

# Transport II $\Rightarrow$ Metals (6.)

1

$\Rightarrow$  Metals (follow, "Physics of Materials" Yves Quere)

- free electrons essential,
- but QM also essential. Drude is dubious

i.e. if  $d \sim$  lattice scale, for metal

$$p \sim \hbar/d \Rightarrow E_{QM} \sim \hbar^2 / 2md^2$$

( $\sim$  repulsion)

$\therefore$  need  $\sim 10$  eV for  $T > E_{QM}$

so for room temp. conductor

QM is essential to model. (can take  $T=0$ )

- Particular focus of QM treatment is

Pauli Exclusion Principle, and its

effect on electron response  $\Rightarrow$  conductivity.  
n.b. Exclusion sets distribution function.

so review some basics of:

- QM for free electrons
- density of states

i) - Fermi distribution, energy, etc.  
 $\Rightarrow$  scale,  $\nu_e$

ii) - conductivity, and Drude redux.

iii) - strength, etc.

Aside:

1a. ~~1a~~

Example of Fermion Exclusion Driven

Pressure: Chandrasekhar Mass

Takes  $M > M_{\odot}$  to collapse to white dwarf.

Aside: Chandrasekhar Limit - Simple Derivation  
(c.f.: Shapiro, Teukolsky)

→ suppose:  $N$  Fermions in star of radius  $R$   
∴  $n_{\text{Fermion}} \sim N/R^3$

∴ Vol./Fermion  $\sim 1/n$  (Pauli exclusion)

$p \sim \hbar/\Delta x \sim \hbar n^{1/3}$  (Heisenberg Uncertainty)  
↓  
Fermion Momentum  
 $\hbar \sim N^{1/3}/R$

⇒ Fermion energy (per Fermion) =  $E_F = pc \sim \hbar c \frac{1}{R}$  (replaces:  $\frac{1}{n}$  like thermal energy)  
 $\sim \hbar c \frac{N^{1/3}}{R}$  (effective repulsion)

Gravitational Energy (per Fermion) =  $E_{\text{grav}} \sim -\frac{GMm_B}{R}$  (Baryon mass)

$M \sim N m_B$

Pressure → electron  
Mass → Baryon

∴  $E = E_F + E_G$

$$= \frac{\hbar c N^{1/3}}{R} - \frac{GNm_B^2}{R}$$

Note QM effects



Note:  $E = E_F + E_G$   
 $= \frac{\hbar c N^{1/3}}{R} - \frac{GNM_B^2}{R}$

$E > 0$   $\Rightarrow$  decrease  $E_F, E_G$  by increasing  $R$ .

but as  $E_F \downarrow$ , electrons non-relativistic,  
 $\therefore E_F \sim 1/R^2 \rightarrow$  esbism.

$E < 0$   $\Rightarrow$  decrease  $E$  without bound by decreasing  $R \Rightarrow$  collapse  
 binding

$\therefore$  esbism:  $\hbar c N^{1/3} = GNM_B^2$

$N_{Max} = \left( \frac{\hbar c}{Gm_B^2} \right)^{3/2} \sim 2 \times 10^{57}$  (Proton)  
 Max # particles.

$\therefore M_{Chandrasekhar} = N_{max} m_B \sim 1.5 M_{\odot}$

i.e.  $M > M_{Chandrasekhar} \approx 1.5 M_{\odot}$

$\Rightarrow N > N_{crit} \Rightarrow$  collapse

# QM and Density of States

Key point:  $E_{\text{em}} \sim 10 \text{ eV}$ .  $T_{\text{room}} \sim 0.01 \text{ eV}$ .


$\therefore$  can treat metal as zero temperature gas of electrons. (No thermal spread)

$\rightarrow$  distribution set by Pauli Principle.

$\rightarrow \partial f / \partial E \sim \delta(E - E_F) \Rightarrow \nabla$

$\Rightarrow$  Density of states is key concept.  
i.e. Particles fill up available states

Consider 1D, 3D: Temp relevant at boundary of dist. (\*) box  $\rightarrow$  ion field.

