PHYS 460

LECTURE 2

LAST WEEK I INTRODUCED ONE OF THE EARLIEST MODERN THEORIES OF METALS: THE DRUDE MODEL COMING OF THE DISCOVERY OF THE ELECTRON IN 1896, THE DRUDE MODEL ATTEMPTED TO DESCRIBE METALS USING BOLTZMANN'S TRANSPORT EQUATIONS, DEVELOPED FOR GASES. IT WAS CLASSICAL, EMPIRICAL AND RIFE WITH ASSUMPTIONS, BUT WAS AMAZINGLY SUCCESSFUL FOR A FIRST CRACK.

SPECIFICALLY, BUT ASSUMING e^- IN A SOLID OBEYED THE EQUATION

$$\frac{dp(t)}{dt} = -\frac{p(t)}{\tau} - e\vec{E} - e\vec{v}\times\vec{B}$$

$p(t)$ = momentum
τ = relaxation time

DRUDE WAS ABLE TO REPRODUCE

1. OHM'S LAW $\quad \vec{j} = \sigma_0 \vec{E}, \quad \sigma_0 = \frac{ne^2\tau}{m}$

2. HALL EFFECT $\quad R_H = \frac{E_y}{j_x B} = -\frac{1}{ne}$

3. AC CONDUCTIVITY $\quad \sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau}$ $\rightarrow$ PLASMA FREQUENCY $\quad \omega_p = \sqrt{\frac{4\pi n e^2}{m}}$

4. WIEDEMAN-FRANZ LAW

$$L = \frac{K}{\sigma T} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2$$

AMONG OTHER THINGS

EQUATIONS (1) & (2) I WAS ABLE TO ADDRESS LAST LECTURE, AND (3) I WILL LEAVE TO HOMEWORK.

THE W-F LAW IS IMPORTANT ENOUGH, HOWEVER THAT I FEEL I SHOULD TAKE A FEW MOMENTS TO LAY IT OUT. IT IS ALSO A NATURAL LAUNCHING PAD FOR THE NEXT TOPIC: THE SOMMERFELD MODEL.

THE PICTURE BEHIND THE W-F IS RATHER SIMPLE. IT STEMS FROM THE OBSERVATION THAT MATERIALS THAT CONDUCT CURRENT WELL ALSO TEND TO CONDUCT HEAT, AND THE NATURAL CONCLUSION THAT PERHAPS BOTH CURRENT AND HEAT ARE BEING CARRIED BY THE SAME DEGREES-OF-FREEDOM (e^-). THE LAW ITSELF IS EMPIRICAL, AS IT WAS KNOWN FOR ALMOST 50 YEARS THAT $\frac{K}{\sigma T} \simeq 2.2 \times 10^{-8} \frac{W\Omega}{K^2}$ FOR MANY METALS. THERE WAS NO QUANTATIVE MODEL FOR EITHER ELECTRICAL & HEAT CONDUCTION, SO ANY MEANS OF UNDERSTANDING THIS WAS CONSIDERED A HUGE SUCCESS

