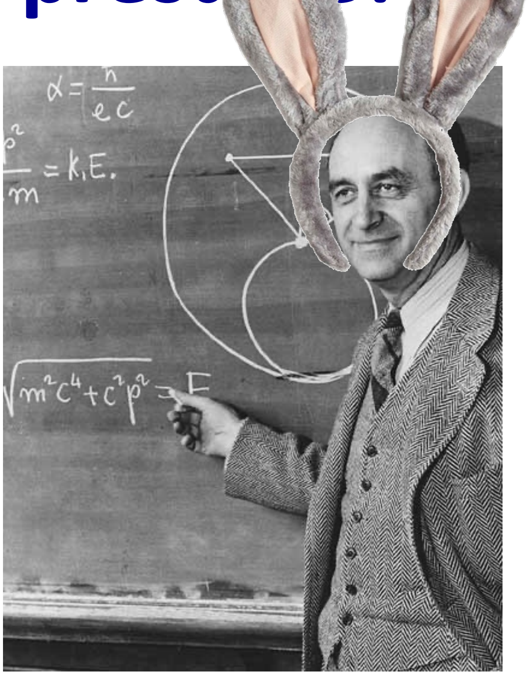
MSE 423 Fall 2024 – Week 11

"Dr. Fermi, I presume?"



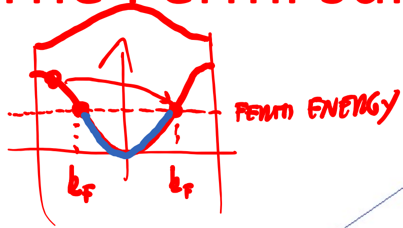
Last week

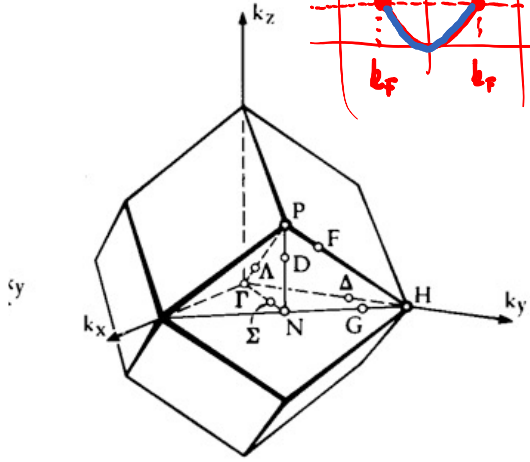
$\frac{2\pi}{a}$ ... $1 \cdot \frac{3}{4}\frac{3}{4}0$ $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Γ, X, K, L

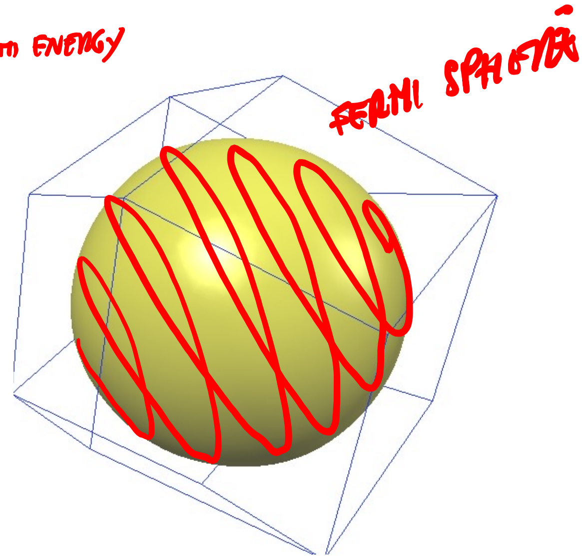
- Diamond/zincblend ~~lattices~~ CRYSTALS and their BZs – special points and paths
- Band structures and ARPES
- Diamond and zincblende semiconductors
- Free electron gas and silicon; silicon vs lead; silicon vs germanium vs GaAs (also, OSSCAR).ORG
- Valence and conduction band minima/maxima – discussion in Si/Ge/GaAs along a path or in 3D BZ
- Band gaps (values), and direct/indirect
- Perovskites, coinage metals, localized vs delocalized

