Lecture 9
Free Electrons

Both “free” and “electron” are loaded terms here.

AC Conductivity and Plasmon

- AC Conductivity and Dielectric Constant

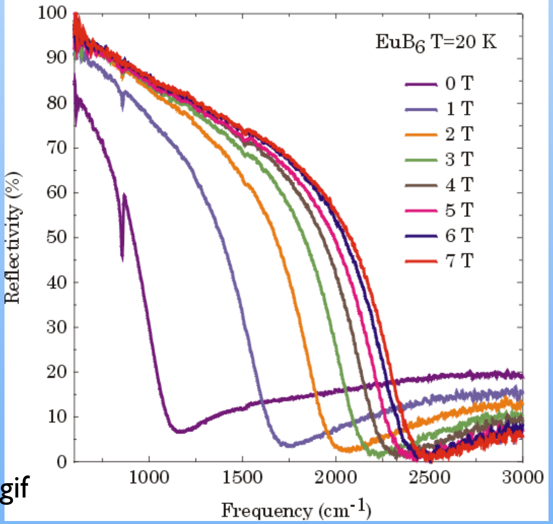
$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}, \quad \sigma_0 = \frac{ne^2\tau}{m}. \qquad \epsilon(\omega) = 1 + \frac{4\pi i\sigma}{\omega}. \qquad \epsilon(\omega) = 1 - \frac{\omega_p{}^2}{\omega^2},$$

cf. Marder 20.2 (lecture)

- Longitudinal, Purely Electric Collective Mode – Plasma Oscillation

$$\omega_p{}^2 = \frac{4\pi ne^2}{m}.$$

Detection by plasma edge in Reflectivity, plasmon loss in Photoemission or Electron Loss Spectroscopy



http://www.solidphys.ethz.ch/spectro/doc/fig/fig103.gif

Quantum Treatment of Free Electrons

Free electrons on a “hyper-ring” or a “hyper-torus”

Born-von Karman boundary condition.
Generalize a ring (1d) to a torus (2d), a cube with periodic boundary (3d) etc.
Define D as spatial dimension.

$$\psi(\boldsymbol{x}) = \psi(\boldsymbol{x} + \boldsymbol{L}) \qquad \boldsymbol{L} = (L, L, \ldots, L) \quad D - vector$$

$$\psi(\boldsymbol{x}) = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{x}}, \qquad k_i = \frac{2\pi n_i}{L}, \quad i = 1..D, \qquad n_i = \text{integer}, \qquad V = L^D$$

Quantum Numbers

$$\boldsymbol{p} = \hbar \boldsymbol{k}, \qquad \varepsilon = \frac{\hbar^2 k^2}{2m}, \quad S_z = \frac{1}{2}\hbar$$

Will consider mainly D=3 in this course.

Fermi Sea at T=0

DOS $$dN = 2\frac{4\pi k^2 dk}{\left(\frac{2\pi}{L}\right)^3} = V\frac{k^2 dk}{\pi^2} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\varepsilon}d\varepsilon = g(\varepsilon)d\varepsilon$$

$$g(\varepsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{\varepsilon} \propto \sqrt{\varepsilon}$$

in 3d

Fermi-Dirac Statistics and Number of particle numbers

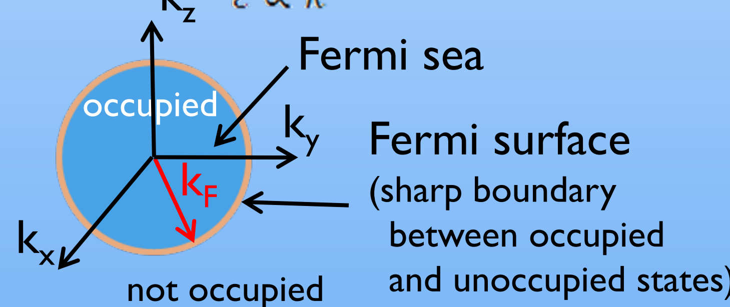
give the energy cutoff (μ): $$N = \int_0^{\varepsilon_F} g(\varepsilon)d\varepsilon = \frac{V}{3\pi^2}\left(\frac{2m\varepsilon_F}{\hbar^2}\right)^{\frac{3}{2}}$$

Fermi energy $$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} \equiv \frac{\hbar^2 {k_F}^2}{2m}$$

