Chapter 7: Energy Bands

Chris Wiebe

Phys 4P70

Nearly-free Electron Model

- Successes of the Free Electron Model:

1. Heat Capacity (~T at low temperatures)
2. Electrical Conductivity
3. Thermal Conductivity

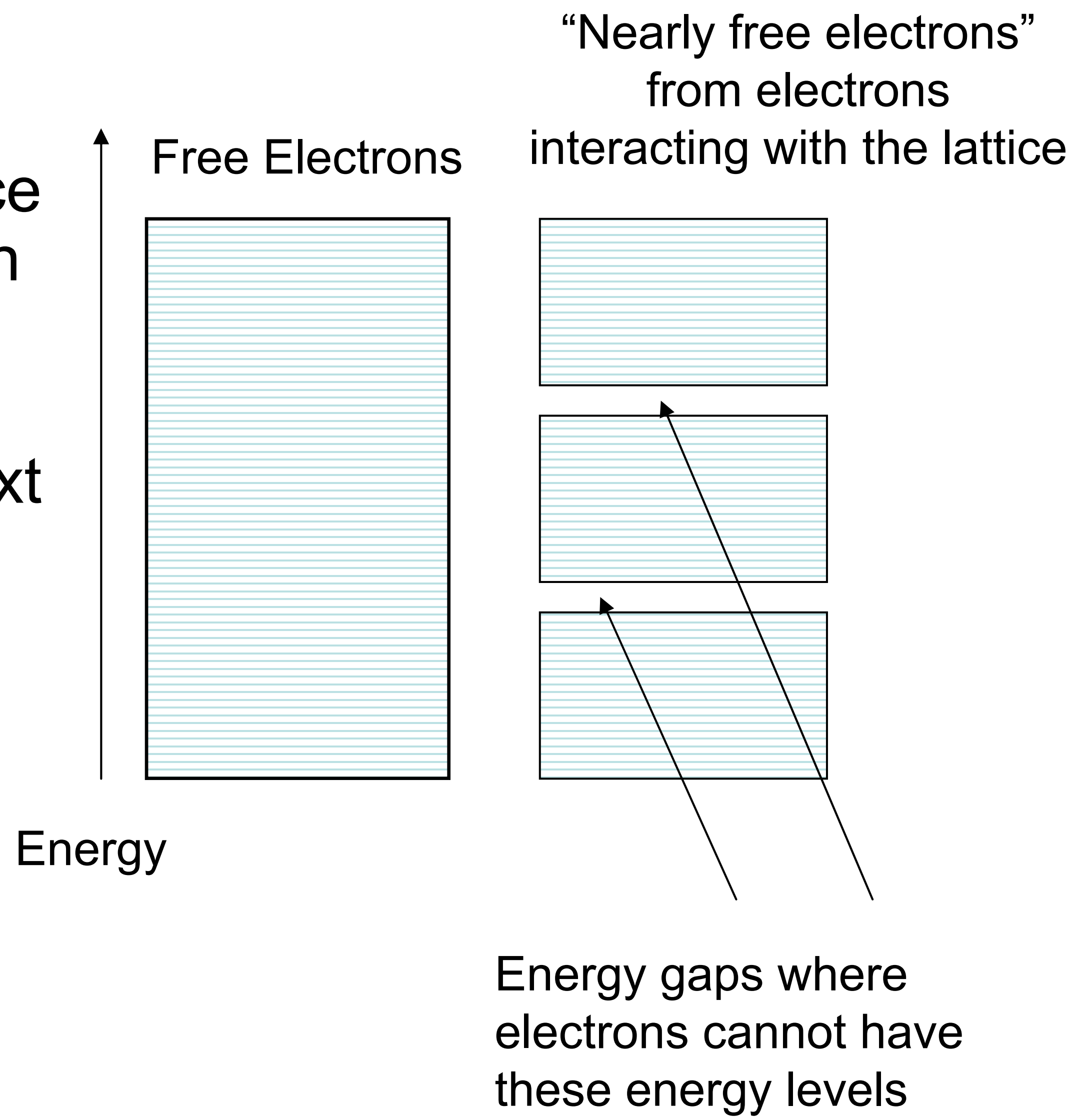
- However, it does not explain:

