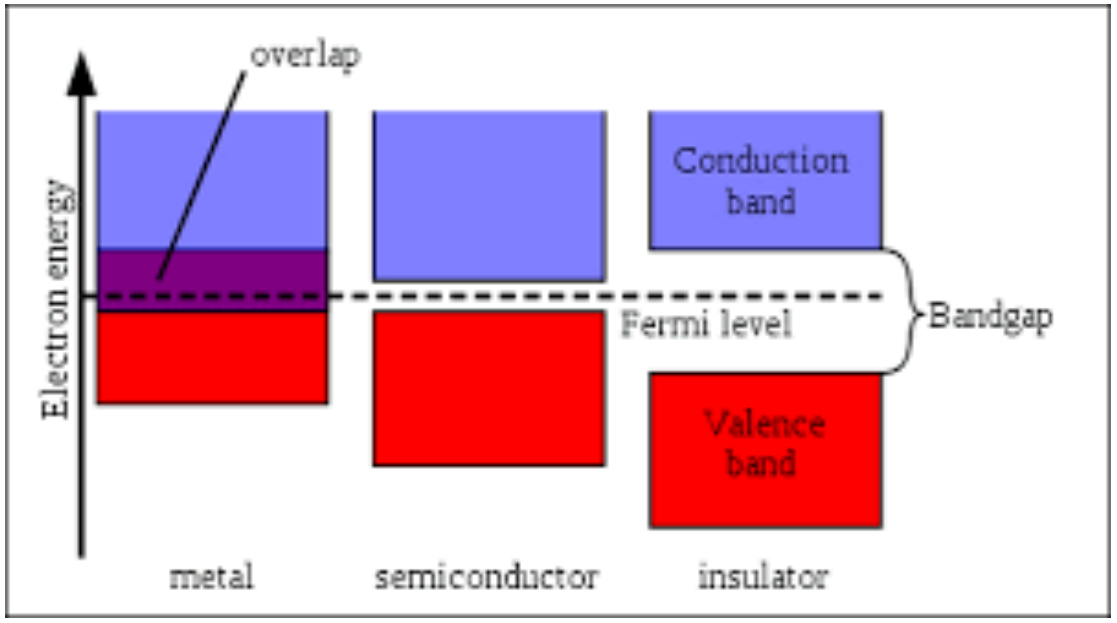
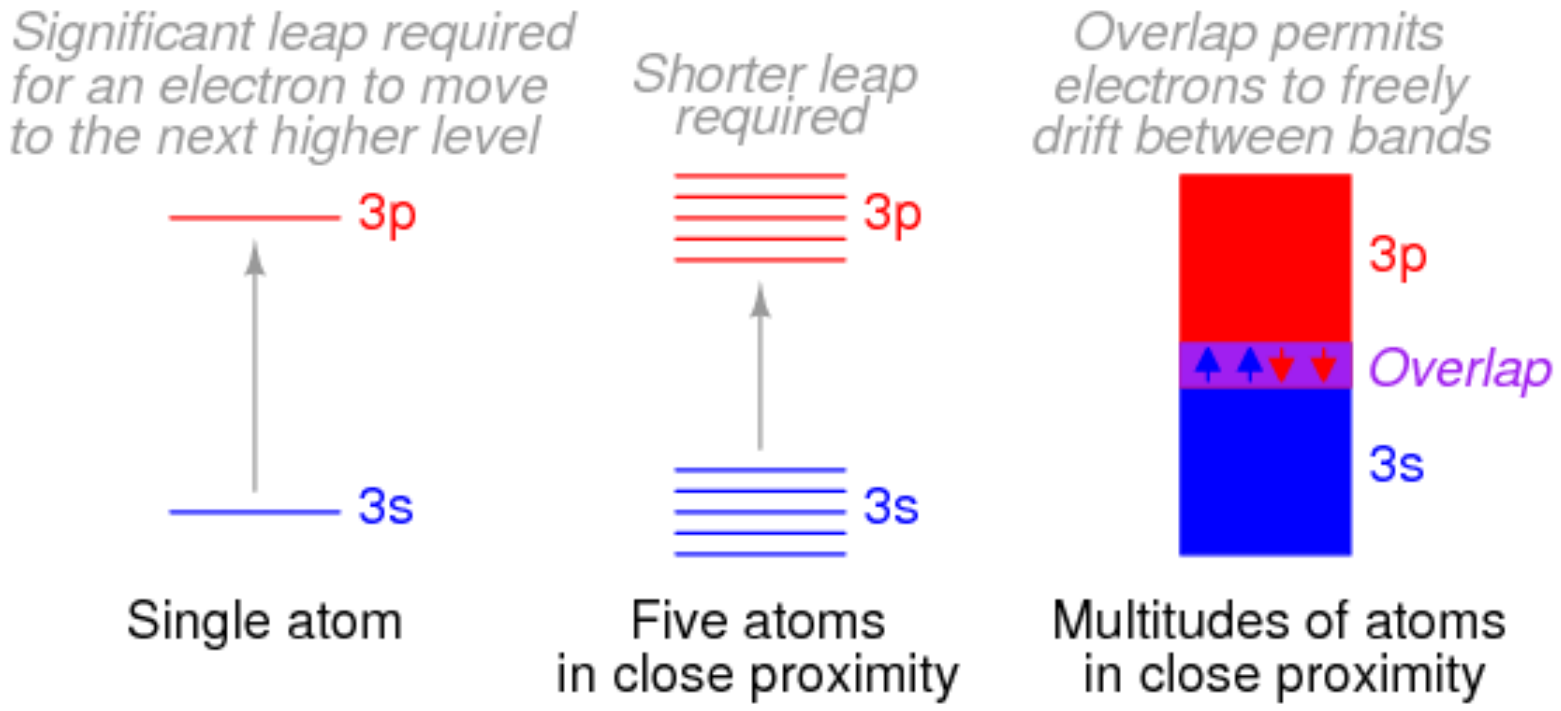
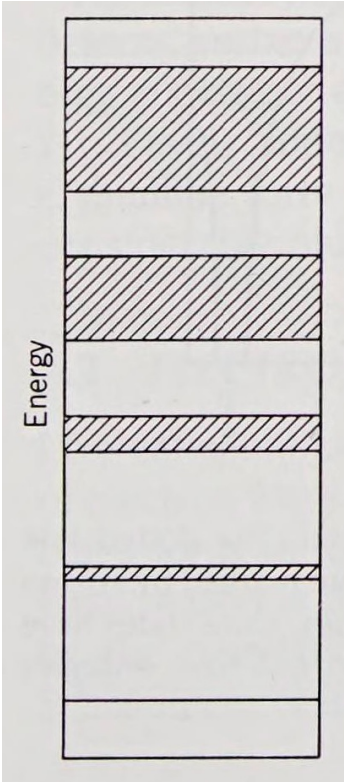
8. Estados electrónicos



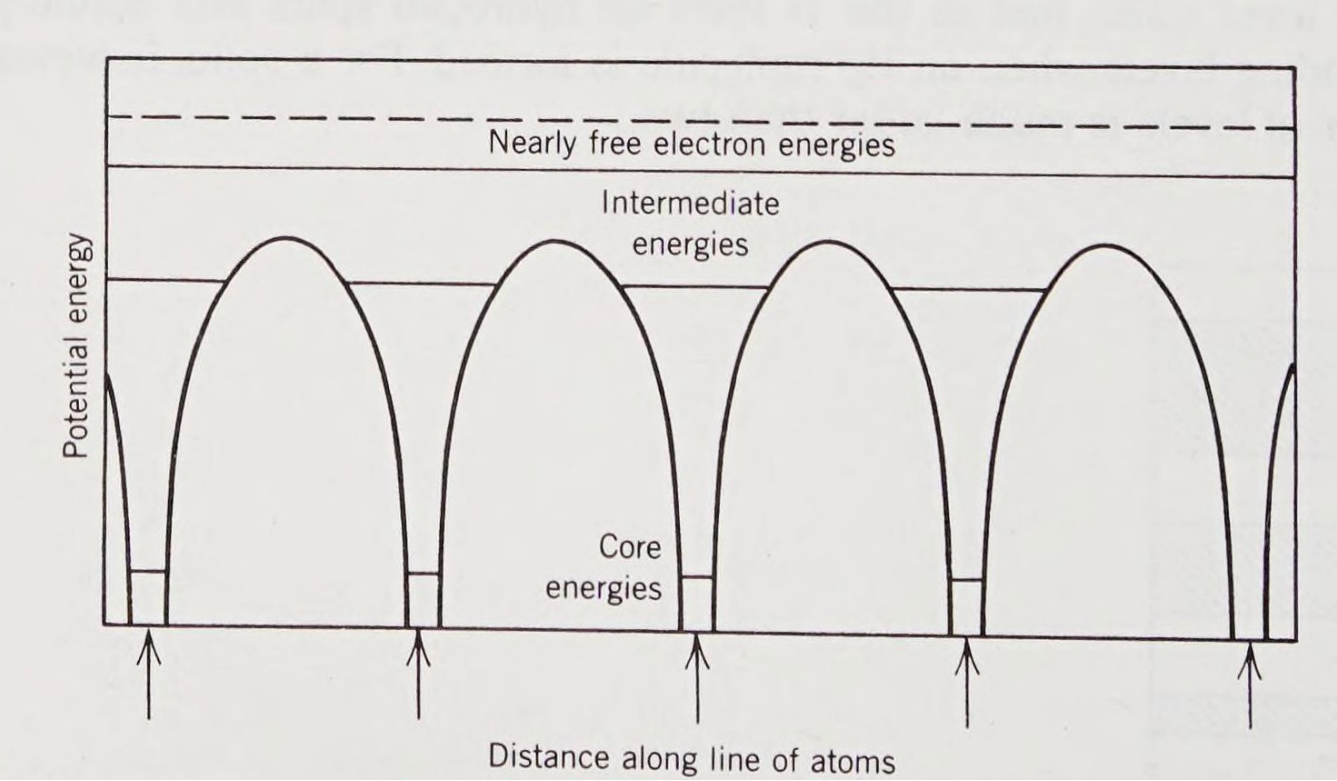
Overlap of atomic states



Bands



Electronic energy along a line of atoms

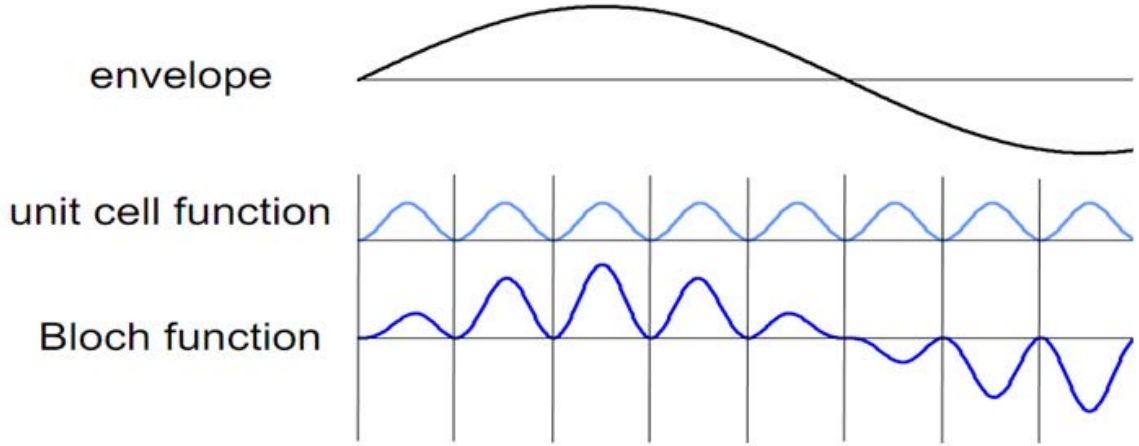


Bloch's theorem

we can rewrite the Bloch theorem equation $\psi(x+a) = \exp(ika)\,\psi(x)$ alternative form

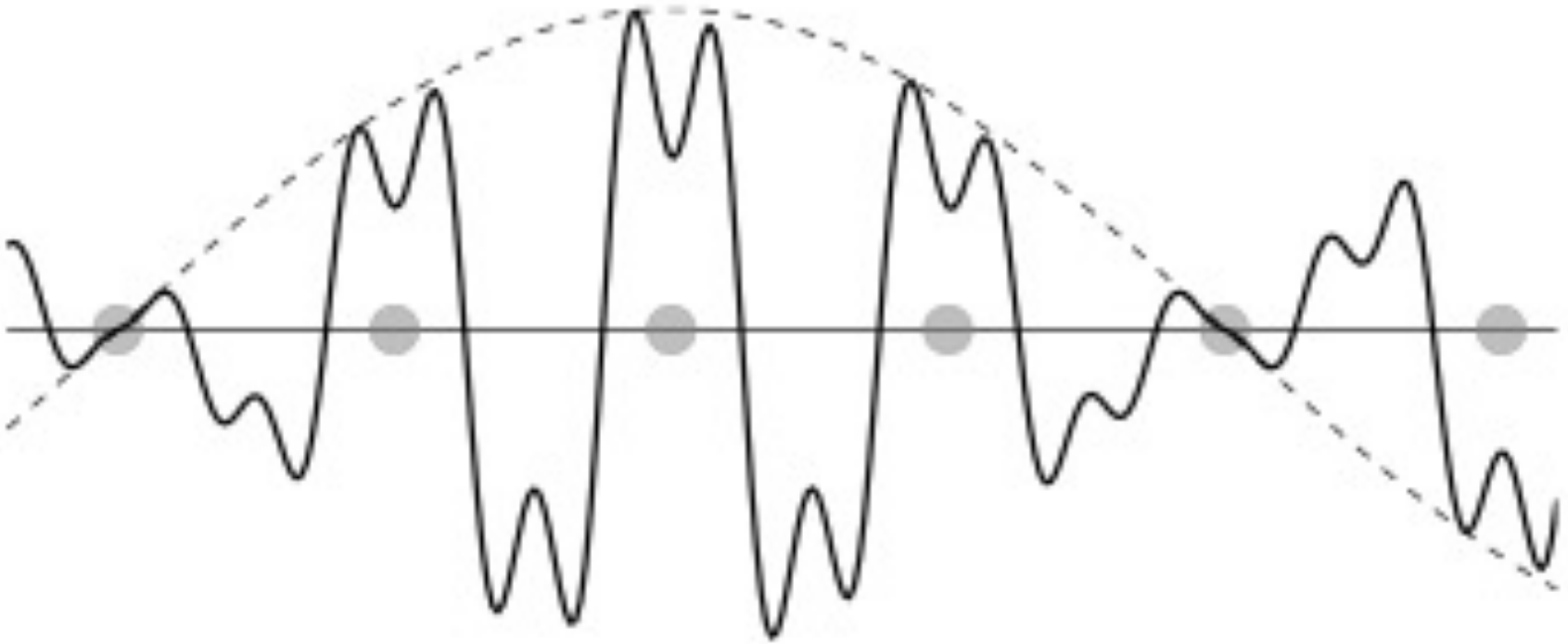
$$\psi(x) = u(x)\exp(ikx)$$

where u(x) is periodic with the lattice periodicity.