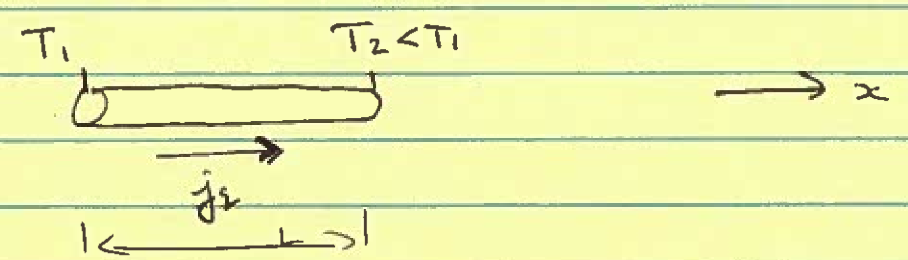
DRUDE PROVIDED THAT ANSWER IN THE FORM OF SCATTERING ELECTRONS

DEFINE "THERMAL CONDUCTIVITY" WITH THE FOLLOWING EQUATION

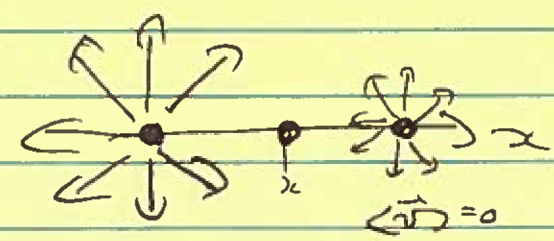
$$\vec{j}_2 = -K \vec{\nabla} T \qquad \text{FOURIER'S LAW}$$

HERE $\vec{j}_2$ IS "THERMAL CURRENT DENSITY" WITH UNITS [ENERGY] / [AREA][TIME] AND THE NEGATIVE JUST TELLS US HEAT GOES FROM HIGH TO LOW T

CONSIDER THE FOLLOWING MEASURMENT, WHERE A TEMP GRADIENT IS ACTIVELY MAINTAINED ON A ROD OF SOME METAL



IN SUCH AN EXPERIMENT, THERE IS NO CLOSED CIRCUIT, SO CURRENT CAN'T FLOW. BUT ENERGY CAN FLOW, SINCE AT ANY POINT, x, ELECTRONS COMING FROM THE HOT SIDE HAVE MORE ENERGY THAN ELECTRONS FROM THE COLD SIDE



1D: $\quad j_E = -k \dfrac{dT}{dx}$

$$j_E = \frac{nv}{2}\,\varepsilon(T(x - v\tau)) - \frac{nv}{2}\,\varepsilon(T(x + v\tau))$$

electrons traveling Δx in per sec

HALF GOING RIGHT WAY

energy of single e^-

FOR $l = v\tau \ll L$

$$j_E \approx \frac{nv}{2}\left[\varepsilon(T(x)) + \frac{d\varepsilon}{dx}(-v\tau) - \varepsilon(T(x)) - \frac{d\varepsilon}{dx}(+v\tau)\right.$$

$$= -nv^2\tau \,\frac{d\varepsilon}{dT}\,\frac{dT}{dx}$$

$\varepsilon(T(x - v\tau)) = \frac{d\varepsilon}{dT}\frac{dT}{dx}\,dx$

SO 1D IS SIMPLE TO VISUALIZE. TO GENERALIZE TO 3D, WE WRITE

$$v_x \to \vec{v}$$

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

Specific heat

ALSO $$n\frac{d\varepsilon}{dT} = \frac{N}{V}\frac{d\varepsilon}{dT} = \frac{1}{V}\frac{dE}{dT} = C_v$$

$$\Rightarrow \quad \vec{j}_q = -\frac{n v^2 C_v \tau}{3} \vec{\nabla} T$$

OR $$\boxed{K = \frac{1}{3} v^2 \tau C_v}$$

DOES THIS LOOK LIKE W-F? NO, BUT SINCE DRUDE FELT HE WAS LOOKING AT CLASSICAL PARTICLES, HE WENT AHEAD AND APPLIED THE EQUIPARTITION THEOREM

$$\langle \tfrac{1}{2} m v^2 \rangle = \tfrac{3}{2} k_B T$$

$$C_v = \tfrac{3}{2} n k_B$$

$$\Rightarrow \quad \frac{K}{\sigma T} = \frac{\frac{1}{3} \times \frac{3k_BT}{m} \tau \left(\frac{3}{2} n k_B\right)}{\frac{ne^2\tau}{m} T}$$

$$= \frac{3}{2}\left(\frac{k_B}{e}\right)^2 = 1.11 \times 10^{-8} \frac{W\text{-}\Omega}{K^2}$$

$$= L$$ ← LORENTZ NUMBER

IN REALITY

$$L = 2.22 \times 10^{-8} \frac{W\text{-}\Omega}{K^2}$$

BUT PRETTY CLOSE!

