Condensed Matter Physics I

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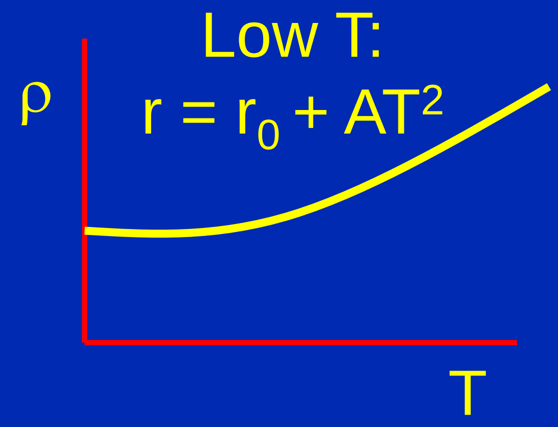
Previously

- Heat conductivity
- Intro second quantization

Today

- Metals

What is a metal ?



<u>Electrical conductivity:</u>

$\rho_{300\,K} \sim 1.7$ (Cu) - 153 $\mu\Omega\cdot$cm (Pu)

<u>Thermal conductivity:</u>

Cu: $K_{300\,K} \sim 3.9$ W/Kcm   Pu: $K_{300\,K} \sim 0.049$ W/Kcm

Wiedemann-Franz: $K/\sigma = \alpha\, T$

Quartz: $K \sim 0.13$ W/Kcm   NaCl: $K \sim 0.27$ W/Kcm

<u>Reflectivity:</u>

Highly reflecting upto plasma-frequency

$\omega < \omega_p \qquad \omega_p^2 = 4\,\pi\, n\, e^2 / m$

FREE ELECTRON MODEL

FEM, overview

- Free electron model (Drude, Sommerfeld theory)
- Statistics and density of states
- Heat capacity
- Electrical conductivity (Ohm's law)
- Influence of a magnetic field (Hall effect)
- Thermal conductivity and Wiedemann-Franz law

Electrons in metals

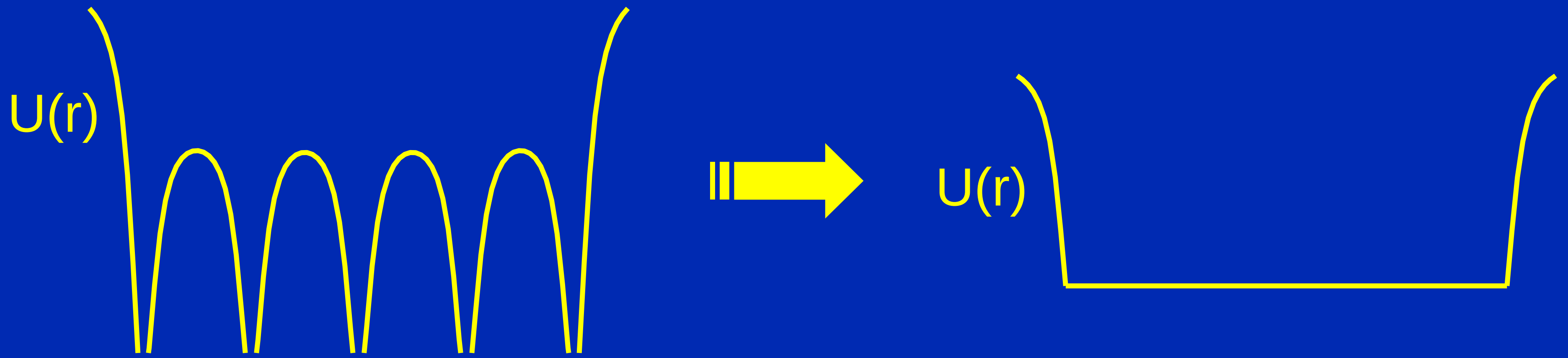
P. Drude: 1900 kinetic gas theory of electrons, classical
Maxwell-Boltzmann distribution
independent electrons
free electrons
scattering from ion cores (relaxation time approx.)

