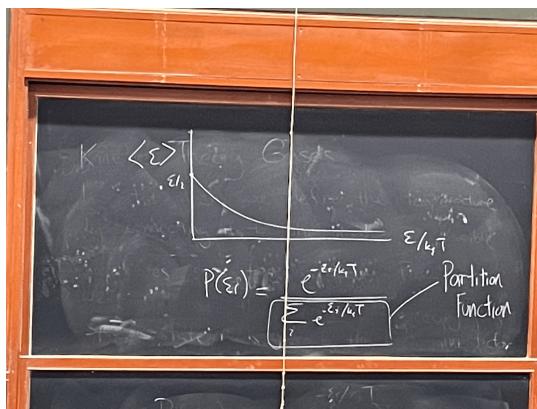
Then, the expected value of the energy of the system is

$$\begin{aligned} \langle \epsilon \rangle &= 0 \cdot P(0) + \epsilon \cdot P(\epsilon) \\ &= 0 + \frac{\epsilon e^{-\beta\epsilon}}{1+e^{-\beta\epsilon}} \\ &= \frac{\epsilon}{e^{\beta\epsilon} + 1} \end{aligned}$$

Notice that if  $T \rightarrow 0$  then  $\langle \epsilon \rangle \rightarrow 0$  and if  $T \rightarrow \infty$  then  $\langle \epsilon \rangle \rightarrow \epsilon/2$

(Include graph of  $\langle \epsilon \rangle$  vs  $T$ )

$$\begin{aligned} W(\epsilon) &= \Omega_0 P(0) + \Omega_1 P(\epsilon) \quad \text{solid?} \\ (\Omega_0 + \Omega_1) e^{-\epsilon/T} &= \frac{\epsilon}{e^{\epsilon/T} - 1} = \frac{\epsilon}{e^{\epsilon/T} - 1} = \frac{\epsilon}{e^{\epsilon/T} - 1} \\ H & \langle \epsilon \rangle = \frac{\epsilon_1}{e^{\epsilon_1/T} - 1} + \frac{\epsilon_2}{e^{\epsilon_2/T} - 1} \end{aligned}$$



The normalization factor in  $P(\epsilon_r)$  is called the **Partition Function**

$$Z = \sum_i e^{-\epsilon_i/k_B T}$$

In our two-state system the energy spectrum is discrete. However, in general, we can have continuous spectra.

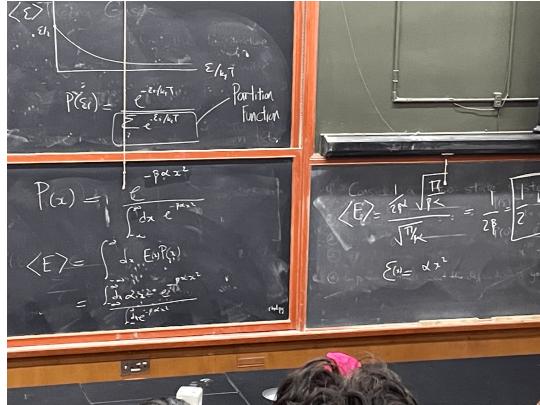
A very useful distribution to be familiar with is the following, where we have a continuous spectrum of states:

$$P(x) = \frac{e^{-\beta \alpha x^2}}{\int_{-\infty}^{\infty} dx e^{-\beta \alpha x^2}}$$

and the energy spectra is dependent on  $x$  i.e. we have  $E(x)$ . Then,

$$\langle E(x) \rangle = \int_{-\infty}^{\infty} dx E(x) P(x)$$

(Include intermediate steps)



which gives us

$$\langle E \rangle = \frac{1}{2\beta} = \frac{1}{2} k_B T$$

Notice that  $\langle E \rangle$  is **independent of  $\alpha$ !** i.e. it only depends on temperature.

In general, if we have quadratic degree of freedom in the boltzmann factor, it does not impact the average energy.

Suppose we have  $n$  such quadratic degrees of freedom in our expression for energy:

$$\epsilon = \sum_{i=1}^n \alpha_i x_i^2$$

For example,

$$\frac{1}{2}mv^2 + \frac{1}{2}kx^2$$

then, the average energy is

$$\begin{aligned} \langle \epsilon \rangle &= \sum_{i=1}^n \alpha_i \langle x_i^2 \rangle \\ &= \sum_{i=1}^n \frac{1}{2} k_B T \\ &= \frac{n}{2} k_B T \end{aligned}$$

