The Sommerfeld Theory of Metals

-- continued

Fermi-Dirac Distribution

the probability that a electron will have energy ε

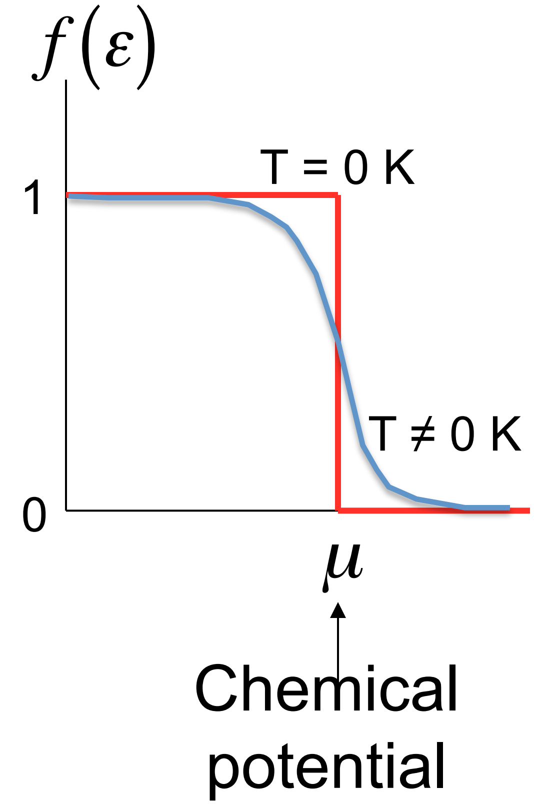
$$f(\varepsilon) = \frac{1}{\exp\left(\varepsilon - \mu \big/ \kappa_B T \right) + 1}$$

due to the kinetic energy of the electron with finite temperature

the quantum difference that arises from the fact That electrons are indistinguishable

Electron Distribution

$$f(\varepsilon) = \frac{1}{\exp\left(\frac{\varepsilon - \mu}{\kappa_B T} \right) + 1}$$



T = 0 K: all electrons stay in the ground state

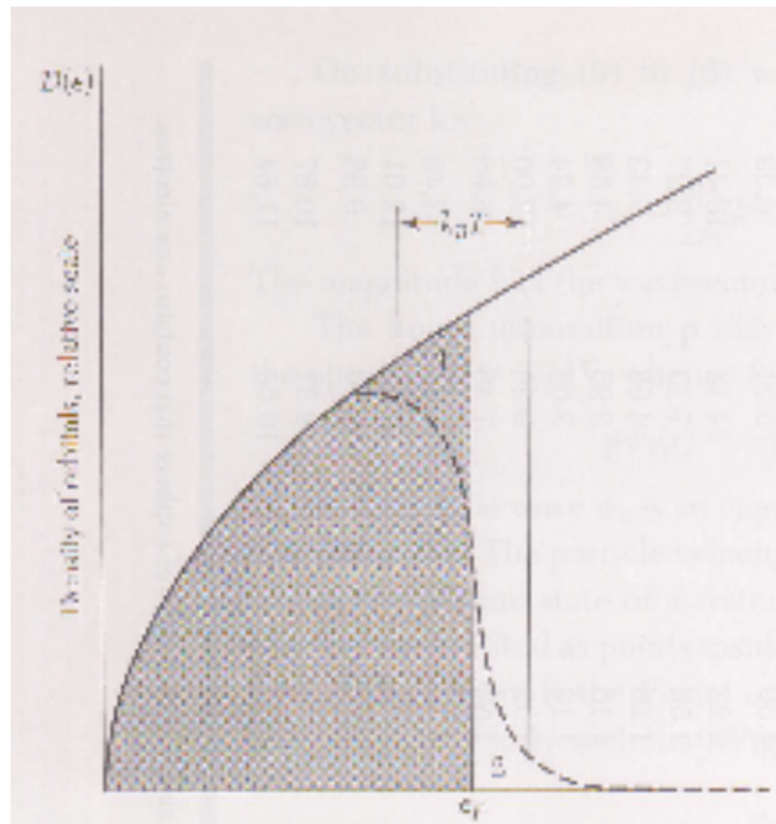
T ≠ 0 K: excitations due to thermal energy

g(ε) versus ε

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

$$= 0 \qquad \varepsilon > \varepsilon_F$$

$$g(\varepsilon_F) = \frac{mk_F}{\hbar^2\pi^2} = \frac{3}{2}\frac{n}{\varepsilon_F}$$