A. Sommerfeld: 1928
Fermi-Dirac statistics

F. Bloch's theorem: 1928
Bloch electrons

L.D. Landau: 1957
Interacting electrons (Fermi liquid theory)

Free electron approximation



Neglect periodic potential & scattering (Pauli)

Reasonable for “simple metals” (Alkali Li,Na,K,Cs,Rb)

Eigenstates & energies

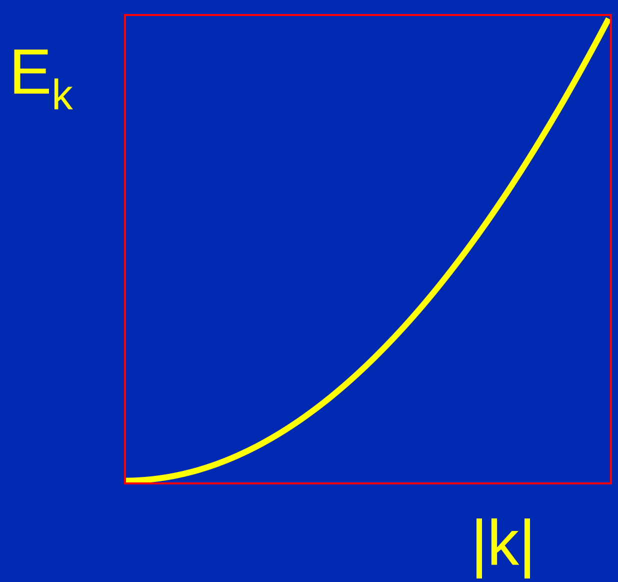
$$\left(\frac{-\hbar^2}{2m}\nabla^2 + \cancel{U}\right)\psi = i\hbar\frac{d\psi}{dt}$$

$$\psi_{\vec{k}}(r,t) = \psi_0 e^{i(\omega t - \vec{k}\cdot\vec{r})}$$

$$E_{\vec{k}} = \frac{\hbar^2}{2m}\left|\vec{k}\right|^2$$

$$\vec{k} = 2\pi(n_x/L_x, n_y/L_y, n_z/L_z)$$

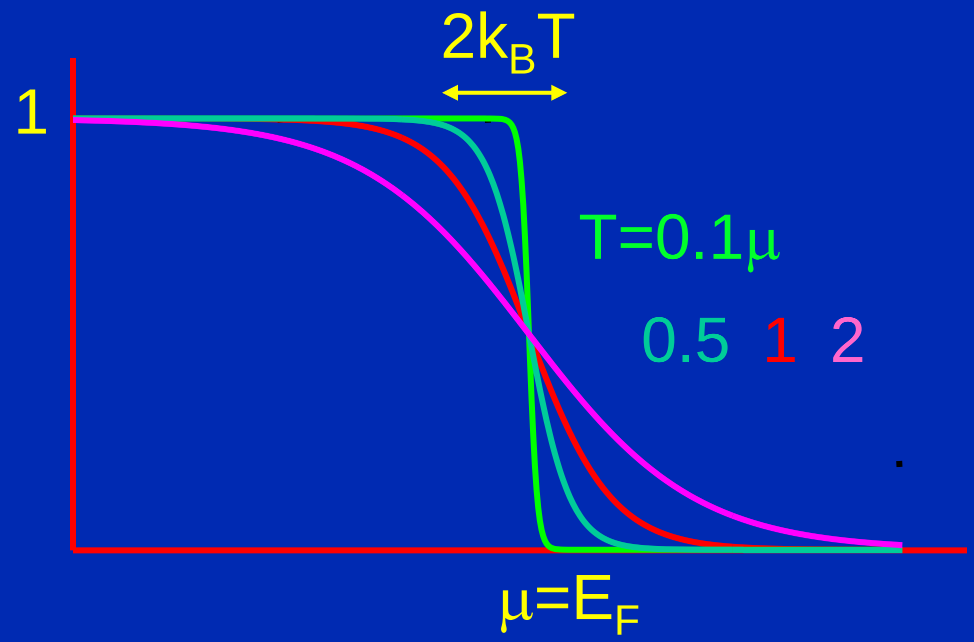
$$D_d(k) \propto L^d \cdot k^{d-1}$$



Statistics & DOS

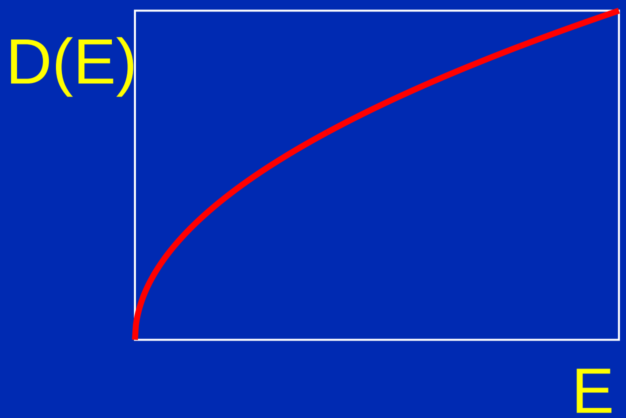
Fermi-Dirac statistics:

