PYL 102

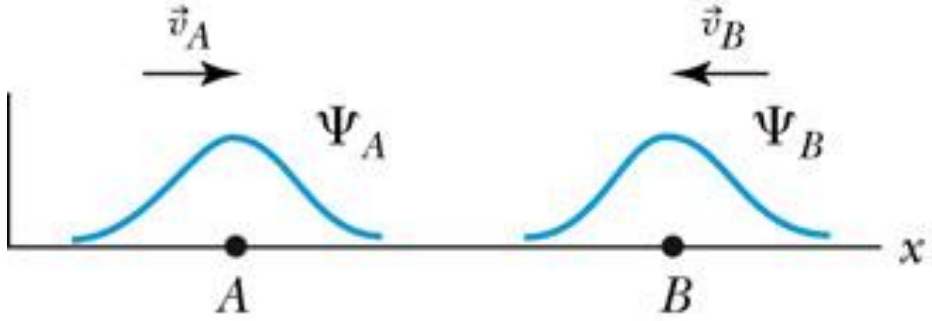
Wednesday, Sept. 25, 2024

Kronig Penney model

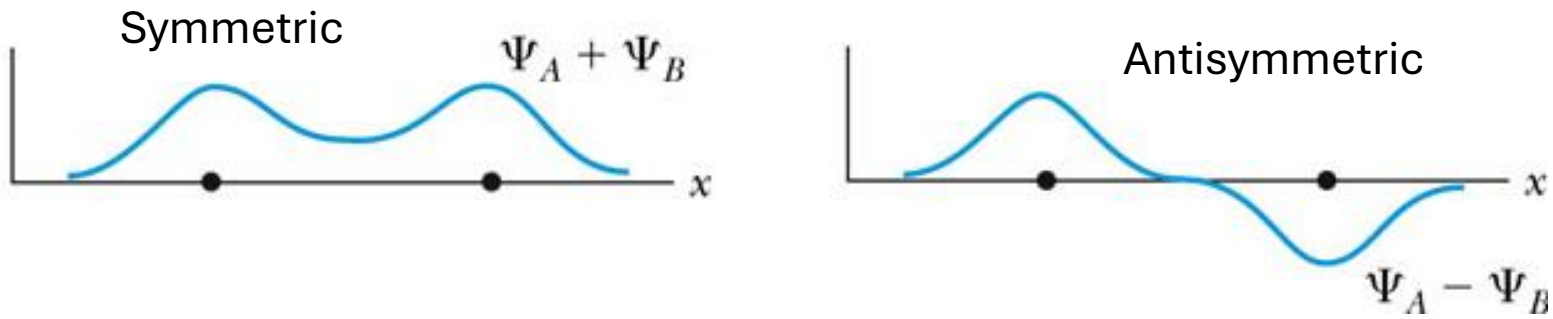
Band Theory of Solids

- The essential feature of the band theory is that the allowed energy states for electrons are nearly continuous over certain ranges, called **energy bands**, with forbidden energy gaps between the bands.

- Consider initially the known wave functions of two hydrogen atoms far enough apart so that they do not interact.



Interaction of the wave functions occurs as the atoms get closer



An electron in the symmetric state has a nonzero probability of being halfway between the two atoms, while an electron in the antisymmetric state has a zero probability of being at that location

- In the symmetric case the binding energy is slightly stronger resulting in a lower energy state.
  - Thus there is a splitting of all possible energy levels (1*s*, 2*s*, and so on).

