Summary of last lecture

- Free electron gas model: application to a metal
  - Fermi energy
  - Heat capacity
  - Electrical conductivity
  - Successes and failures

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Aims of this lecture

- Nearly free electron model:
  - Bragg reflection a the BZ boundary
  - Appearance of energy gaps
  - Understanding metals and insulators

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2) The nearly-free-electron model

Electrons in crystals are waves travelling in a periodic potential

We have seen (Section 3) that such waves should undergo Bragg reflection, at certain wavevectors (the edges of Brillouin zones)

In this section we give a qualitative discussion of the far-reaching consequences of the crystal potential on the behaviour of electrons in solids...

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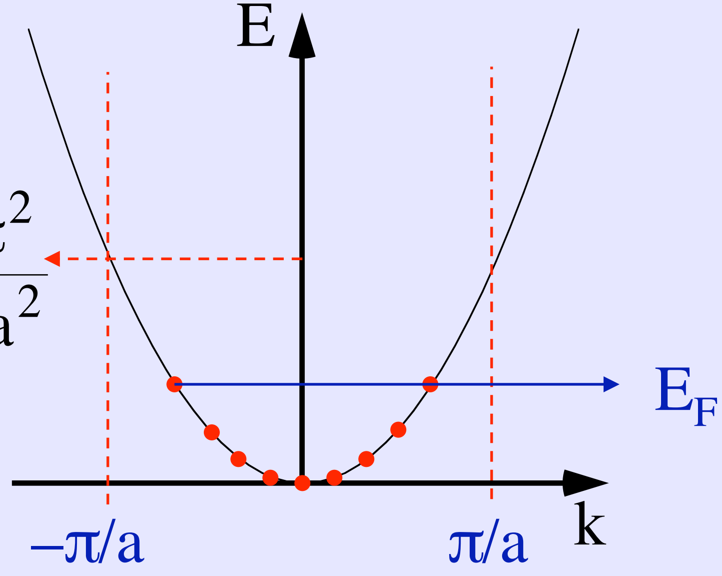
2) The nearly-free-electron model

Free electron dispersion:

...with first Brillouin zone:

$-\pi/a \rightarrow \pi/a$ $E_{BZ} = \dfrac{\hbar^2\pi^2}{2ma^2}$

(a the lattice constant)



We now know that there are discrete states on this curve which we fill up to the Fermi energy

How many electrons do we need for their k-vectors to approach the Brillouin zone edge?

2) The nearly-free-electron model

Remember our cubic array of allowed states in k-space

The volume of k-space per allowed state is $(\pi/L)^3$ (for a cube -shaped crystal, side L, ignoring spin)

Volume per state = $\frac{1}{2}\left(\frac{\pi}{L}\right)^3$ including spin

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2) The nearly-free-electron model

The volume in k-space of a Brillouin zone (assuming a simple cubic lattice, lattice constant a) is $(\pi/a)^3$

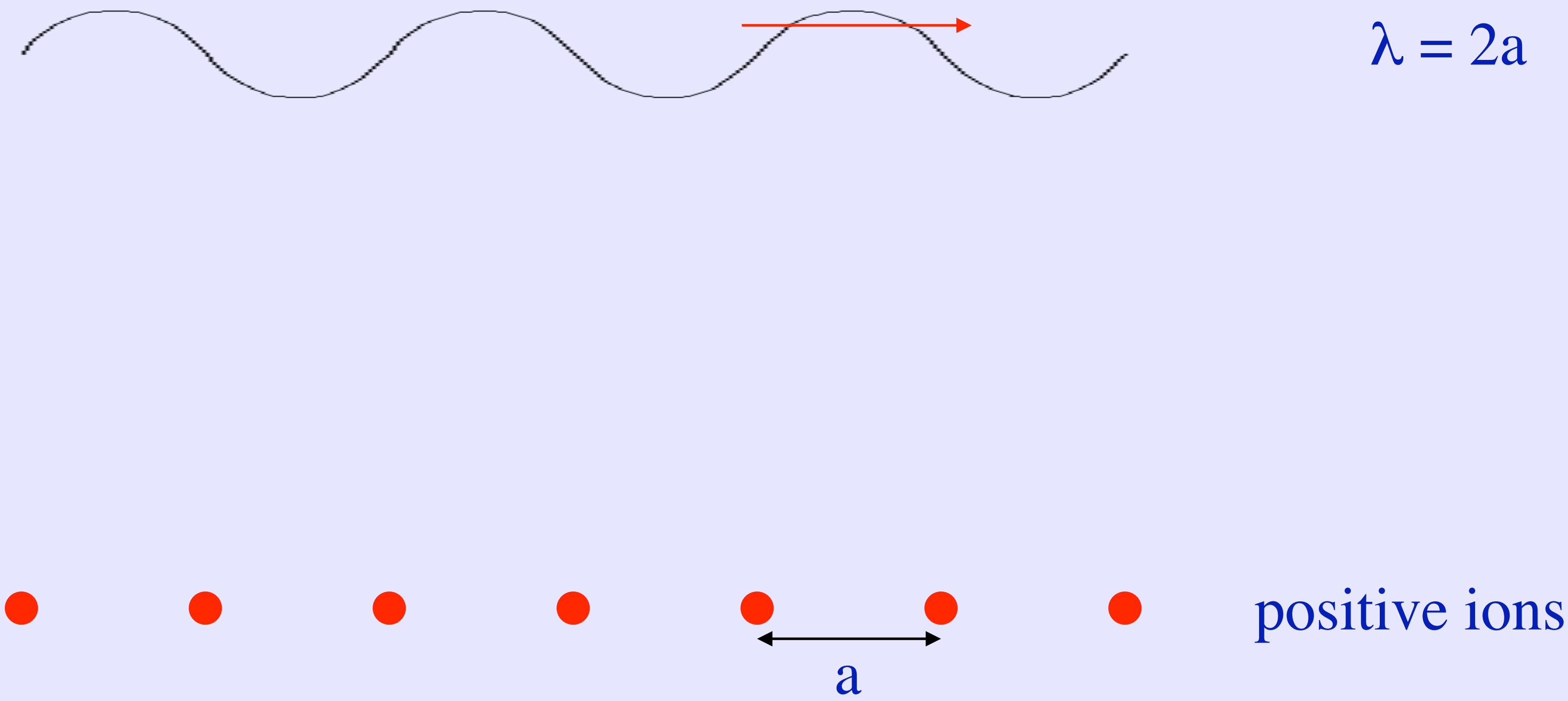
→ number of allowed states in Brillouin zone is $2\frac{(\pi/a)^3}{(\pi/L)^3} = 2\frac{L^3}{a^3}$