Sommerfeld calculation for T ≠ 0 K

Carrier density $n = \int g(\varepsilon) f(\varepsilon) d\varepsilon$

$$= n_{0(GS)} + \left\{ (\mu - \varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) \right\}$$

Energy density $u = \int g(\varepsilon) f(\varepsilon) \varepsilon d\varepsilon$

$$= u_{0(GS)} + \left\{ (\mu - \varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) \right\} + \frac{\pi^2}{6} (k_B T)^2 g(\varepsilon_F)$$

Chemical Potential vs Fermi Energy

$$n = n_0 + \left\{ (\mu - \varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) \right\}$$

$n = n_0$ -- it is assumed to be T-independent

$$\mu = \varepsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)} = \varepsilon_F \left(1 - \frac{1}{3} \left(\frac{\pi k_B T}{2 \varepsilon_F} \right)^2 \right)$$

$\mu = \varepsilon_F$ **When T = 0 K**

Specific Heat of the Electron Gas

T = 0 K: all electrons stay in the ground state

$C_{electron}$ (T=0K)= ?

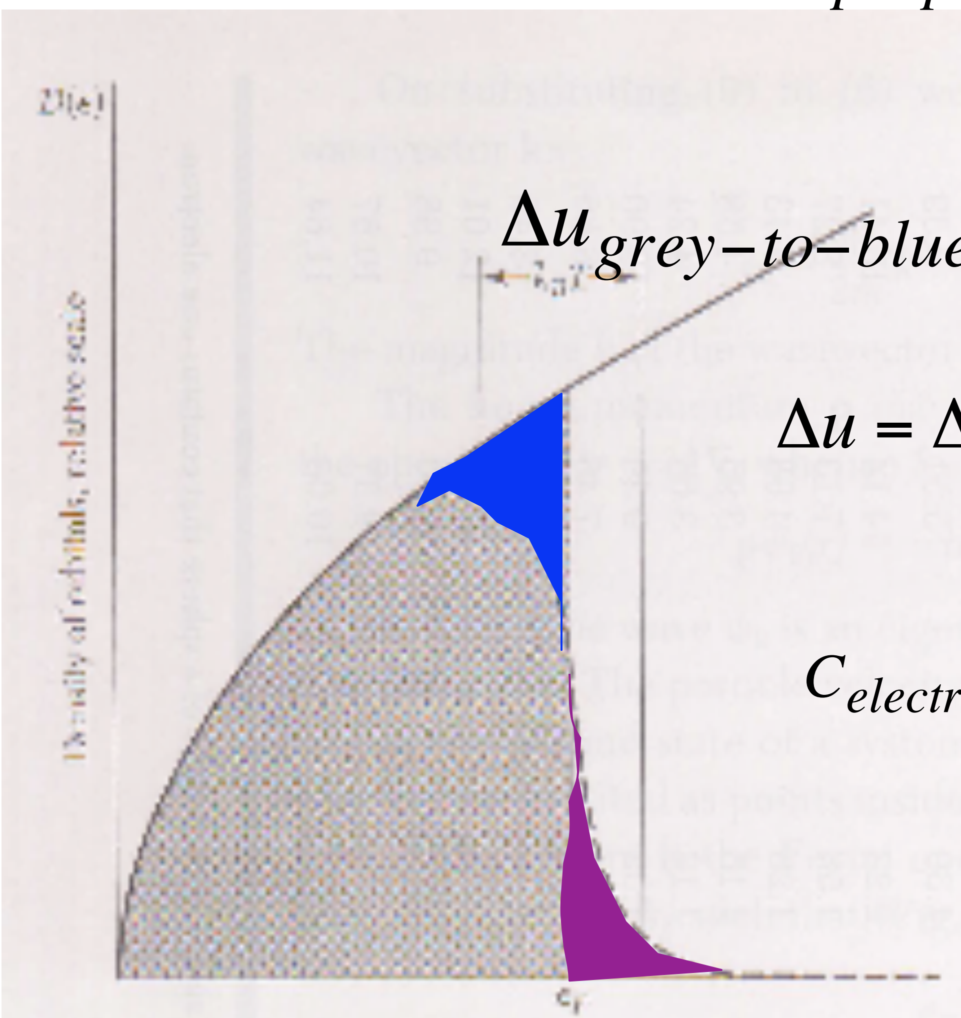
T ≠ 0 K: excitations due to thermal energy

$C_{electron}$ (T≠0K)= ?