$$f_{FD}(E) = \frac{1}{e^{\frac{E-\mu}{kT}} + 1}$$

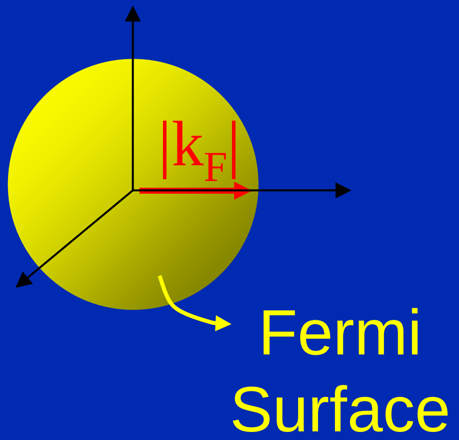


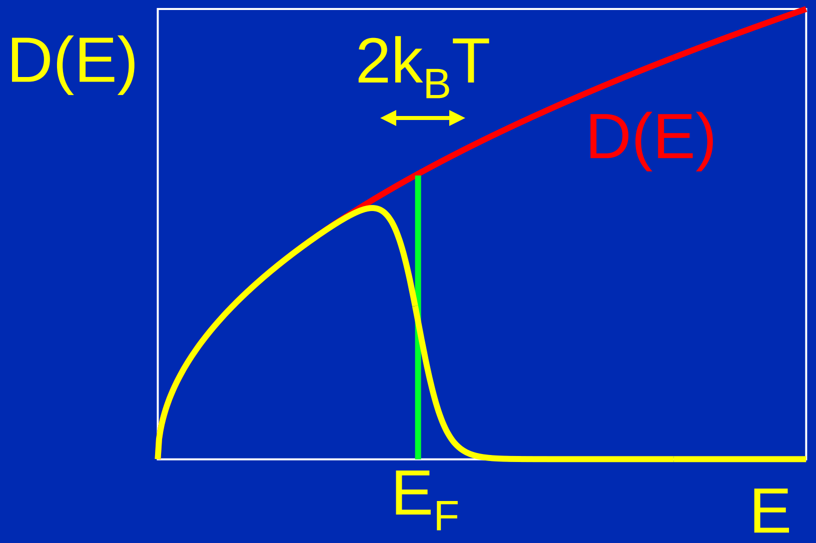
Density of states:

$$D(E) = 2 \cdot D(k) \cdot \frac{dk}{dE} = \frac{Vm}{\pi^2 \hbar^3} \sqrt{2mE}$$



Occupation of states





Free electron gas parameters

$$N = \int_0^\infty D(E)\cdot f_{FD}(E)\, dE$$

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

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

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

$$E_F = \frac{1}{2} m v_F{}^2$$

$$v_F = \frac{\hbar k_F}{m}$$

$$T_F = E_F / k_B$$

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

$$D(E_F) = \frac{Vm}{\pi^2\hbar^3}\sqrt{2mE_F}$$

$$D(E_F) = \frac{V}{\pi\hbar^2}\cdot\left(\frac{3}{\pi}n\right)^{1/3} m$$

Sodium

Na $1s^2 2s^2 2p^6 3s$ = [Ne]3s

r_{ion} = 0.98 Å d_{nn} = 1.83 Å

$$n = 2.65 \cdot 10^{22}\ \text{cm}^{-3}$$

$$E_F = 3.23\ \text{eV}$$

$$k_F = 2.65 \cdot 10^{22}\ \text{cm}^{-1}$$

$$v_F = 1.07 \cdot 10^{8}\ \text{cm/s}$$ → Non relativistic

$$T_F = 3.75 \cdot 10^{4}\ \text{K}$$ → Degenerate quantum gas

E_F hardly depends on T

So far

- Free electrons, i.e. no periodic potential
- Independent electrons, i.e. no e^- - e^- interactions
- Relaxation time approximation (scattering time τ)
- Classical statistics (Drude)
- Fermions (Sommerfeld)

→
- Density of states (1D, 2D, 3D)
  - Fermi energy (E_F, k_F v_F, T_F)

t.b.d.