**Example, Mass on a spring:**  $\langle \epsilon \rangle = 2 \cdot \frac{1}{2} k_B T = k_B T$

Now, solids are 3D objects comprised of a bunch of atoms, which we can imagine as being joined together with **springs**. Suppose we have such a solid with  $N$  atoms. Then, the mean energy is

$$\begin{aligned} \langle \epsilon \rangle &= \underbrace{3}_{\text{dimension}} \cdot \underbrace{2}_{2 \text{ d.o.f's}} \times \frac{1}{2} k_B T \times N \\ &= 3Nk_B T \end{aligned}$$

Then, the Heat Capacity of the solid is

$$C = \frac{d\langle \epsilon \rangle}{dt} = 3Nk_B$$

or, for a mole of the solid,

$$C_{\text{mole}} = 3N_A k_B = 3R$$

Nothing in this derivation depended on the material being considered. So, we've shown that **every solid has the same heat capacity!**

Well, this is wrong. But at high enough temperatures, it does hold pretty well.

**6** 2. August 30: Missed lecture. Ask in Office Hours.

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**2 August 30: Missed lecture. Ask in Office Hours.**

7 3. September 2: Labor Day! No class

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### **3 September 2: Labor Day! No class**

## 4 September 4: Debye Model

Today we'll begin studying the Debye Model (Ch. 2 in the textbook).

From studying the Einstein Model, we realized that in order to better understand solids we must treat them *Quantum Mechanically*.

Debye asked "What if sound in solids was like light, and was quantized & dispersed like light?". When we say "dispersed" we mean, written as a function of momentum

$$\underbrace{\omega}_{\text{freq.}} = \underbrace{v}_{\text{vel. of sound}} \underbrace{|\vec{k}|}_{\text{wavevector}}$$

### 4.1 1D case

Let's analyze this in one-dimension. Consider sound traveling along a 1-D solid (a string) of length  $L$ . In order to analyze our string, we'll use **Born-von Karman** boundary conditions to turn our string of length  $L$  into a *circle* of circumference  $L$ .

Include picture

#### Why is it fine to assume periodicity?

Simple waves generally tend to be periodic in nature, and even if we do have to deal with aperiodic waves, we can almost always decompose them into sums of periodic waves using **Fourier Analysis**, so we just assume periodicity to save effort.

With these boundary conditions, a sound wave at  $x$  has the same value at  $x + L$ . So, suppose

$$\begin{aligned} e^{ikx} &= e^{ik(x+L)}, \text{ so } e^{ikL} = 1 \\ \implies kL &= n(2\pi) \\ \implies k &= n \cdot \frac{2\pi}{L} \text{ for } n = \dots, -1, 0, 1, 2, 3, \dots \end{aligned}$$

Often (eg. when calculating average energies) we'll need to sum over the  $k$ -states. If we have a continuum solid, we can convert our sums to integrals as

$$\sum_k \rightarrow \frac{1}{\Delta k} \int_{-\infty}^{\infty} dk$$

### 4.2 3D case

Assuming we now have a cuboid of *sidelength*  $L$ , our wavevectors have the form

$$\begin{aligned} \vec{k} &= (k_1, k_2, k_3) \\ &= \frac{2\pi}{L} (n_1, n_2, n_3) \end{aligned}$$

for  $n_1, n_2, n_3 \in \mathbb{N}$

So, we convert our sums into integrals as

$$\sum_i \rightarrow \frac{1}{(2\pi/L)^3} \int d^3 \vec{k} = \left(\frac{L}{2\pi}\right)^3 \int d^3 \vec{k}$$

### 4.3 Debye's Calculation following Planck

We have the dispersion relation

$$\omega(\vec{k}) = v_s |\vec{k}|$$

and so, with the Einstein model,

$$\langle E \rangle = 3 \times \sum_k \hbar \omega(\vec{k}) \left( n(\vec{k}) + \frac{1}{2} \right)$$

(we have th factor of 3 becayse that's how many *modes* we have for sound waves: 2 transverse modes and 1 longitudinal mode)

and the Bose Occupation Factor is

$$n_s(\vec{k}) = \frac{1}{e^{\beta n \omega(\vec{k})} - 1}$$

So,

$$\langle E \rangle = 3 \left( \frac{L}{2\pi} \right)^3 \int_{-\infty}^{\infty} d^3 \vec{k} \hbar \omega(\vec{k}) \left( n_s(\vec{k}) + \frac{1}{2} \right)$$

Each excitation made is a **Boson** of frequency  $\omega(\vec{k})$  and occupied  $n_s(\vec{k})$  times.

Using spherical coordinates in  $k^3$  space,

$$\int d^3 \vec{k} \rightarrow \int_0^{\infty} 4\pi k^2 dk$$

where now  $k$  just refers to the magnitude of  $\vec{k}$ .