Specific Heat of the Electron Gas

T≠0K

$$\Delta u_{blue-to-purple} = \int_{\varepsilon_F}^{\infty} (\varepsilon - \varepsilon_F) f(\varepsilon) g(\varepsilon) d\varepsilon$$



$$\Delta u_{grey-to-blue} = \int_{0}^{\varepsilon_F} (\varepsilon_F - \varepsilon)[1 - f(\varepsilon)] g(\varepsilon) d\varepsilon$$

$$\Delta u = \Delta u_{blue-to-green} + \Delta u_{grey-to-blue}$$

$$C_{electron} = \frac{du}{dT} = \int_{0}^{\infty} (\varepsilon - \varepsilon_F) \frac{df(\varepsilon)}{dT} g(\varepsilon) d\varepsilon$$

Electron Specific Heat at low temperatures

$$k_B T << \varepsilon_F$$

$$C_{electron} = \int_0^{\infty} (\varepsilon - \varepsilon_F) \frac{df(\varepsilon)}{dT} g(\varepsilon) d\varepsilon$$

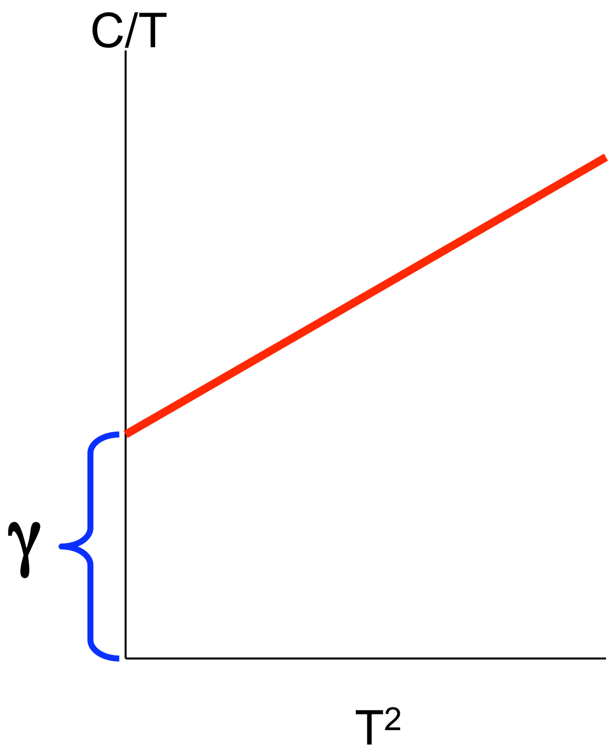
$$\sim g(\varepsilon) \int_0^{\infty} (\varepsilon - \varepsilon_F) \frac{df(\varepsilon)}{dT} d\varepsilon$$