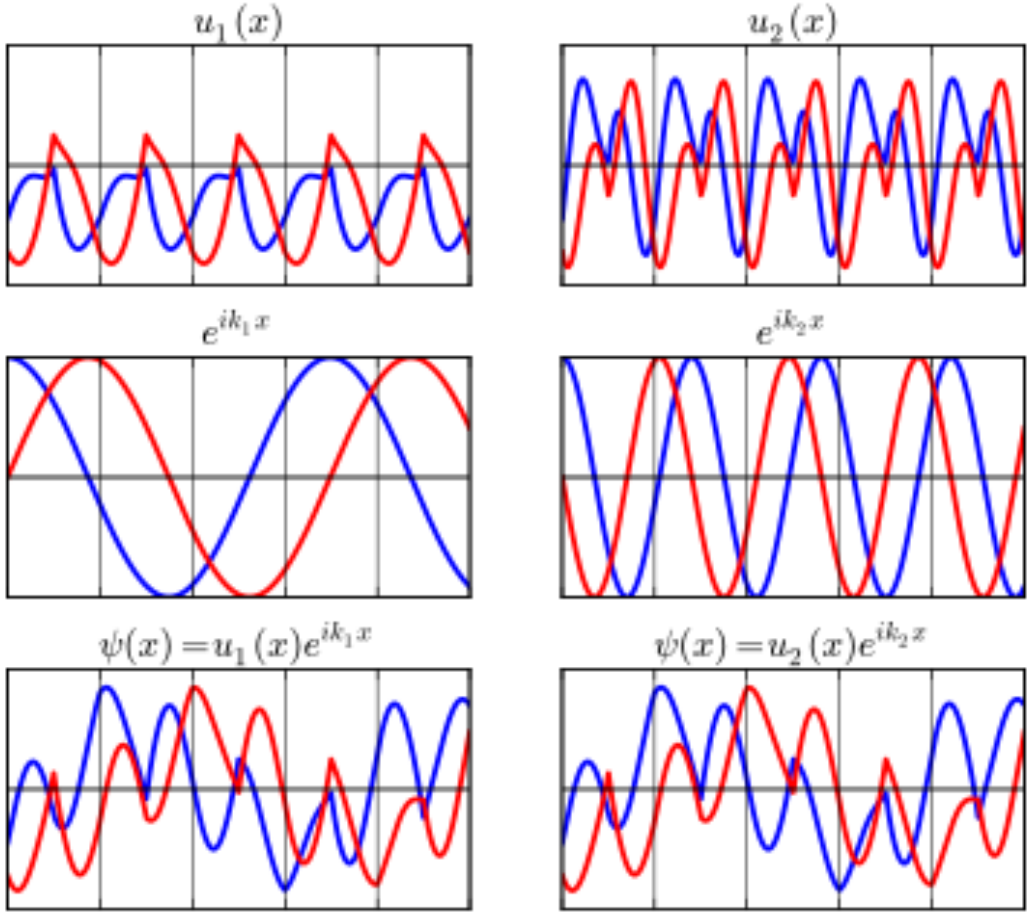


Concept of the Bloch functions. We can think of the exp(ikx) as being an example of an "envelope" function that multiplies the unit cell function u(x)