- Sommerfeld
  - Compressibility
  - Heat capacity
  - Conductivity, Hall effect, 1D conduction
  - Thermal conductivity, Wiedemann-Franz law
- FAILURES of the free electron models
- Including the periodic potential the e^- live in.

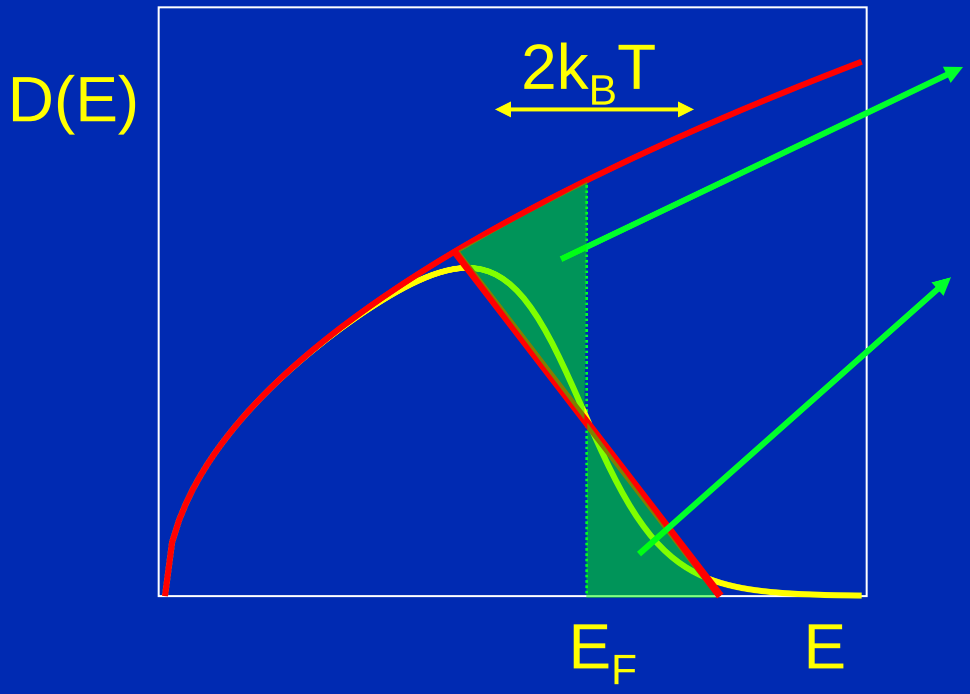
Compressibility

$$B = 1/K = -V\, dP/dV = V\, d^2U/dV^2$$

	$B_{f.e.}$ (Gpa)	B_{obs} (Gpa)
Li	24	12
Na	9	6.5
K	3	3
Rb	2	2
Cs	1.5	1.5
Cu	64	134
Ag	35	100
Al	228	76

Heat capacity: Quick&Dirty

$$C_{el} = \frac{dU_{el}}{dT} = \frac{d}{dT}\int_0^\infty E \cdot D(E) \cdot f_{FD}(E,T)\, dE$$



$$-\frac{1}{2}k_B T \times \frac{1}{2} D(E_F) \cdot (E_F - \frac{k_B T}{2})$$

$$+\frac{1}{2}k_B T \times \frac{1}{2} D(E_F) \cdot (E_F + \frac{k_B T}{2})$$

$$\Delta U = \frac{k_B^{\,2} T^2}{2} D(E_F)$$

$$C_{el} = k_B^{\,2} D(E_F) \cdot T$$

$$\Rightarrow \mathbf{C_{el} \propto T}$$

Heat capacity

Electronic contribution

$$C_{el} = \frac{1}{3}\pi^2 \cdot D(E_F) \cdot k_B{}^2 T = \frac{1}{2}\pi^2 N k_B \frac{T}{T_F} << \frac{3}{2} N k_B$$

Electrons + lattice (low T): $C_v = \gamma \cdot T + A \cdot T^3$

$$\gamma = \frac{1}{3}\pi^2 \cdot D(E_F) \cdot k_B{}^2 \propto m$$

$$\frac{\gamma_{exp}}{\gamma_{f.e.}} \neq 1 \quad \Rightarrow \quad m^*_{th} \equiv \frac{\gamma_{exp}}{\gamma_{f.e.}} m_0$$