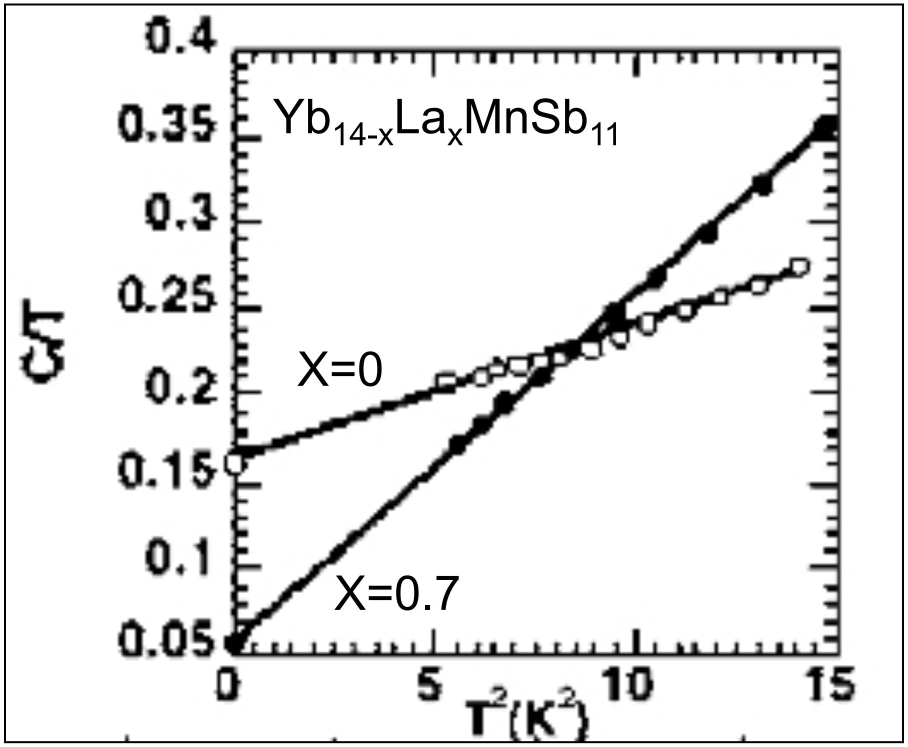
$$\sim \frac{1}{3} \pi^2 g(\varepsilon) k_B^2 T$$

Note $C_{electron} \propto T$

Total Specific Heat at Low Temperatures

$$C_{total} = C_{electron} + C_{phonon} = \gamma T + \beta T^3$$



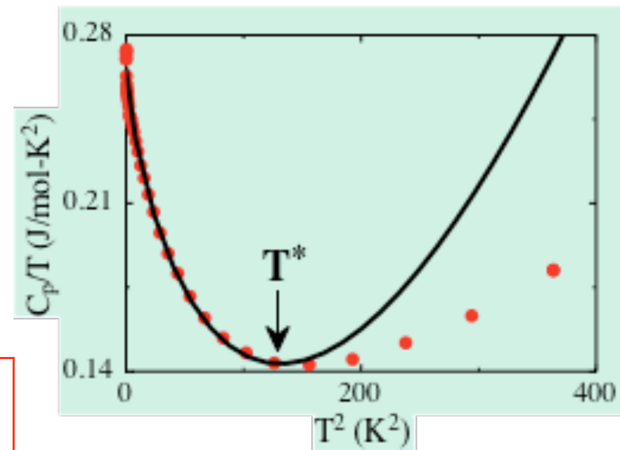


Heavy Electrons (Fermions)

γ(observed) ≠ γ(free-gas model) -- Why?

The effective mass of electrons are different from that of free electrons

$$\frac{m_{eff}}{m_{free}} = \frac{\gamma(observed)}{\gamma(free)}$$



Heavy Electrons (Fermions)

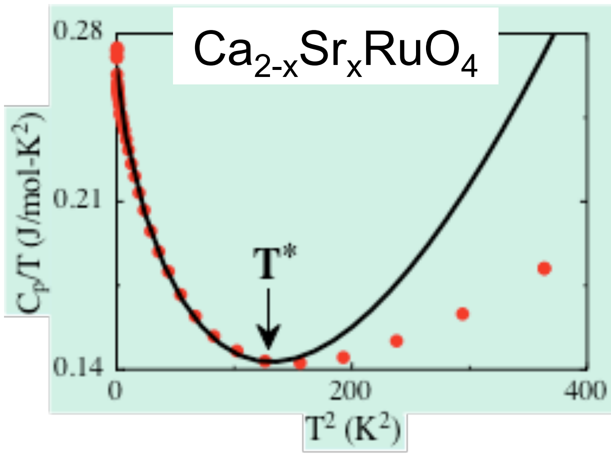
$$T<T^*: \quad \frac{C_p}{T} = \gamma + \beta T^2 + \delta T^2 \ln(T/T_{fl})$$