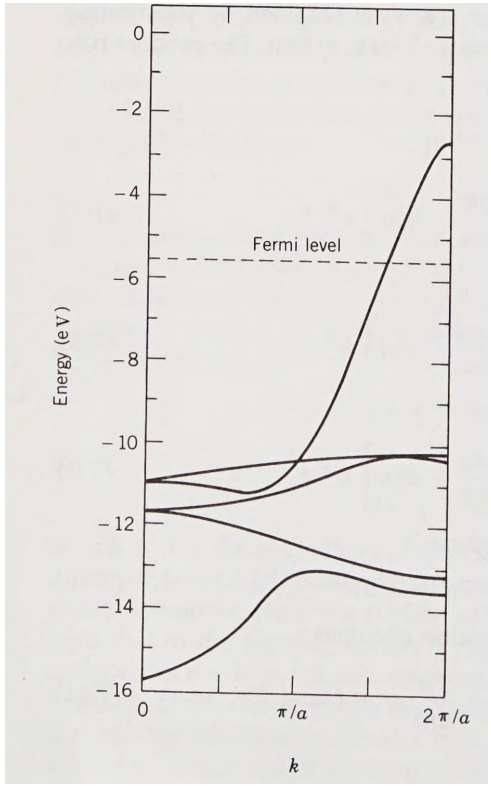
Bloch function



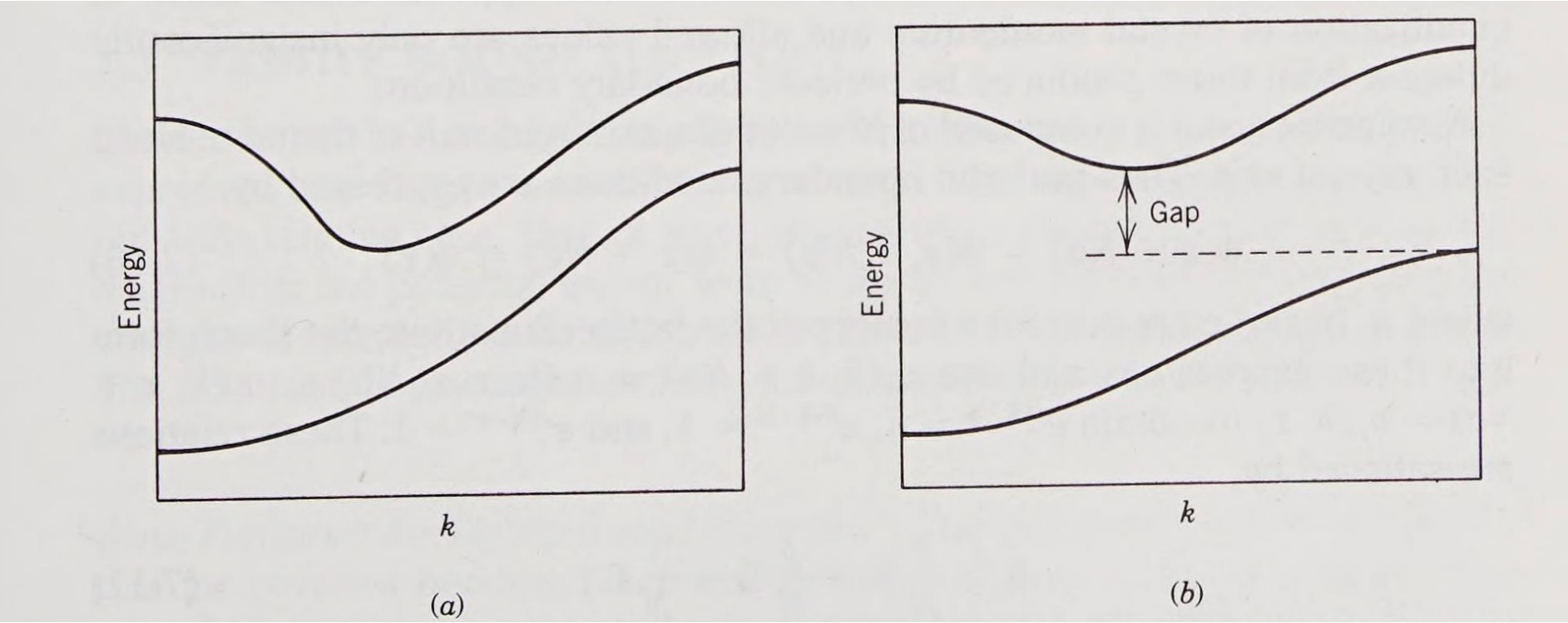
Bloch functions



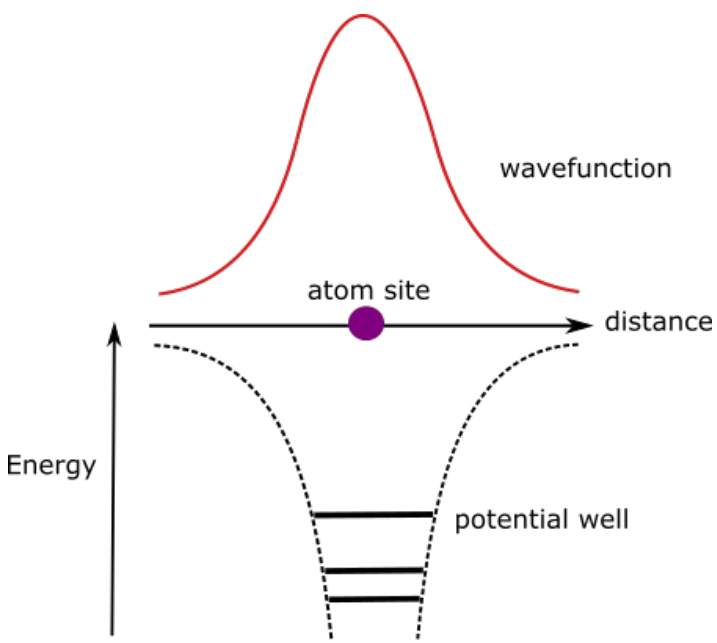
Bands of copper in the 100 direction

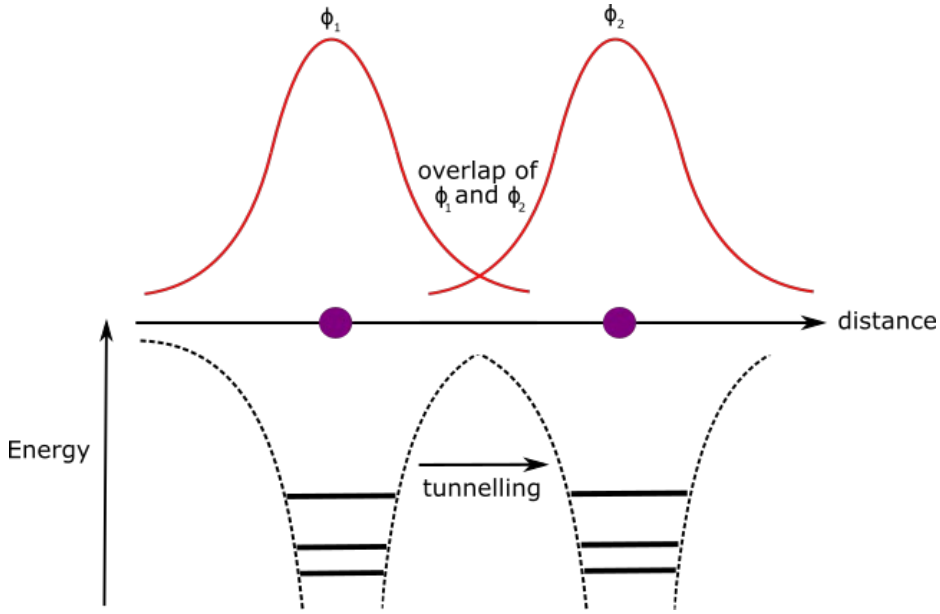


Band overlap

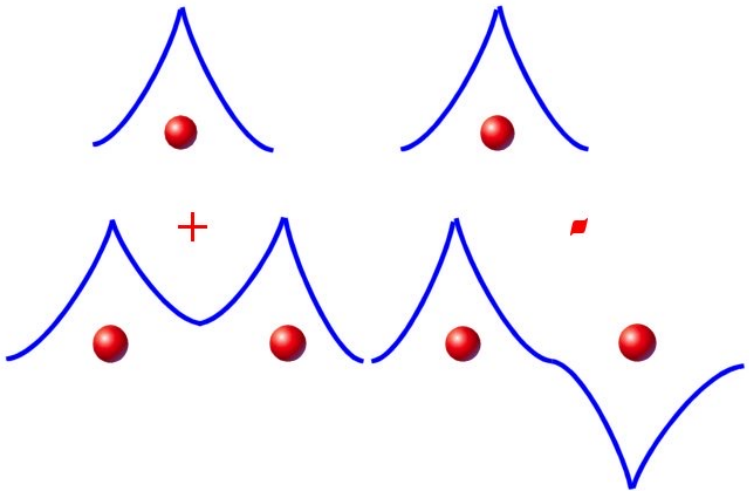


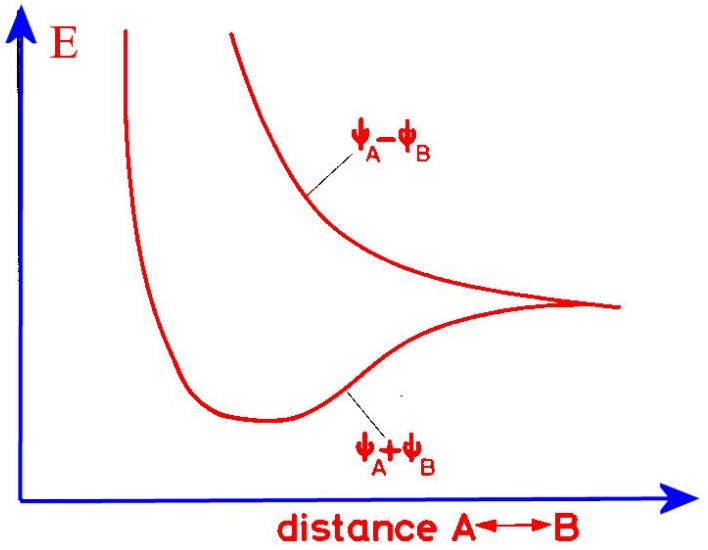
Recall: Covalent Bonding



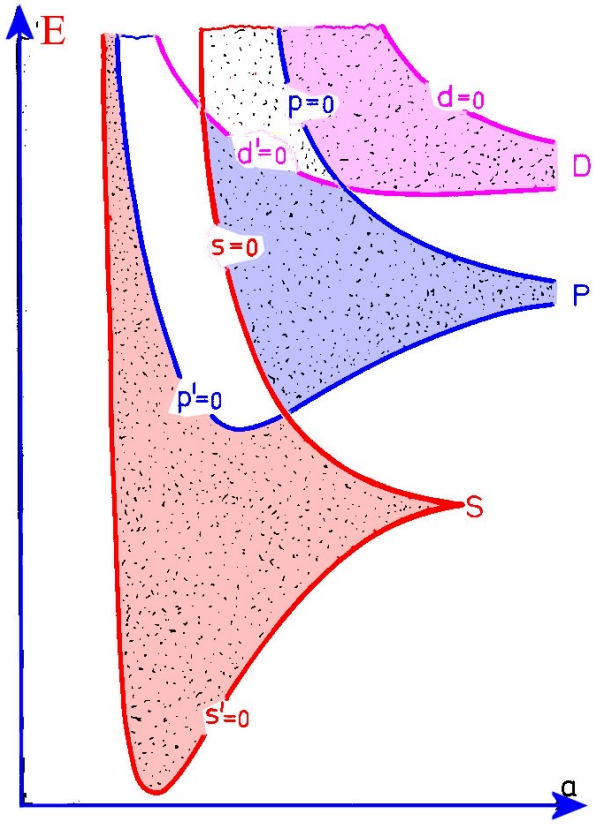


Bonding and anti-bonding states & energies

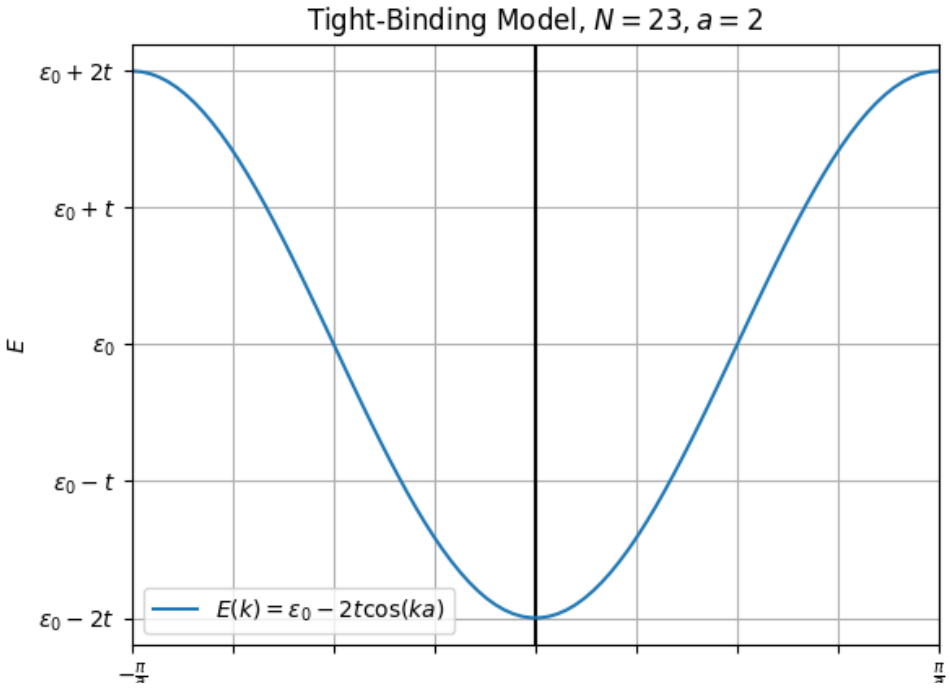


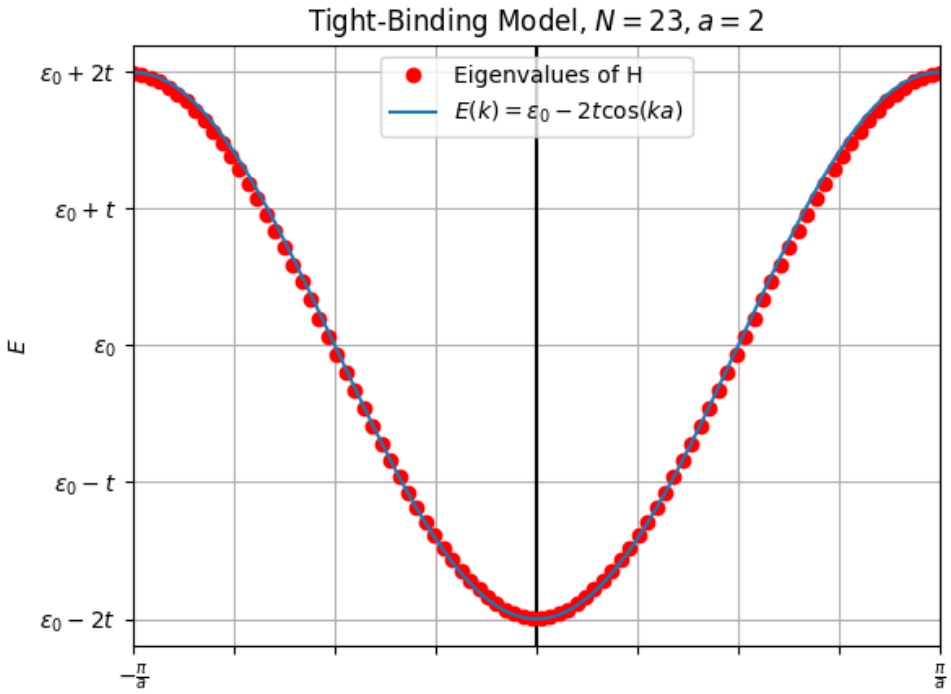


Many atoms: bands



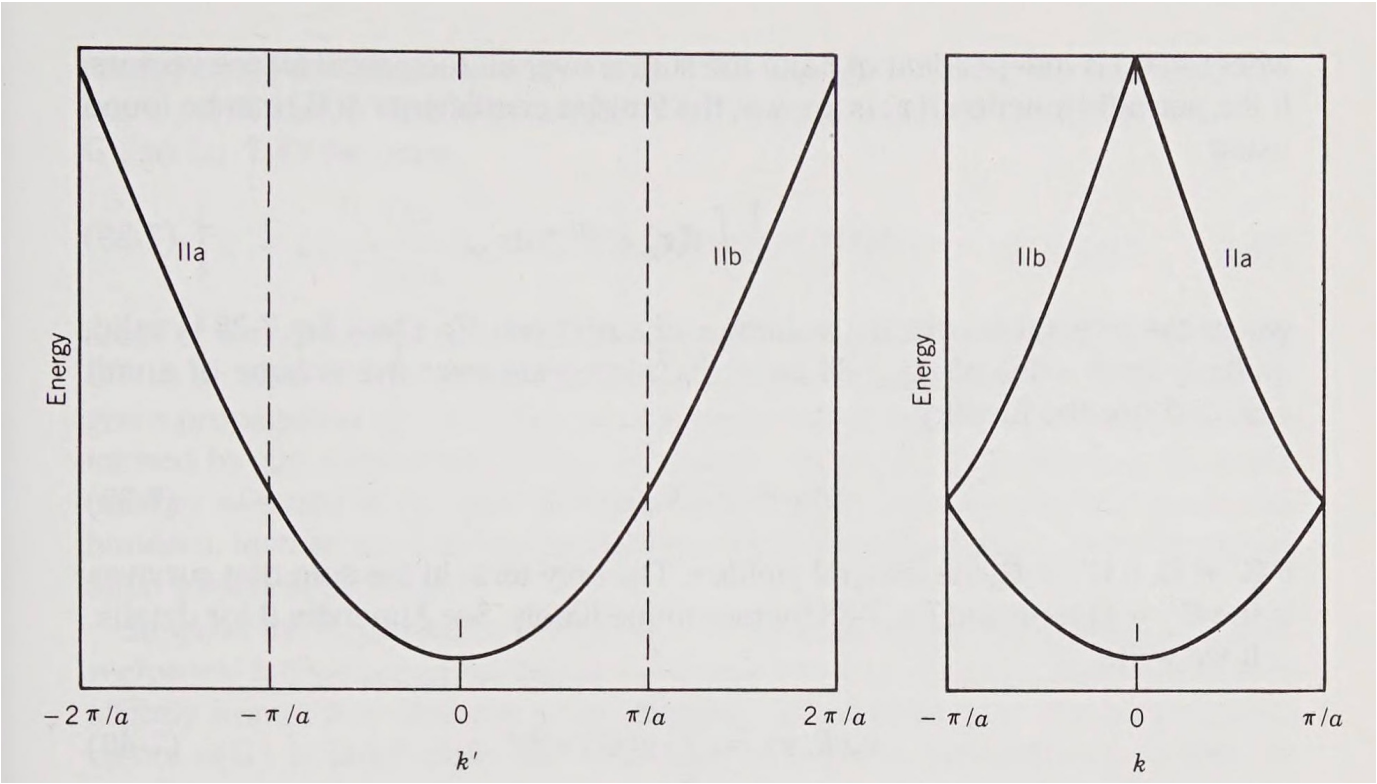
Exercise: tight binding model in 1d



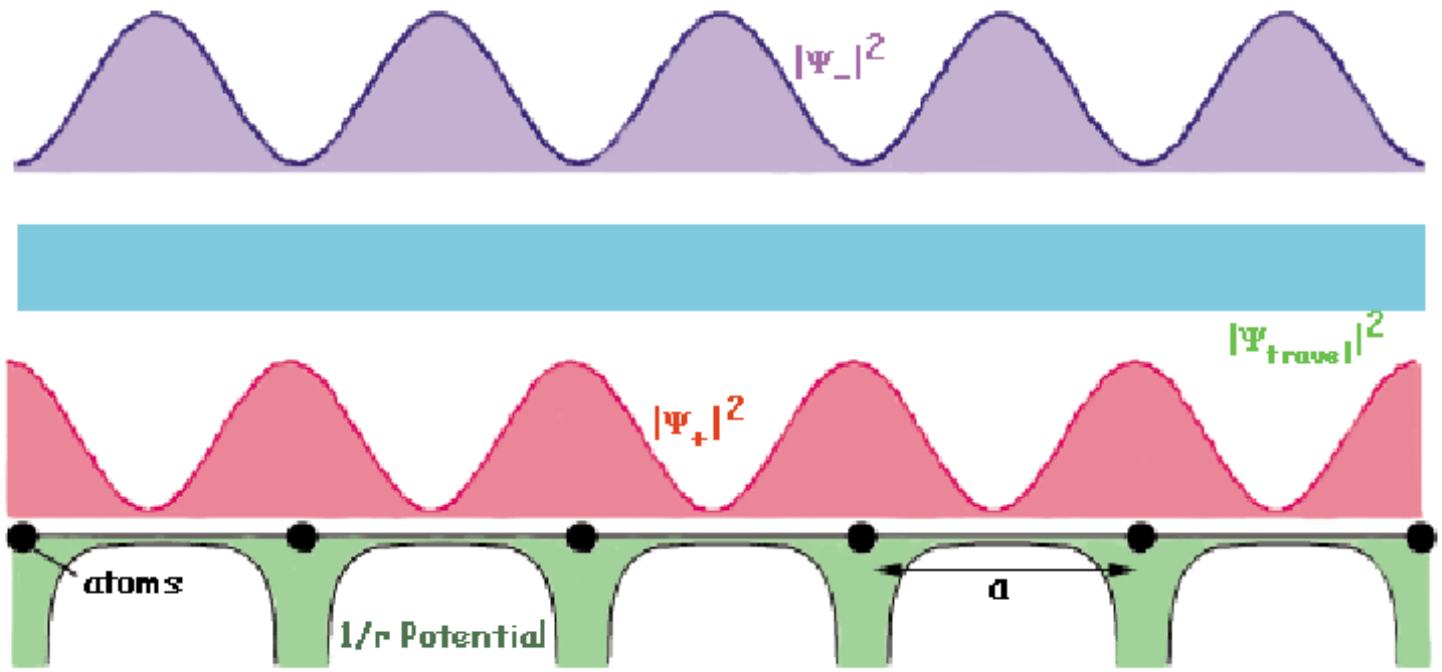


Simon, S. H. (2013). *The Oxford solid state basics*. Oxford, UK: Oxford Univ. Press.

