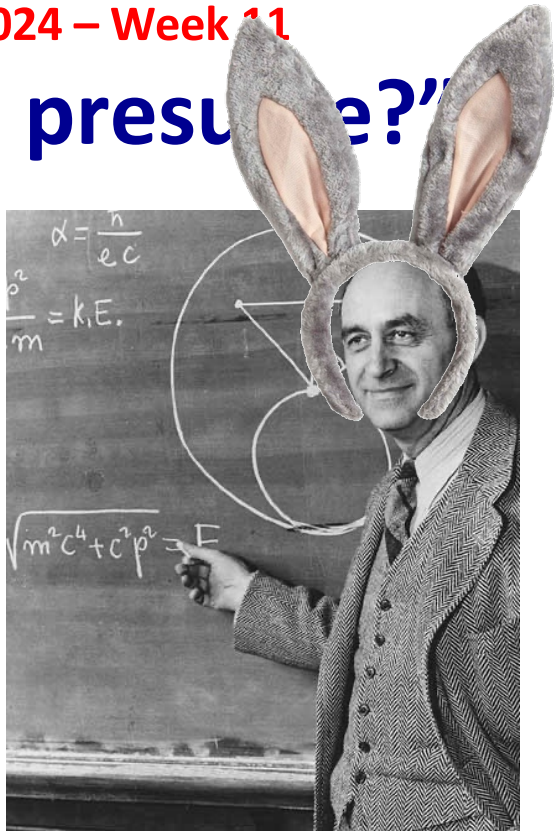
MSE 423 Fall 2024 – Week 11

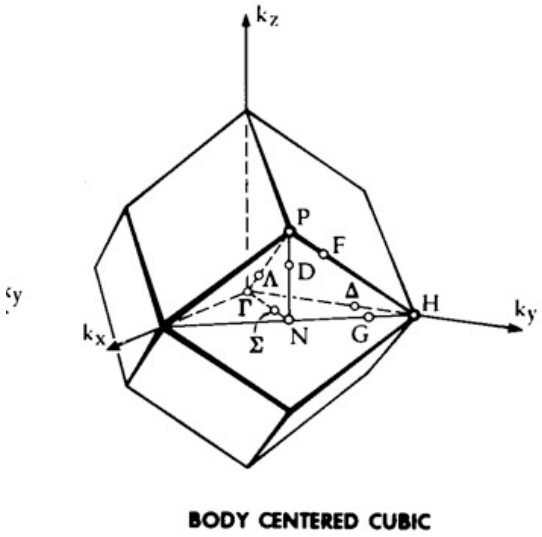
"Dr. Fermi, I presume?"



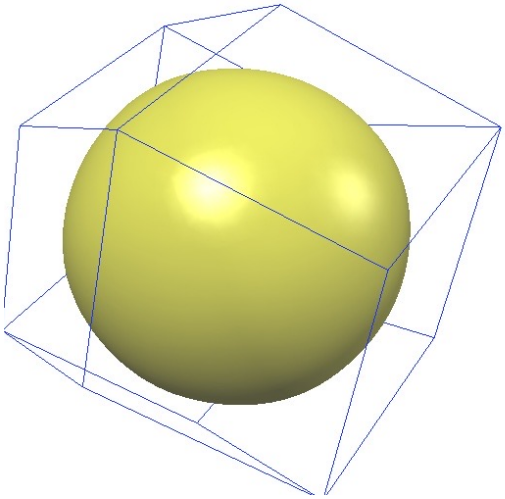
Last week

- Diamond/zincblend lattices 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)
- 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