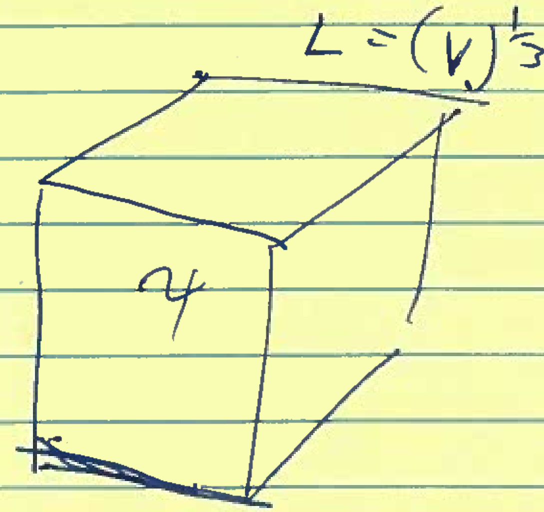
PROBLEM C_v HAD BEEN MEASURED, AND IS NOWHERE NEAR $\frac{3}{2}nk_B$ (TOO LARGE BY FACTOR OF 100!). WE WILL SEE THAT THIS COMPENSATED FOR BUT 100 TIMES UNDER ESTIMATION OF v^2

TO DO THIS PROPERLY, WE NEED QM.

FIRST ATTEMPT: SOMMERFELD THEORY

- INSTEAD OF CLASSICAL PARTICLES, TREAT ELECTRONS AS INDEPENDENT MATTER WAVES

PARTICLES IN A BOX



$$\mathcal{H}\psi = E\psi$$

AND $p = -i\hbar\nabla$

$$\Rightarrow -\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

WE INCLUDE NO POTENTIAL, BUT CONSTRAIN ELECTRONS TO BOX USING BOUNDARY CONDITIONS:

$$\psi(x+L) = \psi(x),\ \psi(y+L) = \psi(y),\ \psi(z+L) = \psi(z)$$

"BORN-VON KARMEN" OR "PERIODIC" BOUNDARY CONDITIONS DO NOT AFFECT SOLUTION, BUT HAS BENEFIT OF MATHEMATICAL SIMPLICITY AND ALLOWS US TO DISCUSS MOVING WAVES

SOLUTION IS $\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

WITH $\varepsilon(\vec{k}) = \frac{\hbar^2 k^2}{2m}$

<u>NOTES</u>: • PREFACTOR INCLUDED TO ENSURE PROPER NORMALIZATION $\left(1 = \int d\vec{r}\, |\psi(\vec{r})|^2 \right)$

• $\psi_{\vec{k}}$ IS AN EIGENSTATE OF MOMENTUM OPERATOR, SO EACH SOLUTION HAS UNIQUE <u>MOMENTUM</u>

• $\vec{k}$ IS THUS REFERRED TO EITHER AS "WAVEVECTOR" OR "MOMENTUM VECTOR"

SPECIFICALLY, SINCE $\hat{p} = -i\hbar\nabla$

$$\hat{p}\psi = \hbar\vec{k}\psi$$

$$\Rightarrow \vec{v} = \frac{\hbar\vec{k}}{m}$$

$$\varepsilon_{\vec{k}} = \frac{1}{2}mv^2$$

IS JUST KINETIC ENERGY

• IN WAVE INTERPRETATION, ONE ALSO DISCUSSES DE BROGLIE WAVELENGTH

$$\lambda = \frac{2\pi}{k}$$

$\vec{k}$ IS NOT CONTINUOUS! APPLYING B.C.