L^3/a^3 is just the number of primitive unit cells in the lattice

If we assume the simple case of a one-atom basis, we reach the edge of the first Brillouin zone by having two free electrons per atom (e.g. Calcium)

2) The nearly-free-electron model

Consider an electron in a travelling wave quantum state, moving through the crystal, with k=π/a:



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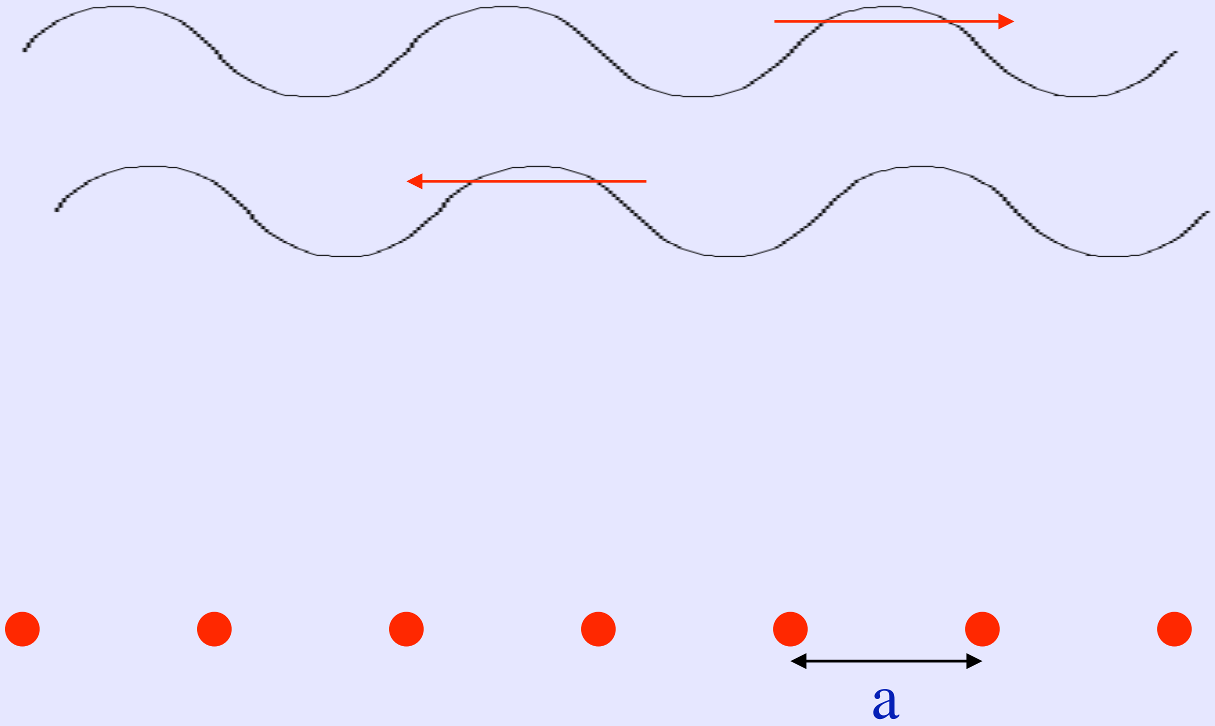
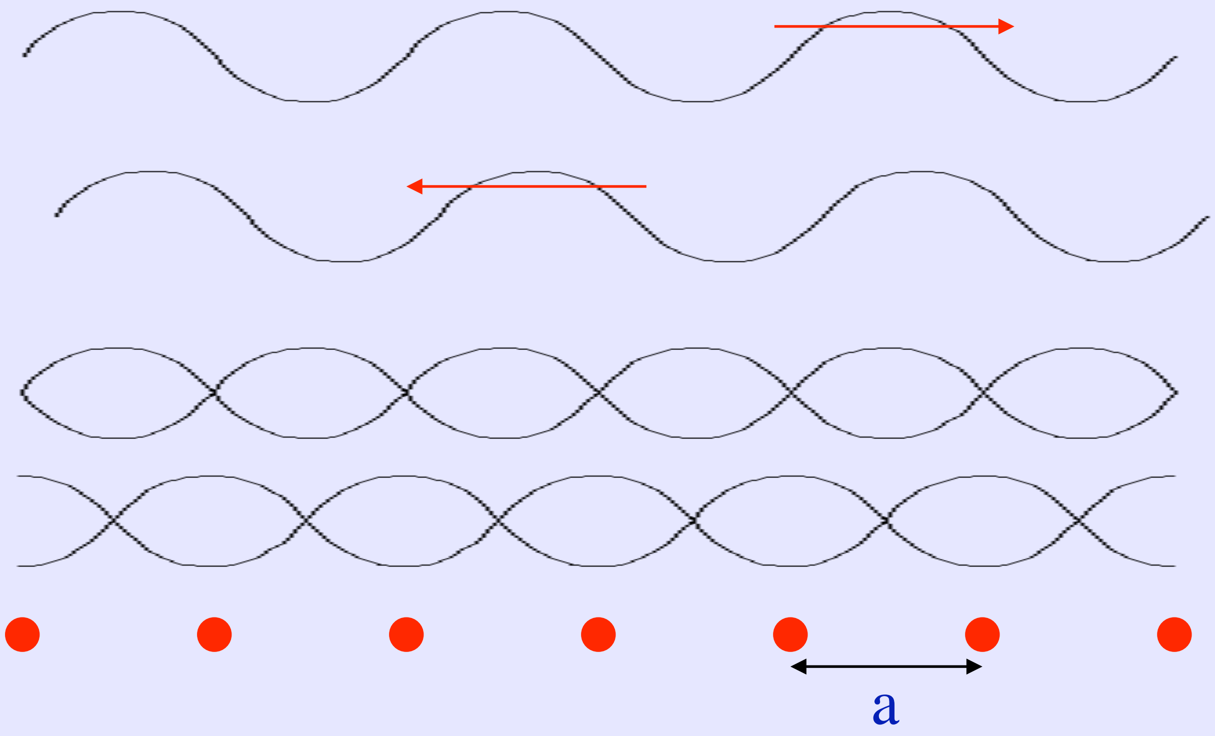
2) The nearly-free-electron model