- 1D Particles in a box, 

$\sim$  i.e. linear dynamics; organic semi-conductors

$\sim \left( \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right) \psi = E \psi$  is TISE

$\therefore E_n = E_0 n^2$

$E_0 = \frac{\hbar^2}{2m} \frac{2\pi^2}{L^2}$  (no spin)

$\psi_n = \sqrt{\frac{2}{L}} \sin \frac{2\pi x n}{L} e^{-i(E_n t) / \hbar}$

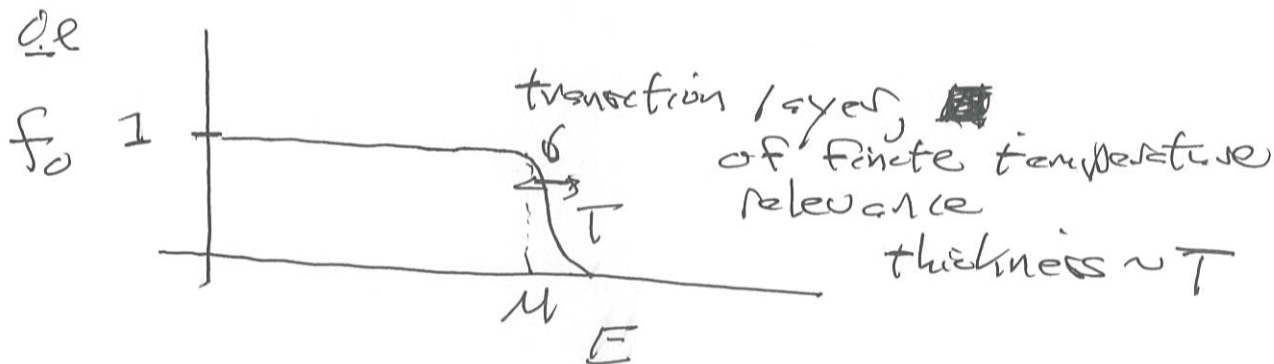
To count # states  $\Rightarrow$

① - count #  $k$ 's  $\Rightarrow$  integrate in  $k$ .

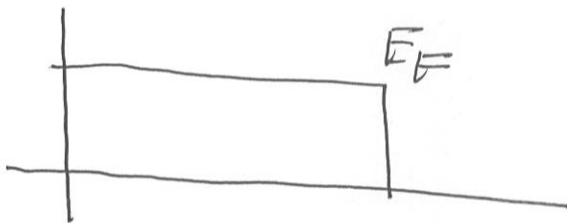
Point is:

- Fermi-Dirac distribution:

$$f(E) = \frac{1}{\exp((E-\mu)/T) + 1}$$



so often, for  $\mu \gg T \Rightarrow$



i.e. zero temp. approximation is used.

Idea, then is that system simply fills up the states  $\left(\frac{L}{2\pi}\right)^3$  per  $d^3k$ , with 2 occupants per state, due spin  $\uparrow \downarrow$ .

$\Rightarrow \Lambda(E) \Rightarrow$  density of states.

... states for

50

$$E = \left(\frac{\hbar^2}{2m}\right) k^2$$

$$dE = \left(\frac{\hbar^2}{2m}\right) 2k dk$$

∴

$$dk = \left(\frac{\hbar^2}{m}\right)^{-1/2} \frac{dE}{2E}$$

$$= \left(\frac{\hbar^2}{m}\right)^{-1/2} \frac{dE}{2E}$$

$$= 2 \left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{dE}{\sqrt{E}}$$

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# states (particles)

$$N = \left(\text{states per } k\right) \int dk = \left(\text{states per } k\right) k_F$$

$$N = 2 \cdot \left(\frac{L}{2\pi}\right) \int 2 \left(\frac{\hbar^2}{2m}\right)^{1/2} \frac{dE}{\sqrt{E}}$$

$$= 2 \cdot 2 \cdot \left(\frac{L}{2\pi}\right) \left(\frac{\hbar^2}{2m}\right)^{1/2} \int \frac{dE}{\sqrt{E}}$$