$$\psi_{\vec{k}}(x+L,y,z) = \frac{1}{\sqrt{V}} e^{i(k_x x + k_x L + k_y y + k_z z)}$$

$$= \psi_{\vec{k}}(x,y,z)\, e^{i k_x L}$$

$$\Rightarrow e^{i k_x L} = 1$$

$$k_x = \frac{2\pi}{L} n_x \qquad n_x \in \mathbb{Z}$$

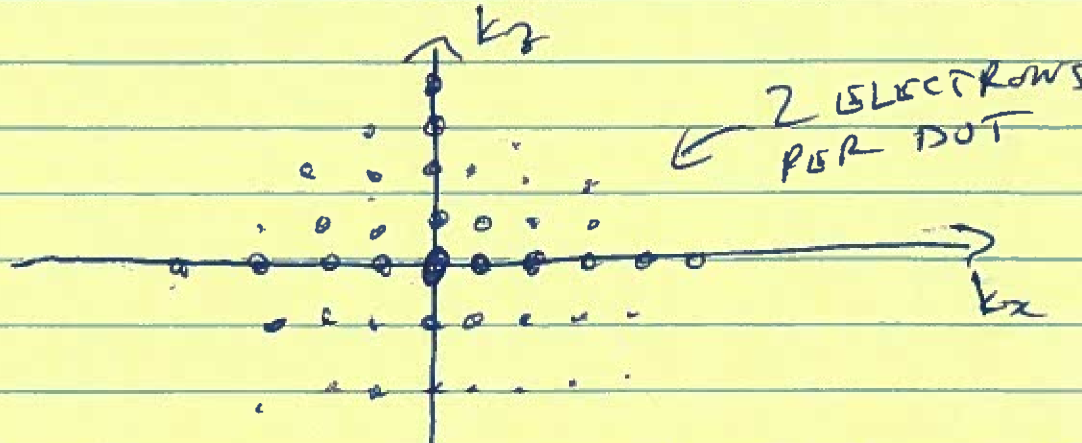
SIMILARLY

$$k_y = \frac{2\pi}{L} n_y \qquad n_y \in \mathbb{Z}$$

$$k_z = \frac{2\pi}{L} n_z \qquad n_z \in \mathbb{Z}$$

INDEPENDENT ELECTRON ASSUMPTION ALLOWS US TO CONSTRUCT MANY BODY STATE SIMPLY BUT FILLING ALL ONE ELECTRON STATES ACCORDING TO PAULI EXCLUSION PRINCIPLE

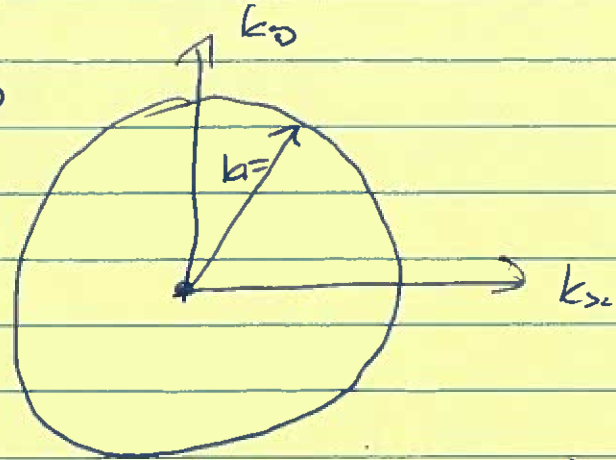
2D EXAMPLE AT $\boxed{T=0}$



KEEP FILLING UNTIL YOU RUN OUT OF ELECTRONS

END UP (IN P-IN-BOX SCENARIO) WITH SOMETHING THAT LOOKS A LOT LIKE A FILLED SPHERE OF STATES

- HIGHEST $|\vec{k}|$ REACHED CALLED "FERMI LEVEL" $\vec{k}_F$
- ASSOCIATED ENERGY CALLED "FERMI ENERGY", ε_F



- ALSO, FERMI MOMENTUM (p_F), VELOCITY (v_F), TEMP (T_F)

- THEORETICAL SURFACE SEPARATING EMPTY AND FULL STATES ~~ARE~~ IS "FERMI SURFACE"

WE CAN ESTIMATE THESE VALUES. WE KNOW A GIVEN VOLUME OF k-SPACE, Ω, CONTAINS

$$\frac{\Omega}{\left(\frac{2\pi}{L}\right)^3} = \frac{\Omega V}{8\pi^3} \quad \text{STATES}$$