1. Physical differences between conductors, semiconductors, insulators
2. Positive Hall Coefficients (R_H values)

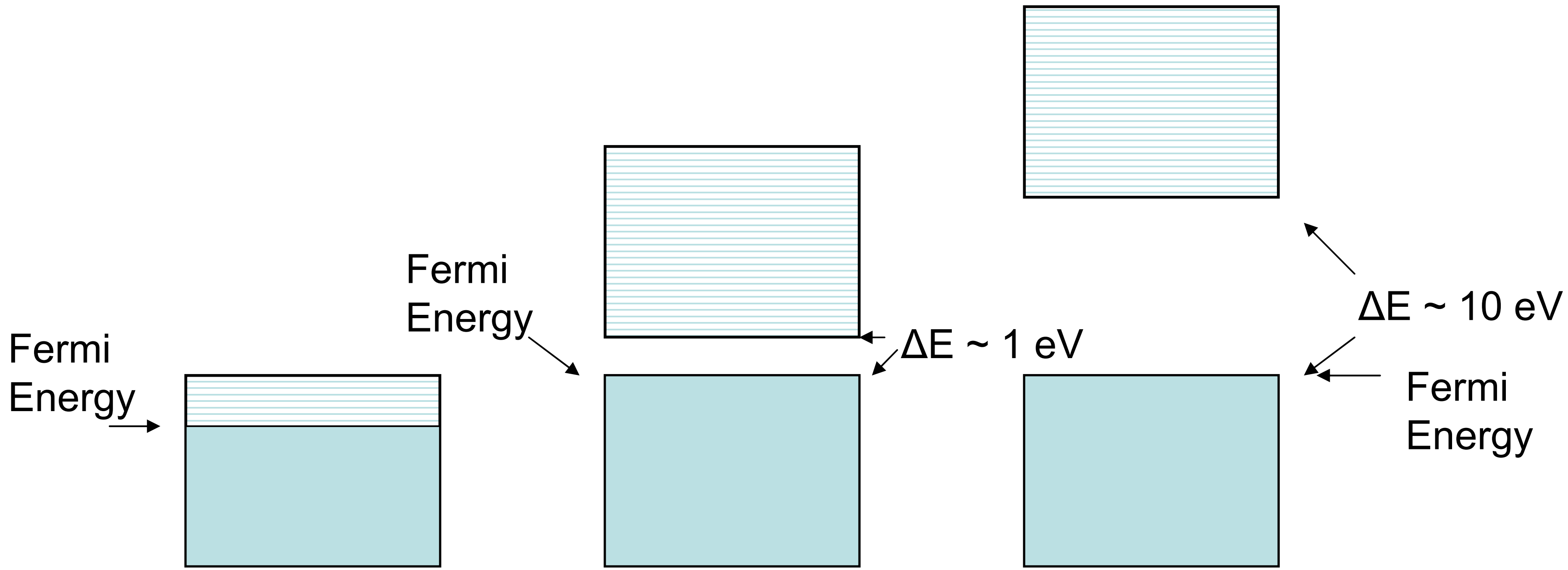
- This gives rise to the nearly-free electron model (the electrons can now interact with the periodic latttice)

Physical Picture

- The interactions of the electrons with the lattice result in energy gaps in the possible electron levels
- We will show in the next section how energy gaps can arise in a simple periodic lattice (much more complicated models exist)



