Notes:

- **Exam next week!** Wednesday in class (22nd)
- Covers: Through ch. 10 (tight binding material, today).
- **Alternative time**: may work by general agreement:
  - Wednesday evening or Thursday evening, e.g. 7:30-9:30.
  - Could also start earlier on weds (or Friday) and go through regular class time, only works if no one has 9:10 class.
  - Thursday 23rd at colloquium time (no talk next week).

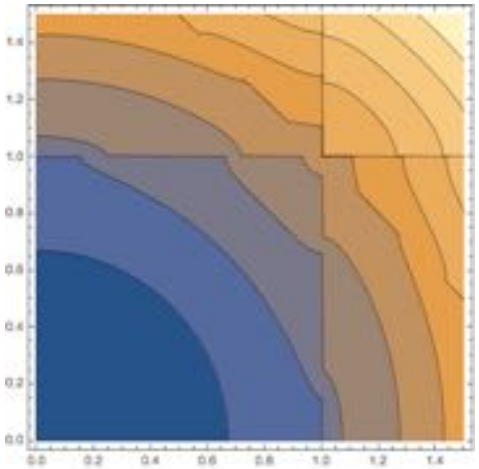
(Plan to decide by end of this week)

Nearly-Free electron bands

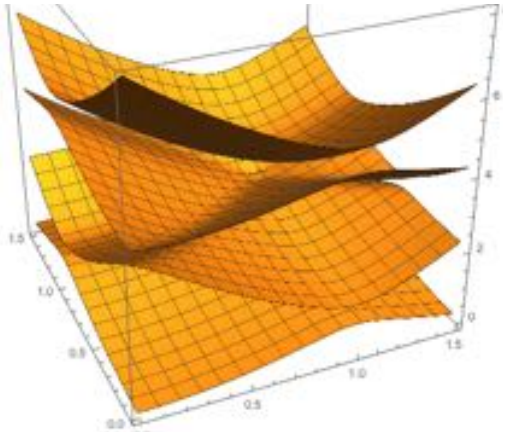
in 2D:

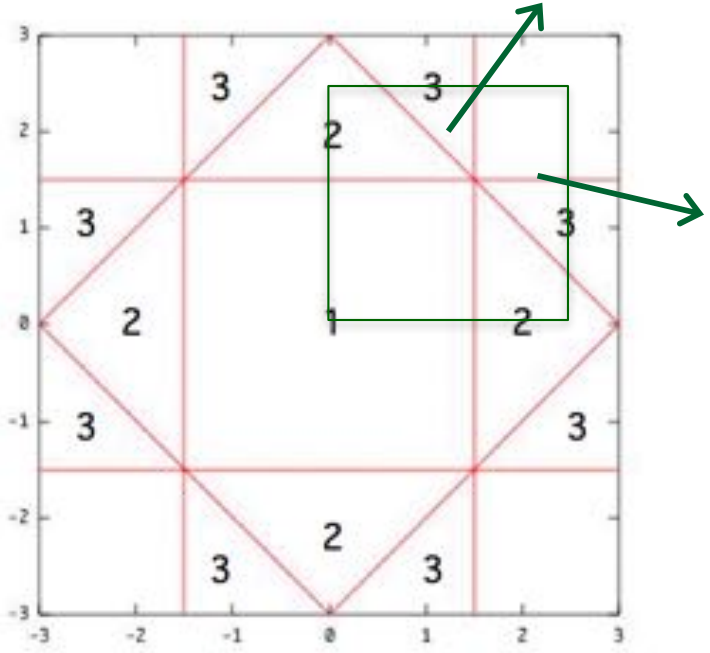
$$\begin{pmatrix} kx^2 + ky^2 & u1 & u1 & u3 \\ u1 & ky^2 + (kx - 2\pi)^2 & u3 & u1 \\ u1 & u3 & kx^2 + (ky - 2\pi)^2 & u1 \\ u3 & u1 & u1 & (kx - 2\pi)^2 + (ky - 2\pi)^2 \end{pmatrix}$$