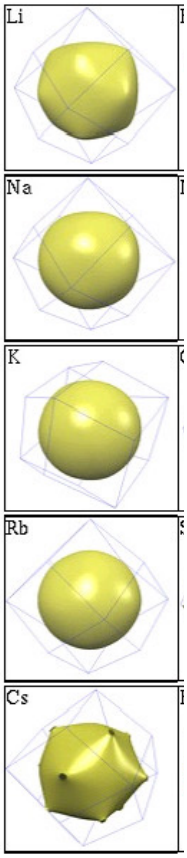
The Fermi surface



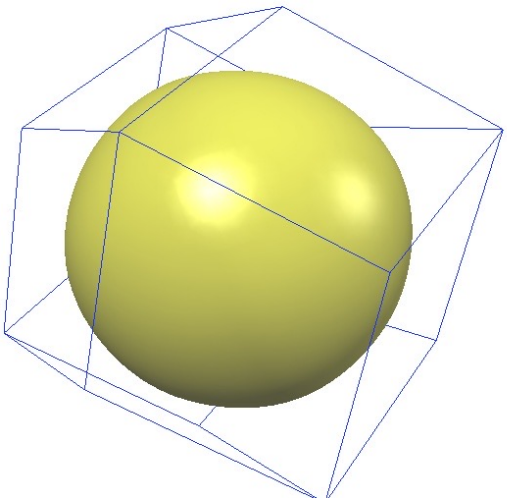
BODY CENTERED CUBIC



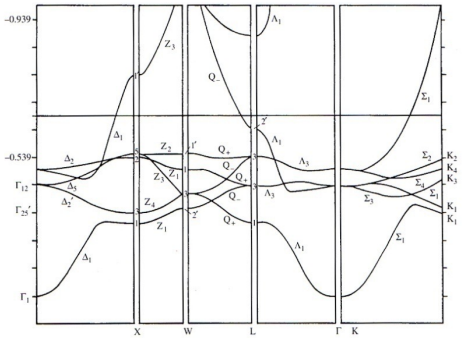
The Fermi surface

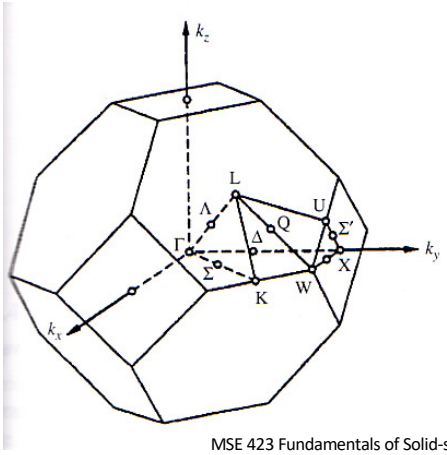


K

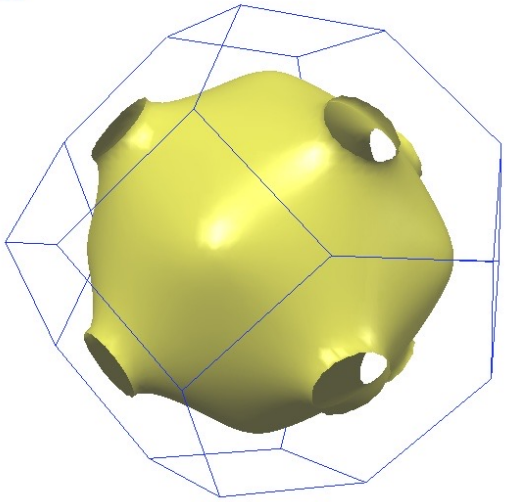


The Fermi surface (fcc)

