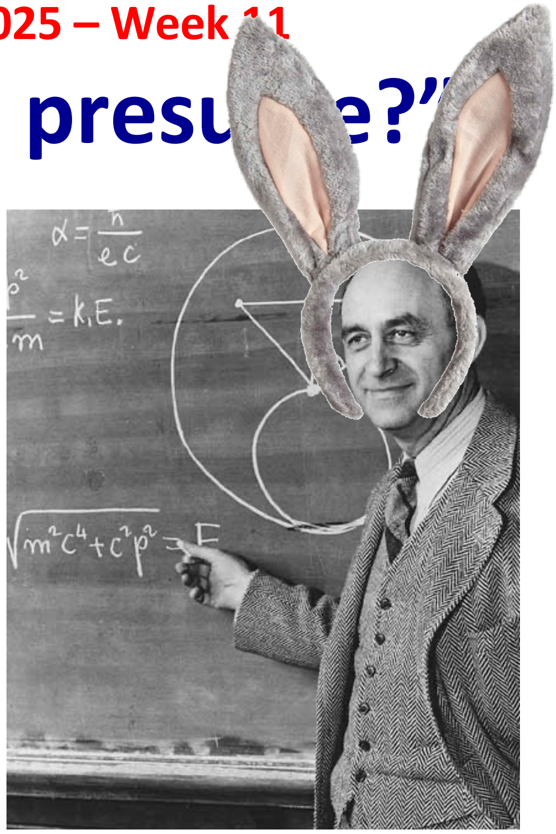
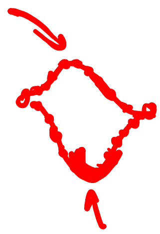
"Dr. Fermi, I presume?"