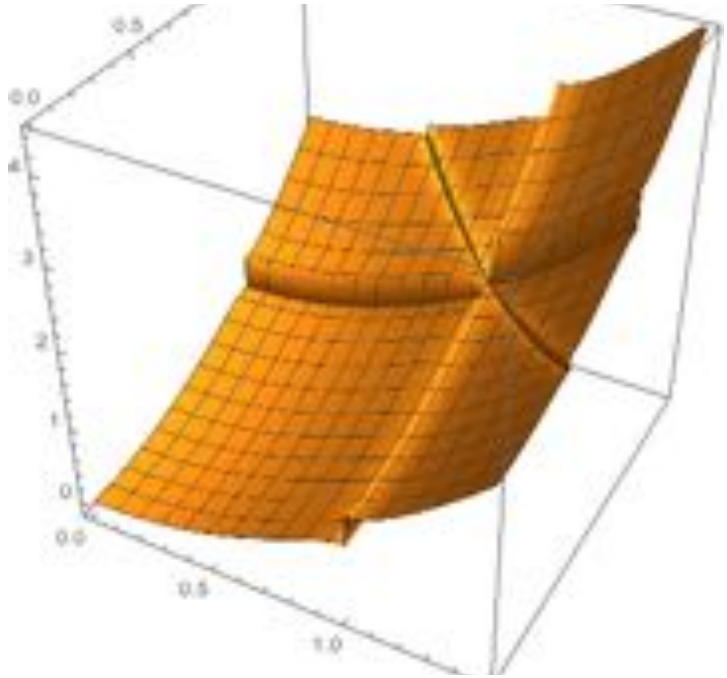
Contours of increasing energy, 1st-3rd zones



eigenvalues







3D bands: FCC Lattice

Note, band-structures typically plotted along representative symmetry lines.

8/cell
(Si or GaAs)

3/cell
(Aluminum)

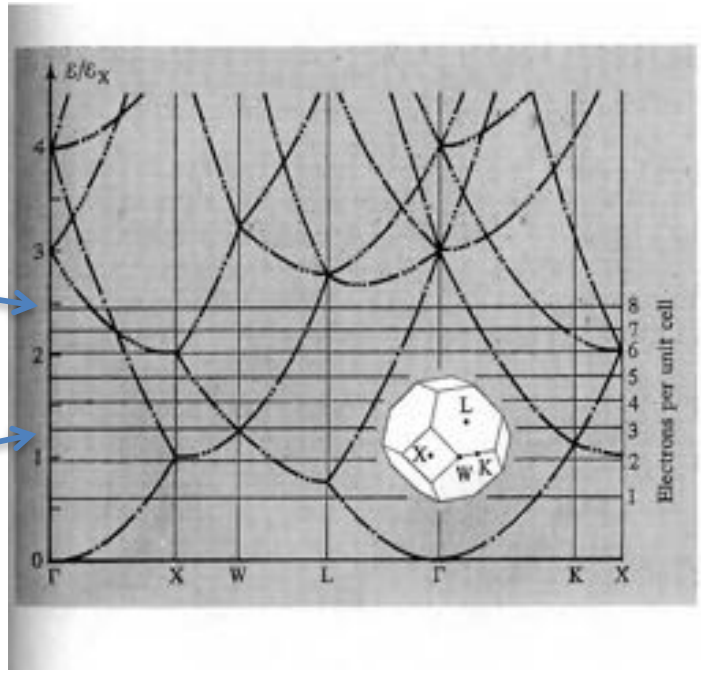


Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = 0)$, K, L, W, and X. ε_X is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

Ashcroft & Mermin picture: Free electron energies.