Then, using the dispersion relation  $\omega = v_s k \implies k = \frac{\omega}{v_s}$ , we can change the variable of integration from  $k$  to  $\omega$  and get

$$\langle E \rangle = 3 \cdot 4\pi \left( \frac{L}{2\pi} \right)^4 \int_0^{\infty} \frac{\omega^2}{v_s^2} \cdot \hbar \omega \cdot \left( n_s + \frac{1}{2} \right) d\omega$$

We can re-write this a little as:

$$\langle E \rangle = \int_0^{\infty} g(\omega) \hbar \omega \cdot \left( n_s + \frac{1}{2} \right) d\omega$$

the function  $g(\omega)$  is the **density of states** in terms of frequency. In this case,

$$g(\omega) = L^3 \frac{12\pi}{(2\pi)^3} \frac{\omega^2}{v_s^3}$$

Defining,

$$\omega_d^3 = 6\pi^2 n v_s^3$$

to be the **Debye Frequency**, the density of states is

$$g(\omega) = N \cdot 9 \frac{\omega^2}{\omega_d^3}$$

### Unpacking this a little:

We have an equation of the form

$$\langle E \rangle = \int d\vec{k} g(\vec{k}) \cdot \hbar\omega(\vec{k}) \cdot \left( n_s(\vec{k}) + \frac{1}{2} \right)$$

In this equation

- $g(\vec{k})$  is the number of states in the with  $d\vec{k}$  in  $\vec{k}$ -space.
- $\hbar\omega(\vec{k})$  is the energy of each mode
- $n_s(\vec{k})$  is the probability of occupation.

### Density of States (D.O.S.)

Consider a sphere of constant radius  $k$  in the  $\vec{k}$ -space (include picture) which are all occupied.

Then, the volume of occupied  $k$ -states is

$$\frac{4}{3}\pi k^3$$

and then Number of states in this volumem is

$$N = \frac{(4/3)\pi k^3}{(2\pi/L)^3} \cdot \underbrace{3}_{2 \times \text{Trans.}, 2 \times \text{Long.}}$$

Let's define (generally),  $g(k) = \frac{dN}{dk}$ . So,

$$\begin{aligned} g(k) &= \frac{3 \cdot 4\pi k^3}{(2\pi/L)^3} \\ &= L^3 \frac{12\pi k^3}{(2\pi)^3} \\ &= (\text{ fill later}) \end{aligned}$$

So,  $g(\omega)d\omega$  is the number of states between  $\omega$  and  $\omega + d\omega$ .

### The Debye Frequency

We defined the Debye Frequency as

$$\omega_d^3 = 6\pi^2 n v_s^3$$

where  $n$  is the number density of the solid and  $v_s$  is the speed of sound. This is a **Material Dependent quantity**.

For example, the larger the speed of sound  $v_s$  the larger the debye frequency. The speed of sound in a dense, rigid, hard solid like diamond would be bigger than the speed of sound in, say, a polymer. Hence, the value of the debye frequency for a specific material tells us about some of its properties.

## 5 September 6:

### Review of Last Lecture's Results

With SHO Dispersion Relation  $\omega = v_s |\vec{k}|$

- Debye Frequency:

$$\omega_d^3 = 6\pi^2 n v^3$$

- Density of States:

$$g(\omega) = 9N \frac{\omega^2}{\omega_d^3}$$

- Average Energy:

$$\langle E \rangle = \frac{9N\hbar}{\omega_d^3} \int_0^\infty d\omega \frac{\omega^3}{e^{\beta\hbar\omega} - 1} + T\text{-independent terms}$$

Ignoring the  $T$ -independent terms (which includes the zero-point energy) (**Write about this more.**) we can make the substitution  $x = \beta\bar{\omega}$  and solve the integral for

$$\begin{aligned} \langle E \rangle &= \frac{9N\hbar}{\omega_d^3(\beta\hbar)^4} \underbrace{\int_0^\infty dx \frac{x^3}{e^x - 1}}_{=\pi^4/15} \\ &= \frac{9N\hbar}{\omega_d^3(\beta\hbar)^4} \frac{\pi^4}{15} \\ &= \frac{\pi^4}{15} \cdot \frac{9N(k_b T)^4}{(\bar{\omega}_d)^3} \end{aligned}$$

which gives us

$$\begin{aligned} C &= \frac{d\langle E \rangle}{dt} \\ &= \frac{12\pi^4}{5} N k_B \left( \frac{k_b T}{\hbar \omega_d} \right)^3 \end{aligned}$$

and this is lovely because, we find experimentally that  $C \sim T^3$ . Define the **Debye Temperature** (denoted  $\Theta$ ) as

$$\hbar\omega_d = k_B \Theta$$

Then,

$$C = \frac{12\pi^4}{5} N k_B \left( \frac{T}{\Theta} \right)^3$$

$\Theta$  plays the role of the Einstein temperature. (**Explain why.**)

**But we still have a problem.**

$C$ , according to this calculation, grows indefinitely as  $T$  increases. But we know exper-

imentally that at high  $T$ , the heat capacity  $C \rightarrow 3 \cdot Nk_B$  (3  $k_B$  per atom, Dulong-Petit Limit).