Conductors, Insulators, Semiconductors



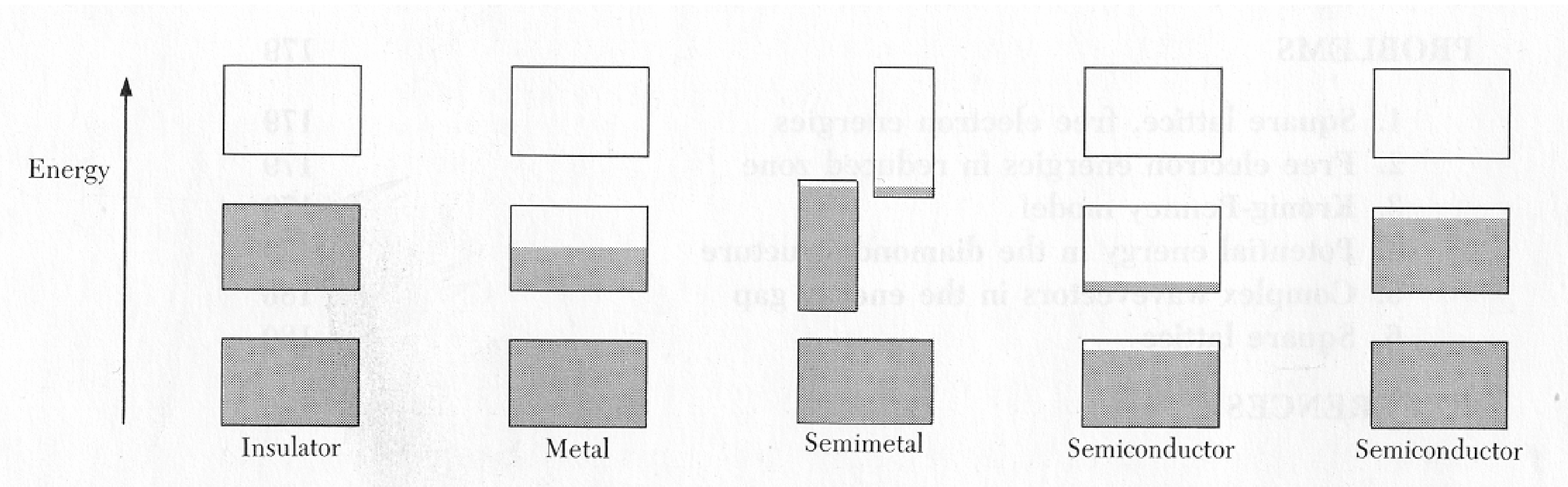
Conductor:
Fermi energy lies within a band of accessible states

Semiconductor:
Fermi energy lies in the gap, gap is relatively small in size (~1 eV) so that some e^-'s can be excited

Insulator: Fermi energy lies in the gap, gap is relatively large in size (~10 eV – electrons cannot be excited to higher states)