$$N = \int dE / \sqrt{E} \sqrt{E_0}$$

$$= \int dE n(E)$$

↓  
density of states

$$n(E) = 1/\sqrt{E} \sqrt{E_0}$$

$$E_0 = \frac{\hbar^2}{2m} \left(\frac{\pi^2}{L^2}\right)$$

$\infty$ , with  
density states  
normalization

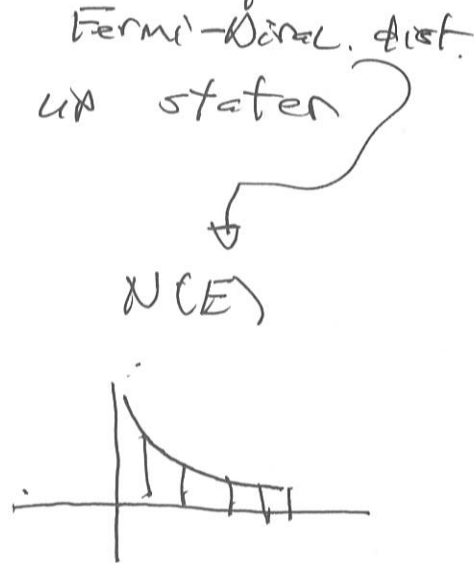
$$N(E) = n(E) F(E)$$

FD  
↑  
Fermi-Dirac dist.

Now, for  $T < \Theta$ , simply fill up states  
so

$$N = \# \text{ particles} = \int_0^{E_F} 1/\sqrt{E} \sqrt{E_0}$$

Fermi energy  
↓  
 $E_F$



$$= 2 (E_F/E_0)^{1/2}$$

$$E_F = (N/2)^2 E_0 = (N/2)^2 \frac{\hbar^2}{2m} \frac{\pi^2}{L^2}$$

↓  
 $\sim \frac{N^2}{L^2}$   
 $\sim N^2$  (concent.)  
(N/L)

$$E_g \sim \frac{\hbar^2}{2m} \Lambda^2$$

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

Fermi wave vector

$$\sim \frac{1}{2} + 2 \frac{1}{2} = 1$$

$k_F \sim \frac{N}{2} \pi / L$  → Fermi wave vector. ↔ Momentum.

5.

and  $v_F \sim \hbar k_F / m$  → Fermi velocity.

Now, in 3D:

→ have spherical shells in  $k$

∴

→ Fermi sphere!

Fermi-Dirac dot.

i.e. distribution now is  $\sim N(E) f_{FD}(E)$

1/50

$$E = \left( \hbar^2 / 2m \right) k^2$$

$$k = \frac{2\pi n}{L}$$

$$dE = \left( \frac{\hbar^2}{2m} \right) 2k dk$$

and

$2 \cdot \left( \frac{2\pi}{L} \right)^{-3}$  states /  $k$  cell  
spin.

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$$N = \int_0^{k_F} 4\pi k^2 dk \left[ 2 \left( \frac{L}{2\pi} \right)^3 \right]$$



Now:  $k^2 = 2mE/\hbar^2$

$$k = (2mE/\hbar^2)^{1/2}$$

$$dk = \left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{1}{2} dE$$

so//

$$N = 2 \left(\frac{L}{2\pi}\right)^3 \int_0^{E_F} 4\pi \frac{2mE}{\hbar^2} \left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{1}{2} dE$$

$$= \frac{L^3}{2\pi^2} \int_0^{E_F} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE$$

$$N = \frac{L^3}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{E_F} \sqrt{E} dE$$

$$= \int_0^{E_F} n(E) dE$$

$$n(E) = \left(\frac{L^3}{2\pi^2}\right) \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{E} dE$$

density  
of  
states

Now, need  $k_F$  for momentum

$$N = \int_0^{k_F} 4\pi k^2 dk \left(2 \left(\frac{L}{2\pi}\right)^3\right)$$

$$= 4\pi \frac{1}{3} L^3 n \dots$$

$$\frac{N}{L^3} \sim \left(\frac{4\pi}{3}\right) \frac{2}{(2\pi)^3} k_F^3$$

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

→ Fermi wave #

$$v_F \sim \frac{\hbar}{m} \left(\frac{3\pi^2 N}{L^3}\right)^{1/3}$$

→ Fermi velocity energy.

$$E_F \sim \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{L^3}\right)^{2/3}$$

observe:

-  $E_F$  indep system size, depends concentration  
i.e.  $\sim \left(\frac{N}{L^3}\right)^{2/3} \sim n^{2/3}$  only.