Free electron bands in 1d



Bragg reflection of free electrons



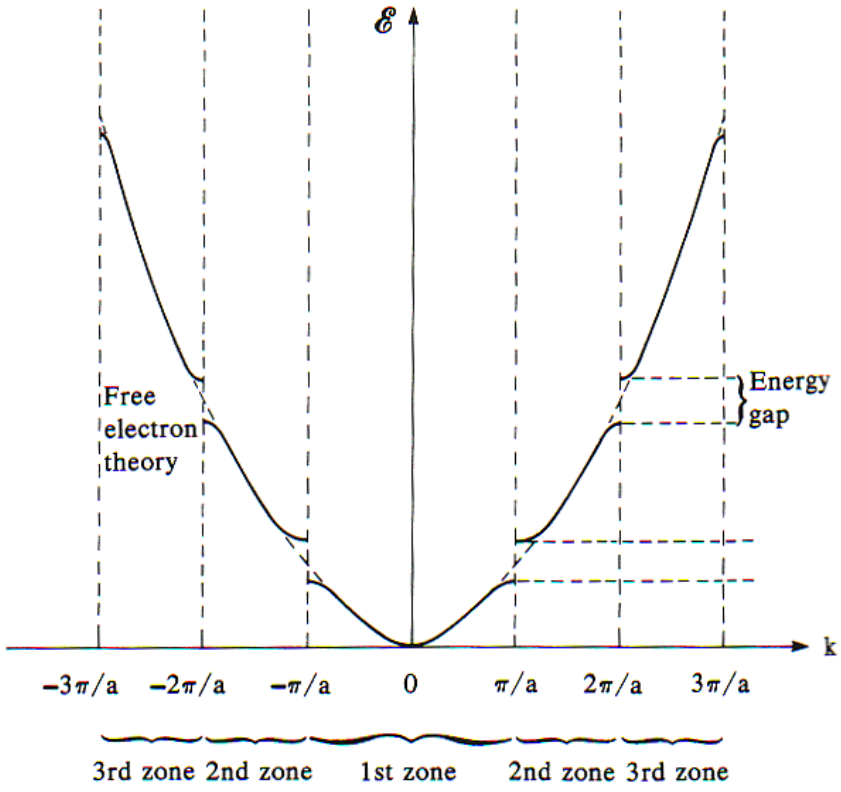
$$e^{ikx} - e^{-ikx}$$

$$\sim \sin(kx)$$

$$e^{ikx} + e^{-ikx}$$

$$\sim \cos(kx)$$

Band gaps of nearly free electrons in 1d



Nearly free electron bands in 1d

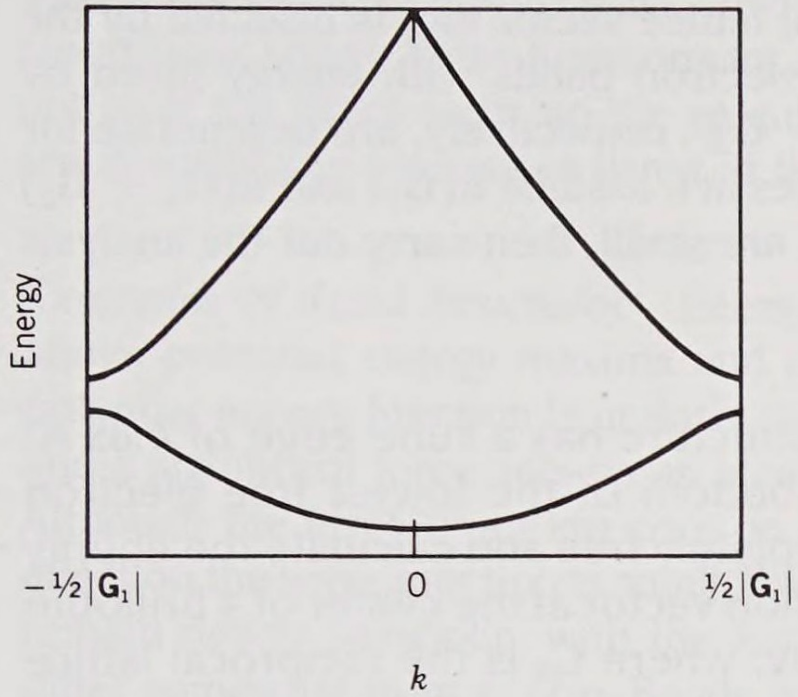
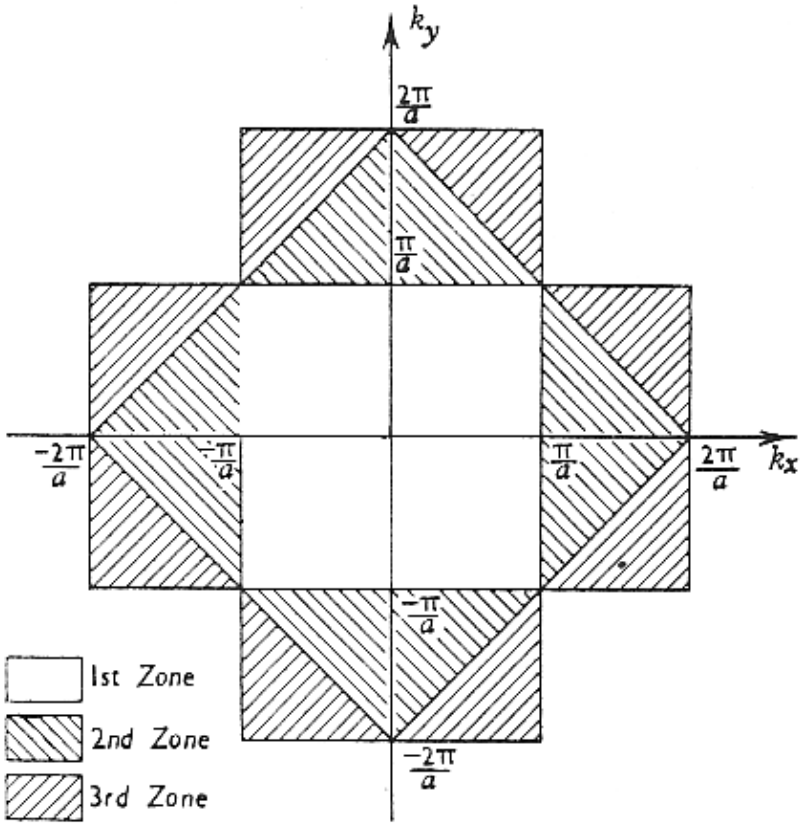
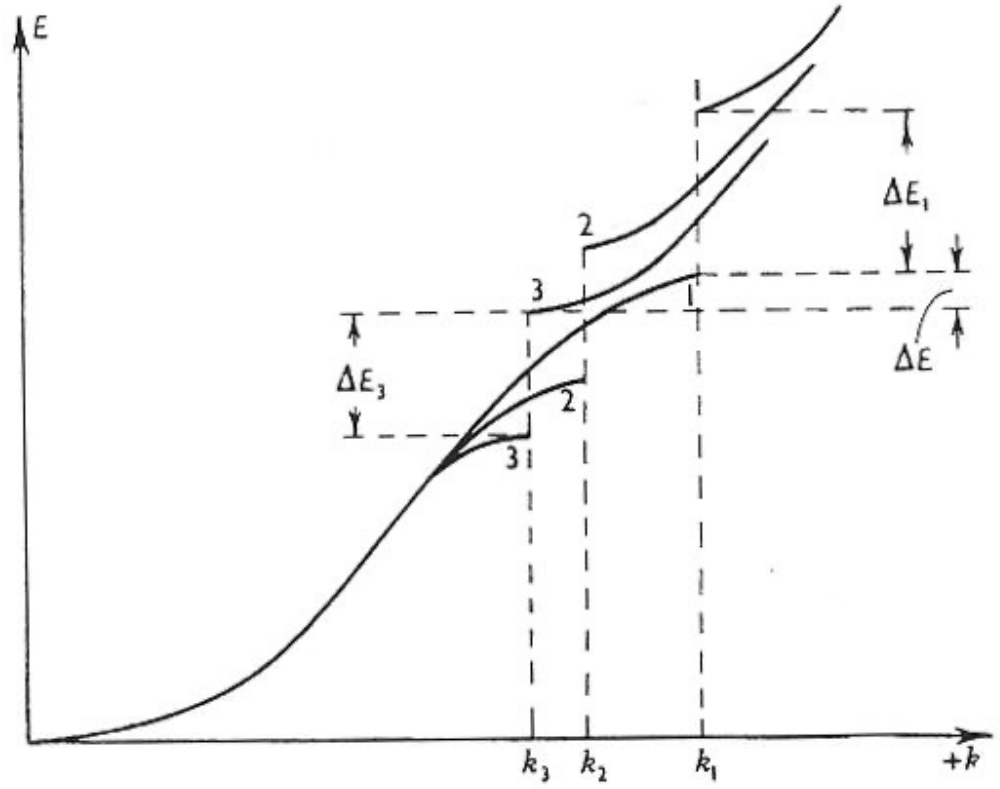


FIGURE 7-7 Energy as a function of propagation vector magnitude for nearly free electrons. The propagation vector is taken to be parallel to reciprocal lattice vector $\mathbf{G}_1$, which is bisected by a Brillouin zone boundary. The curves are similar to those of Fig. 7-6*b* but gaps occur at $\mathbf{k} = \pm\frac{1}{2}\mathbf{G}_1$. The gap width depends on the Fourier component $U(\mathbf{G}_1)$ of the potential energy function.

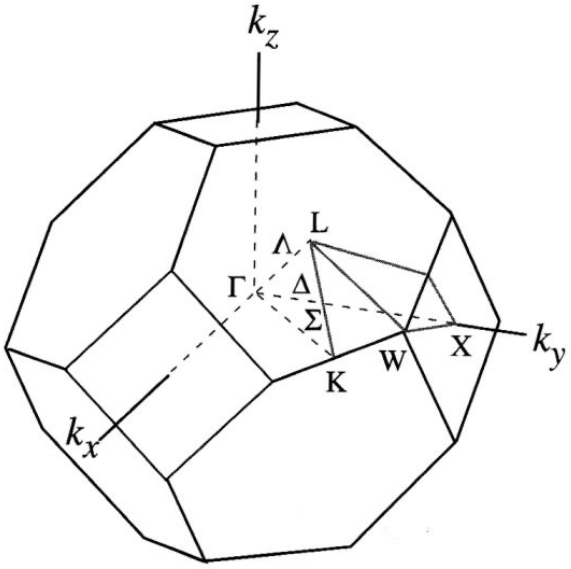
Brillouin zones in 2d

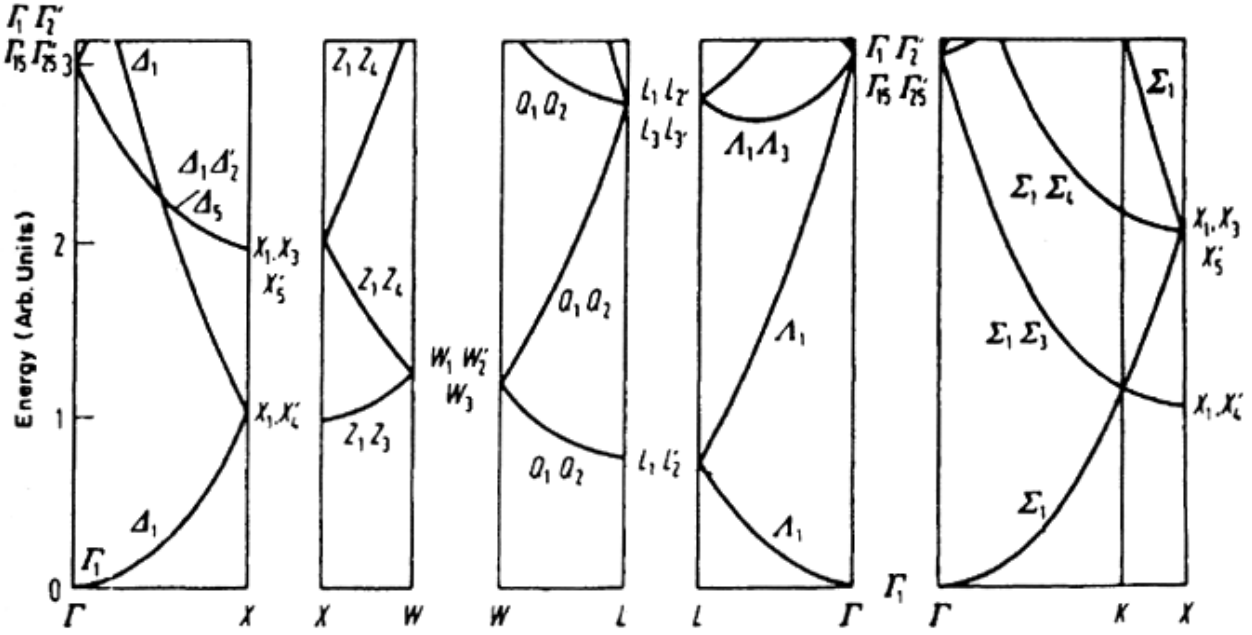


Nearly free electron bands in 2d



Free electron bands in 3d: Al





Nearly free electron bands In 3d: Al

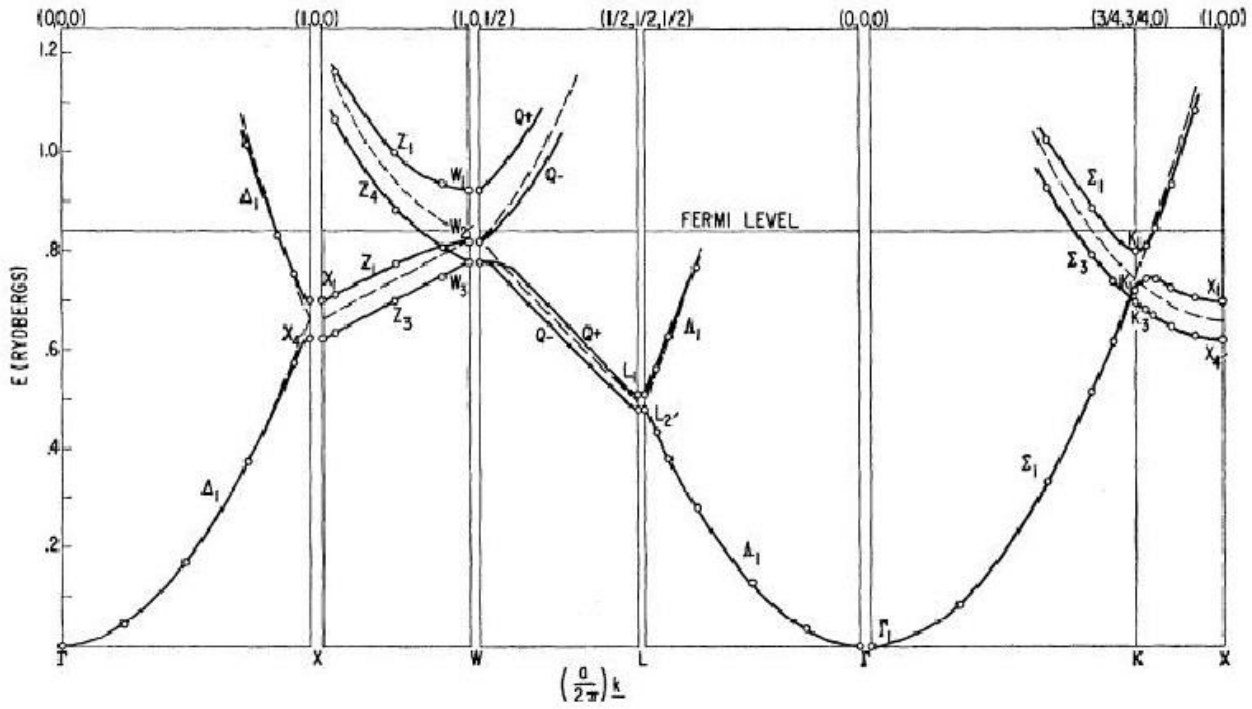
Γ- point: (0,0,0)

X- point: $\frac{2\pi}{a}$ (1,0,0)

L- point: $\frac{\pi}{a}$ (1,1,1)

K- point: $\frac{2\pi}{a}\left(\frac{3}{4},\frac{3}{4},0\right)$

W- point: $\frac{2\pi}{a}\left(1,\frac{1}{2},0\right)$



Bands of potassium in 3 directions

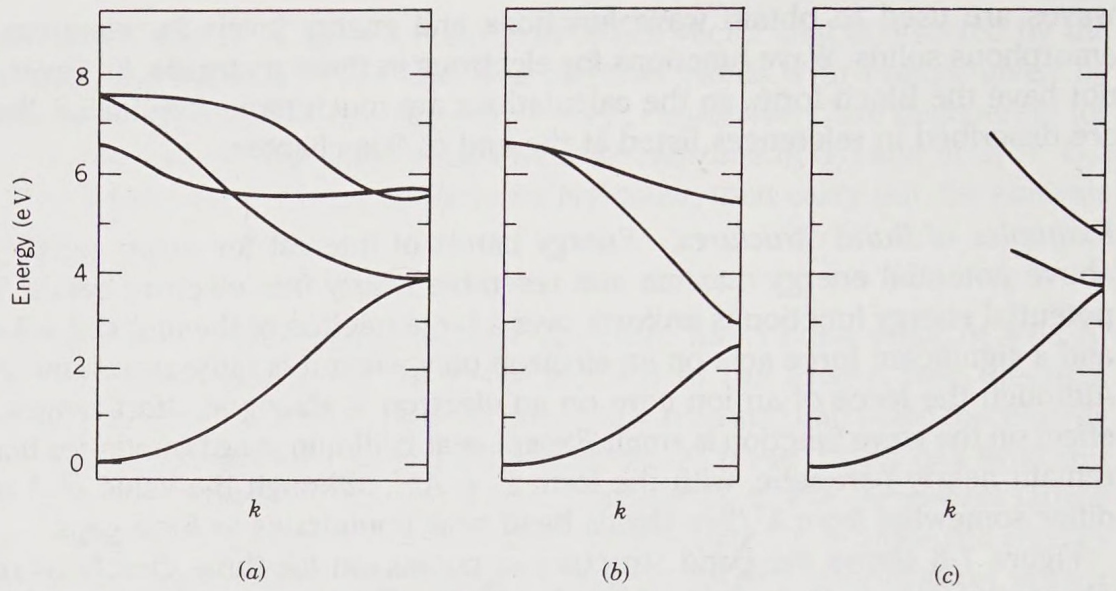


FIGURE 7-8 Electron band structure of potassium for energies near the 4*s* atomic level: (*a*) **k** in the [100] direction; (*b*) **k** in the [110] direction; and (*c*) **k** in the [111] direction. Some curves are incomplete. The bands shown are quite similar in form to those predicted by the nearly free electron model. (From F. S. Ham, *Phys. Rev.* **128**:82, 1962. Used with permission.)