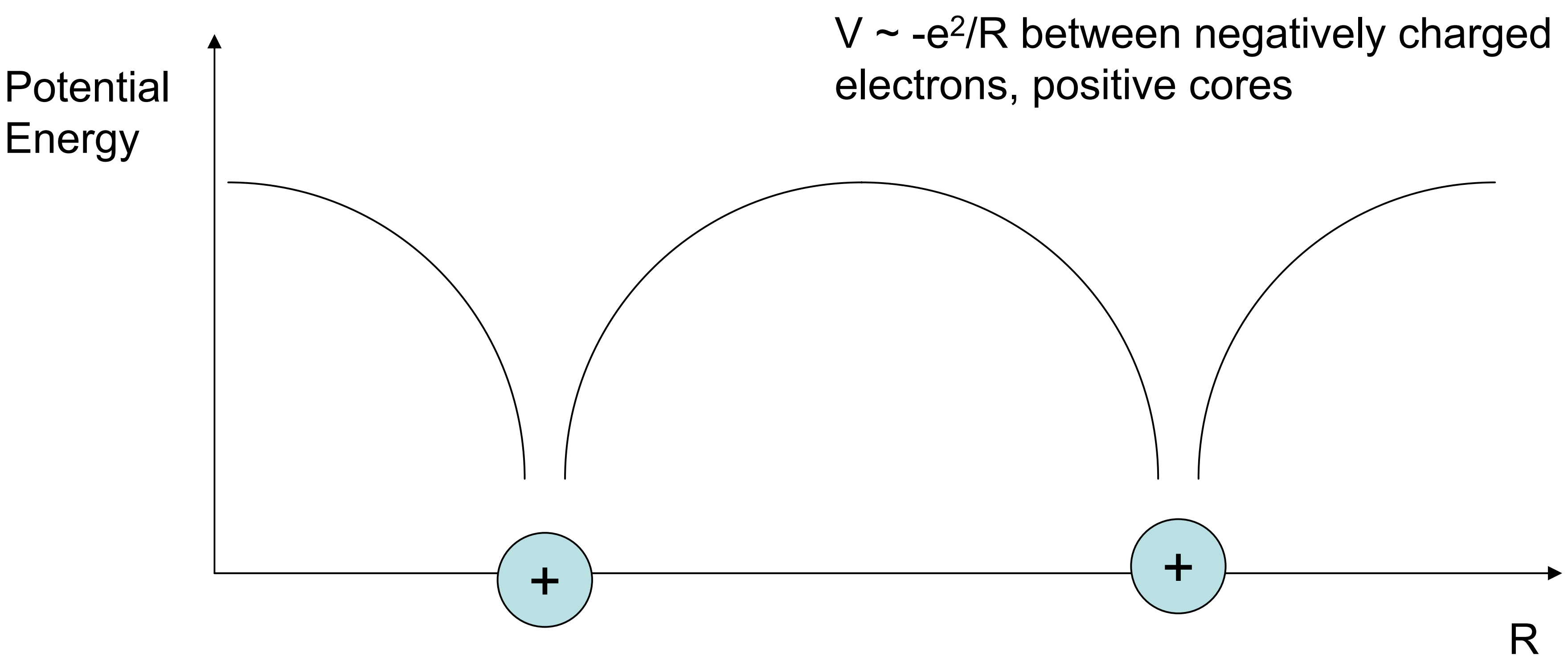
More complicated materials

- Even more complicated energy “band” structures exist:



Physical origin of the gap

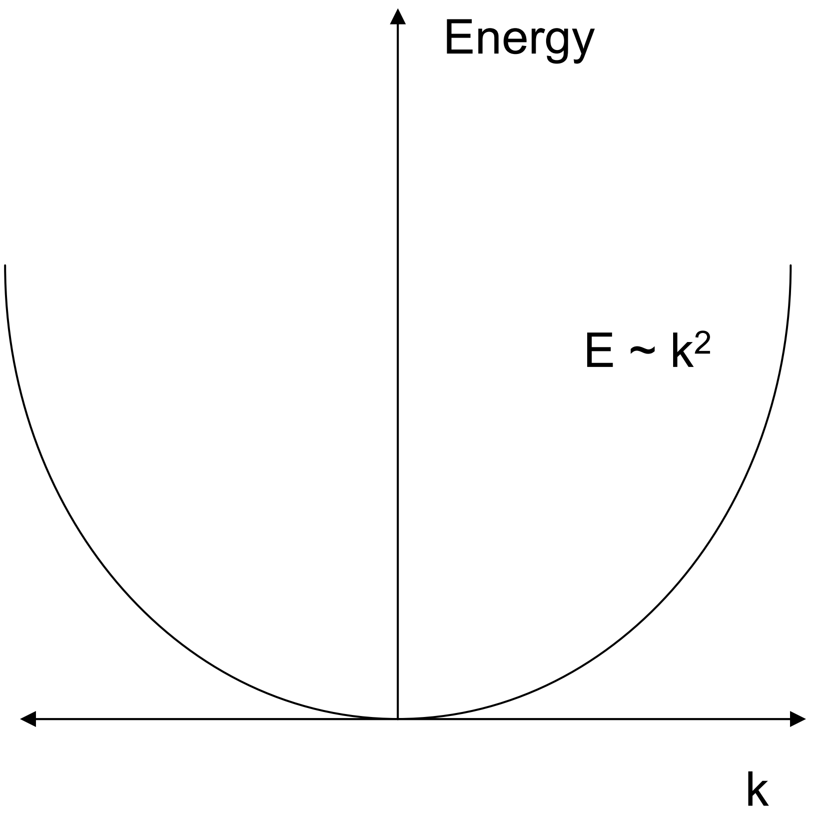
- Where does the gap come from?
- Before, we had the free electron model. Now, we are going to add a periodic potential