The problem with the above calculation is the assumption that there are an infinite number of possible  $k$ -states and sound waves can go to an arbitrarily large  $k$ .

Debye guessed that there shouldn't be more  $k$ -states than there are degrees of freedom in the system, which is set by the number of atoms, "springs", etc.

Debye's trick was to, instead of integrating  $k$ -states from 0 to  $\infty$ , to choose a **cutoff**  $\omega_{\text{cutoff}}$  such that

$$3N = \int_0^{\omega_{\text{cutoff}}} g(\omega) d\omega \text{ and}$$

$$\langle E \rangle = \int_0^{\omega_{\text{cutoff}}} g(\omega) \hbar\omega \left( n_b + \frac{1}{2} \right) d\omega$$

### Why is this justified?

The main concern was to preserve low-temperature behavior while capturing the desired high-temperature behavior.

Now,  $n_B(\omega)$  for low  $T$  naturally plateaus after a certain  $\omega$ , whereas the high  $T$  curves don't. And so, choosing a cutoff doesn't impact the low temperature results but does for high temperature.

Let's investigate the high-temperature case: i.e. temperatures  $T$  for which  $k_B T \gg \hbar\omega_{\text{cutoff}}$

In this case,

$$n_B(\beta\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1} \sim \frac{k_B T}{\hbar\omega}$$

which gives us

$$\begin{aligned} \langle E \rangle &= \int_0^{\omega_{\text{cutoff}}} \hbar\omega \frac{k_B T}{\hbar\omega} g(\omega) d\omega + T - \text{independent terms} \\ &= k_B T \int_0^{\omega_{\text{cutoff}}} g(\omega) d\omega \\ &= k_B T \cdot 3N \end{aligned}$$

That gives us

$$C = \frac{d\langle E \rangle}{dt} = 3Nk_B$$

(Dulong-Petit Limit!)

**So, what is the cutoff frequency?**

$$\begin{aligned}
 3N &= \int_0^{\omega_{\text{cutoff}}} g(\omega) d\omega \\
 &= 9N \int_0^{\omega_{\text{cutoff}}} \frac{\omega^2}{\omega_d^3} d\omega \\
 \implies 3N &= 3N \frac{\omega_{\text{cutoff}}^3}{\omega_d^3}
 \end{aligned}$$

Thus,

$$\boxed{\omega_{\text{cutoff}} = \omega_d}$$

- So, this worked, but Debye and others were still kind of unhappy because introducing an artificial cutoff didn't seem right.
- Another problem with the Debye model was that it was known that some compounds (specifically metals) had a linear specific heat.

### Now we begin CH3 of Simons: Drude, Sommerfeld models

Drude asked, "what is electrons in a metal behaved like a free electron gas?". This wasn't an obvious thing to assume, especially because the Coulomb Interaction between electrons in a metal is *huge*.

Back of the hand calculation:

The coulomb interaction is

$$U \sim \frac{1}{4\pi\epsilon_0} \frac{q^2}{r}$$

and let's guess that  $r$  is around one Angstrom or so. Then the interaction is on the scale... complete this

Regardless, Drude made the assumption, and it turned out to give results that are incredibly accurate. However, it took about 50 years to understand why this unreasonable assumption gives reasonable results for so many metals.

The assumption is that electrons are independent i.e. they don't interact with each other, and they only interact with ions via collisions.

- Electrons have a "scattering time"  $\tau$  determined by these collisions. This roughly characterizes the probability of a collision between an electron and an ion.
- In a time interval  $\delta t$ , the probability of colliding  $\sim \frac{\delta t}{\tau}$ .
- Once a scattering event occurs, an electron with momentum  $\vec{p}$  relaxes on average to  $\vec{p} = 0$  (the momentum after a collision is randomized).
- Between the Collisions, electrons can be accelerated by an electric or magnetic field.

## 6 September 9: Drude Model Continued, Hall Effect

Last time, we left off with the main assumptions of the Drude model. Namely taht electrons do not interact with eac other but do scatter off of the ions of the metal. How does this impact how we think of the motion of the electrons in a metal?