Bands of silicon in 3 directions

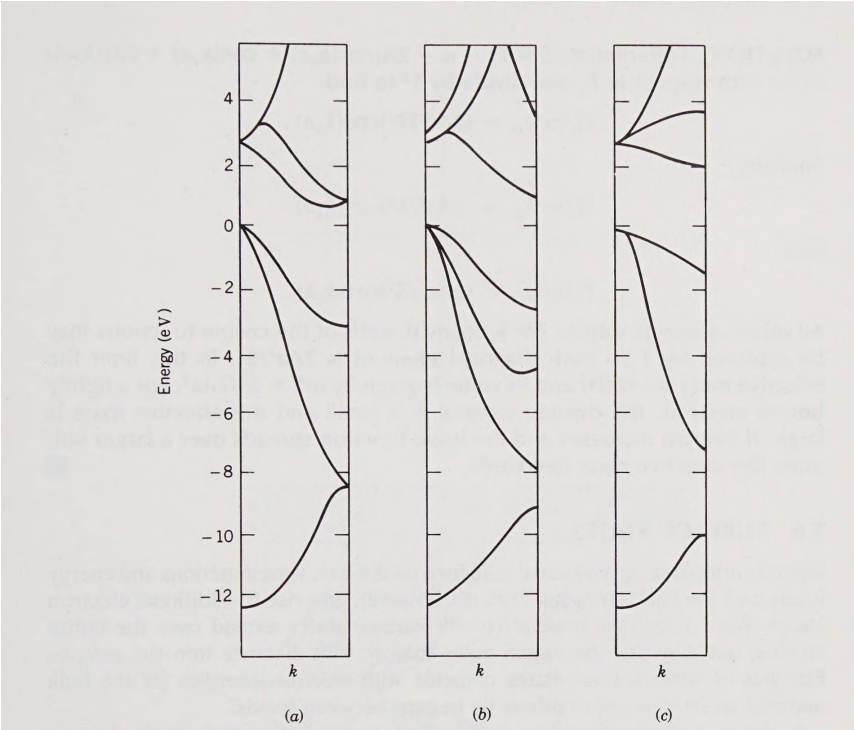
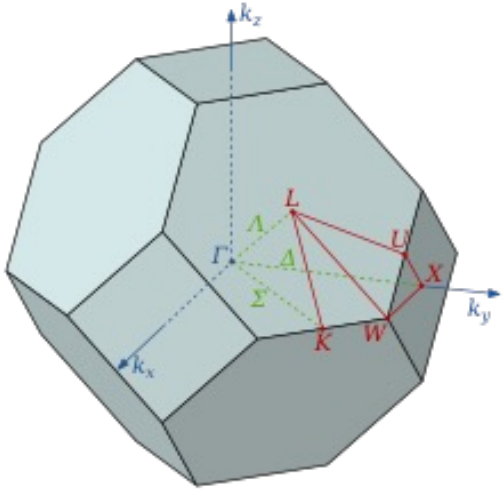
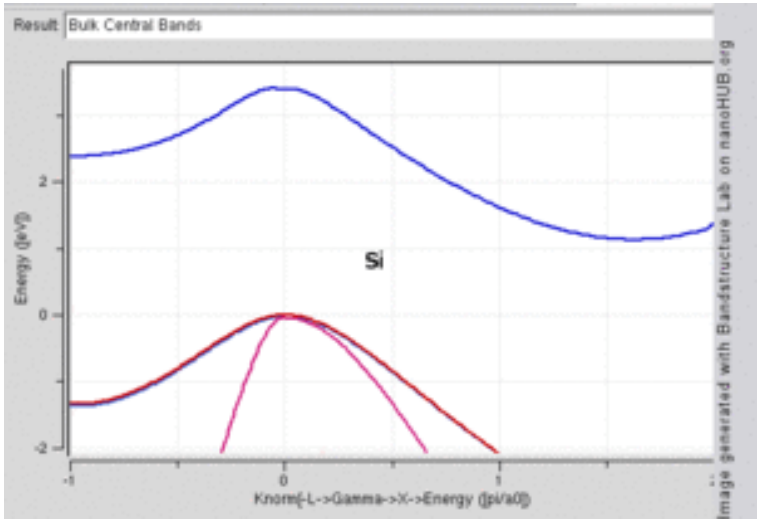


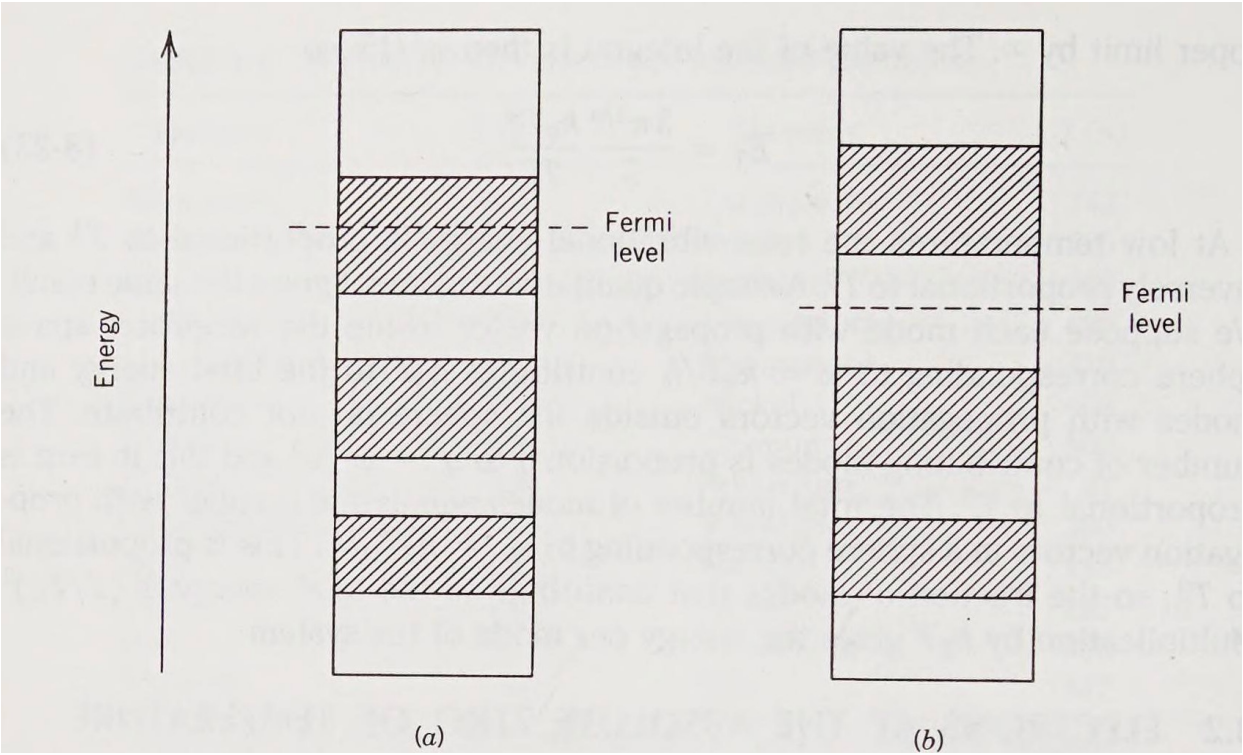
FIGURE 7-9 Electron band structure of crystalline silicon for energies near the 3*s* and 3*p* atomic levels: (*a*) **k** in the [100] direction; (*b*) **k** in the [110] direction; and (*c*) **k** in the [111] direction. Bands below $E = 0$ are valence bands and are associated with bonding. Higher bands are conduction bands and are important for the electrical properties of silicon. A gap exists between the valence and conduction bands. (From A. Zunger and M. L. Cohen, *Phys. Rev.* **B 20:**4082, 1979. Used with permission.)