↓

$\gamma = 266$ mJ/mol-K^2

More than 100 times larger

Specific Heat: more than C_e and C_p

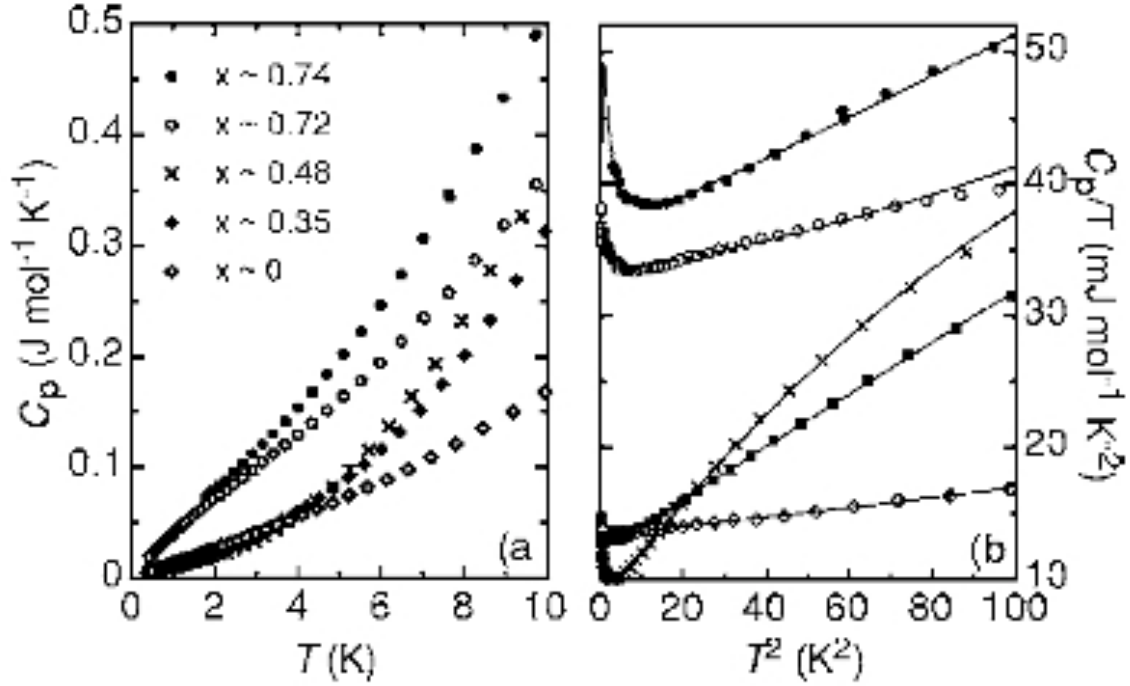


$$T<T^*: \quad \frac{C_p}{T} = \gamma + \beta T^2 + \delta T^2 \ln(T/T_{fl})$$

$$\downarrow$$

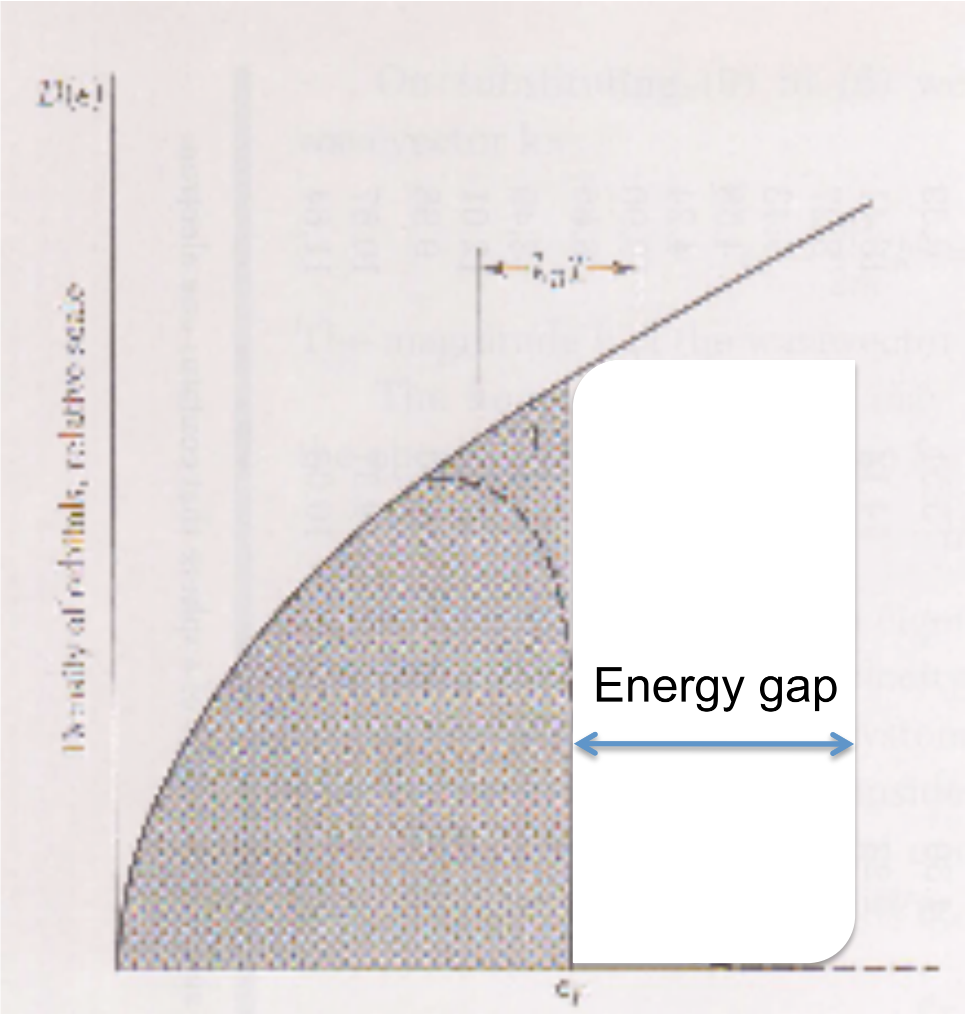
$$\gamma = 266 \text{ mJ/mol-K}^2$$

Na_xCoO_2



Non-linear C/T versus T^2 implies there is/are additional contribution(s)

Localized Electrons
- Cannot be treated as electron gas



$$C_{electron} = \frac{du}{dT} = 0$$

Sommerfeld Approach

$$C_{electron} = \frac{1}{3}\pi^2 g(\varepsilon) k_B^2 T = \frac{1}{2}\frac{\pi^2 n k_B^2 T}{\varepsilon_F}$$

$$\kappa = \frac{1}{3} v^2 \tau c_v = \frac{1}{3}\left(\frac{2\varepsilon_F}{m}\right)\tau\left(\frac{1}{2}\frac{\pi^2 n k_B^2 T}{\varepsilon_F}\right) = \frac{\pi^2 n k_B^2 T}{3m}$$

$$\frac{\kappa}{\sigma T} = \frac{\pi^2 n \tau k_B^2 T}{3m}\left(\frac{m}{ne^2 \tau T}\right) = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 = 2.44 \times 10^{-8} W - \Omega / K^2$$

✔

Sommerfeld Approach

Thermopower $Q = \frac{\Delta V}{\Delta T} = -\frac{c_v}{3ne}$ **(Drude)**

$$C_{electron} = \frac{1}{3}\pi^2 g(\varepsilon) k_B^2 T = \frac{1}{2}\frac{\pi^2 n k_B^2 T}{\varepsilon_F}$$

$$Q = \frac{\Delta V}{\Delta T} = -1.42\left(\frac{k_B T}{\varepsilon_F}\right)\times 10^{-4}\, V/K$$

Homework today (due on Sept. 23, 2010)

1. Problem 3a in page 55 (Ashcroft/Mermin)

Problems with Free Electron Model

- Free electron approximation
(ignore ions)

- Independent electron approximation
(ignore electron-electron interaction)

- Relaxation-time approximation

In reality:

- R_H depends on H and T
- $\rho(H) \neq \rho(0)$
- $\frac{\kappa}{\sigma T}$ depends on T
- σ depends on T

....

Free Electron Model

electrons only

Need to consider lattice (ion) contribution

Prof. Cyrill Slezak