**Question: What average momentum will the electrons have?**

Recall that the probability of an electron scattering off an ion in time-interval  $\delta t$  is  $\delta t/\tau$ . Now, since

$$\vec{F} = \frac{d\vec{p}}{dt}$$

we can say

$$\langle \vec{p}(t + \delta t) \rangle = \left( \vec{p}(t) + \vec{F}\delta t \right) \times \left( 1 - \frac{\delta t}{\tau} \right) + 0 \times \frac{\delta t}{\tau}$$

where  $(\vec{p}(t) + \vec{F}\delta t)$  is the momentum for an electron accelerated by a force  $\vec{F}$  and we multiplied it with  $(1 - \frac{\delta t}{\tau})$  which is roughly the fraction of electrons not scattered, 0 is the (average) momentum after scattering and we multiply it with  $\frac{\delta t}{\tau}$  which is the fraction of electrons scattered.

So, dropping the bars which denote avg. momentum since all our quantities are averages,

$$\begin{aligned} \vec{p}(t + \delta t) &= \vec{p} = \frac{\delta t}{\tau} \vec{p}(t) + \vec{F}\delta t - \vec{F} \underbrace{\frac{(\delta t)^2}{\tau}}_{\approx 0} \\ &= \vec{p}(t) + \vec{F}\delta t - \frac{\delta t}{\tau} \vec{p}(t) \\ \implies \frac{\vec{p}(t + \delta t)}{\delta t} &= \vec{F} - \frac{\vec{p}(t)}{\tau} \end{aligned}$$

So, scattering "reduces" the overall force in a manner just like drag. If we remove  $\vec{F}$  so  $\vec{F} = 0$  and then take the limit  $\delta t \rightarrow 0$  we have

$$\frac{d\vec{p}}{dt} = -\frac{\vec{p}}{\tau}$$

This looks like exponential decay, so we have the solution

$$\boxed{\vec{p}(t) = \vec{p}(0)e^{-t/\tau}}$$

We have **exponential loss of momentum due to scattering**.

Let's use these results to study the movement of electrons in a conducting wire.

### 6.1 Conducting Wire, Drude Conductivity

Consider a conducting wire of cross sectional area  $A$  as shown in the figure below:

Include figure.

Let us add a force  $\vec{F} = -e\vec{E}$ , so

$$\frac{d\vec{p}}{dt} = -e\vec{E} - \frac{\vec{p}}{\tau}$$

and denote the current density  $\vec{j}$ . We have  $\vec{j} = e\vec{v}n$  where  $n$  is the number density of electrons in the wire and  $\vec{p} = m\vec{v}$  where  $m$  is the mass of electron.

Consider the Steady State:  $\frac{d\vec{p}}{dt} = 0$

**Note:** There is a difference between Steady State and Equilibrium State.

A steady state is one in which the rate of change is zero, whereas an equilibrium state is one in which the potential is minimized.

Usually equilibrium states correspond to "global" minima of the potential function, but it's possible to have "meta-stable" equilibrium states which are local minima. For example, diamond is a meta-stable state of carbon, whereas graphene is not.

Then, we have

$$\begin{aligned} e\vec{E} &= -\frac{\vec{p}}{\tau} \\ \implies \delta q &= |\vec{v}| \underbrace{\delta t A}_{\text{vol. of } e^- \text{s flowing in time } \delta t \text{ across } A} \cdot (-en) \\ \implies \vec{j} &= \frac{1}{A} \frac{dq}{dt} \underbrace{\vec{v}}_{\substack{\text{unit vec. in dir. of vel.}}} - ne\vec{v} \end{aligned}$$

and

$$\begin{aligned} e\vec{E} &= -\frac{\vec{p}}{\tau} = -\frac{m\vec{v}}{\tau} \\ \implies \vec{v} &= \frac{e\tau}{m}\vec{E} \end{aligned}$$

Thus,

$$\begin{aligned} \vec{j} &= +ne\vec{v} \\ \implies \vec{j} &= +\frac{ne^2\tau}{m}\vec{E} \end{aligned}$$

We call  $\sigma = \frac{ne^2\tau}{m}$  the **Drude Conductivity**. Physically, this formula for conductivity makes a lot of sense

- The greater the density of electrons ( $n$ ), the greater the conductivity.
- The more time between scattering events ( $\tau$ ), the greater the conductivity.
- The heavier our charged particles are ( $m$ ), the weaker the conductivity.

The last point is more interesting than it may seem. For instance, in heavy-metal systems, we observe spin-orbit effects in which the speeds of electrons approach relativistic speed which can

impact the mass  $m$ .