Nearly Free Electron Model

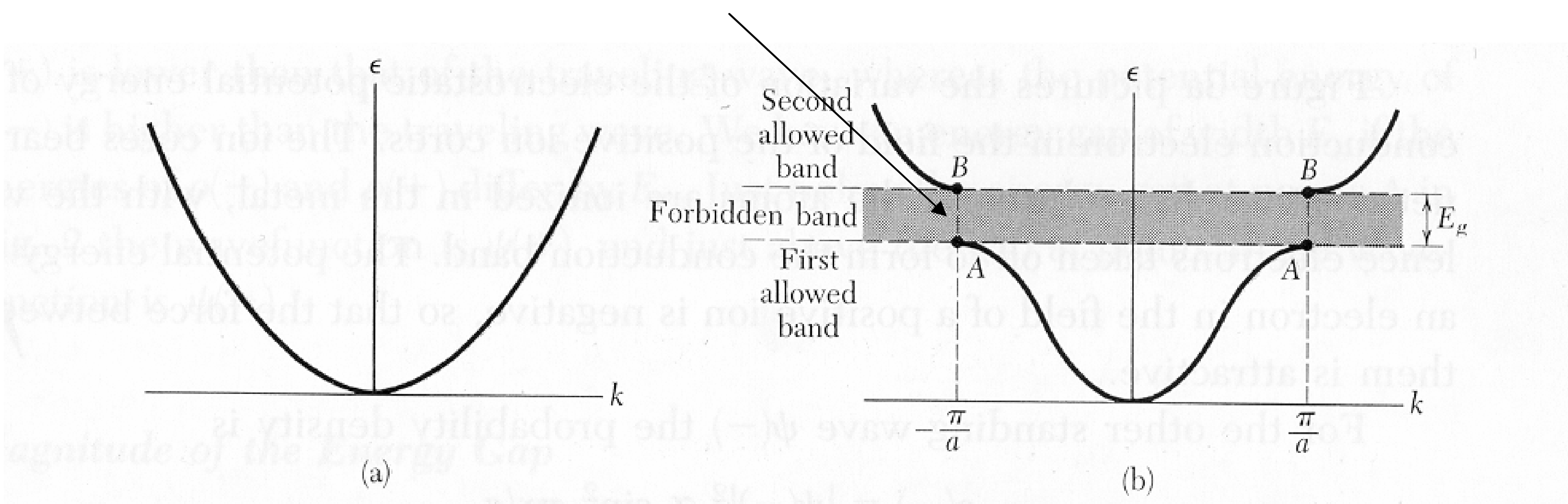
- What is the dispersion curve of the free electron model?
- Electrons have an energy $E = \hbar\omega = (\hbar k)^2/2m$

  (where $k^2 = k_x^2 + k_Y^2 + k_z^2$)
- The free electron wavefunction are plane waves of the form $\psi_k(r) = \exp(i\, k \cdot r)$, which are running waves of momentum $p = \hbar k$
- So, these are particles which can have any k value
- What happens when we add a periodic lattice of lattice constant a?



Periodic Potential

- Effect of the periodic potential: particles (behaving like waves) which are moving through a lattice spaced by lattice constant a
- Electrons diffract from the periodic lattice!
- This is the physical origin of the band gap – there are some electron energy levels which are forbidden because the electron waves cancel themselves out at these wavelengths!
- What wavelengths are these?
- At the zone boundary: k = +/- π/a