Fermi momentum $$k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}}$$

Fermi temperature $$T_F \equiv \frac{\varepsilon_F}{k_B}$$

$\varepsilon \propto k^2$



Fermi Sea at T=0

$$r_s = \left(\frac{3V}{4\pi N}\right)^{\frac{1}{3}}, \qquad \frac{4\pi r_s^3}{3} = \frac{V}{N}$$

$$k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} = \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \frac{1}{r_s} = \frac{1.92}{r_s}$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} = \frac{(\hbar c)^2}{2mc^2} k_F^2 \sim \frac{(2000\ eV\text{Å})^2}{1e6\ eV} k_F^2 \sim 4k_F^2\ (= 3.8\ k_F^2\ )$$

if k_F in Å^{-1} and ε_F in eV

Numbers for typical metals (Au, Cu, Al, Na ...)

$$r_s = 1 \sim 2\ \text{Å}$$

$$r_s \sim a \sim \frac{1}{k_F}$$

$$k_F = 1 \sim 2\ \text{Å}^{-1}$$

$$v_F \sim \frac{\hbar k_F}{m} = \frac{\hbar c\ c}{mc^2} k_F \sim \frac{2000\ eV\text{Å}}{0.5e6\ eV} \times (1-2)\text{Å}^{-1} \times c \sim 10^{-2}\ c$$

$$v_F \sim \frac{c}{100}$$

$$v_s \sim \frac{c}{10{,}000}$$

$$v_s \sim \frac{\omega_D}{\pi/a} \sim 10 - 100 \frac{\text{meV}}{\text{Å}^{-1}} \frac{c}{\hbar c} \sim 10^{-2} - 10^{-1} \frac{c}{1000} \sim \frac{c}{10{,}000 - 100{,}000}$$

$$\varepsilon_F = 1 \sim 10\ \text{eV}$$

$$T_F = \ 10{,}000 \sim 100{,}000\ \text{K}$$

Recall that 300 K is 26 meV, and the Debye T ~ 100 K.

Finite Temperature

Fermi-Dirac function $f(\varepsilon,T)=\dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$ $\beta=\dfrac{1}{k_BT}$

Determine chemical potential μ using $N=\int_0^\infty g(\varepsilon)f(\varepsilon,T)d\varepsilon$

Obtain energy from $E=\int_0^\infty \varepsilon g(\varepsilon)f(\varepsilon,T)d\varepsilon$

After using Sommerfeld Expansion technique:

$$\mu\approx\varepsilon_F\left[1-\frac{1}{3}\left(\frac{\pi k_BT}{2\varepsilon_F}\right)^2\right] \qquad \mu(T=0)=\varepsilon_F$$

$$E\approx\frac{3}{5}N\varepsilon_F+\frac{\pi^2}{6}(k_BT)^2g(\varepsilon_F) \qquad g(\varepsilon_F)=\frac{3N}{2\varepsilon_F}$$

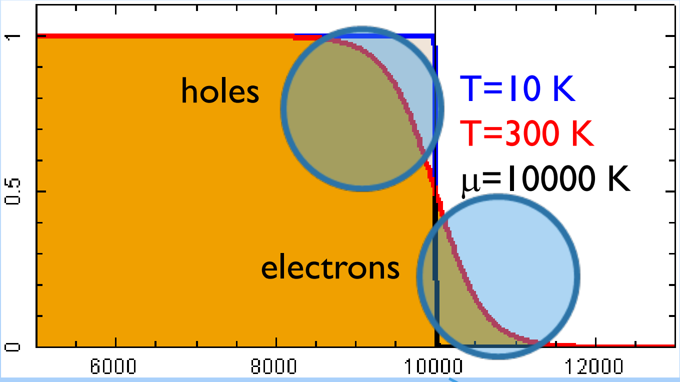
$$C_V=\left(\frac{\partial E}{\partial T}\right)_V=\frac{\pi^2}{3}k_B(k_BT)g(\varepsilon_F)$$

Corrections to T=0 results are of the order, $O\left(\left\{\frac{T}{T_F}\right\}^2\right)$

i.e. very small (10^{-4}) if T ~ RT, compared to T=0 values.

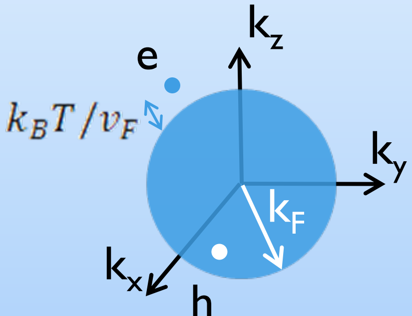
Finite Temperature – Physics

FD function: electron and hole excitation relative to vacuum (i.e. Fermi sea at T = 0)