Now,

$$\begin{aligned}\frac{d\vec{p}}{dt} &= -e\vec{E} - e\vec{v} \times \vec{B} - \frac{\vec{p}}{\tau} \\ &= -e \underbrace{(\vec{E} + \vec{v} \times \vec{B})}_{\vec{F}} - \frac{\vec{p}}{\tau}\end{aligned}$$

In steady state,

$$\begin{aligned}0 &= -e(\vec{E} + \vec{v} \times \vec{B}) - \frac{m\vec{v}}{\tau} \\ \Rightarrow 0 &= -e\vec{E} + \frac{1}{n}\vec{j} \times \vec{B} + \frac{m}{ne\tau}\vec{j} \\ \Rightarrow \vec{E} &= \frac{1}{ne}\vec{j} \times \vec{B} + \frac{m}{ne^2\tau}\vec{j} = \frac{1}{ne}\vec{j} \times \vec{B} + \frac{1}{\sigma}\vec{j}\end{aligned}$$

Let's analyze what this means. Our electric field is the sum of two vectors which are perpendicular to each other. So, the effective electric field is directed in a skewed angle.

Include picture

The angle between  $\frac{1}{\sigma}\vec{j}$  and  $\vec{E}$  is called the **Hall Angle**,  $\theta_H$  and the coefficient of  $\vec{j} \times \vec{B}$  is called the **Hall Coefficient**,  $R_H$

$$R_H = -\frac{1}{ne}$$

If  $\vec{B} = 0$  then for

$$\vec{E} = \begin{pmatrix} E_x \\ 0 \\ 0 \end{pmatrix}$$

we have

$$\vec{j} = \begin{pmatrix} j_x \\ 0 \\ 0 \end{pmatrix}$$

. However, introducing the magnetic field causes the current (density) to become skewed and gain  $j_y, j_z$  components.

A slightly nicer way to view this is by defining the **resistivity tensor** as  $\rho$ :  $\vec{E} = \rho\vec{j}$  where ( $\rho$  is antisymmetric - explain why)

$$\rho = \begin{pmatrix} \frac{1}{\sigma} & B_z/ne & B_y/ne \\ B_z/ne & \frac{1}{\sigma} & B_x/ne \\ B_y/ne & B_x/ne & \frac{1}{\sigma} \end{pmatrix}$$

and denoting

$$\vec{B} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix}$$

we find

$$E = \left[ \frac{1}{ne} \begin{pmatrix} 0 & B_z & B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{pmatrix} + \frac{1}{\sigma} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right]$$

Example: If we have a magnetic field pointing purely in the  $z$ -direction,

fill in later.

The components that are off-diagonal i.e.  $\rho_{ij}$ ,  $i \neq j$  connect the electric field seen in the " $i$ " direction when a current is applied in the " $j$ " direction. This will be measured as a voltage (a potential drop in the " $i$ " direction).

Include picture.

Write the rest from picture.

## 7 September 11:

### Plan for today

- Brief recap of Hall Physics
- Thermal Conductivity
- Wiedeman-Franz Law

### Hall Voltage

Fill from image

When studying the Alkali-metals for example, people found that some of the metals with 2+ valence (Be, Mg) gave values of  $n/n_{\text{atoms}}$  which were anomalous in two ways: they were too small, and they were *negative* - which would indicate that they have *positive* Hall current carriers rather than negative ones - which doesn't make sense in the Drude Model.

To really understand what's going on here, we'll have to use **Band Theory**. We'll come back to this.

#### Ball-park estimates:

Let's try to get a feel for the average free path,  $l$ , travelled by an electron. We know

$$\sigma = \frac{ne^2\tau}{m} \implies \frac{m\sigma}{ne^2} = \tau$$

and we can obtain a value for  $\sigma$  experimentally. Usually, this is done by measuring  $\rho \approx 10^{-5}\Omega m$

Fill this out.

Thus we find that  $l = v\tau \approx 10^5 \text{m/s} \cdot 10^{-15} \text{s} = 10^{-10} \text{m}$  i.e. one Angstrom, which is roughly the spacing between atoms in a crystal. And this matches up with the assumption made in the Drude model!

### 7.1 Thermal Conductivity

The Thermal conductivity of a material is related to how well it conducts heat, so often it's denoted with a  $Q$  subscript. Intuitively, we know that heat flows "hot to cold" i.e. in direction opposite to that of increasing temperature. So, we expect that

$$\vec{j}_Q = -\kappa \nabla T$$

where  $\kappa$  is a constant of proportionality called the **Thermal Conductivity**.

Let's do a loose derivation of a formula for  $\kappa$  (following the one in Simons).

We know electrical current is described as

$$\vec{j} = en\vec{v}$$

where  $n$  is the number of charge carriers per unit volume, and  $\vec{v}$  is the (avg) velocity of the charge carriers.