- this defines a length scale

$$\text{i.e. } \frac{4\pi}{3} r_e^3 = L^3/N$$



↓  
effective volume for single electron

or

$$v_F \sim \hbar/m \left(1/r_e\right)$$

$$\sim \frac{\hbar^2}{2m} \sim \frac{1}{2}$$

18

$$V_F \sim 2/r_e^{-1} \text{ (a.u.)} \quad (\text{eV})$$

$$E_F \sim 1.8 r_e^{-2} \text{ (a.u.)}$$

50

Na	$r_e$ 3.2	$V_F$ 0.5 x 10 <sup>6</sup> m/sec.	$E_F$ 3.2 eV
Al	2	2 x 10 <sup>6</sup> m/sec.	11.7 eV.

(clearly well above room temp.)

and can calculate avg<sup>kinetic</sup> energy:

i.e.

$$\bar{E} \approx \frac{\int_0^{E_F} dE E N(E)}{\int_0^{E_F} dE N(E)}$$

$$\sim 1.1 / r_e^2 \text{ (a.u.)} \quad \left( \sim \frac{\hbar^2}{2m} k_F^2 \right)$$

in eV.

→ note now have scales:

$V_F, k_F, E_F$  of metal. ( $\sim \sigma T$ )

all in terms  $\hbar, m_e, n$ .

Now, what of better discussion of energy?  $\frac{9}{-}$

So far, have:

- Kinetic/repulsive energy

$$E \sim 1.1 / r_e^2$$

$$N_e^3 \sim L^3$$

- Coulombic energy

idea (Drude-equivalent) is that conduction electrons ~ uniform so

e.g. energy cancels, i.e. attraction

$\Rightarrow$  this leaves KE.

vs  
e-e repulsion

} cancel

- but, electrons undergo Pauli's repulsion, i.e. so  $\uparrow \downarrow$  repulsion for opposite spins reduced.

$\Rightarrow$  Exchange Term

$$\Rightarrow \Delta E_{\text{Pauli}} = - \frac{.5}{r_e} \text{ (au)}$$

really decrease repulsion, opp. spins  
 $\downarrow$   
 $1/r_e$  attractive force

thermal exchange

$\Rightarrow$  lowers energy

$$\boxed{E \approx 1/r^2 - .5}$$

# → Transport

~ heuristics: For transport, need:

- velocity
- length, time

Here:  $v \rightarrow v_F$

$\lambda_{MFP} \rightarrow v_F \tau_{relax}$

Point: - only electrons on surface of Fermi sphere can move, in response  $E$ . For  $k < k_F$ , all states occupied. Thus can't accelerate electrons, as states occupied. opposing force is Pauli repulsion



To estimate:

$$\hbar \frac{dk}{dt} = +eE$$

$$p = \hbar k$$

$$\Delta k \approx +eE \Delta t \approx +eE \tau$$

Now  $\underline{J} = Ne V_F \frac{\delta N}{N}$  = current carried by displaced surface Fermi electrons -  $\delta N/N$   
 - speed is  $V_F$ , f.o.

$$\frac{\delta N}{N} \sim \frac{\Delta k}{k_F} \approx \frac{\Delta E_F}{k_F} \sim \frac{e E \tau_{ix}}{\hbar k_F}$$

$$\hookrightarrow \frac{v_F^2 \Delta k}{k_F^3}$$

$$v_F \approx \frac{\hbar k_F}{m_e}$$

$$\therefore \underline{J} \sim \frac{Ne^2 E \tau_{ix} \hbar k_F}{\hbar k_F m_e}$$

$$\underline{J} \sim \frac{Ne^2 \tau_{ix}}{m_e} E$$

$$J = \frac{Ne^2 \tau_{ix}}{m_e} E$$

back to Drude, in form of answer!