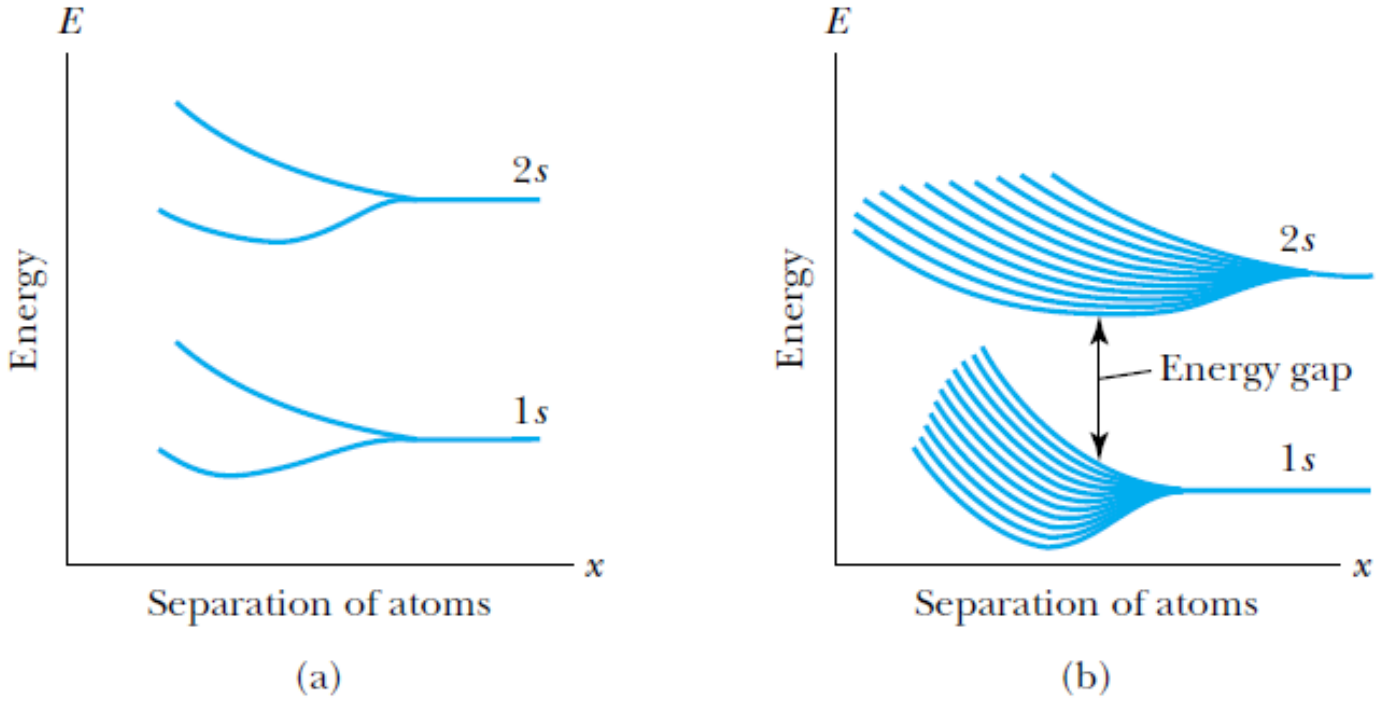
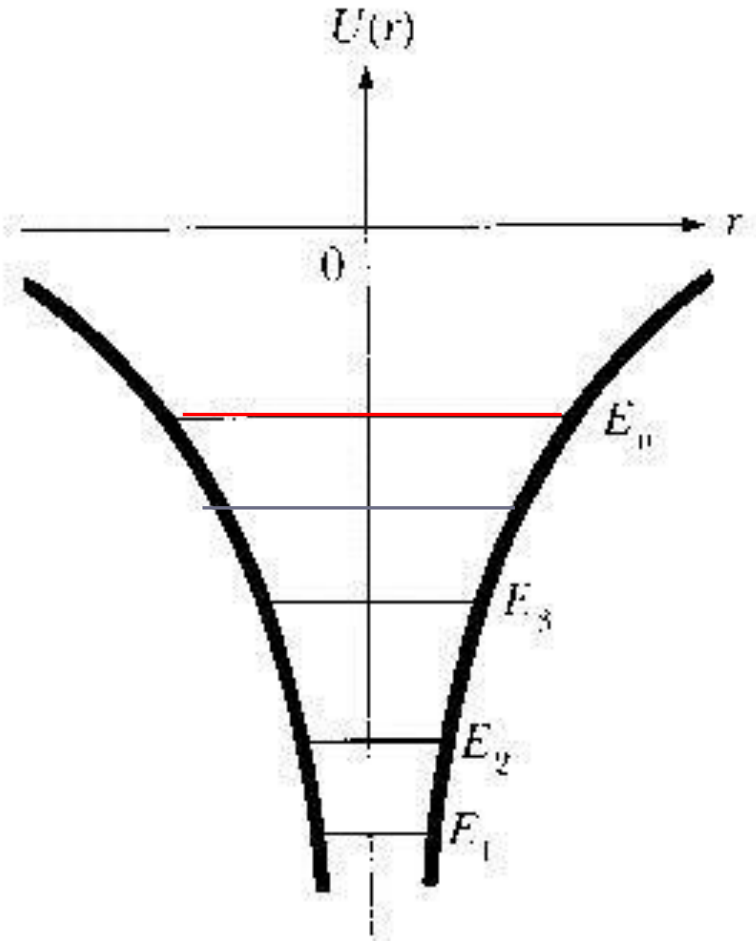
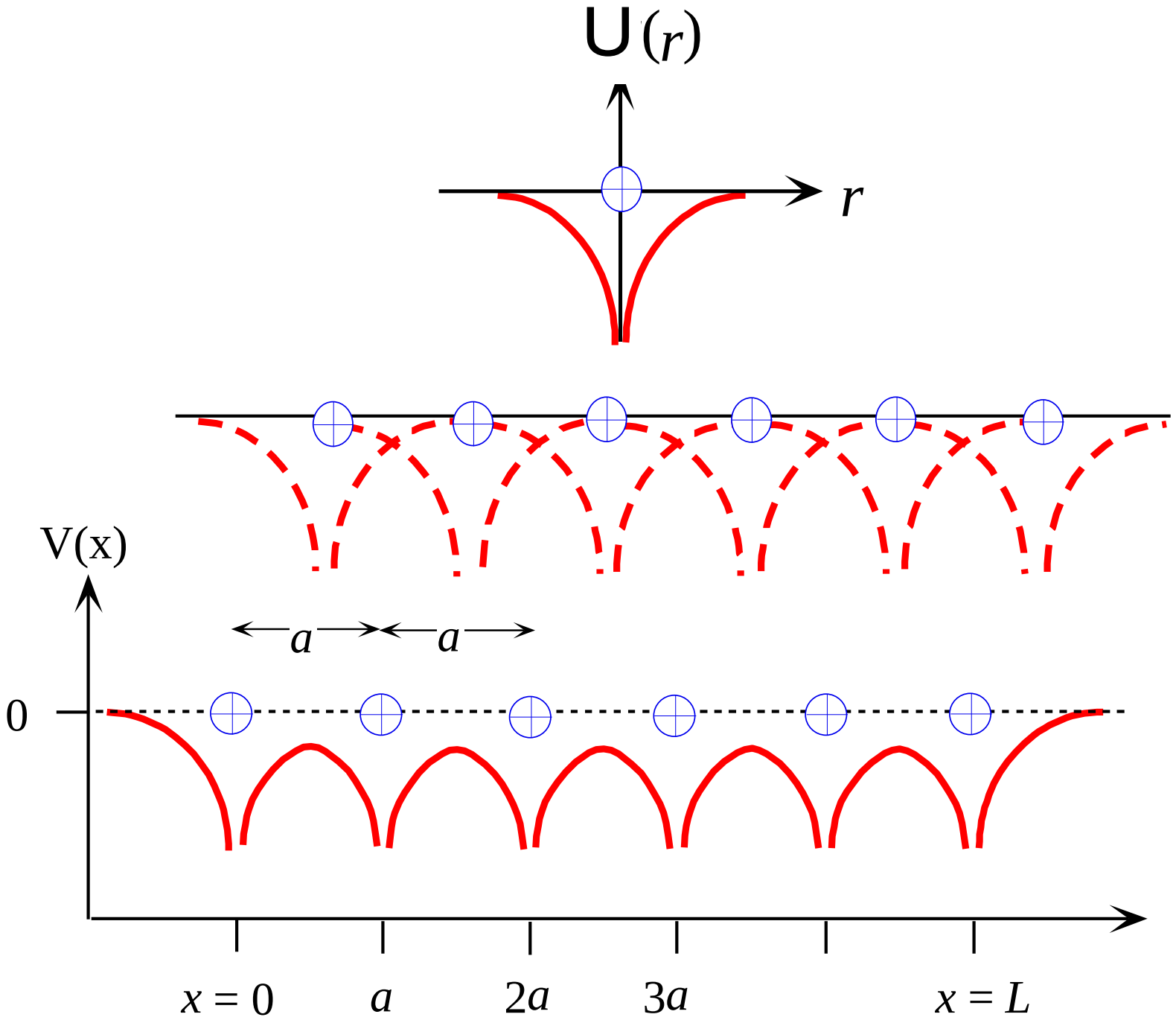