Last week

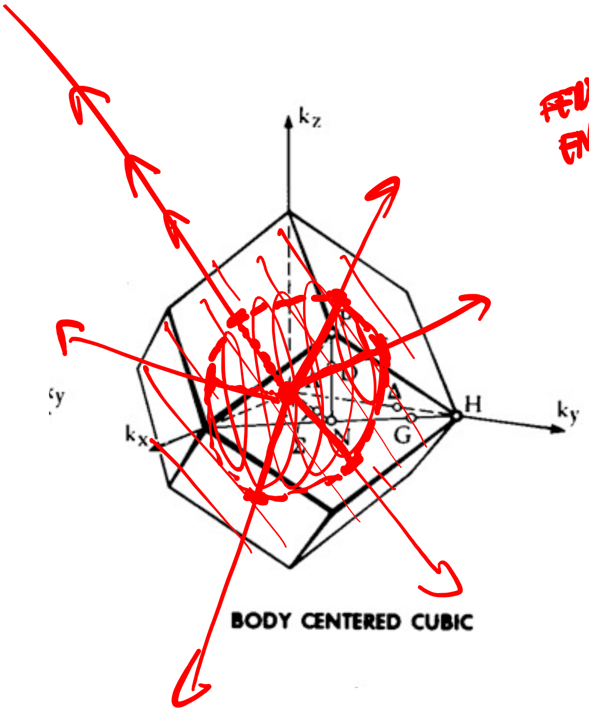
FERMI ENERGY

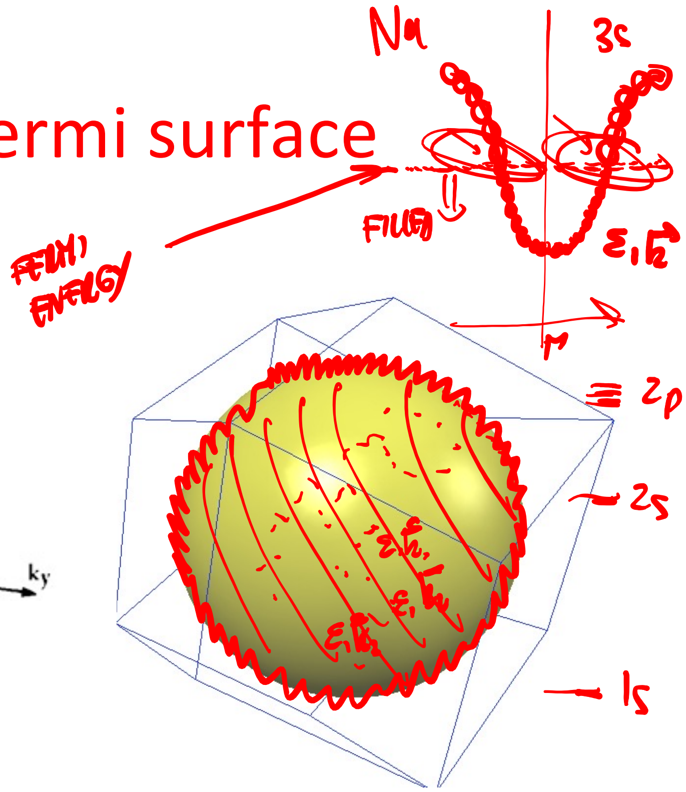
- Diamond/zincblend lattices and their BZs – special points and paths
- Band structures and ARPES ε_{nk}
- Diamond and zincblende semiconductors
- Free electron gas and silicon; silicon vs lead; silicon vs germanium vs GaAs (also, OSSCAR)
- Valence and conduction band minima/maxima – discussion in Si/Ge/GaAs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



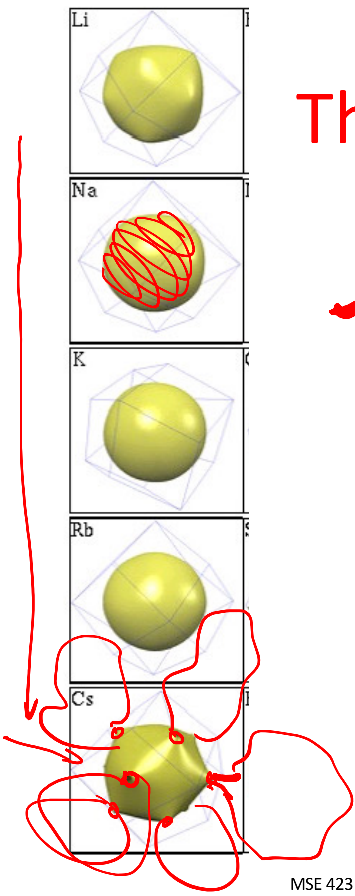
MSE 423 Fundamentals of Solid-state Materials - Nicola Marzari (EPFL, Fall 2025)