But:

- current carried by <sup>Fermi sphere</sup> surface electrons, only.
- $v \rightarrow v_F$
- $\tau_{ix} \rightarrow$  Fermi Golden Rule, QM transitions!

i.e.


$$\frac{1}{\tau_{ix}} \sim \Gamma_F \approx \frac{2\pi}{\hbar} \sum_{k'} | \langle k | V_{int} | k' \rangle |^2 \rho(E_k - E_{k'}) * (f_{k'} - f_k)$$

interaction
energy cons.

↓
↓

transition
 $(f_{k'} - f_k)$

Where:

  $\rightarrow \frac{A}{4} \quad \text{with } |k| \sim |h'|$

$\Rightarrow$  assumed:  $E_h \sim E_{gr}$

$f_h \neq f_{gr}$ , as outside sphere.  
 $f \approx 1$  to  $f = 0$  transition

Similarly, for  $\lambda$ :

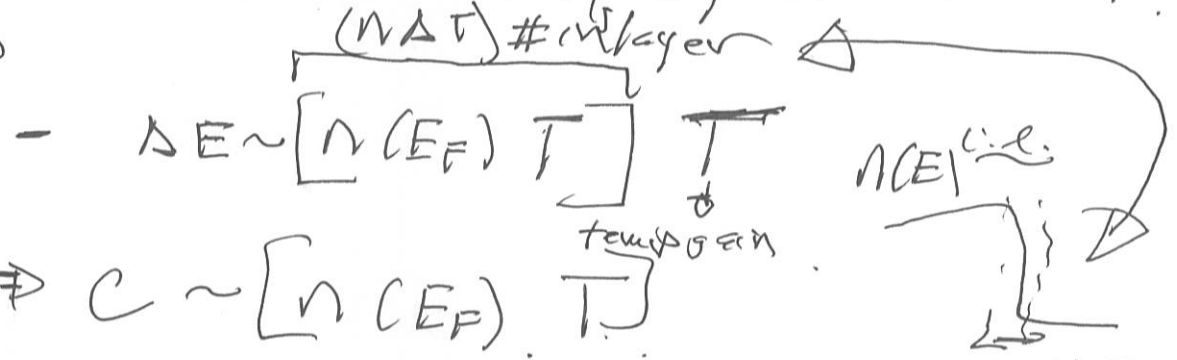
$\lambda \sim n v l_{mp} = \underbrace{C}_{\text{specific heat/vol.}} v_{th} l_{mp} \rightarrow C v_F^2 T_{rx}$   
 $\rightarrow$  does temp matter?  $\sim \frac{C}{m_e} E_F T_{rx}$

Now,  $\frac{d}{dt} = \partial \Delta E / \partial T$ , defn.

spec. heat

- when thermal excitation applied, only a few electrons excited, those at Fermi energy by increment  $T$ .

so



$\therefore \Rightarrow C \sim [N(E_F) T]$

$\hookrightarrow$  specific heat is temp. dependent.

$N(E_F) T$  - shell thickness

$\Rightarrow \lambda \sim \frac{N(E_F) T E_F}{m_e v} T_{rx}$

So

13

$$\lambda \sim \frac{n(E_F) E_F T}{m_e v}$$

For Weidemann-Franz:

$$\lambda / \sigma \sim \frac{n(E_F) E_F T}{v m_e n e^2 \frac{L^3}{m_e}} \rightarrow$$

$$\sim \frac{n(E_F) E_F T}{v n e^2}$$

$$v \sim L^3$$

but

$$\frac{n(E_F) E_F}{L^3} \sim E_F \frac{L^3}{L^3} (E_F)^{1/2} \left(\frac{2m}{\hbar^2}\right)^{3/2}$$

need spec. heat/volume

$$\sim (E_F)^{3/2} \cancel{L^3}$$

$$(2m/\hbar^2)^{3/2}$$

$$\sim \frac{N}{L^3} L^3$$

$$\left(\frac{2m}{\hbar^2}\right)^{3/2} \left(\frac{\hbar^2}{2m}\right)^{3/2}$$

$$\sim N \rightarrow n$$

$$c = c/v$$

$$\lambda / \sigma \sim \frac{NT}{Ne^2}$$

→ recover Weidemann-Franz!