How do we express the *thermal current*? Let's say it's of the form

$$\vec{j}_Q = (\delta E)n\vec{v}$$

where  $n$  is the number of *carriers of energy* per unit volume, and  $\delta E$  is the **average energy carried** in the direction of  $\vec{v}$ .

Suppose we have a slab of material as in the picture below:

Include picture of material

### "Fast & Loose" derivation

Suppose we have particles from two collision sites, each a distance  $v\tau$  away from our point of interest  $x$ .

Include picture of particles and points  $x$

Let's denote the energy of particles coming from the point  $x - v\tau$  as  $E(x - v\tau)$  and the energy of particles coming from  $x + v\tau$  as  $E(x + v\tau)$ . Then, if we think about the "energy landscape", we can imagine the following picture:

Include pic of energy landscape

Then, we can estimate  $\delta E$  as the difference between them, so

$$\vec{j}_Q = n\vec{v} \left( \frac{1}{2}E(x - v\tau) - \frac{1}{2}E(x + v\tau) \right)$$

(We subtract them because they're travelling in opposite directions)

Taylor expanding the Temperature and Energy at the points  $x - v\tau$  and  $x + v\tau$  we get

$$T(x - v\tau) \approx T(x) + \frac{dT}{dx}(-v\tau)T(x + v\tau) \approx T(x) + \frac{dT}{dx}(+v\tau)$$

and

$$\begin{aligned} E(x - v\tau) &\approx E(x) - v\tau \frac{dE}{dx} = E(x) - v\tau \frac{dE}{dT} \frac{dT}{dx} \\ E(x - v\tau) &\approx E(x) + v\tau \frac{dE}{dT} \frac{dT}{dx} \end{aligned}$$

So,

$$\begin{aligned} \vec{j}_Q &= \frac{1}{2}n\vec{v} \left( -2 \cdot \frac{dE}{dT} \frac{dT}{dx} \right) \vec{v}\tau \\ &= -n\vec{v}^2 \tau \frac{dE}{dT} \frac{dT}{dx} \end{aligned}$$

and notice that  $\frac{dE}{dT}$  is the Heat Capacity,  $\frac{dT}{dx}$  is the direction of the temperature gradient.

Now, we're going to do a slightly sus substitution:  $\vec{v}^2 \Leftrightarrow \langle \vec{v}^2 \rangle$ . We're dealing with the 1D case, but in 3D we can verify that

$$\langle v_x^2 \rangle = \langle v_x^2 \rangle = \langle v_x^2 \rangle = \frac{1}{3} \langle v^2 \rangle$$

So, we see that

$$\vec{j}_Q = -\frac{1}{3} n \langle v^2 \rangle C_v \nabla T \tau$$

Thus,

$$\vec{j}_Q = -\kappa \nabla T$$

where

$$\kappa = \frac{1}{3} n \langle v^2 \rangle C_v \tau$$

**Why does this make sense?** Let's compare this expression for thermal conductivity with the familiar expression for electrical conductivity.

$$\begin{aligned}\kappa &= \frac{1}{3} n \langle v^2 \rangle C_v \tau \\ \sigma &= \frac{e^2 n \tau}{m}\end{aligned}$$

- Write from picture
- Heat capacity essentially measures the number of degrees of freedom that carry energy, so  $nC_v$  measures the "number of ways we can carry heat".

Sometimes thermal conductivity is written in terms of free path as

$$\kappa = \frac{1}{3} n \langle v \rangle \tau = \frac{1}{3} n C_v l$$

since  $l = \langle v \rangle \tau$ .

## 7.2 Wiedemann-Franz Law

Note that

$$\begin{aligned}L &= \frac{\kappa}{\sigma T} = \\ &= \dots \\ &= \frac{3}{2} \frac{k_B^2}{e^2}\end{aligned}$$

The quantity  $L$  is known as the **Lorenz Ratio**. It was known experimentally that this ratio was essentially the same for every metal, and the Drude model (though off by a factor of 2) showed that indeed  $L$  is a number relating two fundamental constants.

**How could this derivation possibly be valid when  $C_v$  is actually temperature dependent?**

The reason turns out to be a happy accident - due to the cancellation of two big numbers. However, there are in fact other thermal quantities we can measure to show that the Drude Model is not complete.

Still, the point holds. The Drude model still gave us a lot of good information about metals:

- It showed that, for most purposes, electrons really do behave like a gas.
- It also indicated that, for materials that satisfy the WF-law, the  $n$  in  $\kappa$  and the  $n$  in  $\sigma$  were the same - i.e. the *number* of carriers of charge and the carriers of thermal energy were the same! This strongly indicated that the carriers were in fact the same.