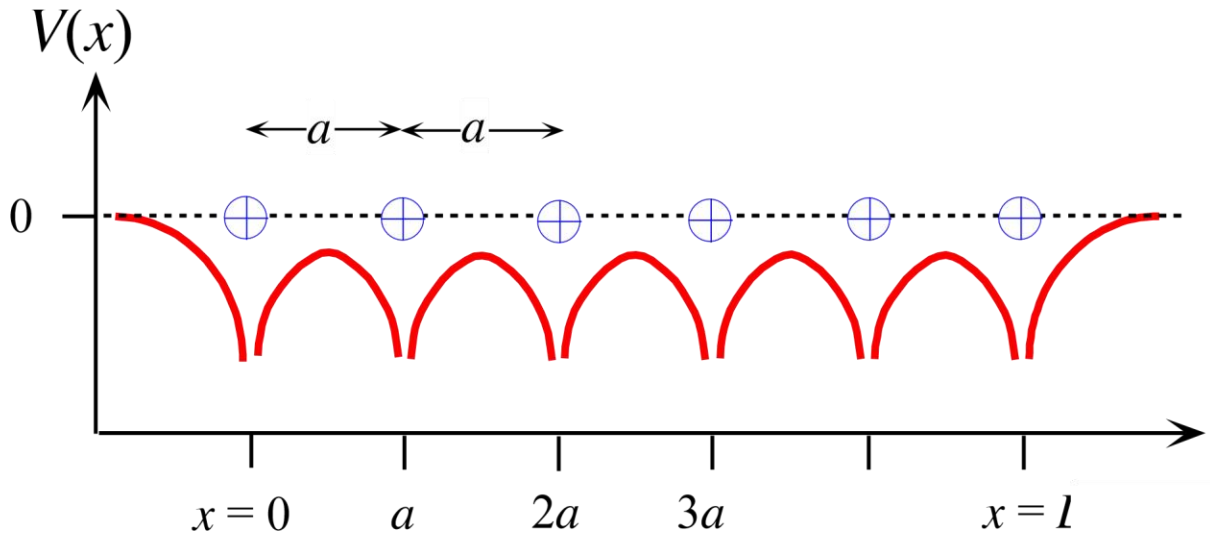
Figure 11.3 The 1*s* and 2*s* energy-level splittings of approaching hydrogen atoms for (a) 2 atoms and (b) 11 atoms. Notice the splitting of each energy level into a nearly continuous band.