or

$$\lambda / \sigma \sim \frac{T}{e^2} k_B^2 \frac{\pi^2}{3}$$

$$\sim T k_B^2 \pi^2 \rightarrow \text{Lorentz factor}$$



So - recover Weideman-Franz!

14.

Key: -  $\tau_{nlx}$  concepts

but - essential to note that transport dominated/due to electrons on surface of Fermi-Sphere.

From Chapman-Enskog perspective:

recall for  $\nabla$ :

(MB)

$$-\frac{e}{m} \underline{E} \frac{\partial f}{\partial v} = c(f) = -\frac{1}{\tau_n} (f - f_0)$$

$$f = f_0 + \delta f$$

$$\underline{J} = -n_0 e \int d^3v \underline{v} f$$

$$\therefore -\frac{1}{\tau_n} (\delta f) \approx -\frac{e}{m_e} \underline{E} \cdot \frac{\partial f_0}{\partial \underline{v}} \quad (\text{after } c-E)$$

$$\delta f \approx \tau_n \frac{e}{m_e} \underline{E} \cdot \frac{\partial f_0}{\partial \underline{v}}$$

$\Rightarrow$

$$\underline{J} = -\frac{n_0 e^2}{\tau_n} \int d^3v \underline{v} E \cdot \frac{\partial f_0}{\partial \underline{v}}$$

$$\sigma \sim \frac{N_0 e^2}{m_0} \tilde{I}_{nlx}$$

n.b.  $\frac{\partial f_0}{\partial v} \sim -\# f_0$   
 distributed over dist.

Now, for QM particles, really need density matrix  $\sum_{ij} |\psi_i\rangle\langle\psi_j|$ . Can use  $N(\underline{x}, \underline{k}, t)$

$N \Leftrightarrow$  Wigner Distribution  $F(\underline{x}, t)$  wave fctns

Quasi-Particle Picture

$$N = \int d^3p e^{i\mathbf{p}\cdot\mathbf{x}} \psi^\dagger(\mathbf{k} + \mathbf{p}/2) \psi(\mathbf{k} - \mathbf{p}/2)$$

classically  $N \rightarrow$  action density

$\rightarrow$  population density

then

can view  $N$  as a kind of wave/wave function density

$$\frac{\partial N}{\partial t} + (\underline{\omega} + \underline{v}) \cdot \underline{\nabla} N - \frac{\partial}{\partial \underline{x}} (\underline{\omega} + \underline{v} \cdot \underline{v}) \cdot \frac{\partial N}{\partial \underline{k}}$$

$$= -\frac{\Gamma}{\tilde{I}_{nlx}} (N - N_0)$$

Wave Kinetic Equation

$$\frac{\partial N}{\partial t} + \frac{\partial \omega}{\partial k} \cdot \underline{\nabla} N - \frac{\partial \omega}{\partial \underline{x}} \cdot \frac{\partial N}{\partial \underline{k}}$$

now  $\frac{\partial W}{\partial \hbar} \rightarrow \frac{\partial \hbar W}{\partial \hbar} \rightarrow \frac{\partial E}{\partial p}$

$$-\frac{\partial W}{\partial x} \cdot \frac{\partial}{\partial \hbar} \rightarrow -\frac{\partial \hbar W}{\partial x} \cdot \frac{\partial}{\partial \hbar} \rightarrow -\frac{\partial E}{\partial x} \cdot \frac{\partial}{\partial p}$$