9. Termodinâmica de electrões

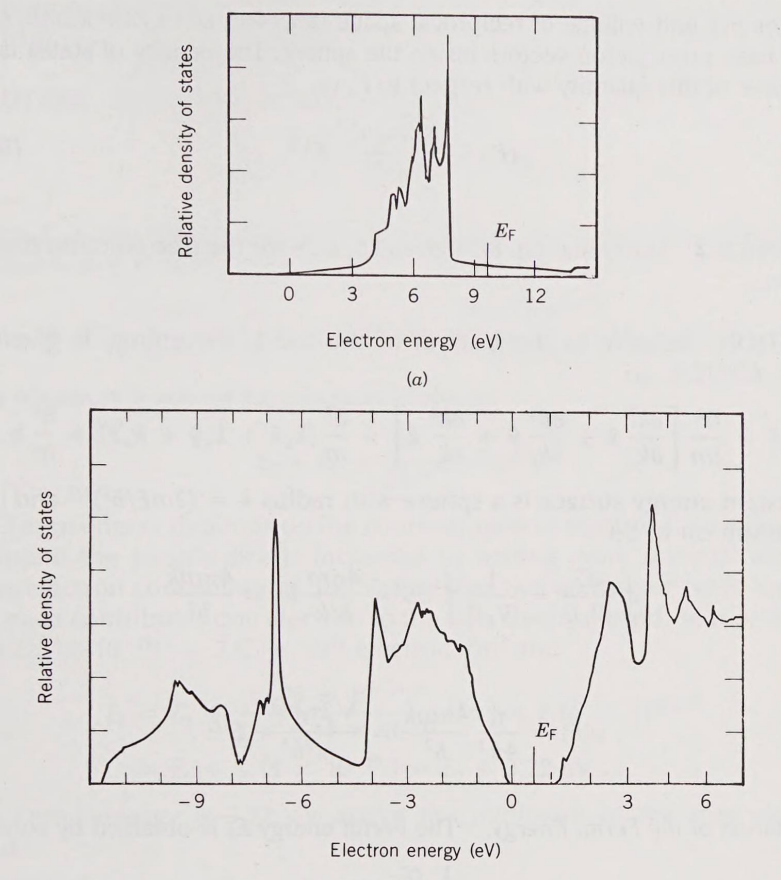




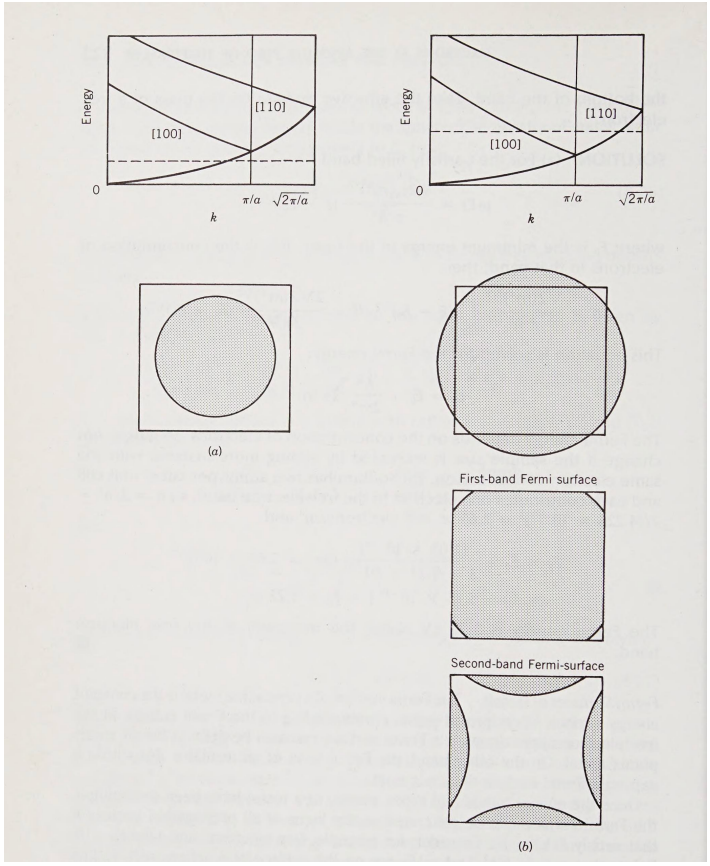
Fermi level



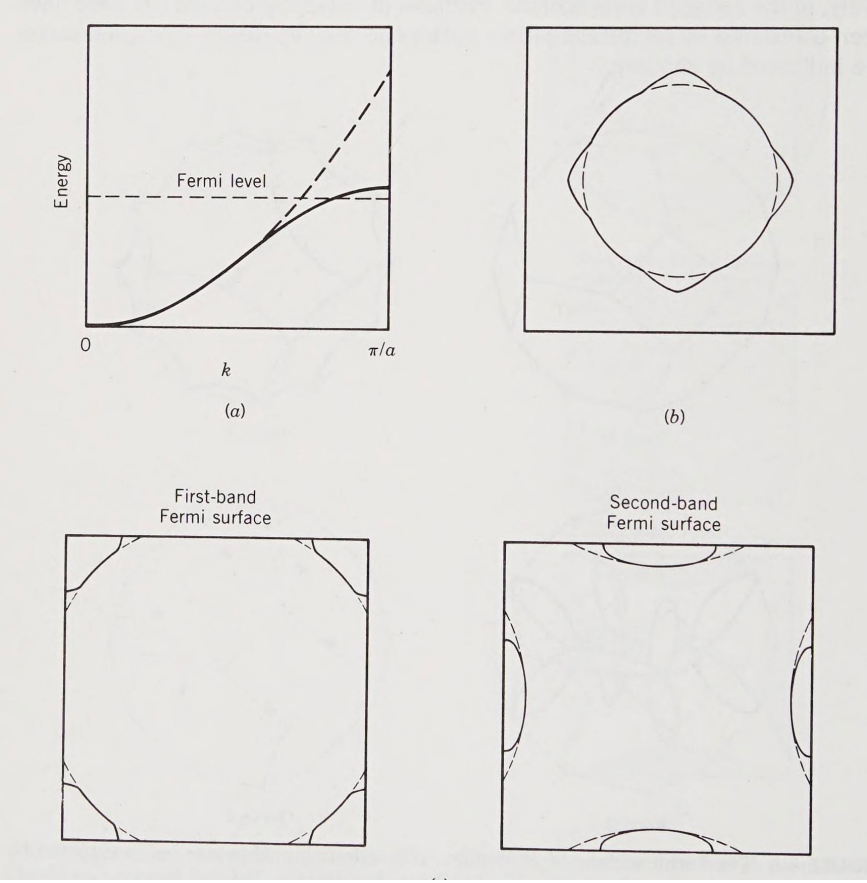
Density of states



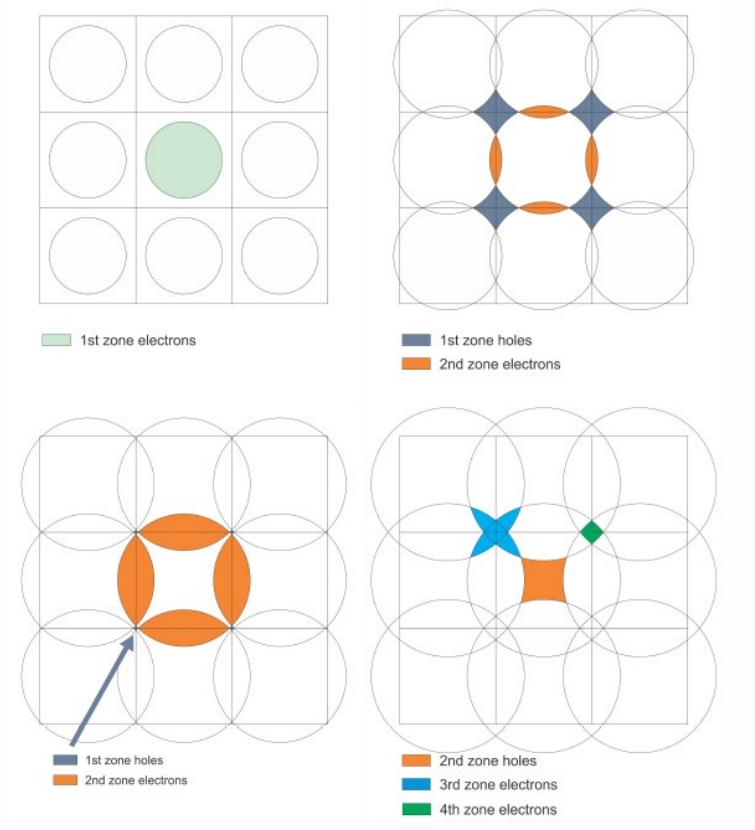
Fermi surface of free electrons in 2d (square)



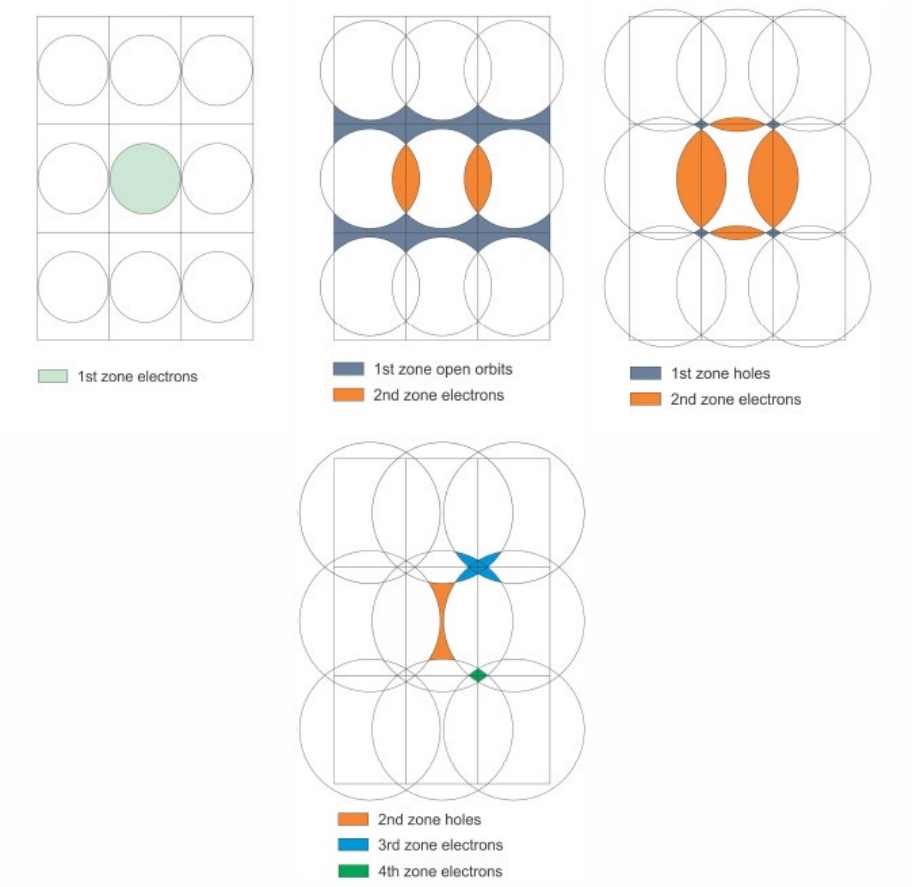
Fermi surface of nearly free electrons in 2d (square)



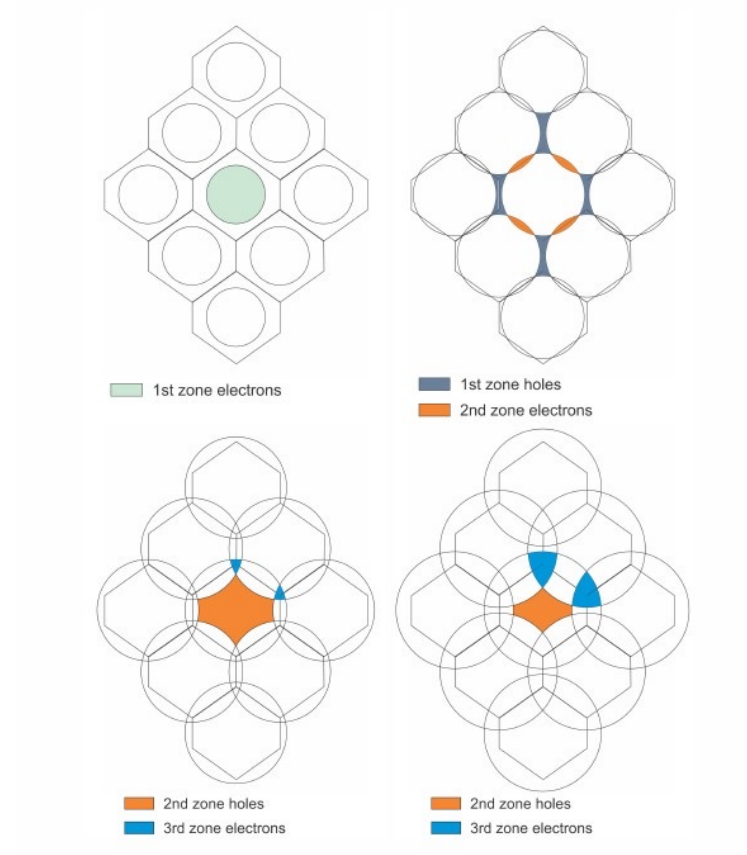
BZ of the square lattice: electrons & holes



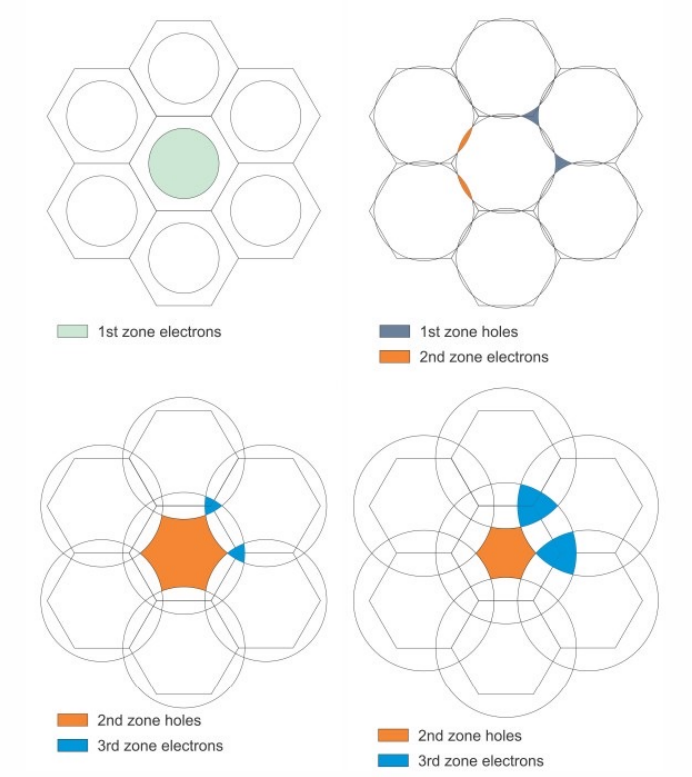
BZ of the rectangular lattice: electrons & holes



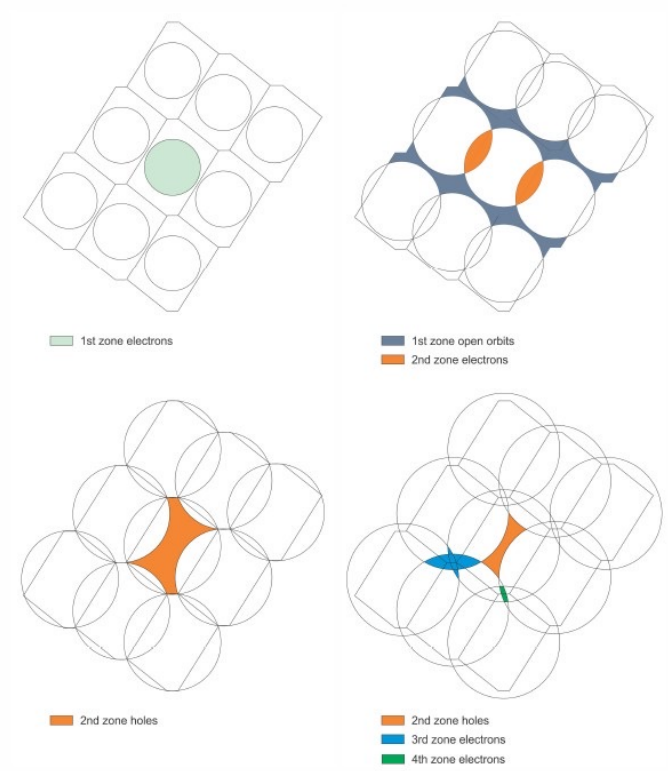
BZ of the face centred rectangular lattice: electrons & holes



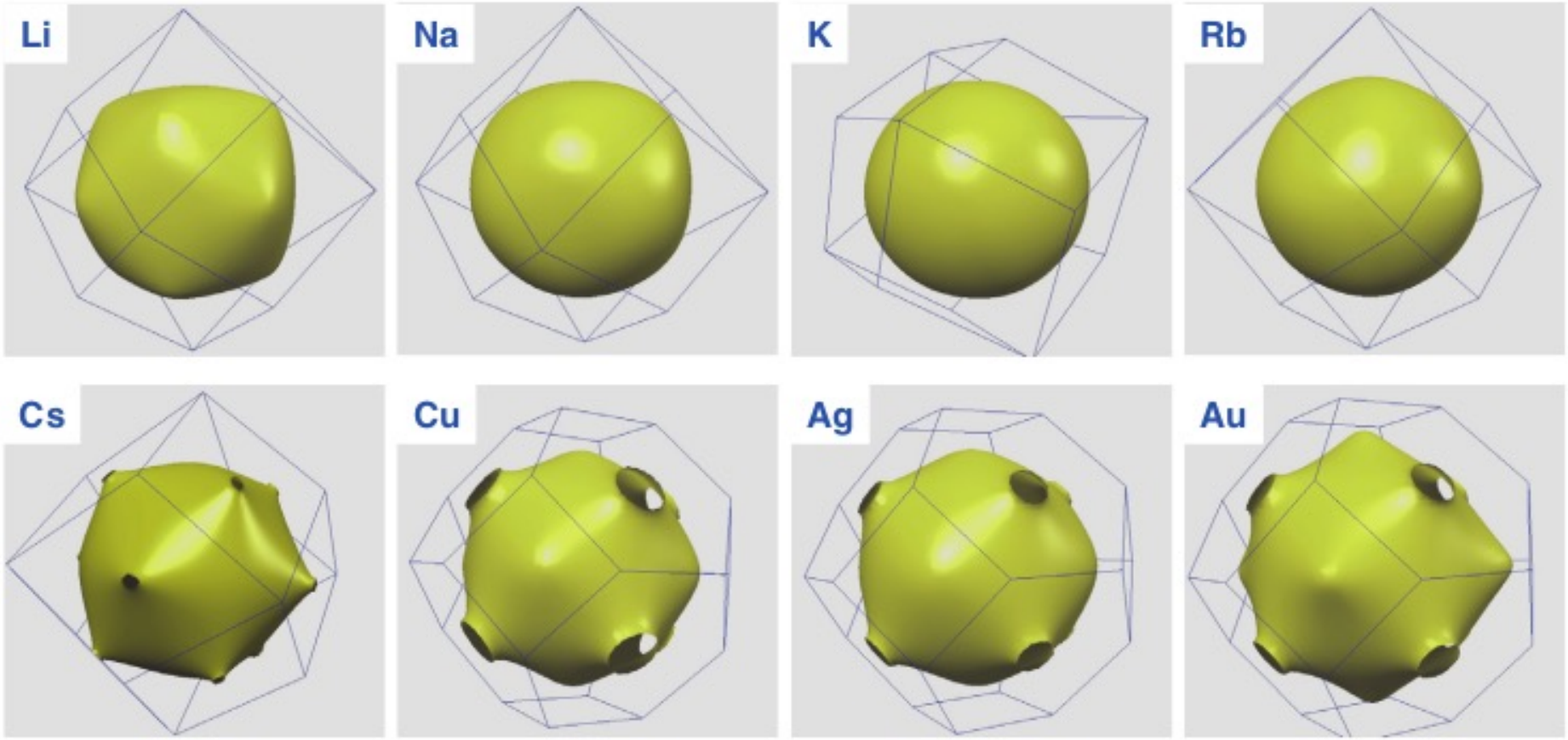
BZ of the hexagonal lattice: electrons & holes