The Fermi surface

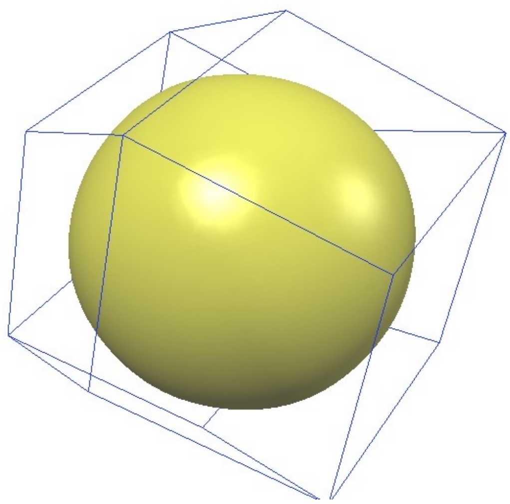




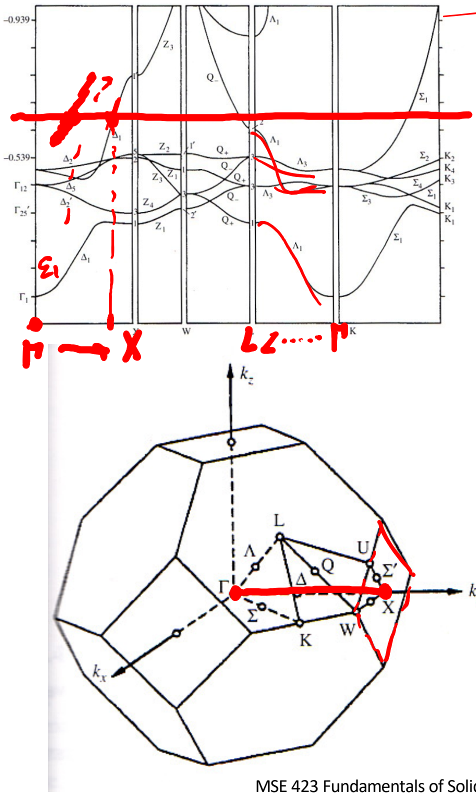
The Fermi surface

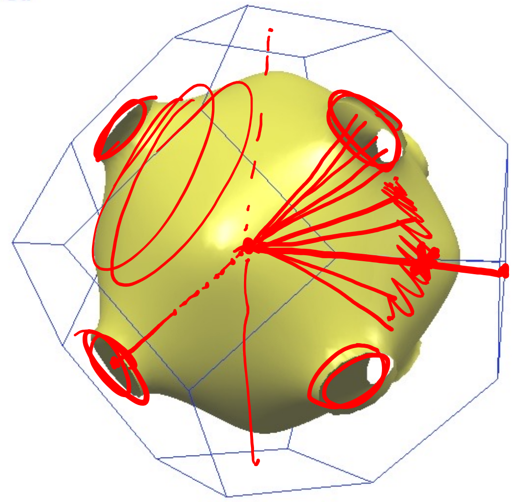


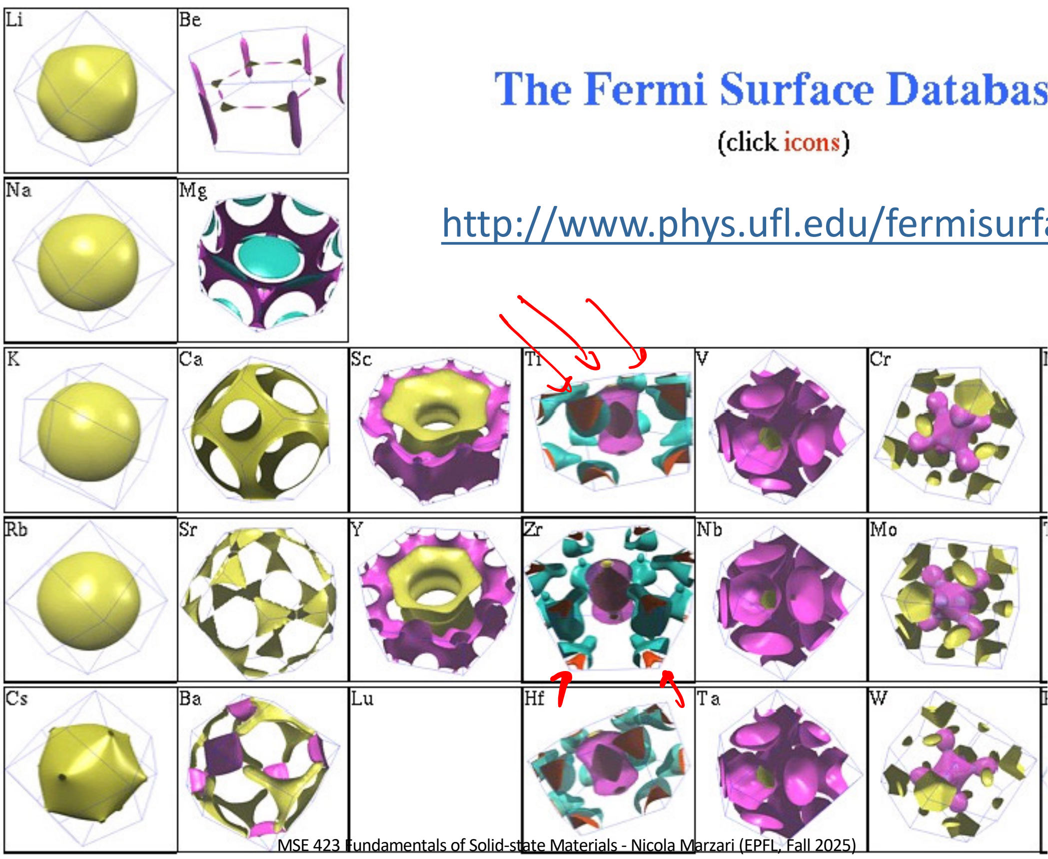
K



The Fermi surface (fcc)







The Fermi Surface Databas

(click icons)

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

The independent-electron gas