OR "DENSITY OF STATES" $= \dfrac{V}{8\pi^3}$

$$\Rightarrow \frac{N}{2} = \left(\frac{V}{8\pi^3}\right)\left(\frac{4}{3}\pi k_F^3\right) = \frac{k_F^3}{6\pi^2} V$$

$$k_F = \left(3\pi^2 n\right)^{1/3}$$

$$\Rightarrow \varepsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} \approx 10\text{-}100 \text{ eV}$$

$(\sim 10^4 \text{ K})$

$$v_F = \frac{\hbar}{m}(3\pi^2 n)^{1/3} \sim 1\text{-}10 \times 10^6 \frac{m}{s} \sim 0.01c$$

AT $T=0$!

FINITE TEMPERATURES

AS AMAZING AS THESE ZERO TEMPERATURE PROPERTIES ARE, PEOPLE CAN'T MEASURE WHAT IS HAPPENING AT ABSOLUTE ZERO. WE NEED TO SEE HOW THINGS VARY WITH TEMPERATURE

CLASSICALLY, # ELECTRONS WITH ENERGY ε IS GIVEN BY BOLTZMANN DISTRIBUTION:

$$f_B(\varepsilon) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\varepsilon/k_B T}$$

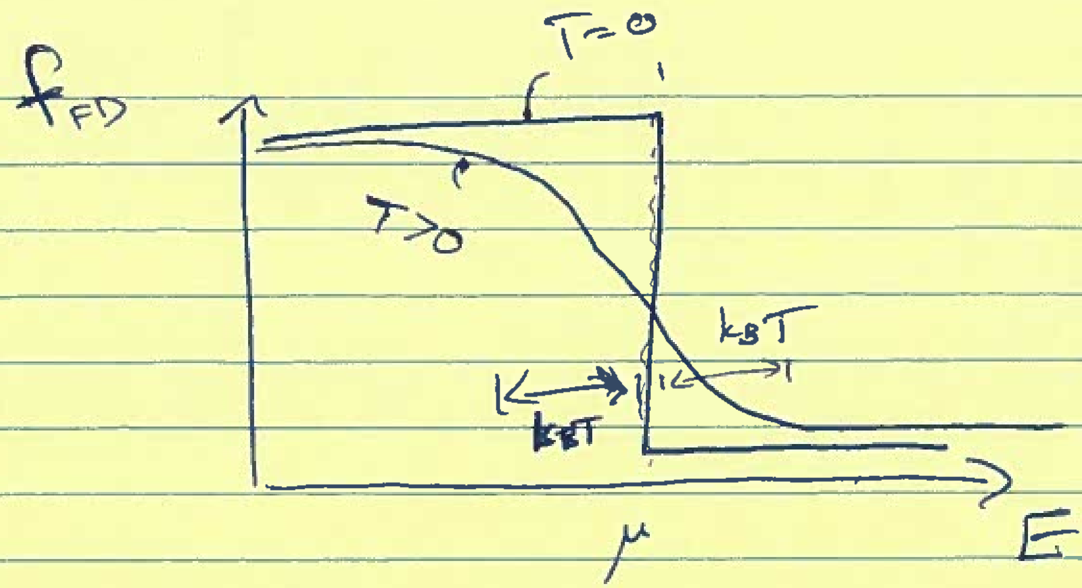
THIS IS WHAT LEADS TO EQUIPARTITION PREDICTION $C_V = \frac{3}{2} k_B$

ONE CAN SHOW (BUT WE WILL NOT) THAT PAULI EXCLUSION PRINCIPLE REQUIRES A DIFFERENT DISTRIBUTION OF PARTICLES:

$$f_{FD} = \frac{1}{\exp\left[\frac{(\varepsilon-\mu)}{k_B T}\right] + 1}$$

WHERE μ = "CHEMICAL POTENTIAL"
= ENERGY REQUIRED TO ADD PARTICLE TO SYSTEM
$\approx \varepsilon_F + \mathcal{O}\left(\left(\frac{T}{T_F}\right)^2\right)$

