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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...

2) The nearly-free-electron model

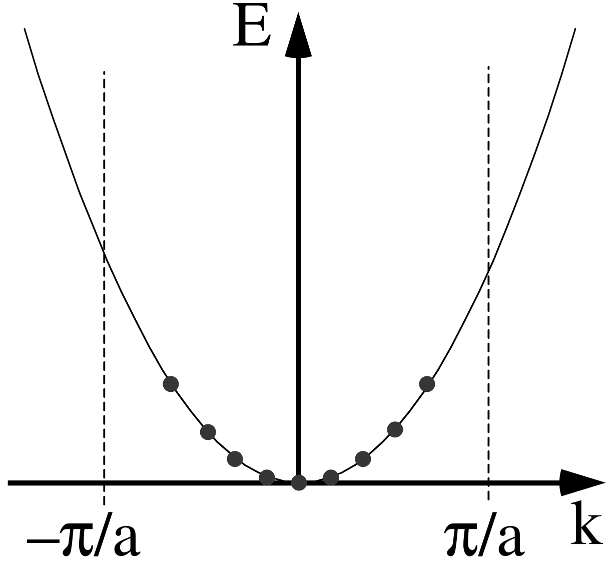
Free electron dispersion:

...with first Brillouin zone:

$-\pi/a \rightarrow \pi/a$

(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?

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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)

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

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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 $(\pi/a)^3$

$\rightarrow$ number of allowed states in Brillouin zone is

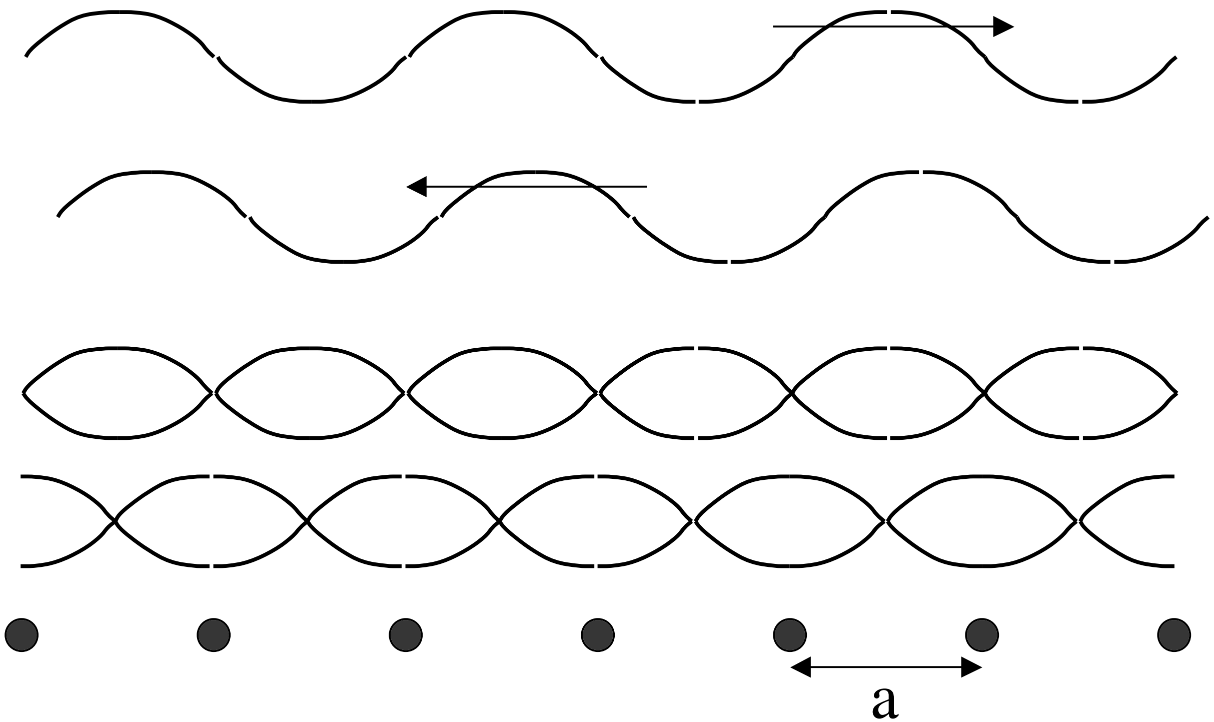
L^3/a^3 is just the number of primitive unit cells in the lattice