- Hamiltonian

$$\hat{H} = -\frac{1}{2}\sum_i \vec{\nabla}_i^2$$

- Eigenvalues and eigenfunctions

$$\psi(\vec{r}) = A\, e^{i\vec{k}\cdot\vec{r}}\, \cancel{u_{\vec{k}}(\vec{r})} = 1$$

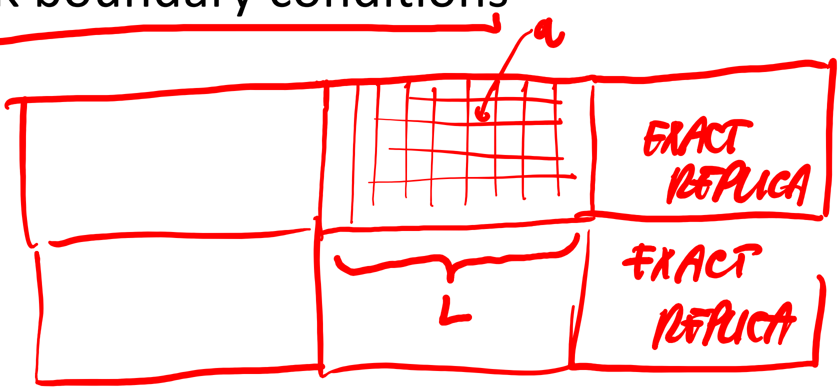
$$\int_{\text{PRIMITIVE CELL}} \|\psi\|^2 = 1 \qquad \int_{\text{PRIMITIVE CELL}} \|A\|^2 = 1 \Rightarrow \|A\|^2 = \frac{1}{V}$$