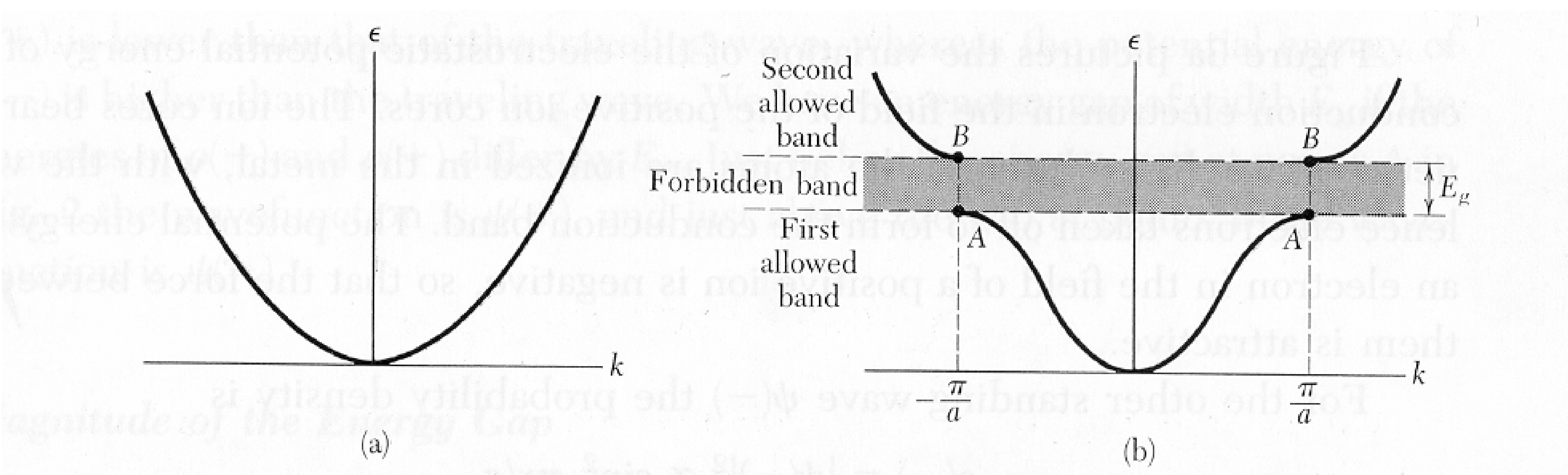


Free electron model

Nearly free electron model

Periodic lattice

- There is an analogy between electron waves and lattice waves (phonons)
- For most value of the dispersion curve, the electrons move freely throughout the lattice (there is a group velocity that is non-zero = dω/dK)
- At the zone boundary (K = +/- π/a) , there are only standing waves (dω/dK = 0).
- What standing wave solutions are stable with these k-values?



Periodic Lattice

- The simplest solution is a combination of wavefunctions of the electrons

$$\Psi_1 = \exp(ikx) = \exp(i\frac{\pi x}{a})$$

$$\Psi_2 = \exp(-ikx) = \exp(-i\frac{\pi x}{a})$$

$$\rightarrow \Psi^+ = \Psi_1 + \Psi_2 = \exp(ikx) + \exp(-ikx) = 2\cos\left(\frac{\pi x}{a}\right)$$

$$\rightarrow \Psi^- = \Psi_1 - \Psi_2 = \exp(ikx) - \exp(-ikx) = 2i\sin\left(\frac{\pi x}{a}\right)$$

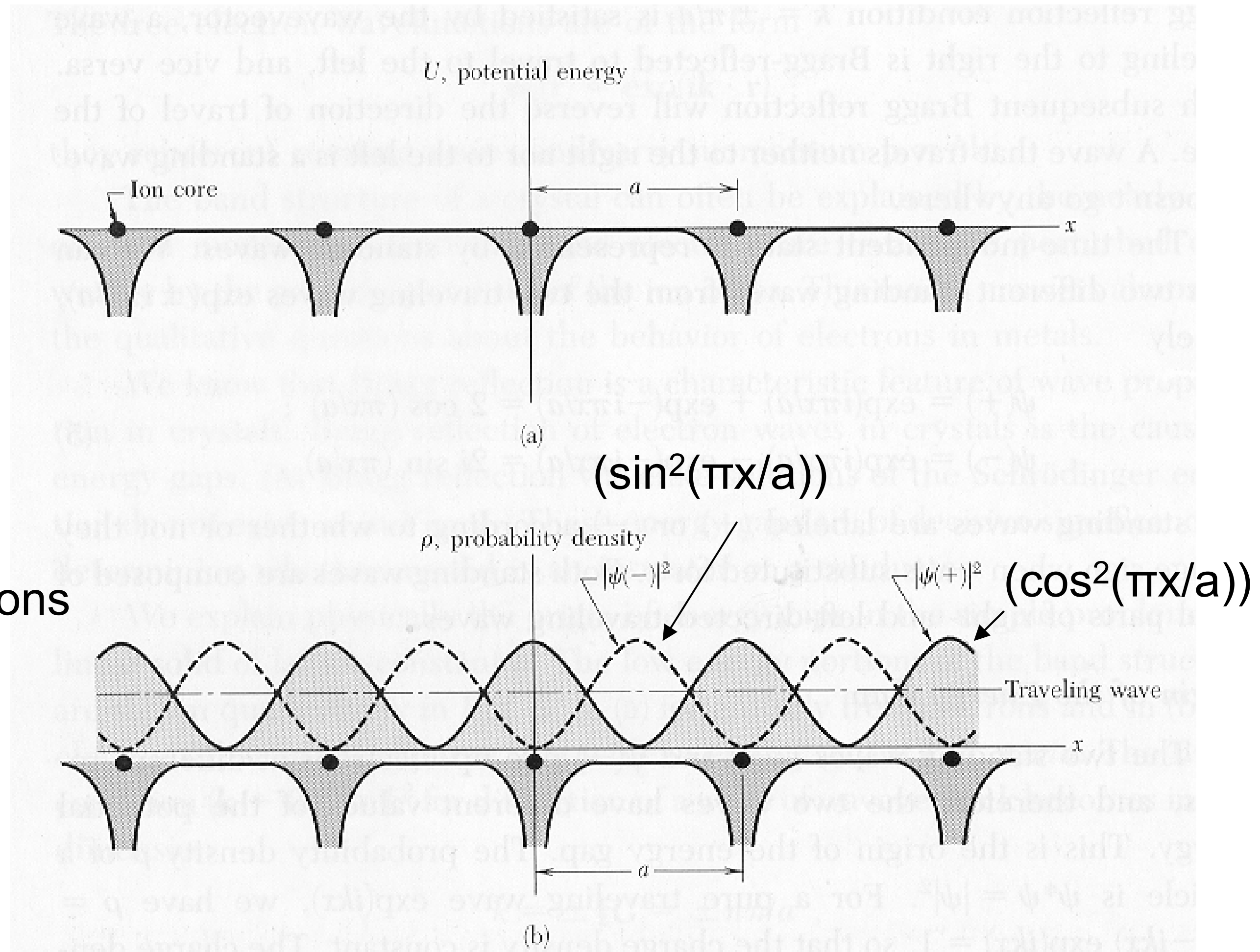
- Note: the combinations of these 2 travelling waves (exp(ikx)) give standing wave solutions (sin and cos)