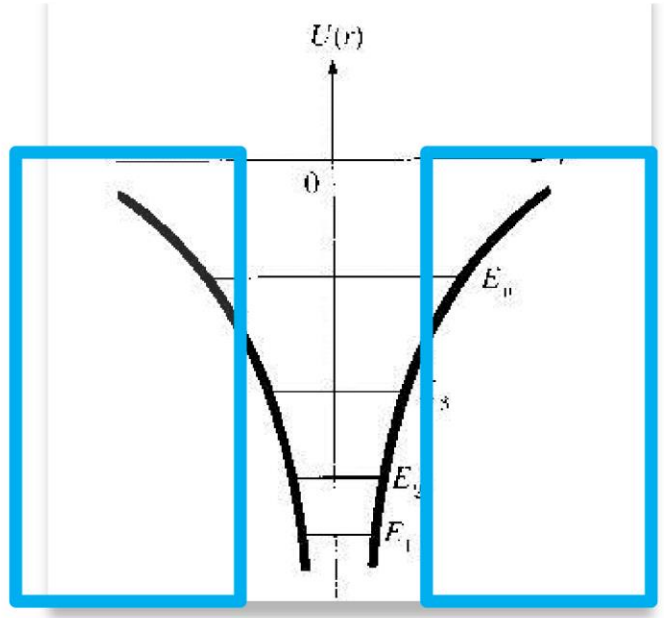
Potential energy of an isolated atom

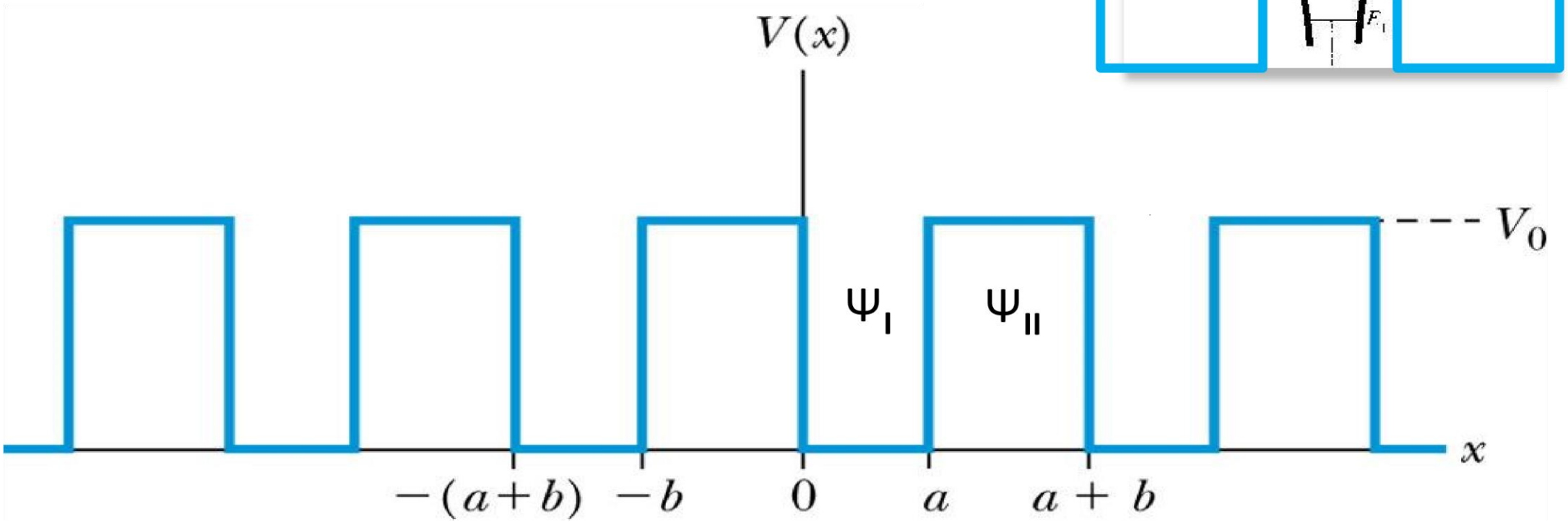


$$U(r) = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$


U(r)
r
V(x)
a
a
0
x = 0
a
2a
3a
x = L

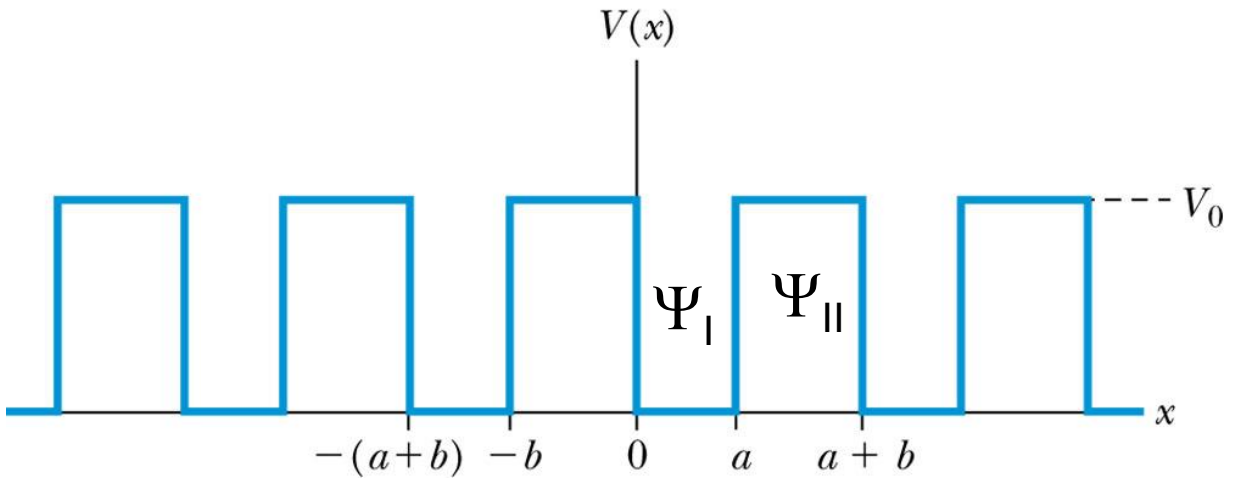

V(x)
a
a
0
x = 0
a
2a
3a
x = l

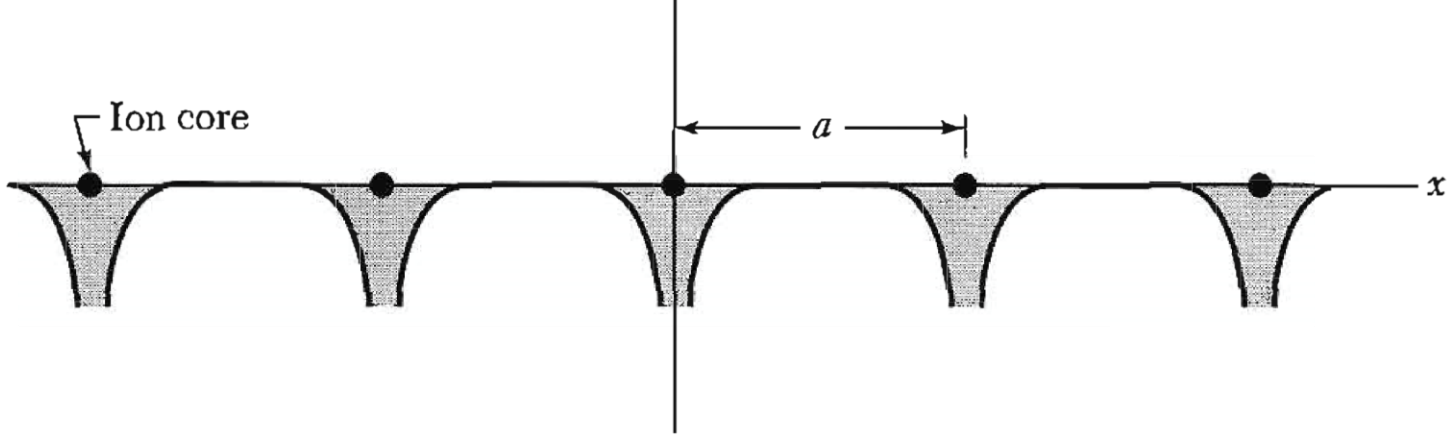

U(r)
0


V(x)
V0
Ψ I
Ψ II
x
−(a+b)
−b
0
a
a + b

Kronig-Penney Model

- Kronig and Penney assumed that an electron experiences an infinite one-dimensional array of finite potential wells.
- Each potential well models attraction to an atom in the periodic structure, so the size of the wells must correspond roughly to the lattice spacing.





Bloch function $\Psi_K(x) = u\ (x) \cdot e^{i K x}$

Bloch's theorem states that solutions to the Schrödinger equation in a periodic potential can be expressed as plane waves modulated by periodic functions (crystal potential here).