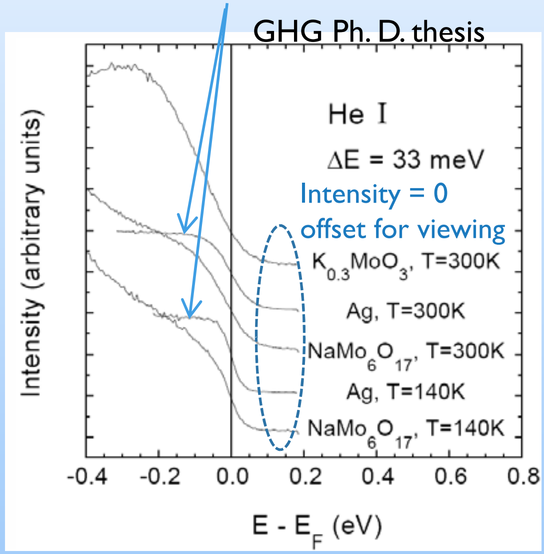
ε(in unit of K) → μ

Deviation from step function (T=0) occurs within the energy range of ~ $k_B T$



Fermi surface becomes blurry due to many e-h pairs.
(only one shown for clarity)

Measured FD function



Physics (expressions good up to numerical factors)

(1) Energy per excited particle ~ $k_B T$
(2) Number of particles ~ $k_B T g(\varepsilon_F)$
(3) E(T) – E(T=0) ~ (1)x(2) ~ $(k_B T)^2 g(\varepsilon_F)$
(4) C(T) = dE/dT ~ $k_B (k_B T) g(\varepsilon_F)$

Heat Capacity due to e⁻'s <u>and</u> lattice

(Often used "specific heat", = heat capacity per volume or mole)

$$C_V(e^-) \approx \frac{\pi^2}{3} k_B (k_B T) g(\varepsilon_F) = \frac{\pi^2}{2} N_e \frac{T}{T_F} k_B \qquad C_V(phonon) \approx \frac{12\pi^4}{5} N_{lattice} \left(\frac{T}{\theta_D}\right)^3 k_B$$

$$C_V \approx \gamma T + \beta T^3$$

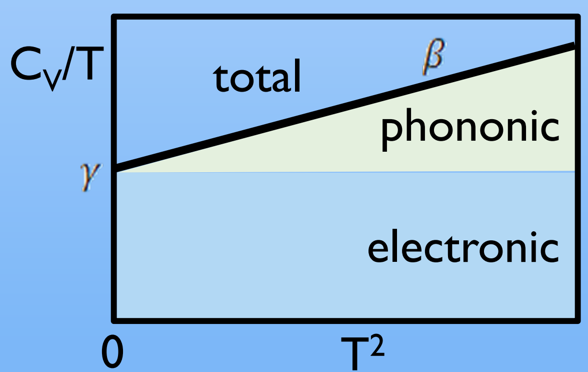
same order in metals (N_e and $N_{lattice}$)

<u>Differences are here!</u> ($\frac{T}{T_F}$ and $\left(\frac{T}{\theta_D}\right)^3$)

Phonon term (cube term) is dominant at high (~ room) temperature (~ θ_D).
Electron term (linear term) is dominant at low temperature.
Rough estimate of the boundary temperaure:

$$\frac{T}{T_F} \sim \left(\frac{T}{\theta_D}\right)^3 \qquad T \sim \theta_D \sqrt{\frac{\theta_D}{T_F}} \sim 100\ K \sqrt{\frac{1}{100}} \sim 10\ K$$

Many Researchers Plot C_V Like this:



$$\frac{C_V}{T} \approx \gamma + \beta T^2$$

γ ~ 1 mJ mol^{-1} K^{-2}
~ free electron value

Many exceptions:
γ can be 1000 times larger!
"Heavy Fermion" system

$$\gamma \sim \frac{k_B}{T_F} \sim \frac{1}{m}$$

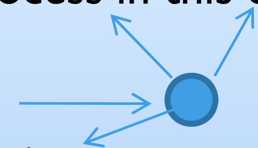
m: <u>effective</u> mass in general

Conduction of Electricity

Source for finite conductivity

NOT ions in static crystal, but impurity, jittering ions (i.e. phonons), and other electrons (but only umklapp process in this case)

A simple model (relaxation time approx.)



Quasi-elastic scattering in random directions

- Relaxation time τ (time between scattering)
- Scattering events wipe out electron's memory (i.e. restores equilibrium)
- Conduction due to a tiny push by electric field between collisions