Periodic Lattice

- What does the electron density (ψ^2) look like?

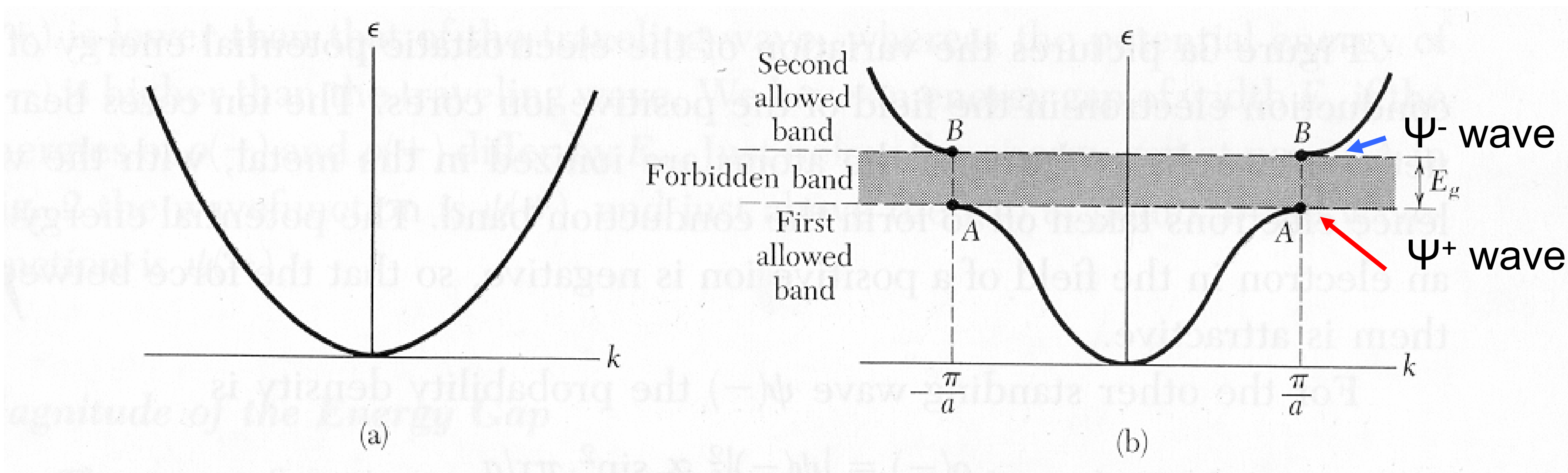
Note: only electrons which have a wavelength commensurate with the lattice ($k = \pi/a$) feel the periodic potential, and they form standing wave patterns

One of these (+) has electrons near the positive cores, the other has the electrons in netween the cores
(so they have different energies)



The Energy Gap

- So, there are 2 solutions for the energies at this K-value
- This is what gives rise to the energy gap



$$E_g = \int U(x)[|\psi^+|^2 - |\psi^-|^2]dx$$

(difference between the expectation values of these 2 energy levels)