Since the electrons are not free their energies are less than the height V_0 of each of the potentials, but the electron is essentially free in the region $0 < x < a$, where it has a wave function of the form

$$\psi = Ae^{ikx} + Be^{-ikx}$$

where the wave number k is given by the usual relation:

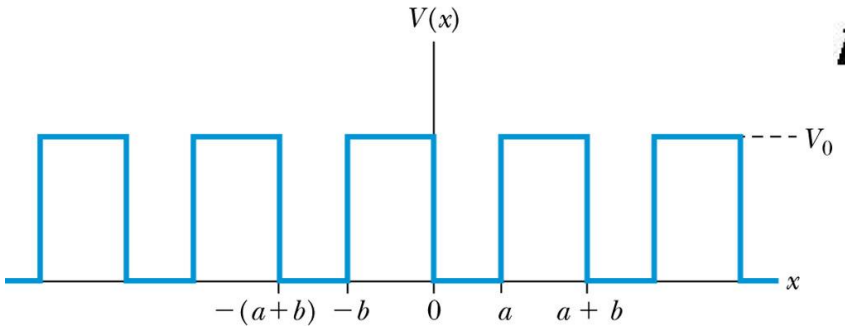
$$k^2 = 2mE / \hbar^2$$

Tunneling

- In the region between $a < x < a + b$ the electron can tunnel through and the wave function loses its oscillatory solution and becomes that of an evanescent wave

$$\psi = Ce^{\kappa x} + De^{-\kappa x}$$

$$\kappa^2 = 2m(V_0 - E)/\hbar^2$$



Boundary conditions: Field continuity and periodic structure to solve for A,B,C and D coefficients

$$\Psi_I(x = 0) = \Psi_{II}(x = 0)$$

$$\frac{d\Psi_I}{dx}(x = 0) = \frac{d\Psi_{II}}{dx} \quad (x = 0)$$

$$\Psi_I(x = a) = \Psi_{II}(x = -b)$$

$$\frac{d\Psi_I}{dx}(x = a) = \frac{d\Psi_{II}}{dx} \quad (x = -b)$$

- Matching solutions at the boundary:

$$\frac{\kappa^2 b}{2k}\sin(ka)+\cos(ka)=\cos(Ka)$$

Right-hand-side of equation is bounded $-1<\cos(Ka)<1$

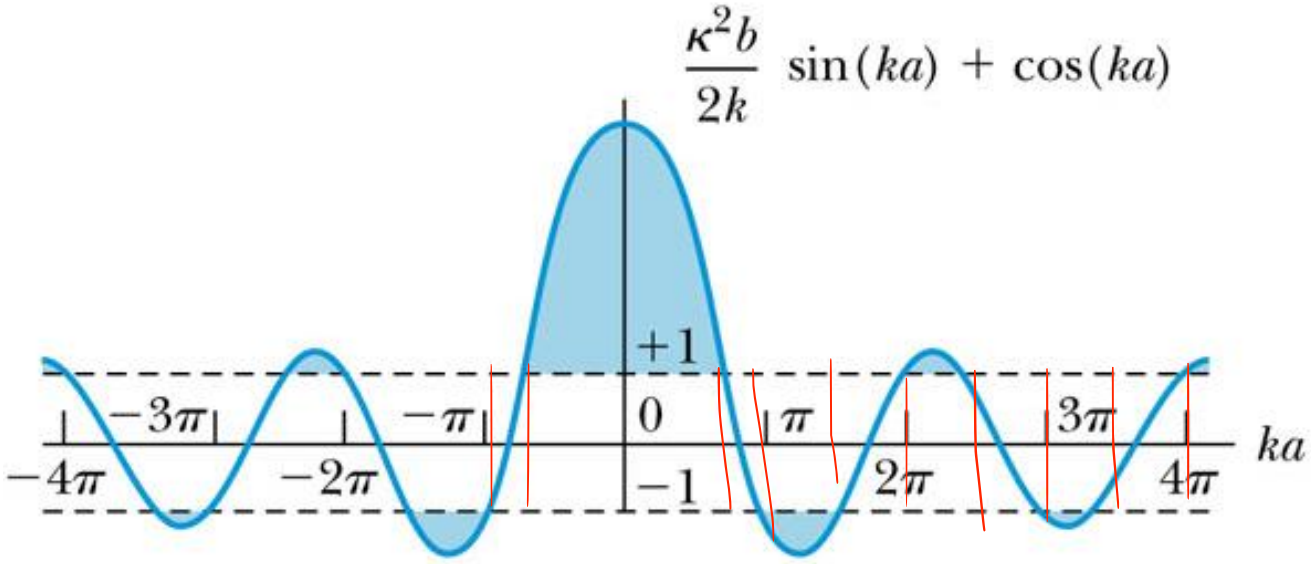
While on the left-hand-side of equation is not bounded within ±1.

Therefore, in order to have non-trivial solution of equation, the parameter *k* or ultimately the electron energy E only has certain allowed values, while other values are forbidden. This gives an explanation of allowed and forbidden energy bands.

Allowed energy band: $\left| \frac{\kappa^2 b}{2k} \sin(ka) + \cos(ka) \right| \leq 1$

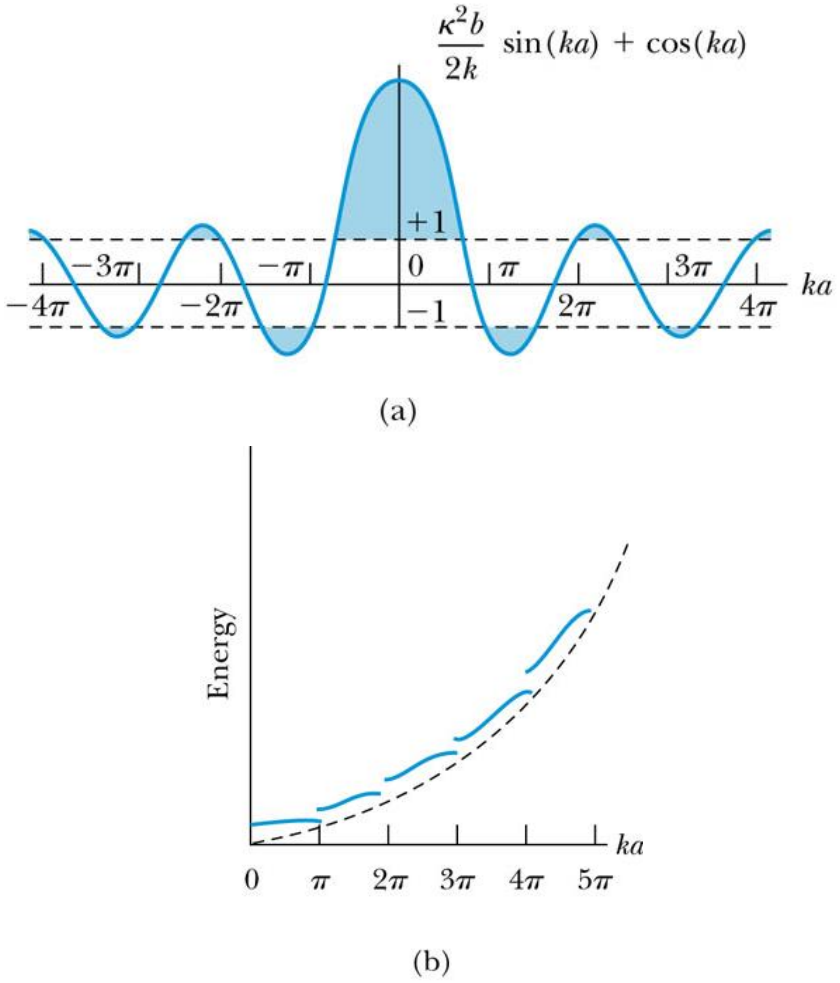
Forbidden energy band: $\left| \frac{\kappa^2 b}{2k} \sin(ka) + \cos(ka) \right| > 1$

- Plotting this it is observed there exist restricted (shaded) **forbidden zones** for solutions.