$\mu = \left.\frac{\partial G}{\partial N}\right|_{T,P}$



AT FINITE TEMPERATURE, f_{FD} IS STEP FUNCTION. STATES BELOW ε_F FULL, ABOVE EMPTY. ONE CAN CALCULATE μ IF YOU KNOW NUMBER OF ELECTRONS

AT FINITE TEMPERATURE, THE NUMBER OF STATES DOESN'T CHANGE, BUT OCCUPATION OF THESE STATES DOES. BUT ONLY STATES WITHIN k_BT OF FERMI SURFACE CAN BE THERMALLY EXCITED TO STATES WITHIN k_BT (BUT ABOVE) FERMI SURFACE. THE OTHER ELECTRONS HAVE NOWHERE TO GO! THE FUNDAMENTALLY RESTRICTS HOW MUCH HEAT THE ELECTRON GAS CAN ACCEPT (i.e. ITS HEAT CAPACITY)

ROUGHLY SPEAKING, IF $N\frac{T}{T_F}$ ELECTRONS CAN TAKE k_BT OF THERMAL ENERGY, THEN ELECTRONIC THERMAL KINETIC ENERGY

$$\mathcal{U} \approx \left(\frac{NT}{T_F}\right) k_BT$$

AND THUS

$$C_V \simeq n k_B \frac{T}{T_F}$$

SINCE $T/T_F \simeq 0.01$ AT R.T., THIS ACCOUNTS FOR DISCREPANCY SEEN IN DRUDE MODEL

MORE GENERALLY, ONE NEEDS TO INSERT FERMI DISTRIBUTION INTO YOUR CALCULATIONS. FOR EXAMPLE

$$u = \frac{U}{V} = 2\int_0^\infty \frac{4\pi k^2}{8\pi^3}\, \varepsilon(\vec{k})\, f(\varepsilon(\vec{k}))\, dk$$

AND $$n = 2\int_0^\infty \frac{4\pi k^2}{8\pi^3} f(\varepsilon(\vec{k}))\, dk$$

THE LATTER OF WHICH ACTUALLY DEFINES THE CHEMICAL POTENTIAL

~~OR~~ A MORE COMMON REPRESENTATION ~~IS~~ INTEGRATES OVER ENERGY

$$\boxed{\begin{aligned} u &= \int_0^\infty \epsilon\, g(\epsilon)\, f(\epsilon)\, d\epsilon \\ n &= \int_0^\infty g(\epsilon) f(\epsilon)\, d\epsilon \end{aligned}}$$

WHERE WE HAVE DEFINED "DENSITY OF STATES" $g(\epsilon) \equiv \frac{1}{V}\frac{dN}{d\varepsilon}$

FOR FREE ELECTRONS, WE CAN USE

$$n = \frac{1}{3\pi^2}\left(\frac{2mE}{\hbar}\right)^{3/2}$$

$$\ln n = \frac{3}{2}\ln E + \text{const}$$

$$g(E) \equiv \frac{dn}{dE} = \frac{3n}{2E} \quad \propto E^{\frac{1}{2}}$$

ONE CAN USE THESE EQUATIONS, AND THE FACT THAT $T/T_F \ll 1$ TO DO A LOW TEMPERATURE TAYLOR EXPANSION OF FERMI DISTRIBUTION (SOMMERFELD EXPANSION), BUT I WILL JUST GIVE THE FINAL RESULT

$$C_v \approx \frac{1}{3}\pi^2 D(E_F) k_B^2 T = \frac{\pi^2 n}{2E_F} k_B^2 T$$

FOR FREE ELECTRONS

NOTE THAT SINCE $E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$, AND EVERYTHING ELSE IS CONSTANT, THE COEFFICIENT OF THE LINEAR TERM IN THE SPECIFIC HEAT IS ACTUALLY A MEASURE OF THE ELECTRON MASS

ONE SEES THAT $m^* \neq m_e$ IN A METAL, WHICH IS REAL AND IS ATTRIBUTED TO A NUMBER OF DEEP PHENOMENA