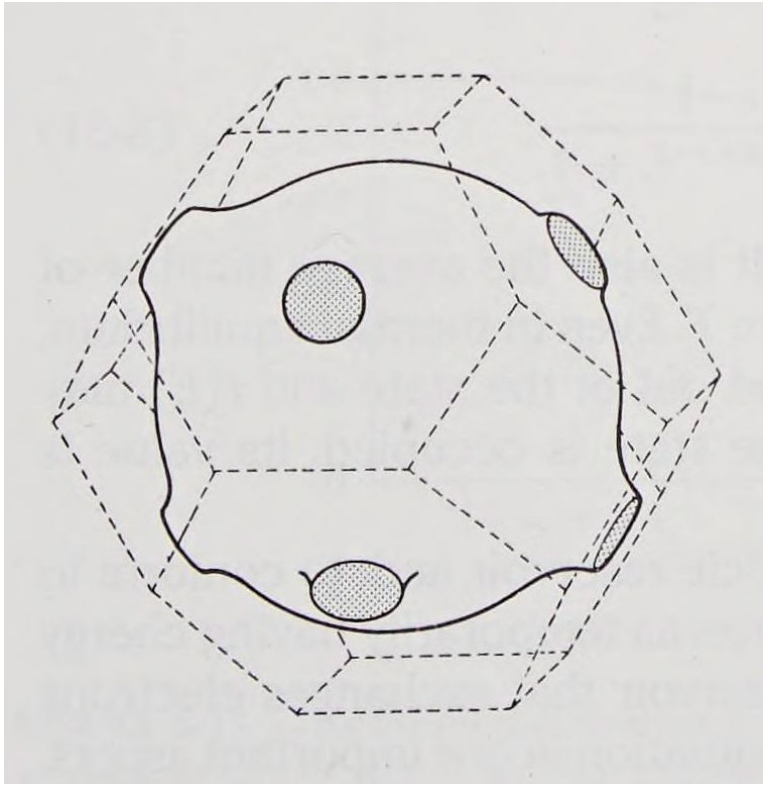
BZ of the oblique lattice: electrons & holes

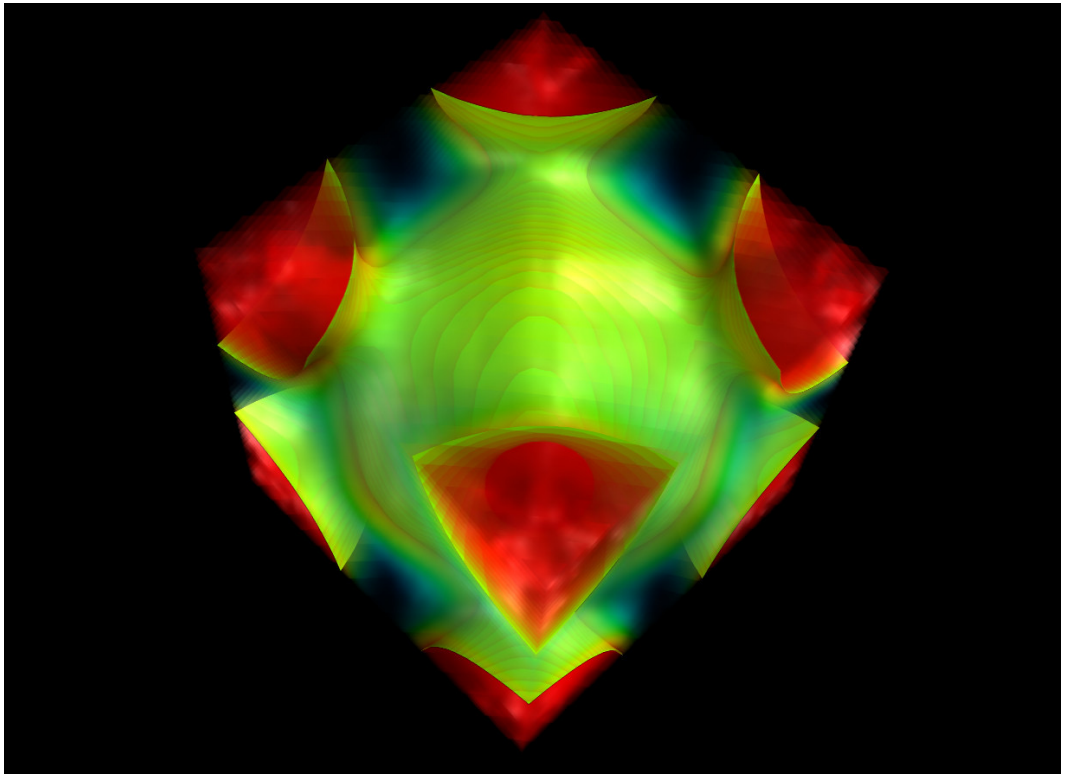


Fermi surface of alkali (bcc) and noble (fcc) metals of valence 1

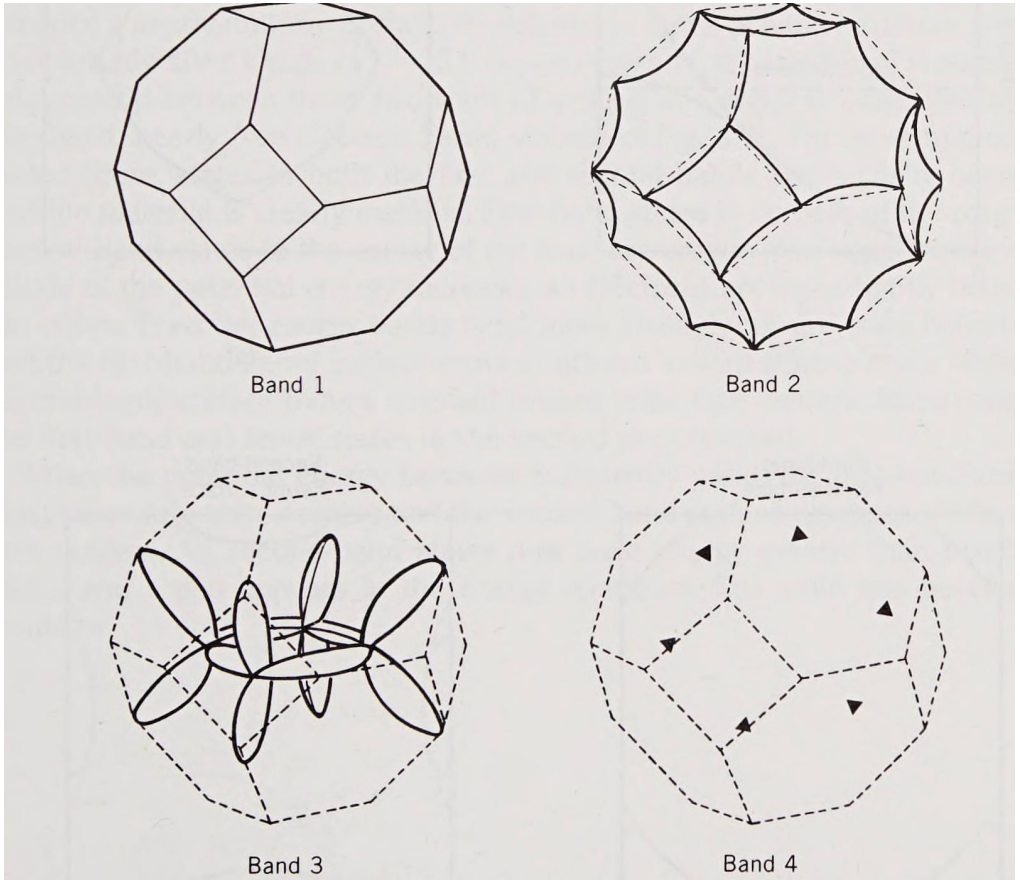


Fermi surface of Cu (fcc valence 1)

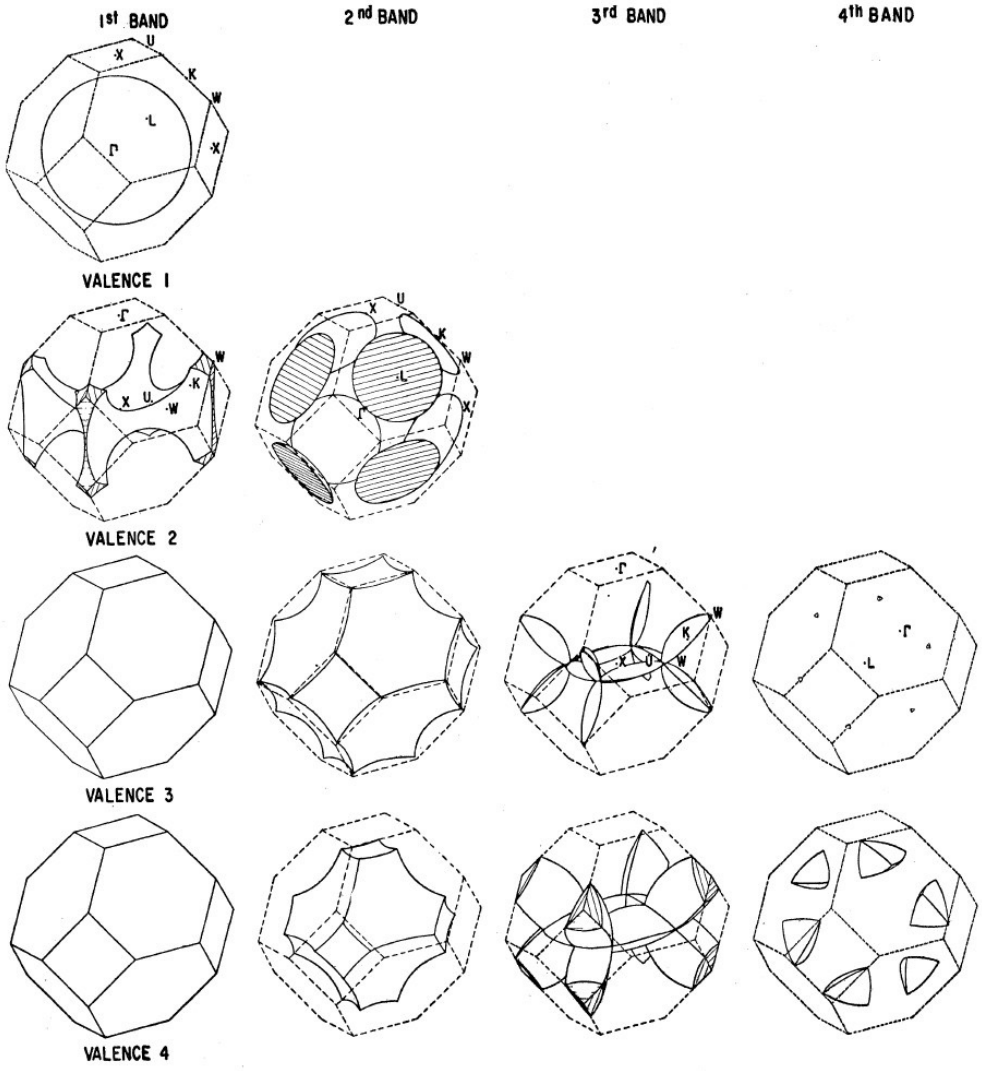




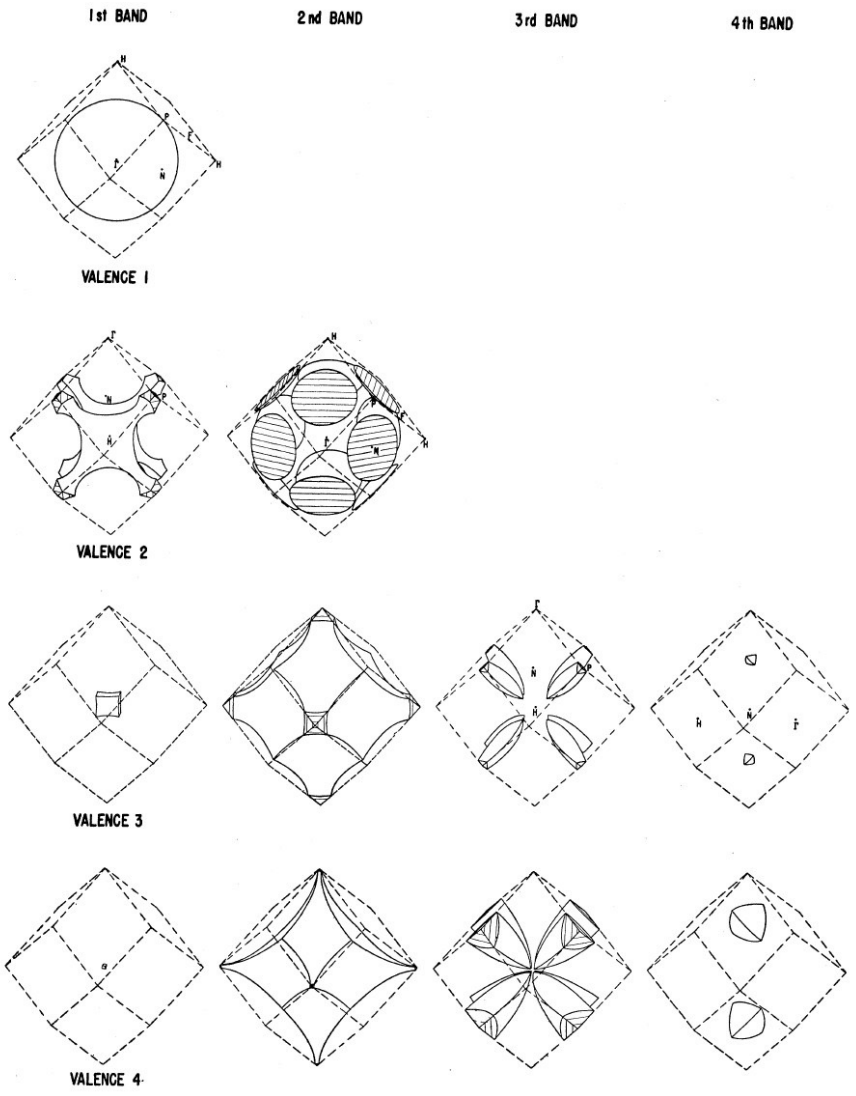
Fermi surface in 3d of Al (fcc valence 3)



