

1 Mott transition

Mott transition describes the transition from insulating to metallic state of a material. It appears if the electron density and therefore the electron screening of the coulomb potential changes.

1.1 Electron screening

The next simplest step after neglecting electron-electron interactions in a material is to consider electron screening.

In this model the electrons don't interact directly, but the positive potential of the nuclei is modified. Normally the coulomb potential has a large range and decreases with $1/r$. In the screening model the negative electrons closer to a nucleus shield its potential so it decreases exponentially and loses its long-range character. Therefore electrons far from the nucleus will see less positive charge.

The characteristic length is described by the screening parameter k_s .

1.2 Metal-insulator transition

Normally we consider a material either to be a metal or an insulator, depending on the position of the Fermi energy within the band structure. But due to screening a transition can take place.

To understand this we consider an electron in a finite quantum well. There is only a finite number of bound states inside the well. If its width is decreased all states move up in energy and the highest ones move outside the well. Therefore the number of bound states decreases until a critical value is reached. Below this width there are no more bound states.

An insulating material with a certain lattice and long distances between the atoms is considered. If the atoms are moved closer together the electron density increases, screening of the coulomb potential appears and the energy levels move up. After a certain point there are no more bound states for the outer electrons and the material becomes a metal.

The important value is the electron density. If it gets high enough and the ground state wave functions of the electrons of neighbouring atoms overlap the material undergoes a Mott transition:

- small electron density -> weak screening -> the electrons are bound and the material is an insulator
- large electron density -> strong screening -> no bound states and the material is a metal

There is a critical electron density, corresponding to a critical screening length k_s where the last electron state is no longer bound:

$$k_s < \frac{1.19}{a_0} \quad (1)$$

a_0 ... Bohr radius

Therefore a material needs to have an electron density which is close enough to the critical density and can be changed to undergo a Mott transition.

The electron density may be changed by temperature, pressure, external fields or doping levels in semiconductors.

2 Peierls Transition

A Peierls transition is a transition from metallic to insulating state at low temperature which appears in one-dimensional conducting structures.

These one-dimensional conducting structures appear in three-dimensional crystals with certain atom chains in one direction which are responsible for the electrical conductivity. Normally, at high temperature, the atoms in the 1D chains are uniformly distributed. If the material has half-filled bands, the periodicity of the chains will spontaneously change below a certain temperature. Atoms will pair together and the period changes from a to $2a$. This means a change in the size of the unit cell and therefore the Brillouin zone boundary moves.

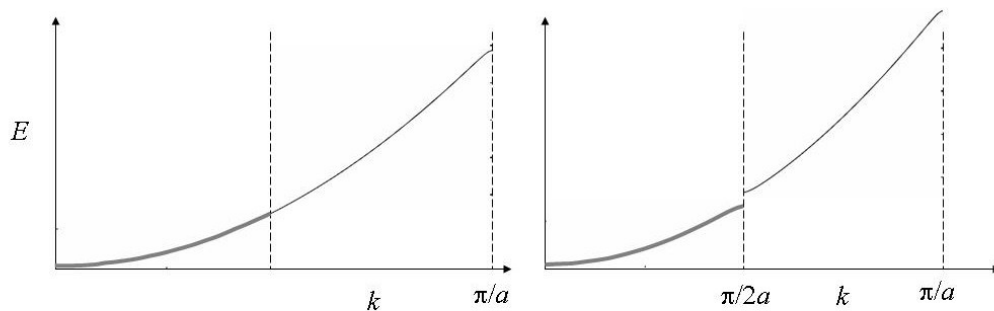


Figure 1: Dispersion relation for a 1D-material with half filled bands and a periodicity of a (left) and $2a$ (right) from <http://lamp.tu-graz.ac.at/hadley/ss2/lectures11/may23/slide19.html>

The dispersion relation of the material helps to explain why this pairing of atoms occurs. Fig. 1 shows the lowest band of the periodic chain. It is parabolic and bends down at the brillouin zone boundary (at π/a for the uniform atom distribution) to cross it at an angle of 90° (due to diffraction of electrons at the boundary). The states are filled up to the first dashed line.

If all electrons are close to the ground state, the pairing of atoms appears and the brillouin zone boundary moves to $\pi/2a$. The filled states next to the brillouin zone boundary bend down while the states on the other side bend up (but as they are empty, it doesn't matter). A gap appears at the fermi surface and the energy of the filled states gets lower. Due to the pairing the system gains electronic energy, which is proportional to the amplitude of the periodic potential while elastic energy is needed for the deformation Δ . The elastic energy increases like Δ^2 , but the electronic energy decreases like Δ . This means as long as Δ is small, the pairing causes an energetic advantage.

To perform a Peierls transition the material needs to be quasi one-dimensional and have half-filled bands.

It becomes insulating below a certain temperature because a gap appears at the fermi surface due to the spontaneous pairing of atoms.

The periodic fluctuations in electron density which are caused by the rearrangement of the ions are called *charge density waves*.