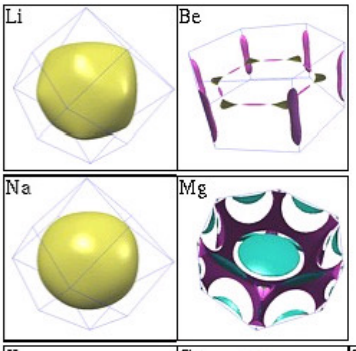




Cu



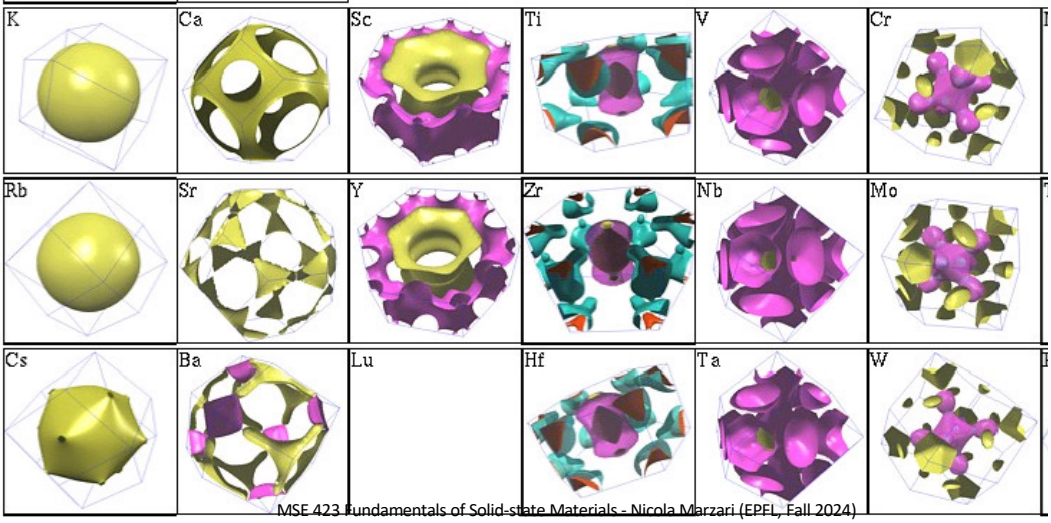
D (VRML) Fermi Surface Database http://www.phys.ufl.e



The Fermi Surface Databas

(click icons)

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



Group velocity, effective mass

The independent-electron gas

- Hamiltonian

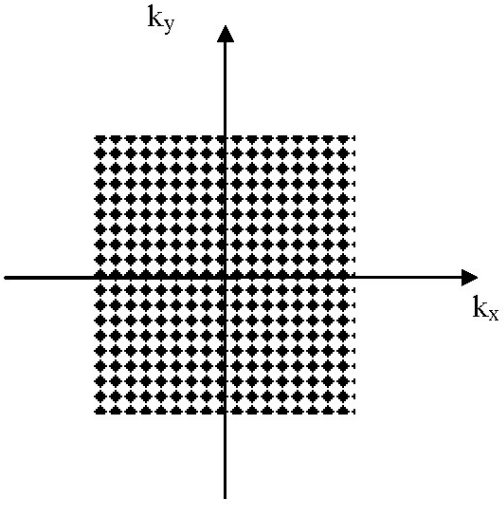
- Eigenvalues and eigenfunctions

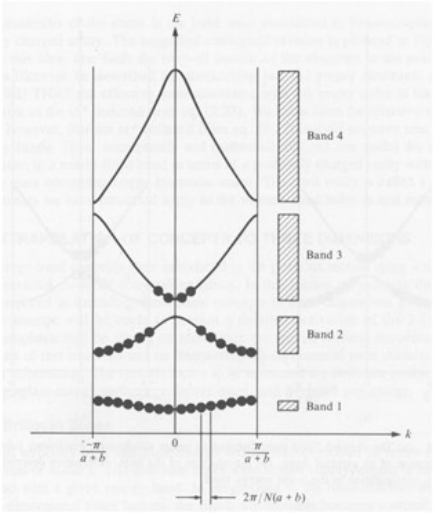
The independent-electron gas

- BvK boundary conditions

The independent-electron gas

- Counting the states





The independent-electron gas

- Particle density

The independent-electron gas

- Energy density

Density of states (for any solid)