$$A = \frac{1}{\sqrt{V}}$$

The independent-electron gas

→ BORN - VAN KÁRMÁN

- BvK boundary conditions



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

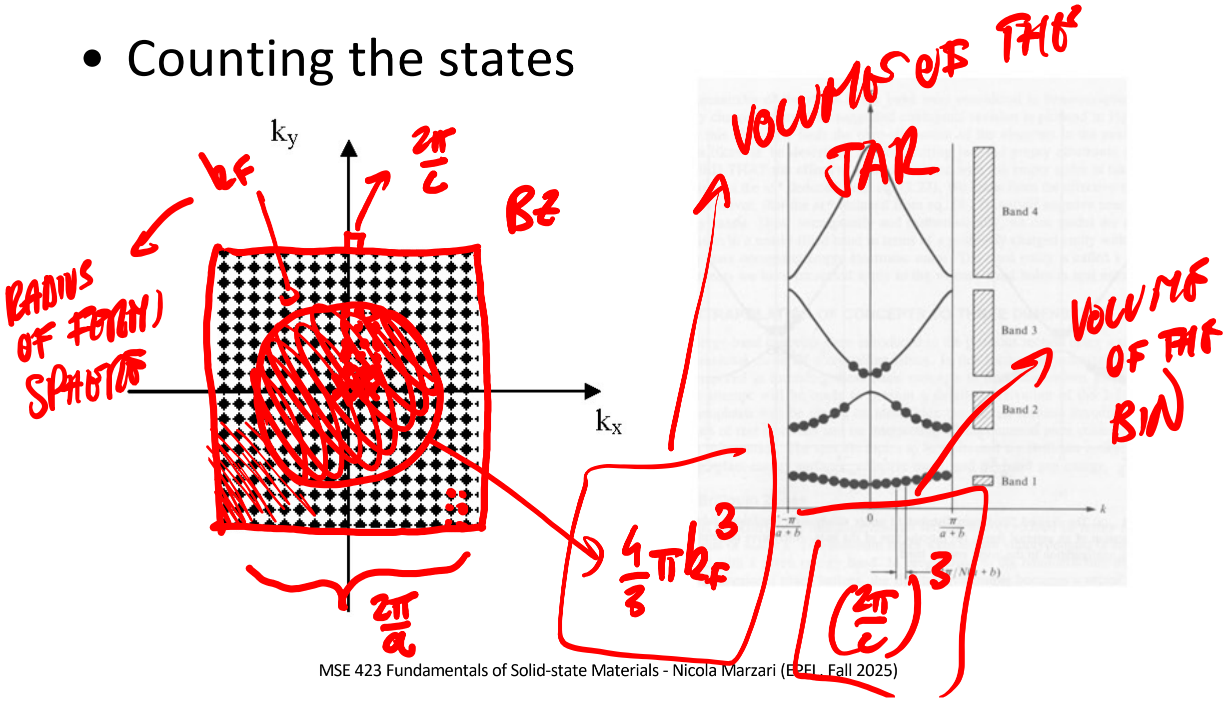
$$e^{i\vec{k}\cdot L} = 1$$

$$\psi_{\vec{k}}(x,y,z) = \psi_{\vec{k}}(x+L,y,z) \quad (1) \text{ FROM BvK}$$

$$\overset{!}{=} e^{i\vec{k}\cdot L}\, \psi_{\vec{k}}(x,y,z) \quad (2) \text{ FROM BLOCH TH.}$$

The independent-electron gas

- Counting the states



The independent-electron gas

DUE TO SPIN DEGENERACY

- Particle density $= \frac{\#\text{ ELECTRONS}}{\text{VOLUME}} = \frac{2\left(\frac{4}{3}\pi k_F^3\right)/\left(\frac{2\pi}{L}\right)^3}{L^3}$

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

$$= \frac{8\pi}{3\cancel{8}\pi^3} k_F^3 = \frac{1}{3\pi^2} k_F^3$$

The independent-electron gas

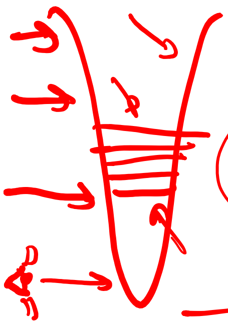
- Energy density $= \dfrac{E}{V} = \dfrac{2\sum_{\vec{k}\,\mathrm{occ}} \frac{\hbar^2}{2m}k^2}{L^3} = \dfrac{8\pi}{8\pi^3}\dfrac{\hbar^2}{2m}\int_0^{k_F} k^4 = \dfrac{1}{\pi^2}\dfrac{\hbar^2}{2m}\dfrac{k_F^5}{5}$

$$= \frac{2\int d^3k \,\frac{\hbar^2}{2m}k^2 / \left(\frac{2\pi}{L}\right)^3}{L^3} = \frac{2\int_0^{\pi} d\vartheta \int_0^{2\pi} d\varphi \int_0^{k_F} dk\; k^2\, \frac{\hbar^2}{2m}k^2 / \left(\frac{2\pi}{L}\right)^3}{L^3} = \frac{2\frac{\hbar^2}{2m}\, 4\pi \int_0^{k_F} k^4 \cdot \left(\frac{L}{2\pi}\right)^3}{L^3}$$