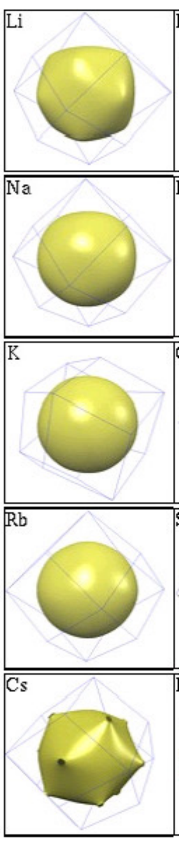
The Fermi surface





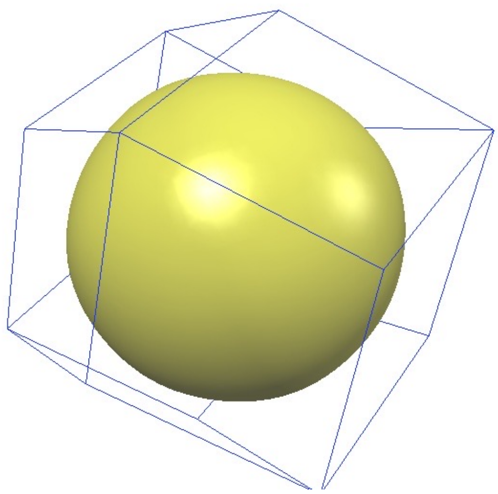
BODY CENTERED CUBIC



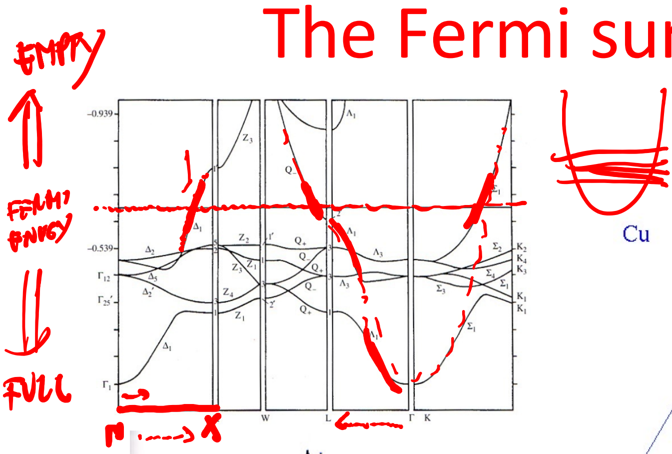


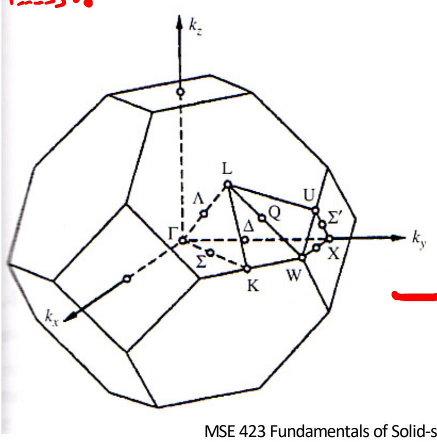
The Fermi surface

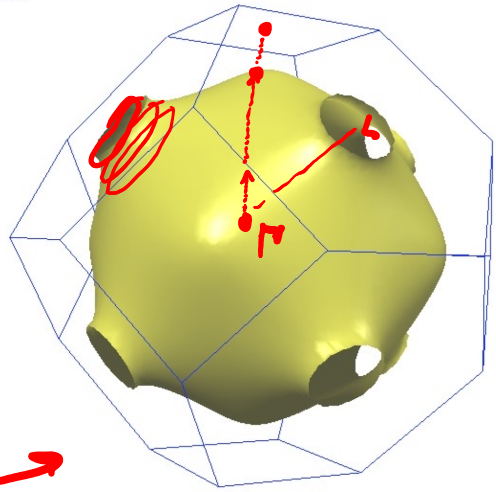
K



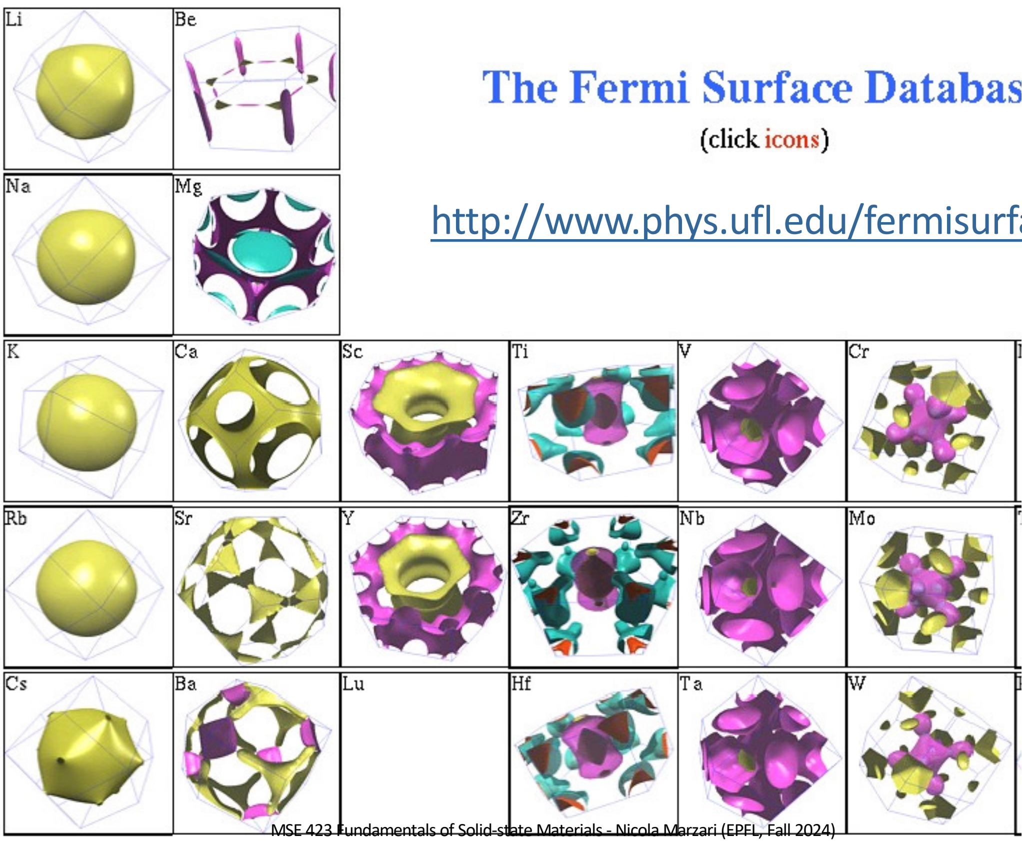
The Fermi surface (fcc)







D (VRML) Fermi Surface Database http://www.phys.ufl.e



The Fermi Surface Databas

(click icons)

http://www.phys.ufl.edu/fermisurface/

Group velocity, effective mass

FOR A FREE EL., $\mathcal{E} = \frac{\hbar^2 k^2}{2m}$

$\mathcal{E}_n(\vec{k})$

FOR AN EL. IN A SOLID → $\mathcal{E} = \mathcal{E}_n(\vec{k})$