This wave keeps Bragg-reflecting, which eventually sets up a counter-propagating travelling wave



2) The nearly-free-electron model

These then combine to form a standing wave. depending on the relative phases, two distinct standing waves are possible:



Either: Nodes at ions

Or: Nodes midway between ions

2) The nearly-free-electron model

Two standing waves have same k, but clearly their energies are different:

Either:

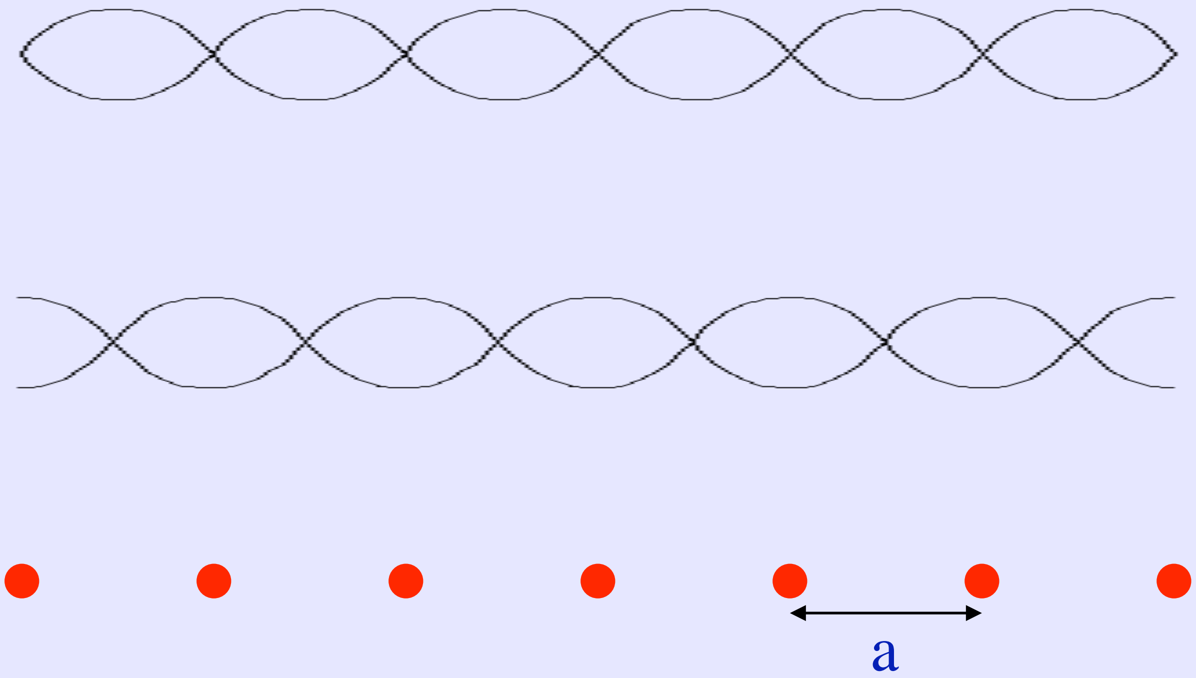
Nodes at ions:

HIGHER energy

Or:

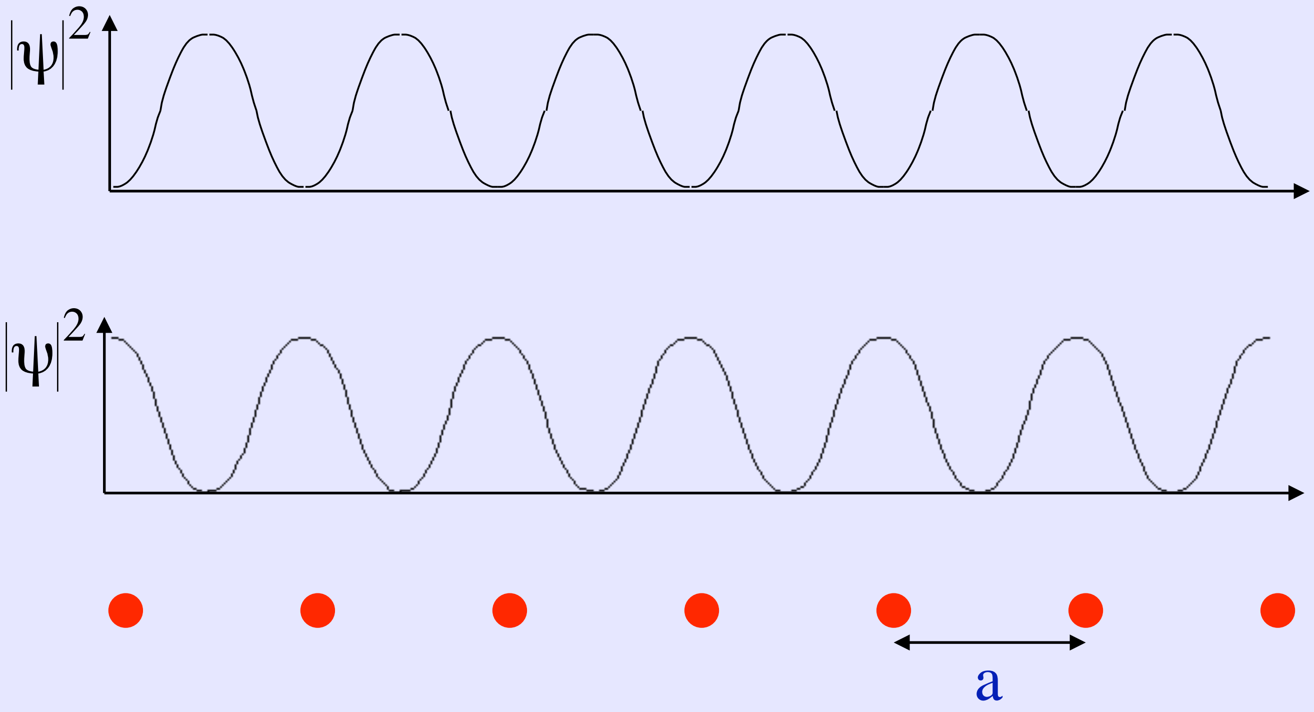
Nodes midway between ions:

LOWER energy



2) The nearly-free-electron model

Strictly speaking we should have looked at the probabilities $\sim |\psi|^2$ before coming to this conclusion:



zero probability at ions:

HIGH ENERGY

max probability at ions:

LOW ENERGY

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2) The nearly-free-electron model

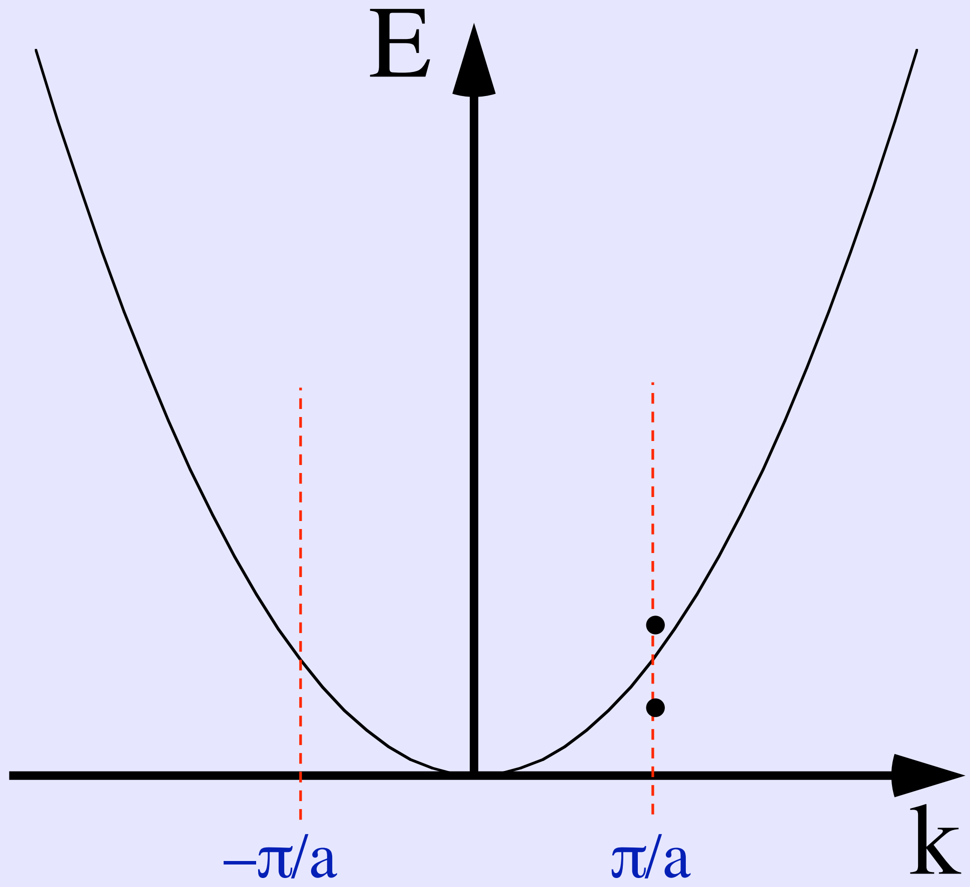
What effect does this have on the dispersion relation:

Two possible energies at
 the BZ edge:

Standing waves:

zero group velocity

$$\rightarrow \frac{dE}{dk} = 0$$



2) The nearly-free-electron model

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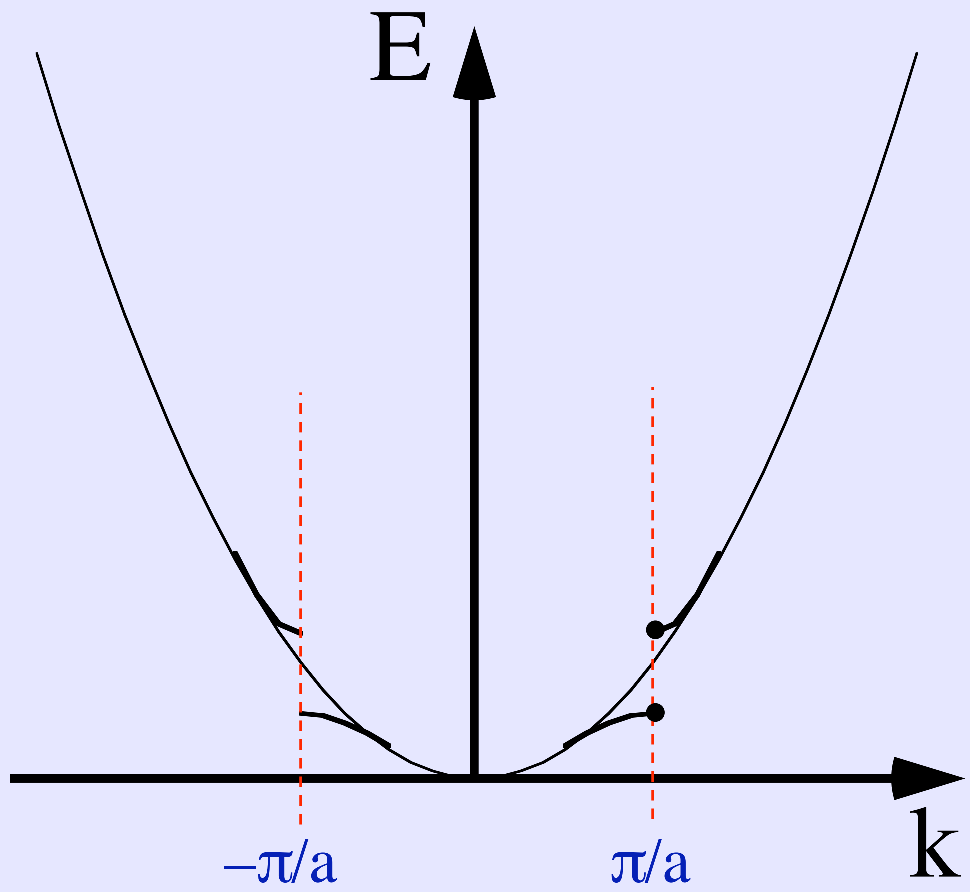