↘

Periodic potential (band mass)
e-p interaction (polarons)
e-e interaction

Heat capacity: Na & K

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Heat Capacity of Sodium and Potassium at Temperatures below 1°K

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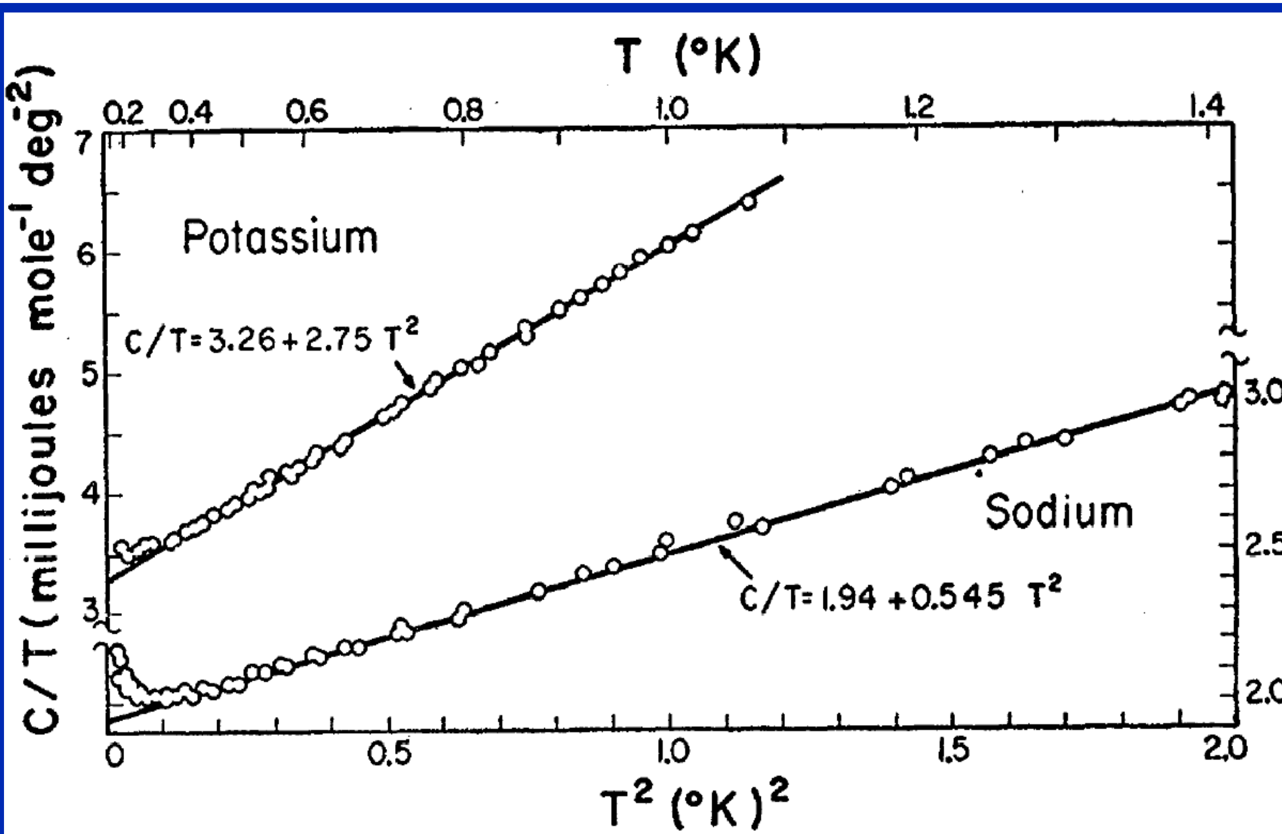
(Received December 17, 1959)



$C = \gamma T + AT^3$

$m_{th} = 1.25\ m_0$

γ & thermal effective mass

Element	Free e^- γ	Expt. γ	m_{th}^*/m_0
	10^{-4} cal/mol K^2		
Li	1.8	4.2	2.3
Na	2.6	3.5	1.3
K	4.0	4.7	1.2
Cu	1.2	1.6	1.3
Be	1.2	0.5	0.42
Fe	1.5	12	8
Mn	1.5	40	27
Bi	4.3	0.2	0.047