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

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

Massive vs massless bands

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

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

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

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

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

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

Probability and partition function

Chemical potential

Fermi-Dirac distribution

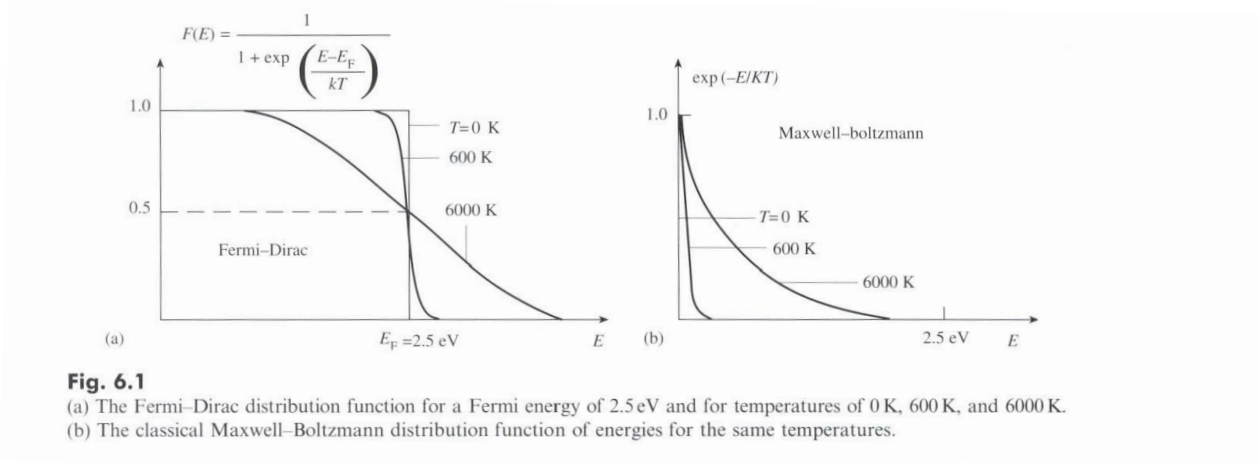


Fig. 6.1
(a) The Fermi–Dirac distribution function for a Fermi energy of 2.5 eV and for temperatures of 0 K, 600 K, and 6000 K.
(b) The classical Maxwell–Boltzmann distribution function of energies for the same temperatures.

Tight-binding (LCAO for solids)

- Hamiltonian $\hat{H} = \hat{H}_{at} + \Delta\hat{U}\left(\vec{r}\right)$

Tight-binding (LCAO for solids)

- Bloch eigenstates of an ATOMIC CRYSTAL

$$\Psi_{n\vec{k}}\left(\vec{r}\right) = \sum_{\vec{R}} \exp\left(i\vec{k}\bullet\vec{R}\right)\varphi_n\left(\vec{r}-\vec{R}\right)$$

Tight-binding (LCAO for solids)

- Bloch eigenstates of a REAL CRYSTAL

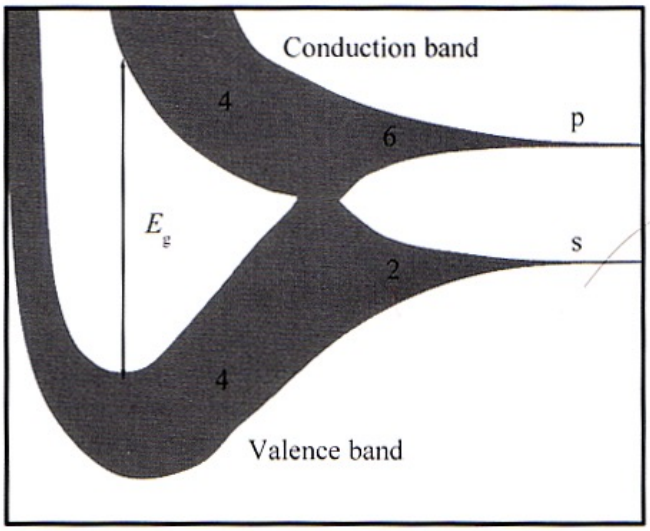
$$\Psi_{n\vec{k}}\left(\vec{r}\right)=\sum_{\vec{R}}\exp\left(i\vec{k}\bullet\vec{R}\right)\phi\left(\vec{r}-\vec{R}\right)$$

$$\phi\left(\vec{r}\right)=\sum_{n}b_{n}\varphi_{n}\left(\vec{r}\right)$$

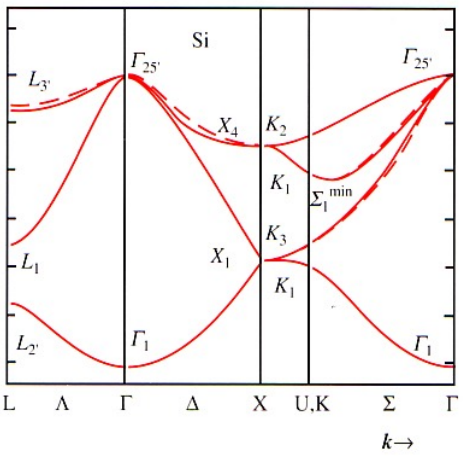
From levels to bands

$$\varepsilon\left(\vec{k}\right)=E_{m}-\beta-\sum_{\substack{nearest\\neighb.}}\gamma\left(\vec{R}\right)\cos\left(\vec{k}\bullet\vec{r}\right)$$

From levels to bands



How many bands in silicon ?