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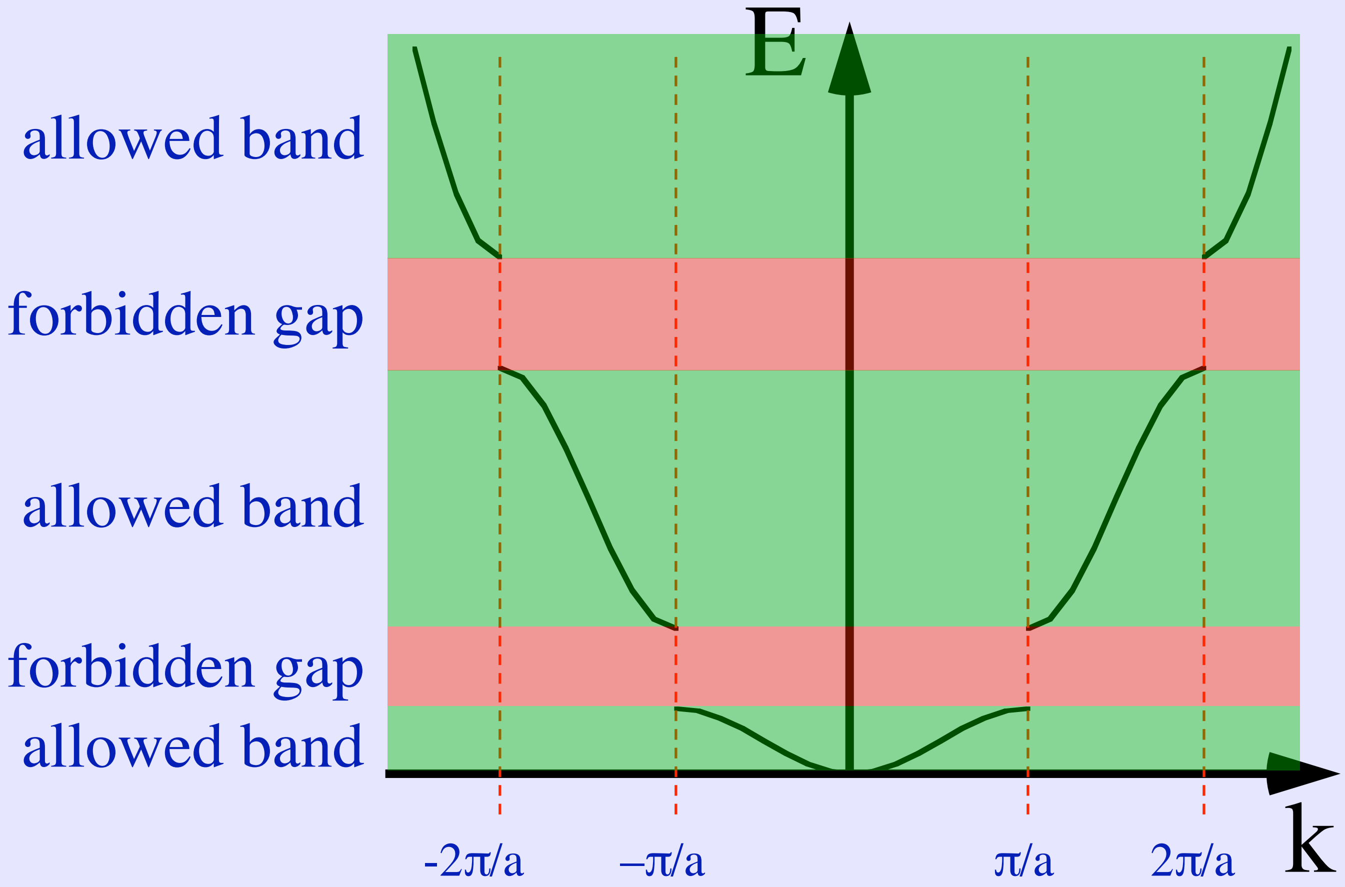
2) The nearly-free-electron model

BAND GAPS APPEAR AT EACH BRILLOUIN ZONE EDGE

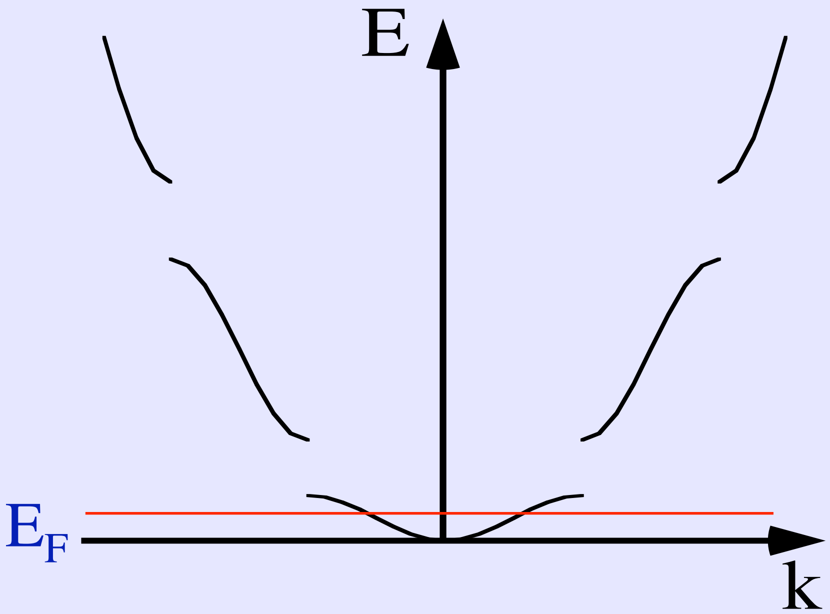


2) The nearly-free-electron model

Comments

- as we increase the number of electrons per atom (or per PUC), E_F moves up the dispersion relation:

1 electron per atom:



2) The nearly-free-electron model

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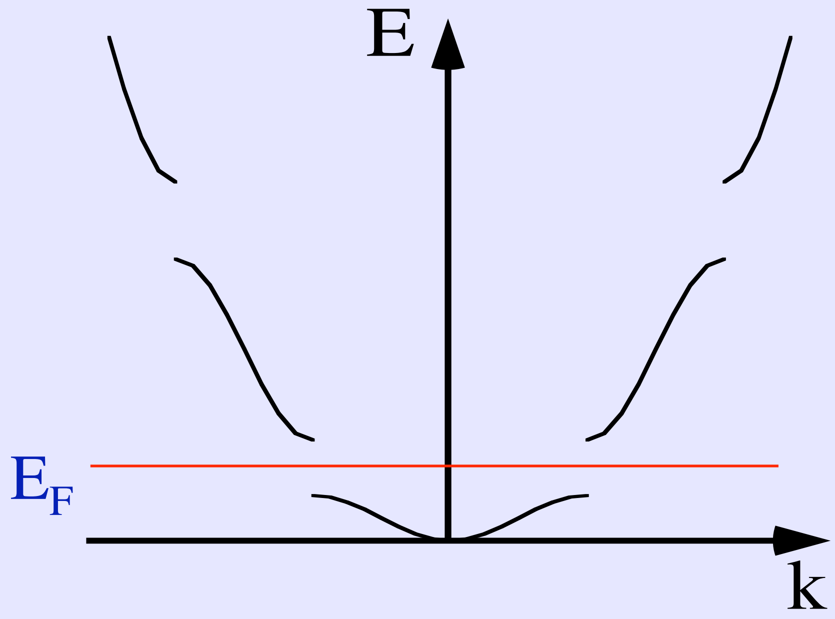