FCC examples

8/cell
(Si or GaAs)

3/cell
(Aluminum)

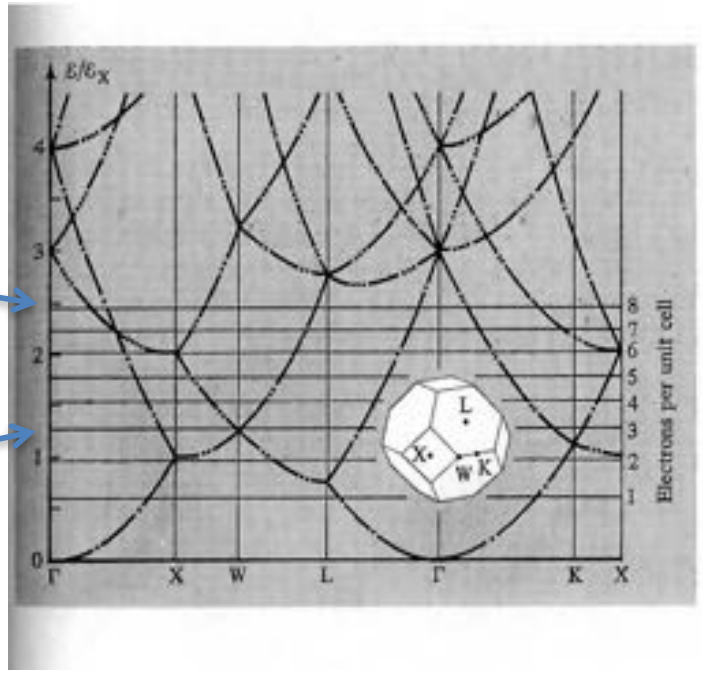
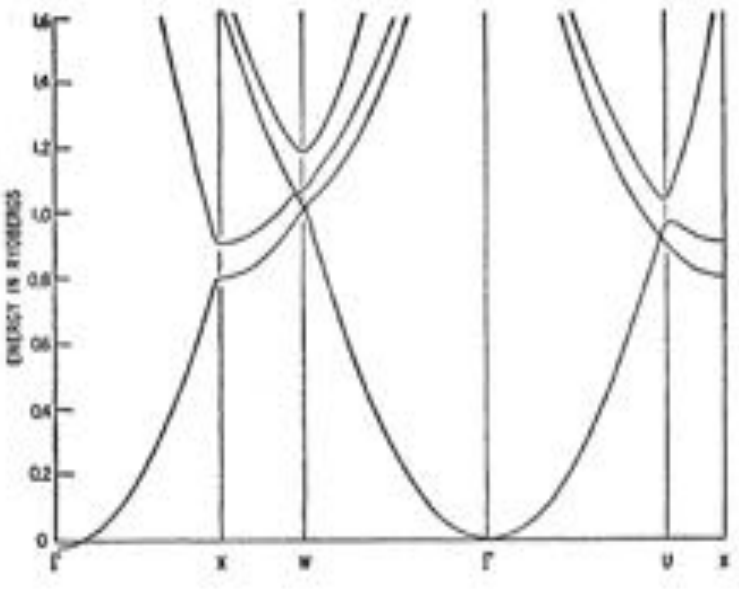
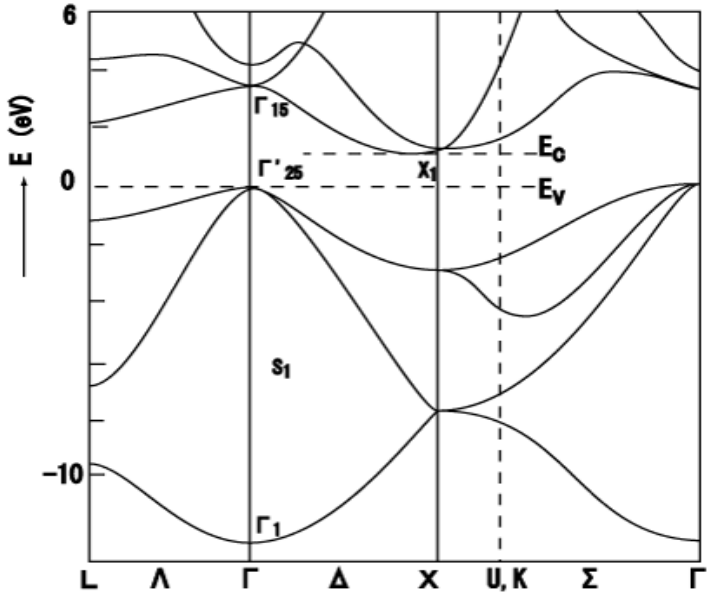


Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points Γ(k = 0), K, L, W, and X. $\mathcal{E}_x$ is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)



Aluminum

[W. A. Harrison, Phys. Rev. 118, 1182 (1960)]



Silicon

[LDA calculation, http://th.fhi-berlin.mpg.de/th/fhi98md/doc /main/node19.html]

FCC examples

8/cell
(Si or GaAs)

3/cell
(Aluminum)

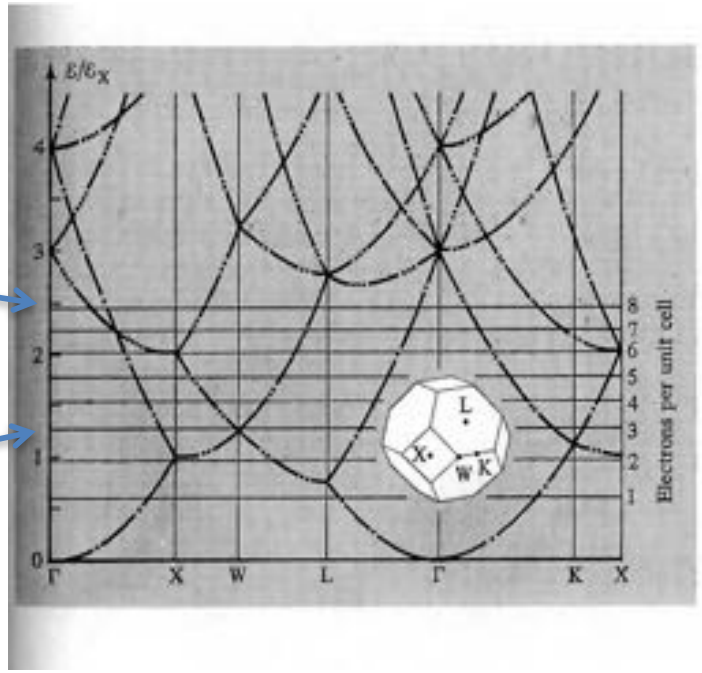
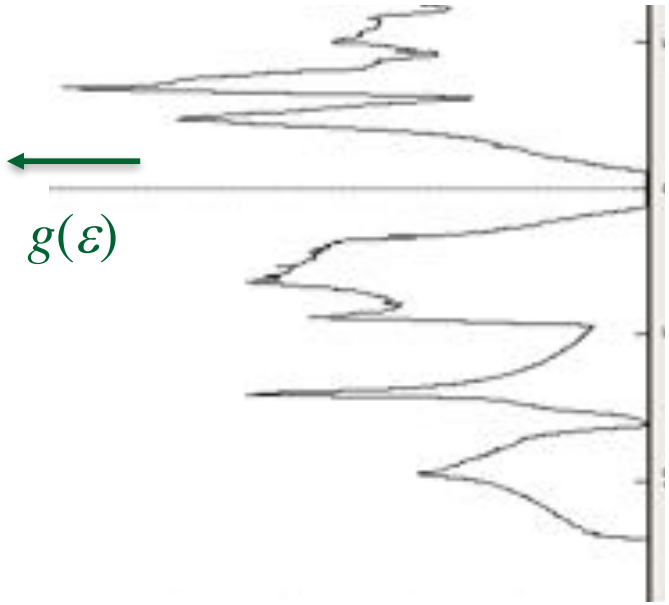
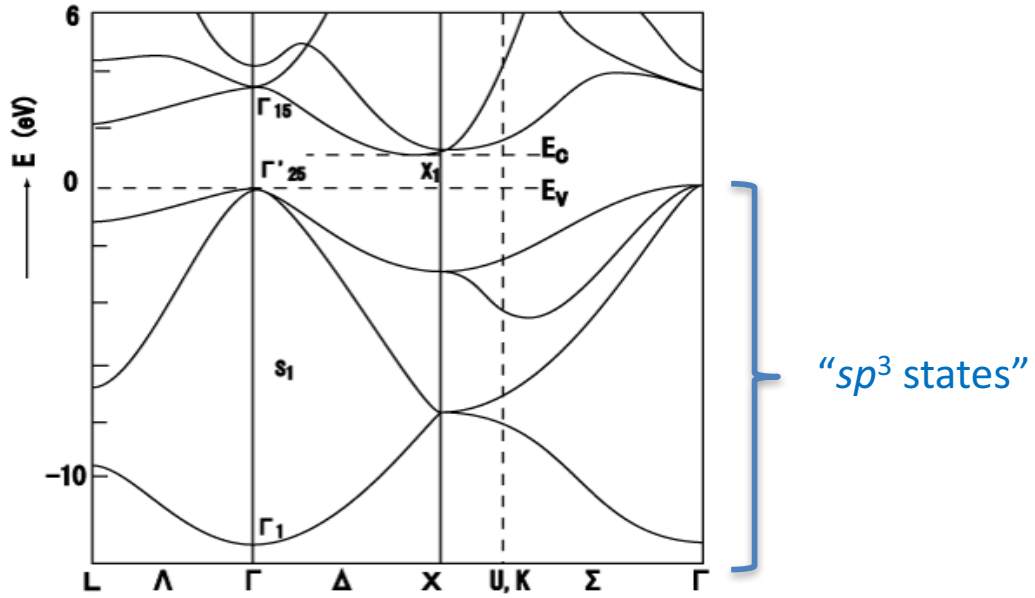


Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points Γ(k = 0), K, L, W, and X. ε_x is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)





"sp^3 states"

Silicon Density of States

[quantumwise.com metaGGA calculation]

Silicon

[LDA calculation, http://th.fhi-berlin.mpg.de/th/fhi98md/doc /main/node19.html]

Tight binding model

Reading: ch. 10

$$\psi_{\vec{k}}(r) = \frac{1}{\sqrt{N}} \sum_R \varphi_n(r-R) e^{i\vec{k}\cdot\vec{R}}$$

Bloch state with localized states as basis set

- LCAO (or "Hückel") model; basis = atomic orbitals.
- More general tight binding: mutually orthogonal local orbitals; "Wannier functions" complete orthonormal set.
- May converge more quickly than plane waves for insulators & more localized systems.

$$H\psi_{\vec{k}}(r) \approx \frac{E_n}{\sqrt{N}} \sum_R \varphi_n(r-R) e^{i\vec{k}\cdot\vec{R}}$$

1st order: E_n energy of isolated state

$$\varepsilon_{\vec{k}} = \left\langle \psi_{\vec{k}} \middle| H \middle| \psi_{\vec{k}} \right\rangle \qquad \varepsilon_{\vec{k}} = E_n + \frac{1}{N} \sum_R \sum_i \left\{ \left\langle \varphi(r-R) \middle| H \middle| \varphi(r-R_i) \right\rangle + c.c. \right\} e^{i\vec{k}\cdot(\vec{R}-\vec{R}_i)}$$

$$\Rightarrow \quad \varepsilon_{\vec{k}} = E_n - \gamma \sum_i e^{i\vec{k}\cdot(\delta\vec{R}_i)}$$

Assume only nearest neighbor matrix elements, all equal to $-\gamma$

$$E_n - 2\gamma\cos(ka)$$

simple 1D case