$$m_n^* = \hbar^2 \left(\frac{\partial^2 \mathcal{E}_n(\vec{k})}{\partial k^2} \right)^{-1} = \hbar^2 \left(\frac{\hbar^2}{2m} 2 \right)^{-1} = \hbar^2 \frac{m}{\hbar^2} = m$$

GROUP VELOCITY

$$\vec{v}_n = \frac{1}{\hbar} \vec{\nabla} \mathcal{E}_n(\vec{k}) = \frac{1}{\hbar} \frac{\hbar^2}{2m} 2k = \frac{\hbar \vec{k}}{m} = \frac{\vec{p}}{m} = \vec{v}$$

The independent-electron gas

- Hamiltonian

$$\hat{H} = -\frac{1}{2} \sum_i \nabla_i^2$$

- Eigenvalues and eigenfunctions

$$\psi(\vec{r}) = A e^{i \vec{k} \cdot \vec{r}} \cancel{u_k(\vec{r})}$$

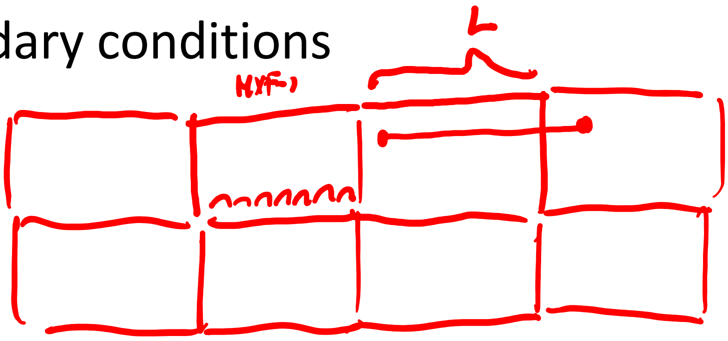
CONSTANT

$$\int_{\text{PRIMITIVE CELL}} \|\psi\|^2 = 1 \Rightarrow \int_V \|A\|^2 = 1 \Rightarrow A = \frac{1}{\sqrt{V}}$$