2 electrons per atom:

2) The nearly-free-electron model

Comments

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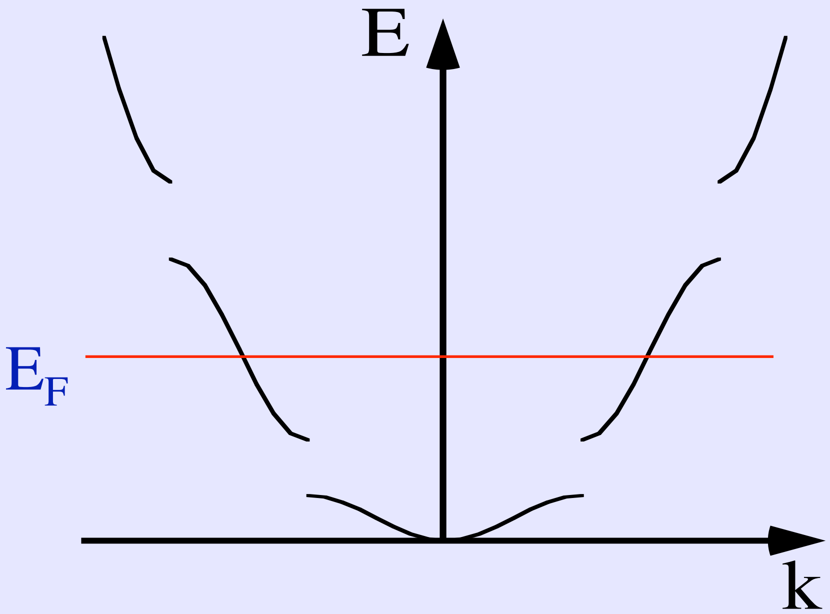
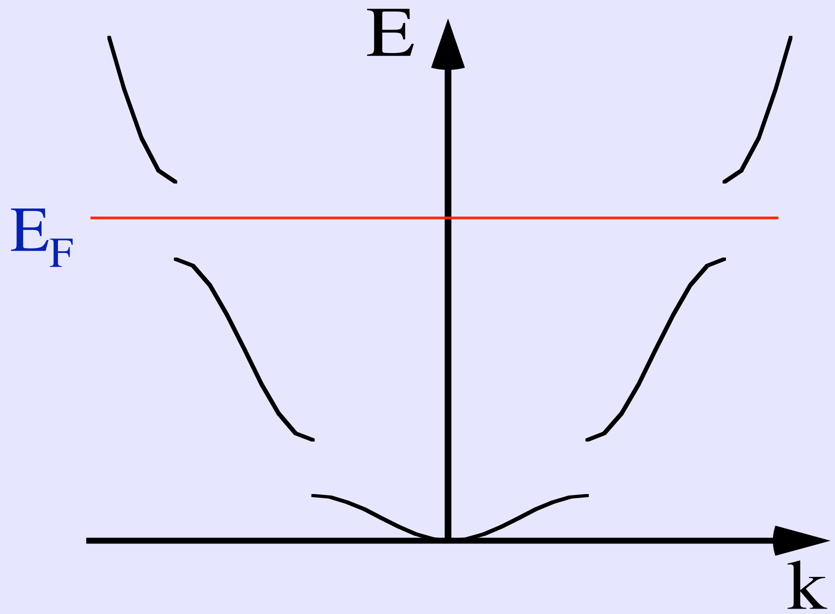


3 electrons per atom:

2) The nearly-free-electron model

Comments

- as we increase the number of electrons per atom (or per PUC), E_F moves up the dispersion relation:

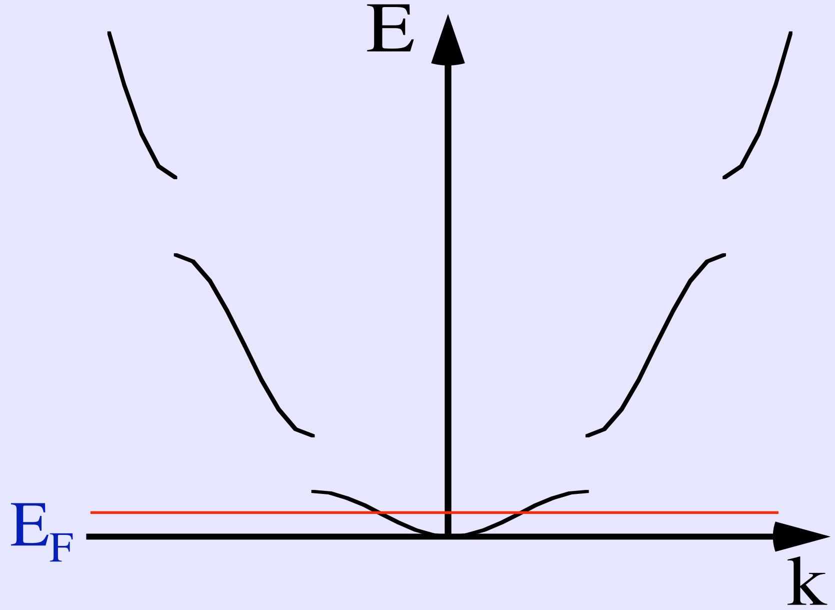


4 electrons per atom:

2) The nearly-free-electron model

Comments

- when E_F is well away from a gap, dispersion is similar to free-electron case, but with slight change in curvature

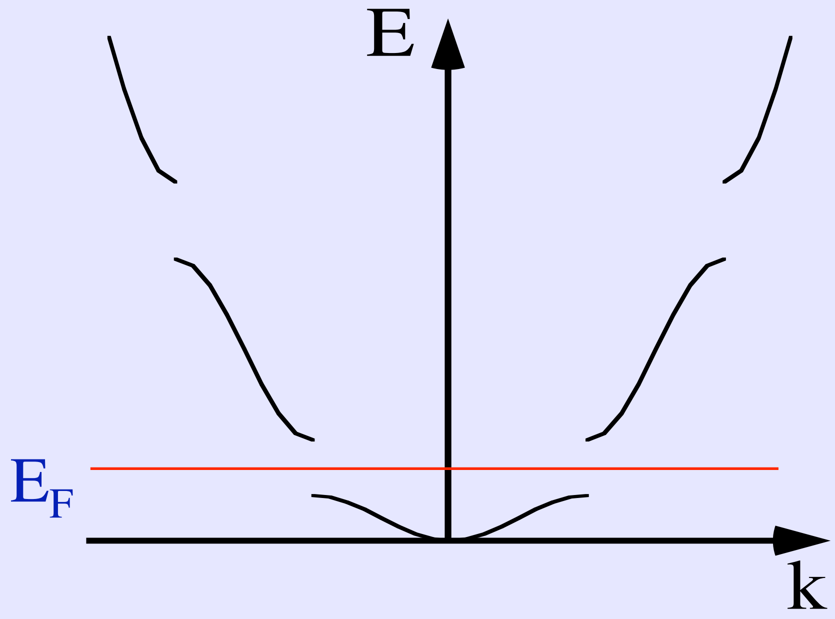


  - remember mass is inversely proportional to curvature
  - behaviour of electrons described by replacing mass with an "effective mass"

2) The nearly-free-electron model

Comments

- when E_F is close to or within a gap, major changes occur...



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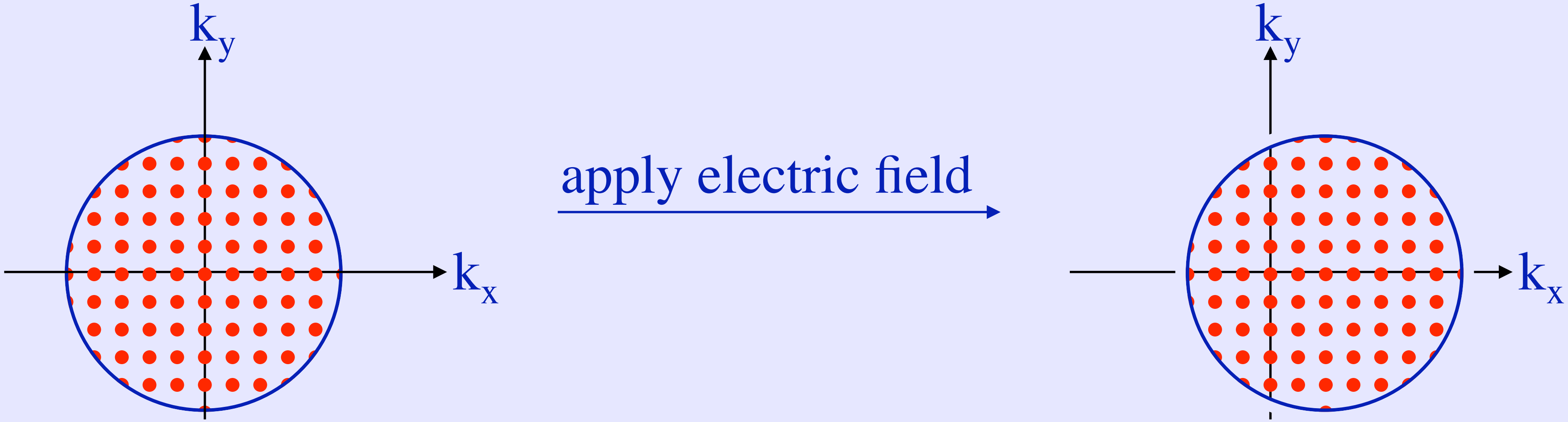
2) The nearly-free-electron model

Metals and insulators

Remember the description of electrical conduction in a metal:



- Electrons on the right move into empty states just above the (equilibrium) Fermi energy – the TINY energy required to do this is supplied by the electric field
- the rest of the electrons then step from left to right filling the states made vacant

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2) The nearly-free-electron model

Metals and insulators

If E_F lies in a forbidden gap, then there are no states near the Fermi energy for electrons to be excited into by the field

→ zero electrical conductivity

– MATERIAL IS AN INSULATOR

If E_F lies in a band of allowed states, then electric field can excite the electrons as described above

→ high electrical conductivity

– MATERIAL IS A METAL

Summary of this lecture

- Nearly free electron model:
  - Bragg reflection a the BZ boundary
  - Appearance of energy gaps
  - Understanding metals and insulators

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Summary

I. Review of Bonding in Solids

II. Crystal Lattices

III. Elastic Scattering of Waves

IV. Atomic Vibrations

V. Electrons in Crystals