We will see why later:

$$F = eE = ma = mv_d/\tau$$

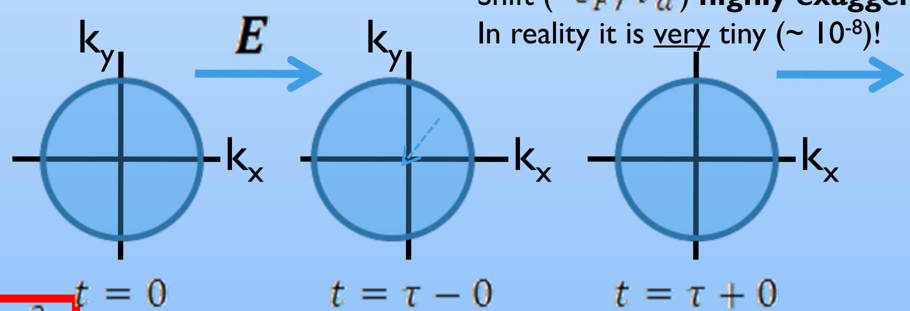
(only magnitude considered)

v_d **Drift velocity**

NOT electron velocity

ONLY a small added velocity

Shift ($\sim \varepsilon_F / v_d$) **highly exaggerated**.
In reality it is very tiny (~ 10^{-8})!



Ohm's law

$$j = nev_d = \frac{ne^2\tau}{m}E = \sigma E$$

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

Drude conductivity=1/Drude resistivity

Equation of Motion

$$m\left[\frac{dv_d}{dt} + \frac{v_d}{\tau}\right] = F$$

Keep in mind that microscopically, electrons are jittering fast (v_F), and the drift velocity is a tiny fraction (10^{-8} v_F) added to it, but it is what makes a difference since drifting adds up while jittering sums to zero.

Conduction of Electricity

- Two common sources of scattering:

  e-ph and e-im (ph=phonon, im=impurity)

$$\frac{1}{\tau} = \frac{1}{\tau_{ph}} + \frac{1}{\tau_{im}} = \frac{1}{\tau_{ph}(T)} + \frac{1}{\tau_{im}}$$

Impurity: no T dependence, elastic

Phonon: T dependence, inelastic (absorption or emission of phonons)

Mattheisen's rule $$\rho = \frac{m}{ne^2\tau} = \rho_{ph}(T) + \rho_{im}$$

- Units, Time scale, drift velocity etc. in typical metals

$$n \sim \frac{10^{23}}{cm^3} \sim \frac{0.1}{\text{Å}^3}$$

$$\sigma \sim (\mu\Omega\,\text{cm})^{-1} = 10^6(\Omega\,\text{cm})^{-1} = 9.000\text{e}17\,(\text{statOhm} - \text{cm})^{-1} = 9.000\text{e}17\,\text{s}^{-1}$$

$$\tau = \frac{m\sigma}{ne^2} = \frac{m\sigma\hbar c}{n\hbar c e^2} \sim \frac{mc^2\sigma}{n\hbar cc^2}\frac{\hbar c}{e^2} = \frac{\text{Å}^3\, 0.5e6\, eV\, 9e17\, s^{-1}}{0.1\, 2e3\, eV\, \text{Å}\, 9e36\, \text{Å}^2\, s^{-2}} 137 \sim 3\times 10^{-14}\, s$$

$$\tau \sim femtosecond\ (R.T.) - 10\ nanosecond\ (low\ T)$$

$$l = v_F\tau = 1e16\frac{\text{Å}}{s} \times \tau \sim 10\ \text{Å} - 1\ \text{mm}$$

Mean free path ~ typically 100 Å – 1 μm

$$v_d = \frac{j}{ne} \sim 1000\frac{\text{A}}{\text{cm}^2}\frac{1}{ne} = \frac{10^3\,\text{A cm}}{10^{23}\times 1.6\times 10^{-19}\text{C}} \sim 1\frac{\text{mm}}{s} \sim 10^{-11}c \sim 10^{-9}v_F$$

Drift Velocity – Slow!

Wiedemann-Franz Law

Thermal conductivity $\kappa = \frac{1}{3} v l \frac{C}{V}$

Fermi velocity $v = v_F$

Electron mean free path $l = v_F \tau$

Electron heat capacity $C = \frac{\pi^2}{2} N \frac{k_B T}{k_B T_F} k_B$ $\quad k_B T_F = \varepsilon_F = \frac{1}{2} m v_F^2$

$$\kappa = \frac{1}{3} v l \frac{C}{V} = \frac{1}{3} v_F^2 \tau \frac{\pi^2}{2} \frac{N}{V} \frac{k_B T}{\frac{1}{2} m v_F^2} k_B = \frac{\pi^2}{3} n\tau \frac{k_B^2 T}{m} = \frac{\pi^2}{3} \frac{n\tau}{m} k_B^2 T \qquad n = \frac{N}{V}$$

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

$$\frac{\kappa}{\sigma T} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$ ≡ Lorenz number

Wiedemann-Franz Law

Holds as long as scattering is τ is similar for σ and κ.
Ok for impurity scattering (low T) or when T >~ θ_D (high T).
It breaks down at intermediate T.