The Forbidden Zones

Plot of the left side of Equation versus *ka* for $\kappa^2 ba / 2 = 3\pi / 2$. Allowed energy values must correspond to the values of *k* for $k = \sqrt{2mE/\hbar^2}$ for which the plotted function lies between -1 and +1. Forbidden values are shaded in light blue. (b) The corresponding plot of energy versus *ka* for $\kappa^2 ba/2 = 3\pi/2$, showing the forbidden energy zones (gaps).



Differences between the Kronig-Penney model and the single potential well

- For an infinite crystal structure (translation periodic lattice) the allowed energies within each band are continuous rather than discrete. In a real crystal the lattice is not infinite, but even if chains are thousands of atoms long, the allowed energies are nearly continuous.

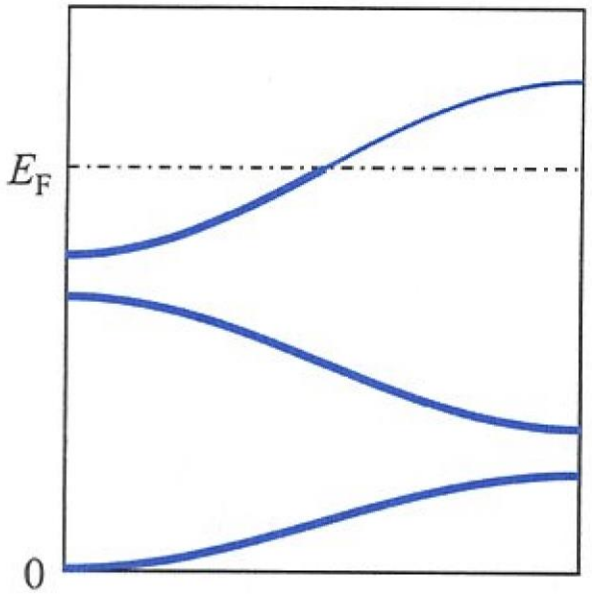
- In a real three-dimensional crystal it is appropriate to speak of a **wave vector** $\vec{k}$ The allowed ranges for $\vec{k}$ constitute what are referred to in solid state theory as **Brillouin zones**.

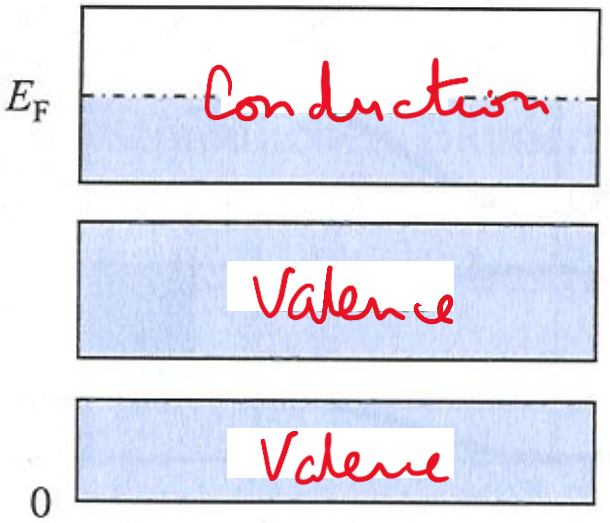
- In a real crystal the potential function is more complicated than the Kronig-Penney squares. Thus, the energy gaps are by no means uniform in size. The gap sizes can be changed by the introduction of impurities or imperfections of the lattice.

- These facts concerning the energy gaps are of paramount importance in understanding the electronic behavior of semiconductors.