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

Either:

Or:

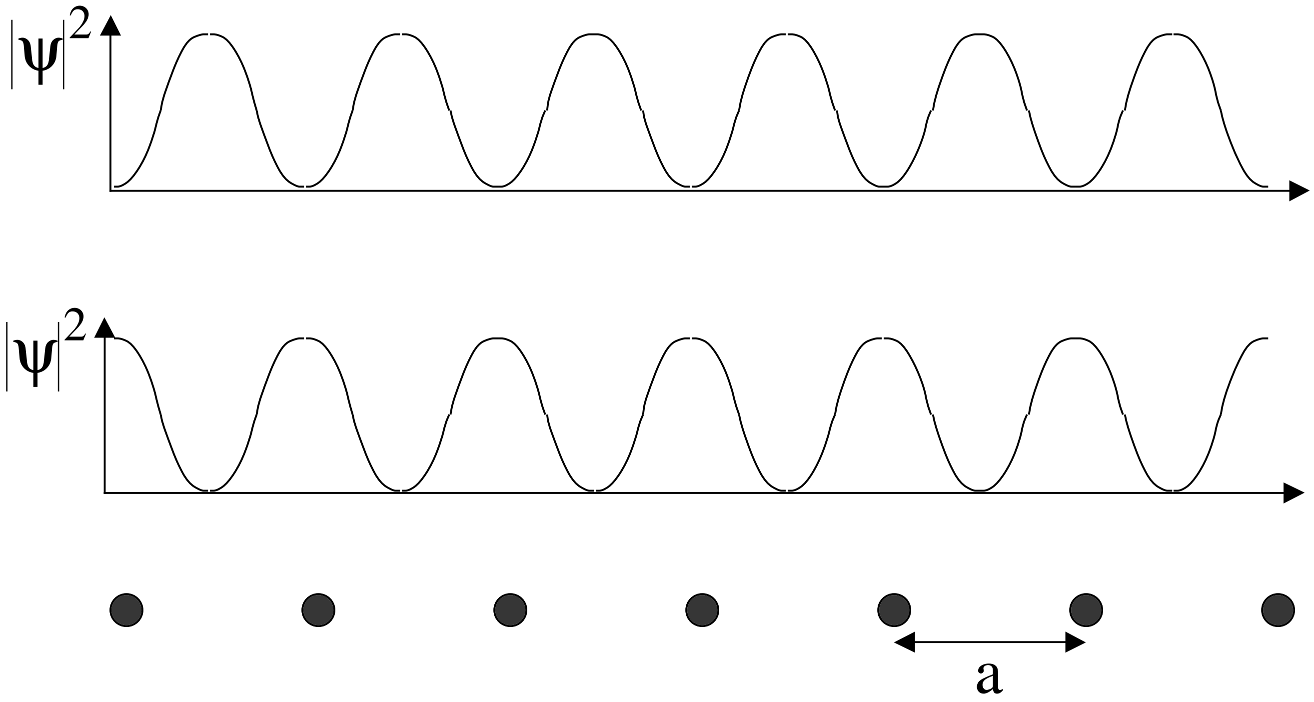


Nodes at ions

Nodes midway between ions

2) The nearly-free-electron model

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



2) The nearly-free-electron model

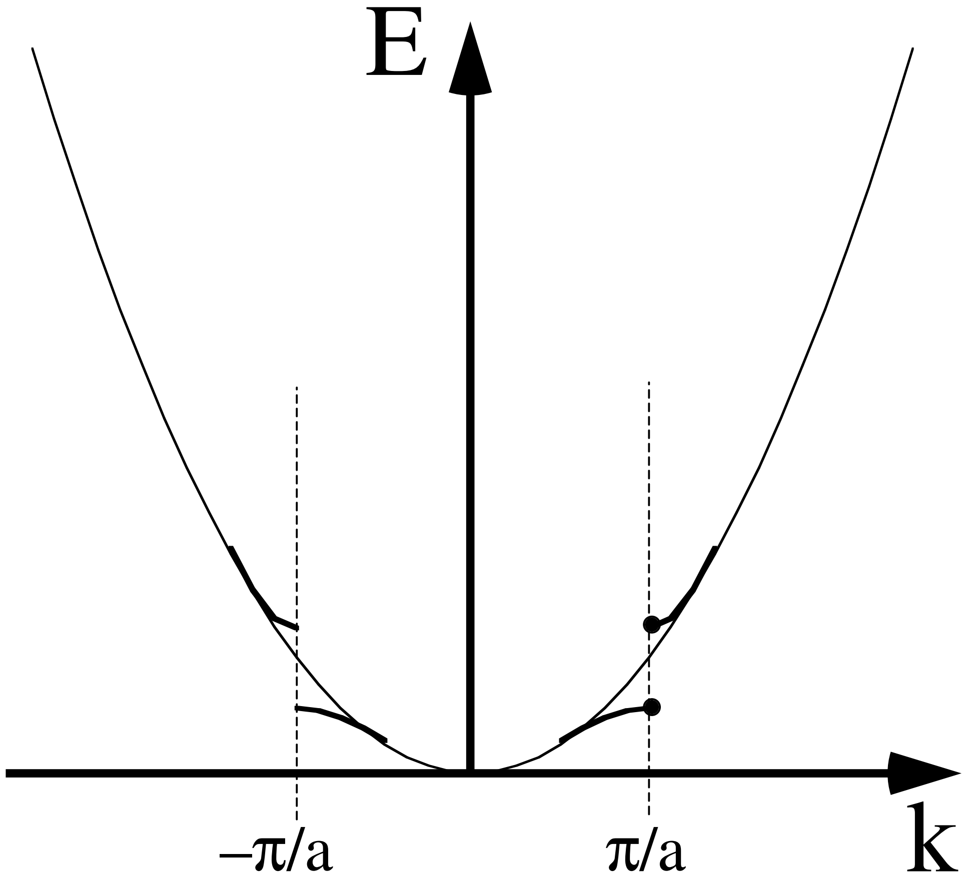
What effect does this have on the dispersion relation:

Two possible energies at the BZ edge:

Standing waves:

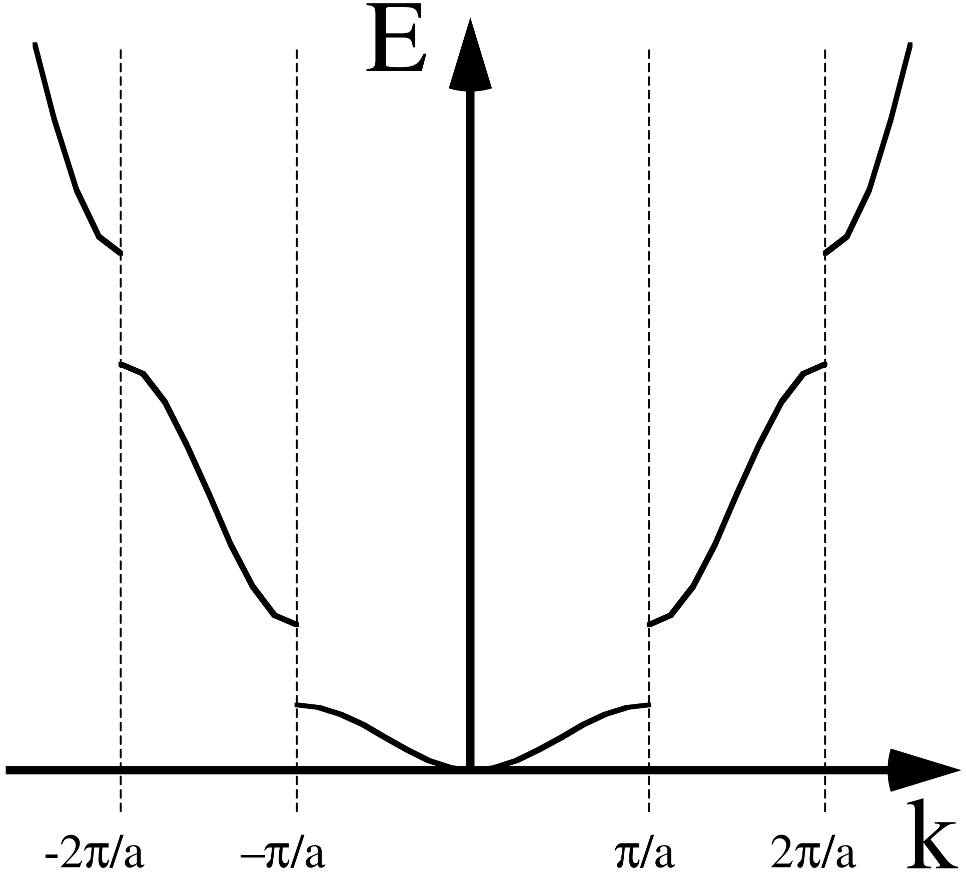
zero group velocity

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



2) The nearly-free-electron model

BAND GAPS APPEAR AT EACH BRILLOUIN ZONE EDGE