OCCUPIED STATES

VOLUME OF THE BZ

Density of states (for any solid)



$$\frac{2\int d\vec{k} \left(\frac{L}{2\pi}\right)^3 \delta(\varepsilon - \varepsilon_n(\vec{k}))}{L^3}$$

#STATES / V

VOLUME INTEGRAL

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

SURFACE INTEGRAL

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

SURFACE ON THE FERMI SURFACE

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)

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

$\varepsilon \sim k^l$

$\varepsilon^{\frac{1}{l}} \sim k$

- $\boxed{\text{S goes as } k^{d-1}}$, where d is the dimensionality

l=2 quadratic l=1 linear

- $\frac{1}{|\nabla \varepsilon(\vec{k})|}$ for a band that has $\boxed{k^l}$ dispersions goes as $\boxed{k^{-(l-1)}}$,

$k^{d-1} \cdot k^{-l+1}$

$k^{d-l} = (\varepsilon^{\frac{1}{l}})^{d-l} = \varepsilon^{\frac{d-l}{l}}$

- the integral goes as $\boxed{k^{d-l}}$
- energy is proportional to k^l, the integral goes as $\boxed{\varepsilon^{(d-l)/l}}$

Statistics of classical and quantum particles

	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

ALICE & BOB ARE CLASS DISTINGUISHABLE

BOSONS

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

ALICE & BOB ARE INDISTINGUISHABLE

QUANTUM

FERMIONS

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

PAULI PRINCIPLES.

$G[P,T,N] \Rightarrow \Omega[P,T,\mu] = G + \mu N$

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

$\Uparrow$

Probability and partition function

$G[P,T] = F + PV$

$\Uparrow$

$F[V,T]$

$$Z = \sum_s e^{-\beta E_s}$$

EXPLORES
EXPONENTIAL

$$p_s = \frac{e^{-\beta E_s}}{Z} \longrightarrow \sum_s p_s = 1$$

$F[V,T]$ $\quad$ $[V,S]$

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

Chemical potential

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

Fermi-Dirac distribution

$$FD(E,T) = \frac{1}{1+\exp\left(\frac{E-\mu}{k_B T}\right)}$$

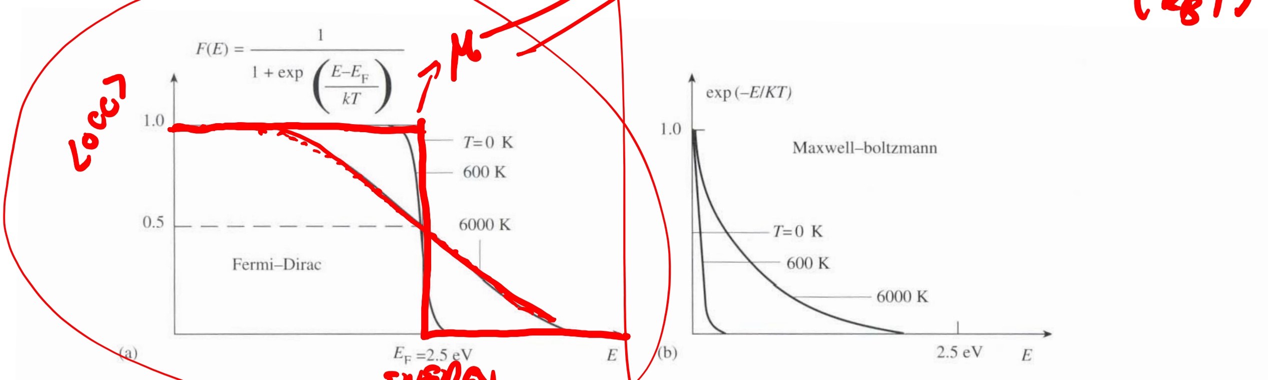


Fig. 6.1
(a) The Fermi–Dirac distribution function for a Fermi energy of 2.5 eV and for temperatures of 0 K, 600 K, and 6000 K.
(b) The classical Maxwell–Boltzmann distribution function of energies for the same temperatures.