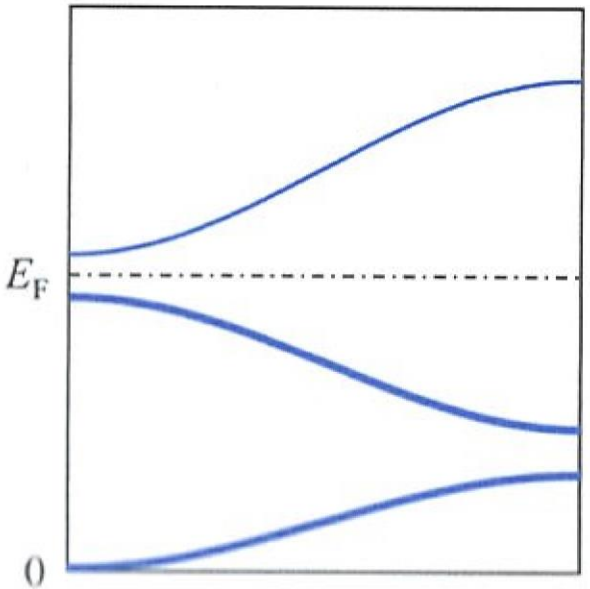
Band Theory and Conductivity

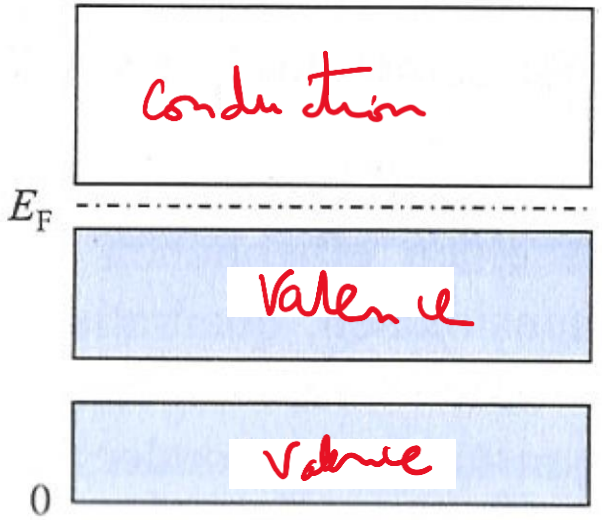
- Band theory helps us to understand what makes a conductor, insulator, or semiconductor.
    1) Good conductors like copper can be understood using the free electron
    2) It is also possible to make a conductor using a material with its highest band filled, in which case no electron in that band can be considered free.
    3) If this filled band overlaps with the next higher band, however (so that effectively there is no gap between these two bands) then an applied electric field can make an electron from the filled band jump to the higher level.
- This allows conduction to take place, although typically with slightly higher resistance than in normal metals. Such materials are known as **semimetals**.



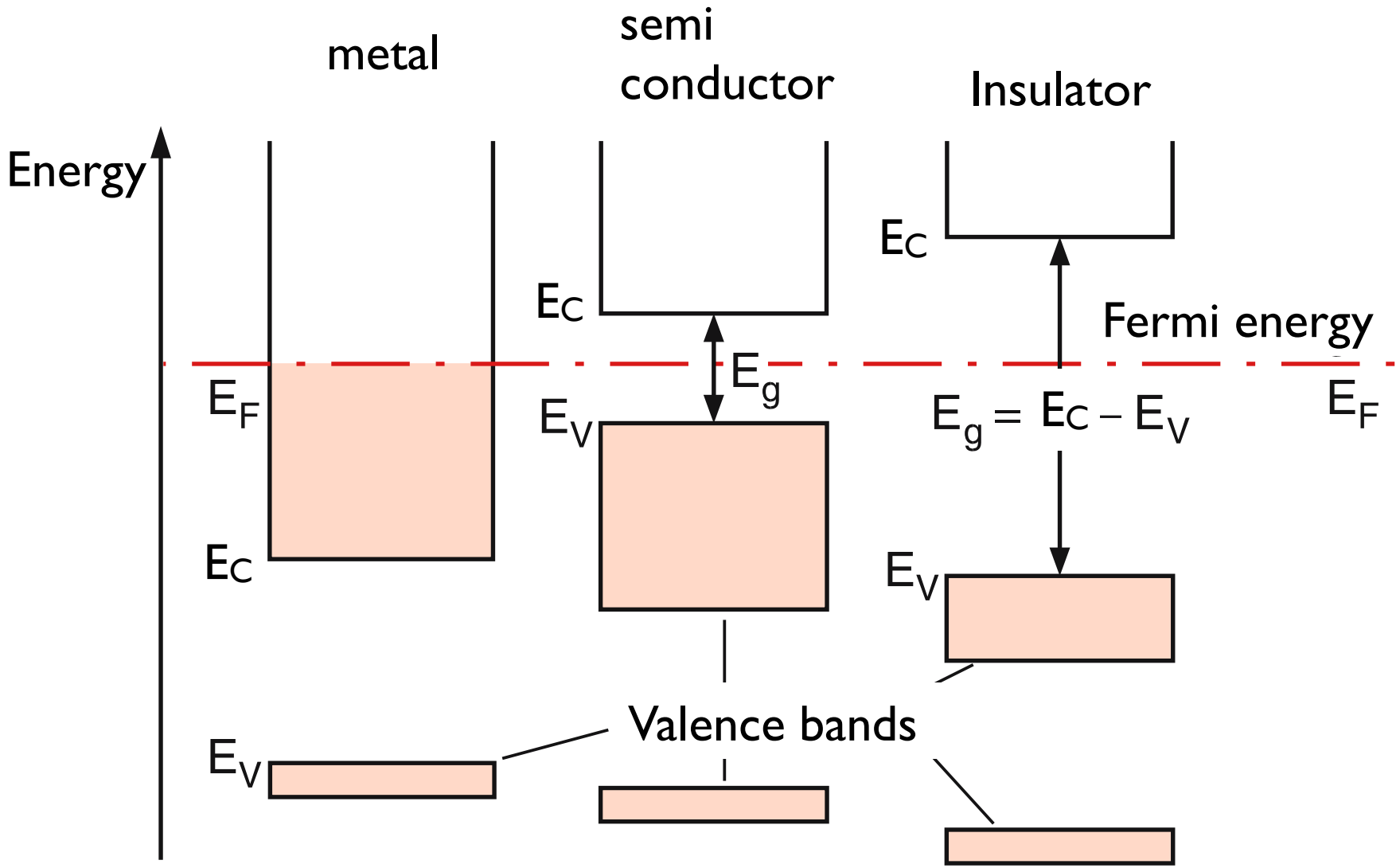


Metal





Insulator


metal
semi
conductor
Insulator
Energy
Ec
Fermi energy
Eg
EF
Ev
Eg = Ec – Ev
EF
Ec
Ev
Valence bands
Ev