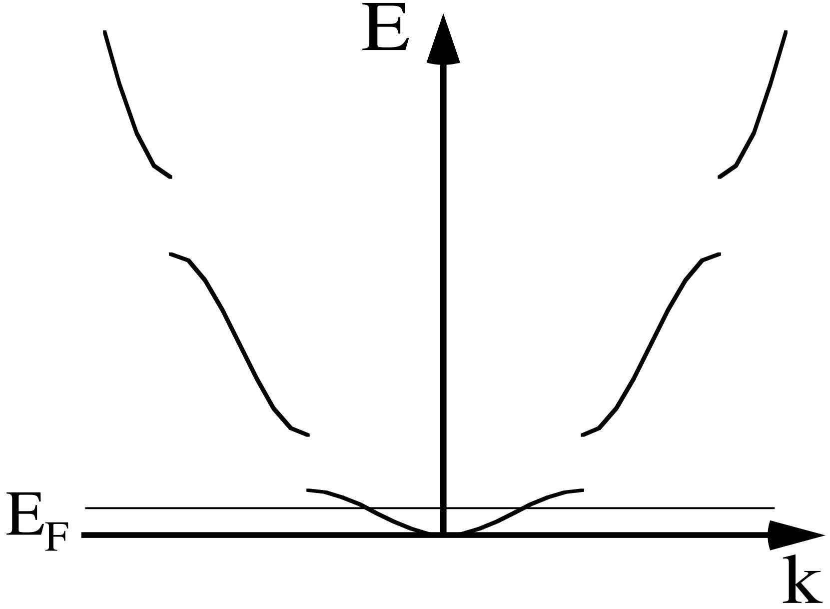


2) The nearly-free-electron model

Comments

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

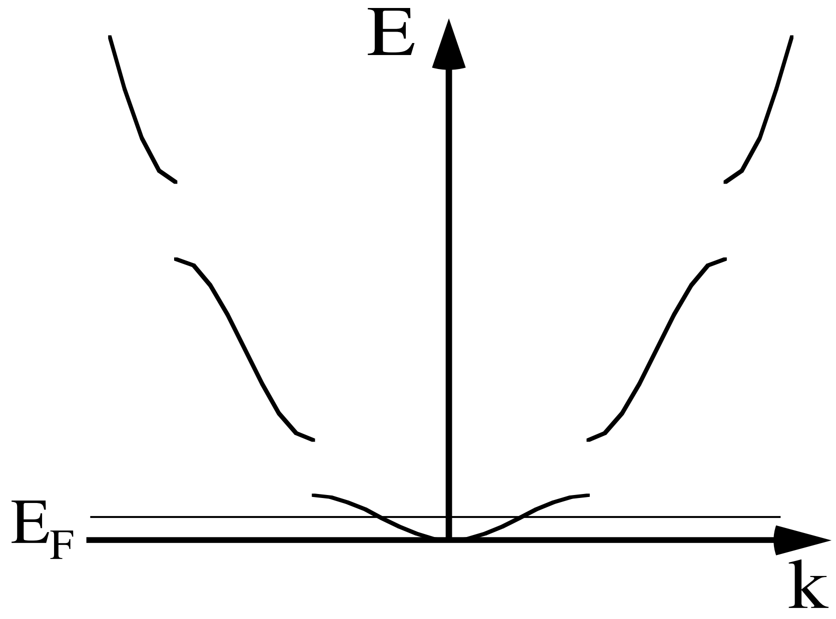
  1 electron per atom:



2) The nearly-free-electron model

Comments

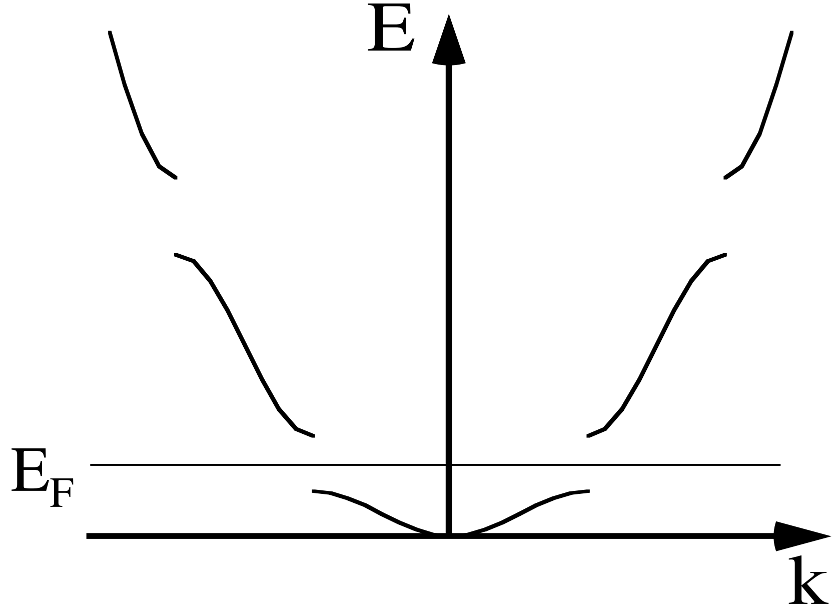
- when E_F is well away from a gap, dispersion is similar to free-electron case, but with slight change in curvature



2) The nearly-free-electron model

Comments

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



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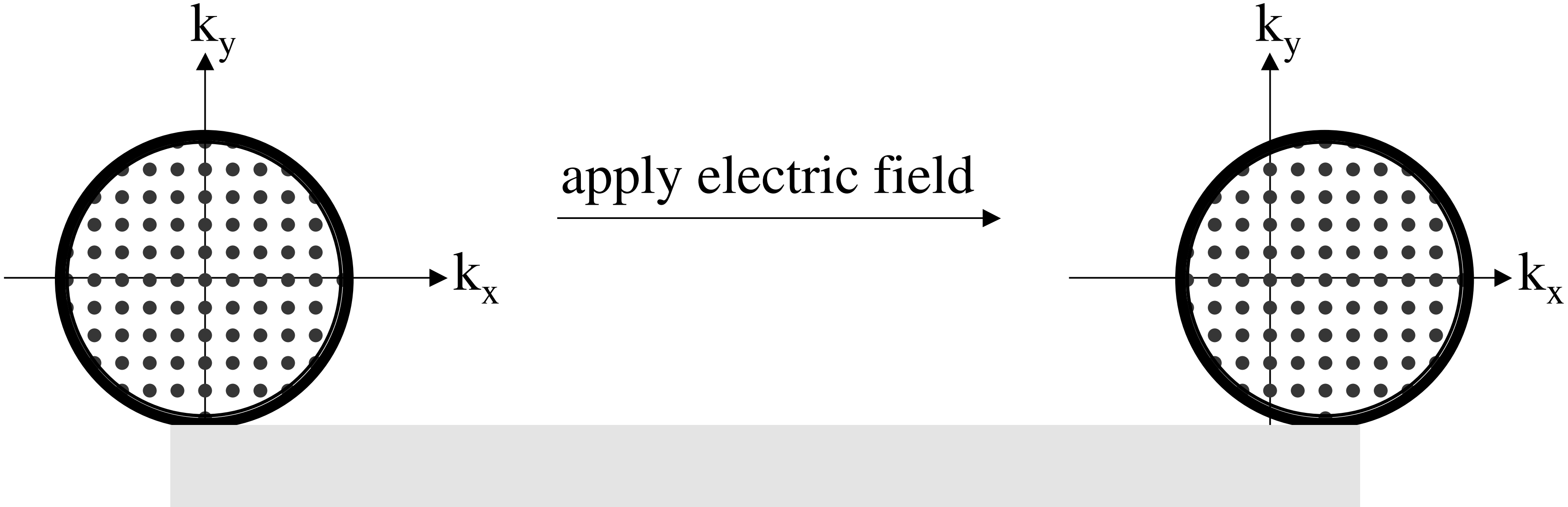
2) The nearly-free-electron model

Metals and insulators

Remember the description of electrical conduction in a metal:



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

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