The independent-electron gas

BORN - VON KÁRMÁN

- BvK boundary conditions



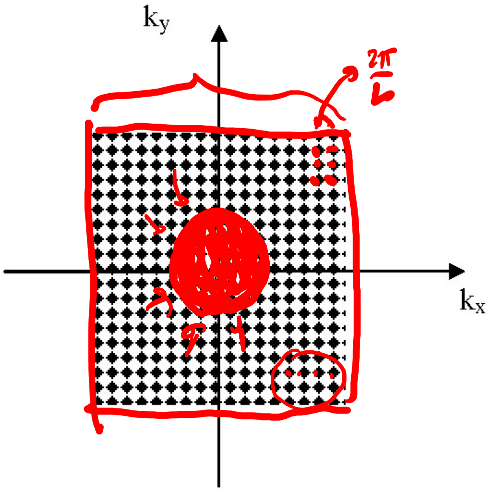
$$e^{ikL}=1$$

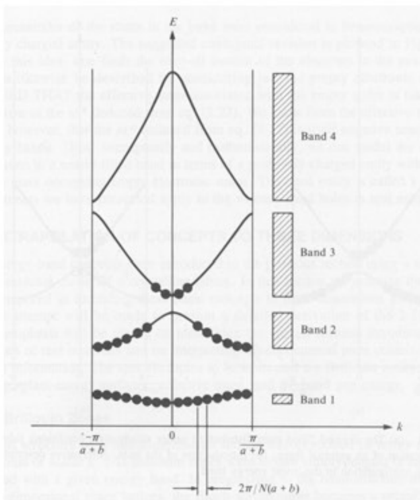
$$k=\frac{2\pi}{L}n$$

$$\psi_k(\vec{r})=\psi_k(x,y,z)=$$
$$=\psi_k(x+L,y,z)=$$
$$=e^{ik\cdot L}\,\psi_k(x,y,z)$$

The independent-electron gas

- Counting the states





The independent-electron gas

- Particle density $= \dfrac{\# EL}{V} = \dfrac{2\left(\frac{4}{3}\pi k_F^3\right)/\left(\frac{2\pi}{L}\right)^3}{L^3} =$

$$= \frac{2 \cdot \frac{4}{3}\pi k_F^3 \left(\frac{8\pi^3}{L^3}\right)^{-1}}{L^3} = \frac{8}{3}\pi k_F^3 \cdot \frac{\cancel{L^3}}{8\pi^3} \cdot \frac{1}{\cancel{L^3}} =$$

$$= \frac{k_F^3}{3\pi^2}$$

$$\frac{2\hbar^2}{2m}\frac{1}{(2\pi)^3}4\pi \cdot \frac{k_F^5}{5} = \frac{\hbar^2}{10 m \pi^2} k^5_{FERMI}$$

The independent-electron gas

- Energy density $= \dfrac{E}{V} = \dfrac{2\sum_{k \in OCCUPIED} \frac{\hbar^2}{2m}k^2}{L^3} =$

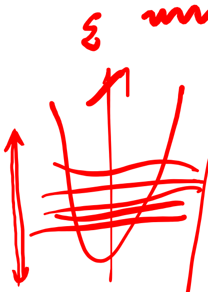
$$= \frac{2\int_{OCCUPIED} d^3k \, \frac{\hbar^2}{2m}k^2 \Big/ \left(\frac{2\pi}{L}\right)^3}{L^3}$$

VOLUME OF A STATE

$$= \frac{2\underbrace{\int_0^\pi d\vartheta \int_0^{2\pi} d\varphi}\int_0^{k_F} dk\, k^2 \frac{\hbar^2}{2m}k^2 \cdot \frac{\cancel{L^3}}{(2\pi)^3}}{\cancel{L^3}} = \frac{2\hbar^2}{2m}\frac{1}{(2\pi)^3}4\pi\int_0^{k_F} dk\, k^4$$

Density of states (for any solid)