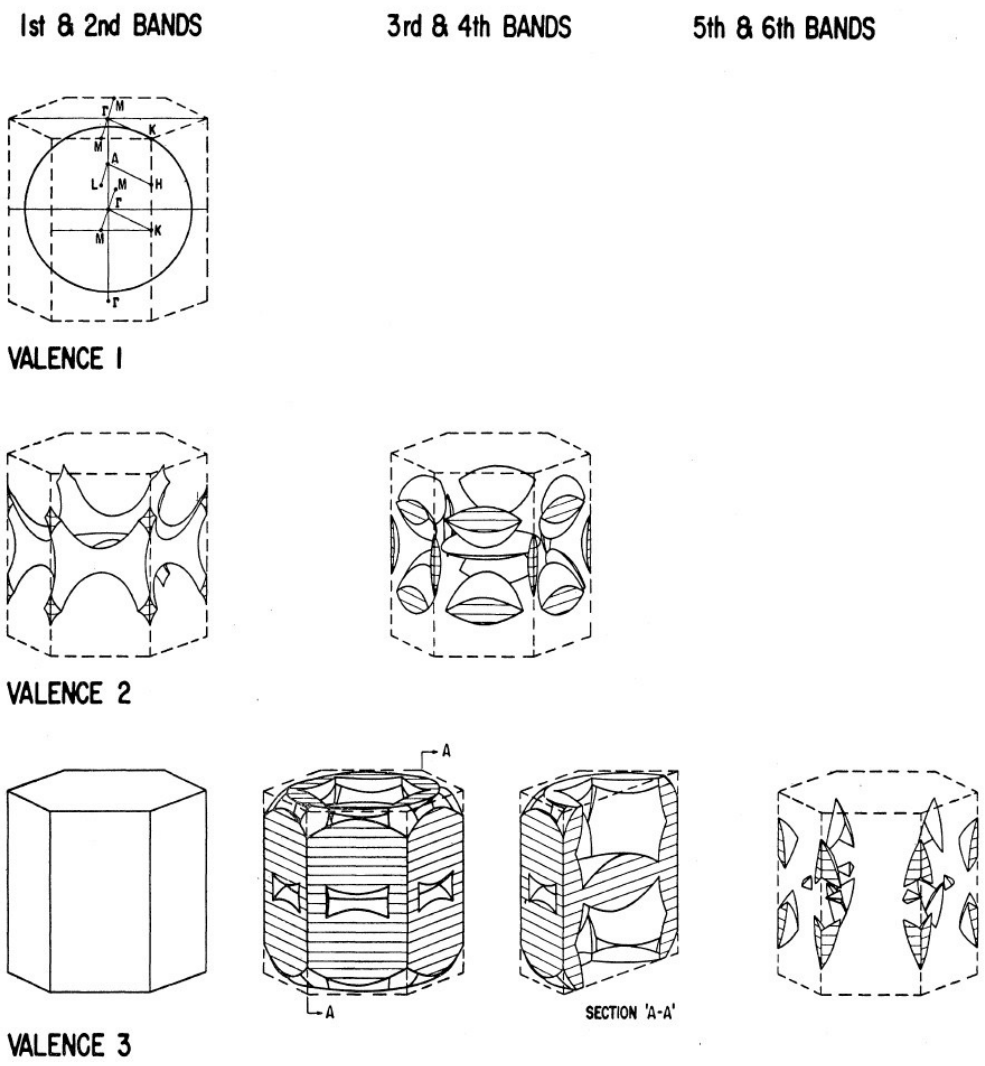
Fcc lattice


1st BAND
2nd BAND
3rd BAND
4th BAND
VALENCE 1
VALENCE 2
VALENCE 3
VALENCE 4

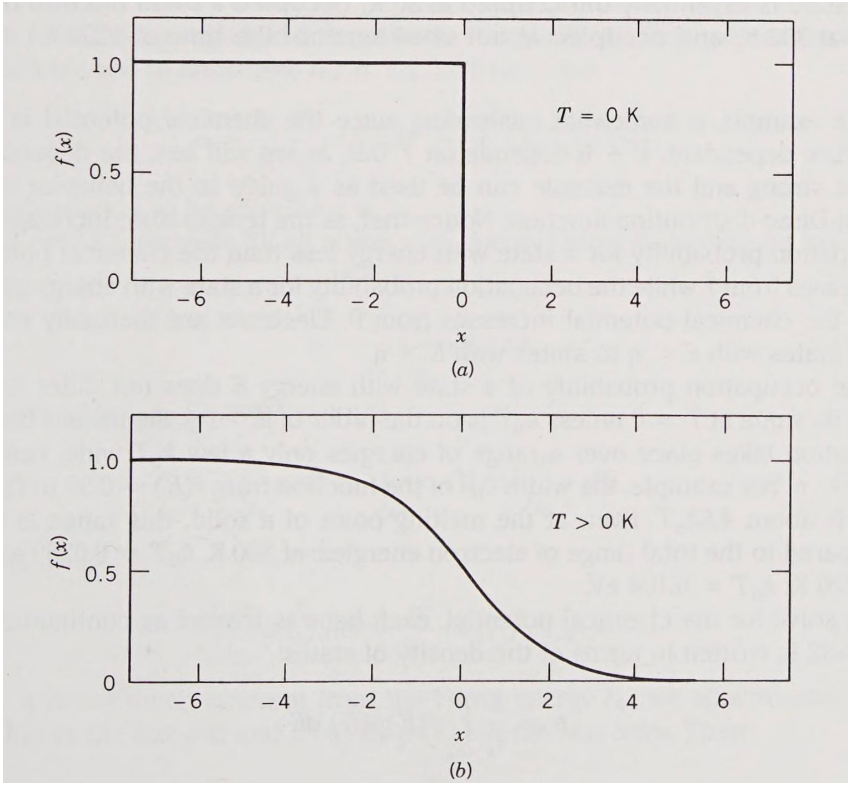
Bcc lattice


1st BAND
2nd BAND
3rd BAND
4th BAND
VALENCE 1
VALENCE 2
VALENCE 3
VALENCE 4

Hexagonal lattice



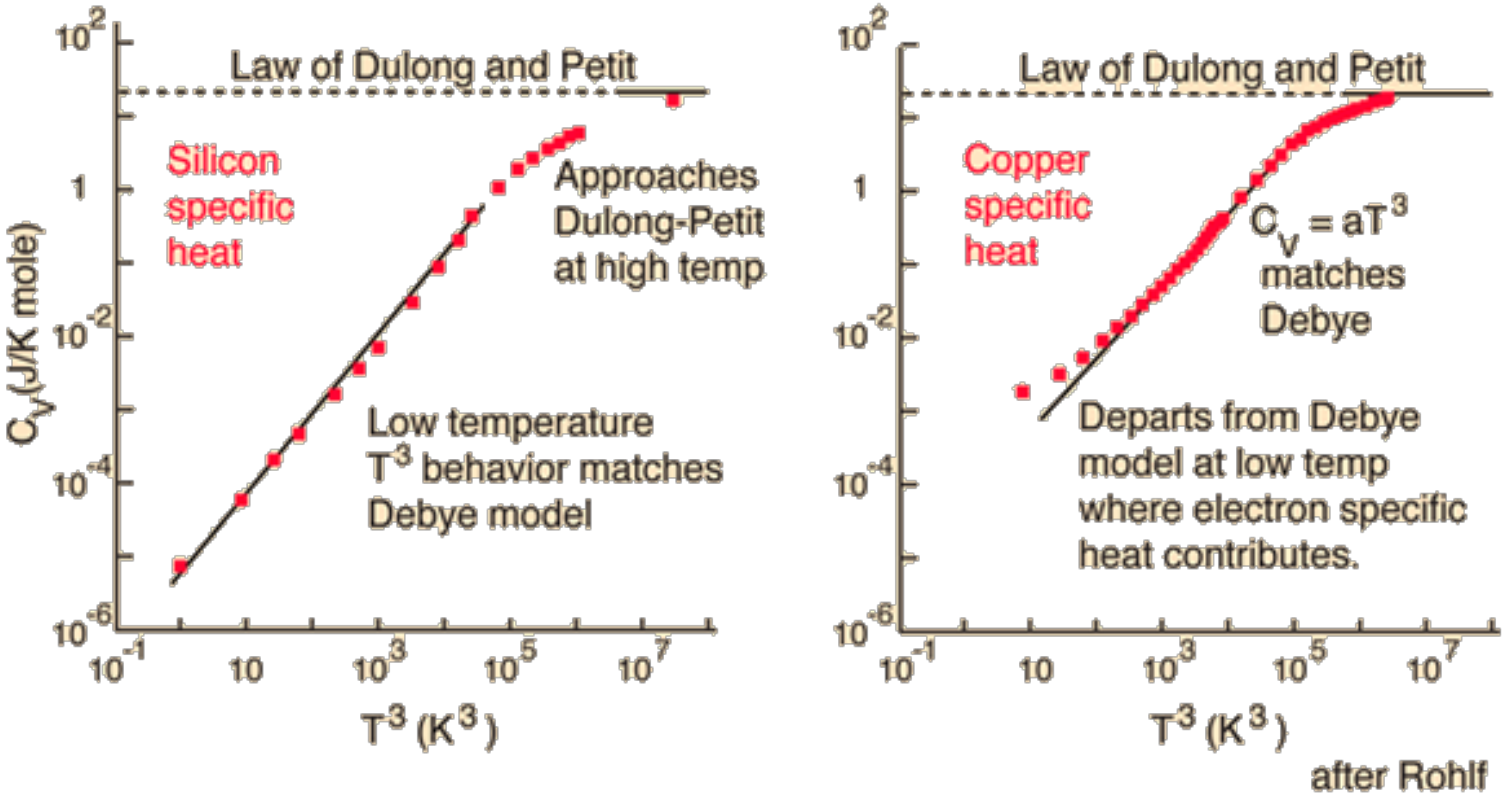
Fermi-Dirac distribution

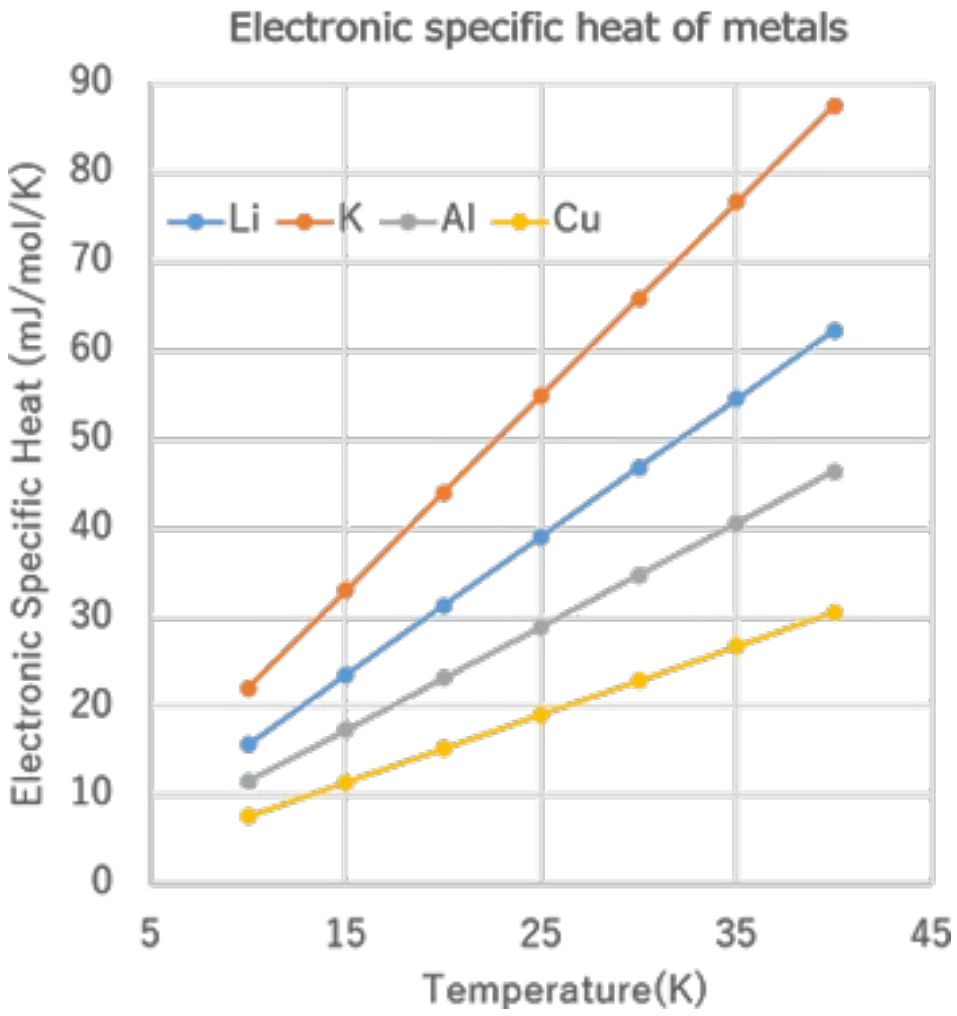


Electronic specific heat

$$C_{electrons} = \frac{\pi^2 N_A k^2 T}{2E_F} mole^{-1}$$

Specific heat of solids




Electronic specific heat of metals
Electronic Specific Heat (mJ/mol/K)
90
80
70
60
50
40
30
20
10
0
Li
K
Al
Cu
5
15
25
35
45
Temperature(K)