## 8 September 13: Sommerfeld Model

In Drude's time, it was reasonable to assume electrons were just gasses and obeyed the Maxwell-Boltzmann statistics. In the 1920s and 30s however, it became well known that electrons are in fact **fermions** - taking this into consideration was the contribution of Sommerfeld.

Instead of a gas, let's suppose electrons behave like a **Fermi Gas** i.e. no more than two electrons (spin up or spin down) can occupy a single energy state.

From Statistical Mechanics, we know that the **Fermi-Dirac** distribution (which gives the distribution of Fermions) looks like

$$n_{FD}(T) = \frac{1}{e^{\beta(E-\mu)} + 1}$$

where  $\mu$  is the **chemical potential** and the **Bose-Einstein** distribution (which gives the distribution of bosons) looks like

$$n_{BE}(T) = \frac{1}{e^{\beta(E)} - 1}$$

### What is the Chemical Potential, $\mu$ ?

The chemical potential determines the maximum energy occupied by electrons at  $T = 0$ .  
**(Write different perspective here later.)**

### How do we determine $\mu$ ?

We figure it out self-consistently. Suppose we have  $N$  electrons in our system.

$$N = 2 \sum_i n_{FD}(E - \mu)$$

The chemical potential is often defined as the energy that is added to the system when add an electron, so

$$\mu = \left. \frac{dE}{dN} \right|_{S,V}$$

This is the Thermodynamic Definition.

The key observation is that **the Chemical Potential and the number of electrons are tied together**.

- Suppose electrons form a free Fermi Gas. Then, each electron has energy described as

$$E = \frac{\hbar^2 |\vec{k}|^2}{2m} = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2)$$

- Now, for a system with a continuous energy-momentum spectrum (like that of a free electron), the chemical potential  $\mu$  really does happen to be the highest occupied state.

include pic

- For a discrete system, however, we define the chemical potential to be the midpoint between the highest-occupied and lowest-unoccupied states. **Why?** The reason is that for  $T \neq 0$ , some states with  $E > \mu$  have a probability of being occupied - and this has to be equal to the probability of unoccupied states with  $E < \mu$  (in order to conserve  $N$ ).

include picture

So,  $\mu$  is between the HOMO and LUMO (-MO stands for "Molecular Orbital").

This discrete behavior will be relevant when we study Band structures later on in the course.

Now, consider a solid as a box of length  $L$  i.e. the boundaries of the solid form infinite potential barriers. We know from QM that an electron in the box has energies

$$E = \frac{\hbar^2 k^2}{2m}, \quad k = \frac{2\pi n}{L}, \quad n = 1, 2, 3 \dots$$

i.e.

$$k_x = n_x \frac{2\pi}{L}, \quad k_y = n_y \frac{2\pi}{L}, \quad k_z = n_z \frac{2\pi}{L},$$

If we think about our momenta in  $\vec{k}$  space, the energy levels are described by points on a lattice, with each lattice point separated by distance  $(\frac{2\pi}{L})$  i.e. each  $\vec{k}$  state occupies a "volume" of  $(\frac{2\pi}{L})^3$ .

The Fermi-Surface is the boundary of occupied and unoccupied states. The Fermi-sphere is the volume of occupied states.

Now, if our box is really large then the spacing between each lattice point is really small since it's  $\sim 1/L$  and we can treat  $\vec{k}$ -space like a continuous space. Then,

$$N = 2 \sum_i n_{FD}(E - \mu) \rightarrow N = 2 \left( \frac{L}{2\pi} \right)^2 \int d\vec{k} n_{FD}(\vec{k})$$

Recall that the Fermi-energy is the maximum occupied-state energy. We denote it as  $E_F$  and define the corresponding Fermi-wavevector as

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

Then, we can calculate

$$N = \left( \int_0^{k_F} d\vec{k} \right) 2 \left( \frac{L}{2\pi} \right)^2$$

Now,

$$\begin{aligned} N &= 2 \cdot \frac{\text{Volume of Fermi-Sphere}}{\text{Volume of each individual } k\text{-state}} \\ &= 2 \cdot \left( \int_0^{k_F} d\vec{k} \right) \left( \frac{L}{2\pi} \right)^2 \\ &= 2 \cdot \frac{4/3\pi k_F^3}{(2\pi/L)} \end{aligned}$$

which gives us

$$\begin{aligned} k_F^3 &= \frac{N}{V} 3\pi^2 \\ \implies k_F &= (n 3\pi^2)^{1/3} \end{aligned}$$

(Write about back of the book calcs for  $v_F$  and  $E_F$ )

General rule: If you can't change energy, you can't see anything. Pretty much all observables are results of changes in the energy.