Tight-binding vs. empirical psp

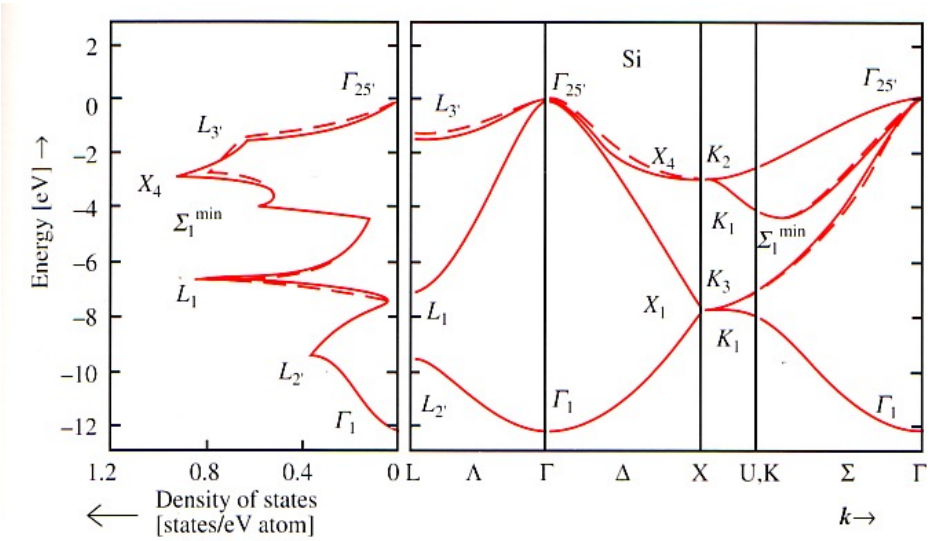


Fig. 2.24. The valence band structure and density of states (see Sect. 4.3.1 for definition) of Si calculated by the tight-binding method (*broken curves*) and by the empirical pseudopotential method (*solid lines*) [2.19]

Tight-binding vs. empirical psp

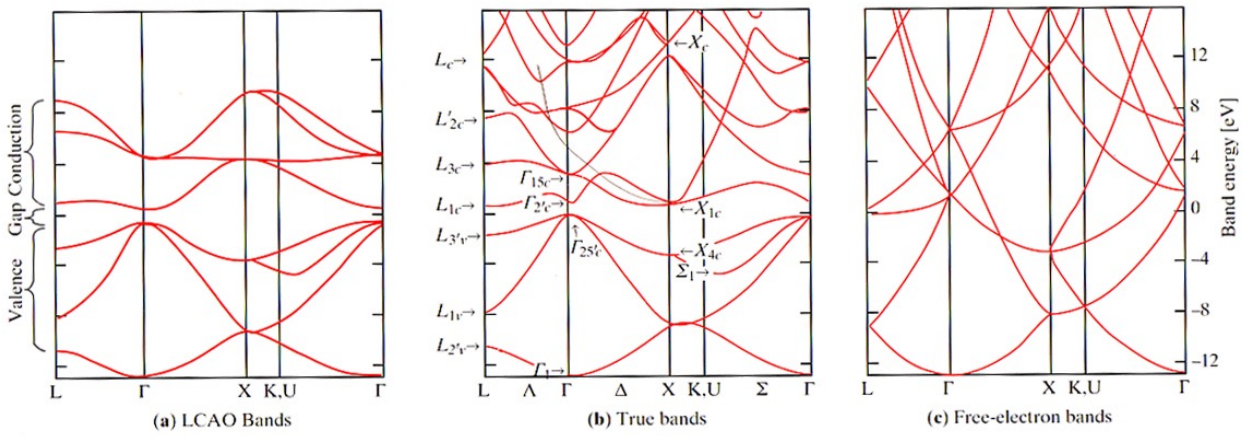


Fig. 2.25. A comparison between the band structure of Ge calculated by **(a)** the tight-binding method, **(b)** the empirical pseudopotential method, and **(c)** the nearly free electron model [Ref. 2.18, p. 79]