ELECTRONS



$\int dk^3 \left(\frac{L}{2\pi}\right)^3$

L^3

$$g_n(\varepsilon) = 2\int \frac{1}{8\pi^3}\, \delta(\varepsilon - \varepsilon_n(\vec{k}))\, d\vec{k}$$

$$g_n(\varepsilon) = 2\int \frac{1}{8\pi^3} \frac{1}{\left|\nabla \varepsilon_n(\vec{k})\right|}\, dS$$

Massive vs massless bands

Dimensions	d=1	d=2	d=3
Massless (E≈k)	const	E	E^2
Massive (E≈k^2)	1/sqrt(E)	const	sqrt(E)

$\varepsilon = k^l$

$$g_n(\varepsilon) = 2\int \frac{1}{8\pi^3} \frac{1}{\left|\nabla \varepsilon_n(\vec{k})\right|}\, dS \Rightarrow k^{-(l-1)}$$

$\varepsilon^{1/l} = k$

- S goes as k^{d-1}, where d is the dimensionality
- $\frac{1}{\left|\nabla \varepsilon(\vec{k})\right|}$ for a band that has k^l dispersions goes as $k^{-(l-1)}$,
- the integral goes as k^{d-l} $\Rightarrow (\varepsilon^{1/l})^{d-l}$
- energy is proportional to k^l, the integral goes as $\varepsilon^{(d-l)/l}$

Statistics of classical and quantum particles

DISTINGUISHABLE

	1	2	3
1	AB		
2		AB	
3			AB
4	A	B	
5	A		B
6		A	B
7	B	A	
8	B		A
9		B	A

INDISTING.

	1	2	3
1	AA		
2		AA	
3			AA
4	A	A	
5	A		A
6		A	A

THEY CAN BE IN THE SAME STATE $\Rightarrow$ BOSON

	1	2	3
1	A	A	
2	A		A
3		A	A

PAULI EXCLUSION

$\Rightarrow$ FERMION

Probability and partition function

$$Z = \sum_{s} e^{-\beta E_s}$$

$$\beta = \frac{1}{k_B T}$$

$$\sum_s P_s = 1 \qquad P_s = \frac{e^{-\beta E_s}}{Z}$$

HELMHOLTZ FREE ENERGY $F = E - TS = F[T,V]$

$$F = -\frac{1}{\beta} \ln Z$$

THERMODYNAMIC

STATISTICAL MECHANICS

Chemical potential

$$\frac{dF}{dN} = \mu$$

Fermi-Dirac distribution

$$F(E) = \frac{1}{1+\exp\left(\frac{E-\mu}{kT}\right)} \qquad \frac{1}{1+\exp\left(\frac{E-\mu}{kT}\right)}$$

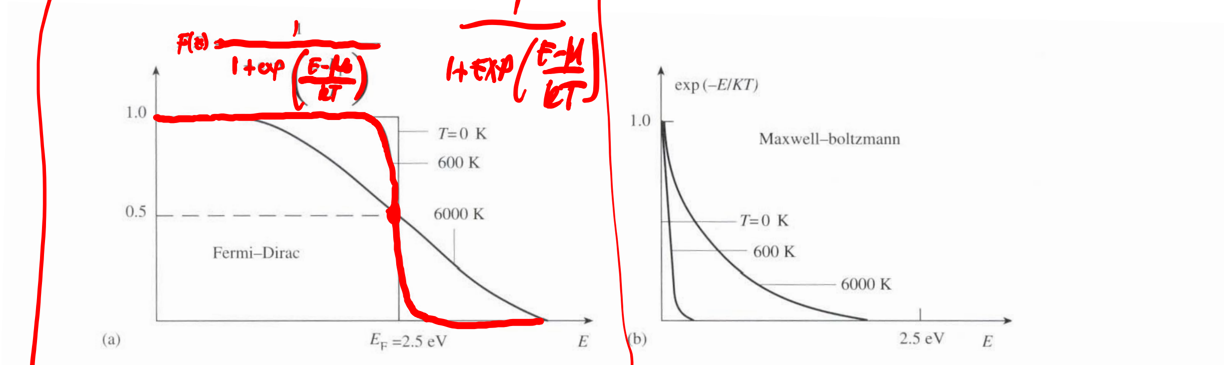


Fig. 6.1
(a) The Fermi–Dirac distribution function for a Fermi energy of 2.5 eV and for temperatures of 0 K, 600 K, and 6000 K.
(b) The classical Maxwell–Boltzmann distribution function of energies for the same temperatures.