but  $E = E_{kin} + V(x)$

$$-\frac{\partial W}{\partial x} \cdot \frac{\partial}{\partial \hbar} \rightarrow -\frac{\partial V}{\partial x} \cdot \frac{\partial}{\partial p} \rightarrow F \cdot \frac{\partial}{\partial p}$$

$$\rightarrow \frac{F}{\hbar} \cdot \frac{\partial}{\partial \hbar}$$

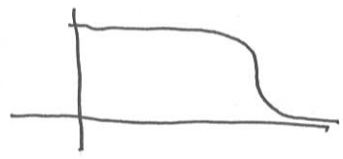
$$N \rightarrow g = g(x, \hbar, t)$$

so

$$\frac{\partial g}{\partial t} + \frac{\partial E}{\partial p} \cdot \frac{\partial g}{\partial x} + \frac{F}{\hbar} \frac{\partial g}{\partial \hbar} = \frac{-1}{T_{Mx}} (g - g_0)$$

For electrons in metals

$$g_0 = F_D(E)$$



and ...

so

$$\frac{\partial g}{\partial t} + \frac{\partial \epsilon}{\partial p} \cdot \frac{\partial g}{\partial \underline{x}} - \frac{e \underline{E} \cdot \underline{\partial} g}{\hbar} = \frac{-\tau}{\tau_{rx}} (g - g_0)$$

and now Chapman - Enskog, as usual.

$$g = g_0 + \delta g$$

$$-\frac{e \underline{E}}{\hbar} \cdot \frac{\partial g_0}{\partial \underline{h}} = \frac{-\tau}{\tau_{rx}} \delta g$$

$$\underline{J} = - \frac{e}{m_e} \int d\underline{h} \hbar \underline{h} \delta g$$

$g_0 \rightarrow$  even.

$$\delta g = + \tau_{rx} \frac{e \underline{E}}{\hbar} \cdot \frac{\partial g_0}{\partial \underline{h}}$$

$$\underline{J} = - \frac{e^2}{m_e} \int d\underline{h} \frac{\hbar \underline{h}}{\hbar} \left( \frac{\partial g_0}{\partial \underline{h}} - \frac{E}{\hbar} \right) \tau_{rx}$$

but where is  $\partial g_0 / \partial \underline{h} \neq 0$  ?  $\rightarrow$  Fermi surface

Now,  $\underline{J} = - \frac{e^2}{m_e} \int d\underline{h} \tau_{rx} \hbar \left[ \frac{\partial g_0}{\partial \underline{h}} \cdot E \right]$

$$\int d\underline{k} = \int 4\pi k^2 dk$$

$$k \rightarrow \left[ \frac{E \cdot \frac{\partial g_0}{\partial k}}{\frac{\partial g_0}{\partial E}} \right] \rightarrow \frac{k}{m} (E - k) \frac{\hbar^2}{m} \frac{\partial g_0}{\partial E}$$

|||

$$\underline{J} = -\frac{e^2}{m_e} \int 4\pi k^2 dk \tau_{rx} \left[ \frac{k}{m} (E - k) \frac{\hbar^2}{m} \frac{\partial g_0}{\partial E} \right]$$

but  $\frac{\hbar^2}{m} k dk = dE$

$$\underline{J} = -\frac{e^2}{m_e} \int dE \tau_{rx} \left[ k (E - k) \frac{\partial g_0}{\partial E} \right] k$$

but  $\frac{\partial g_0}{\partial E} \approx -\delta(E - E_F)$

∴

$$\underline{J} \approx \frac{e^2}{m_e} \tau_{rx} E k_F^3$$

$$\underline{J} \approx \frac{e^2}{m_e} \tau_{rx} k_F^3$$

but  $\approx k_F^3 = 3\pi^2 N = \left( N/L^3 \right)^{1/3}$  19

$$\sigma \approx \frac{ne^2 \tau}{m_e}$$

as usual

Messages:

-  $\partial F_0 / \partial E = -\delta(E - E_F)$

captures idea of localization of ~~electron~~ electron response to Fermi surface.

- result same, physics diff.

- can use WKE for wave transport problems, much like Boltzmann Eqn.

