Solids

Semi-classical electron dynamics

Electrons in crystal lattices

- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Electron dynamics and Electron hole bands
- Photoemission Spectroscopy
- Semi-classical electron dynamics
- Semiconductors
- Ferromagnetism
- Superconductivity

Semi-classical electron dynamics 1

velocity of a wave packet

$$v_x(\vec{k}_0) = \left.\frac{\partial \omega(\vec{k})}{\partial k_x}\right|_{\vec{k}=\vec{k}_0} = \frac{1}{\hbar}\left.\frac{\partial E(\vec{k})}{\partial k_x}\right|_{\vec{k}=\vec{k}_0}$$

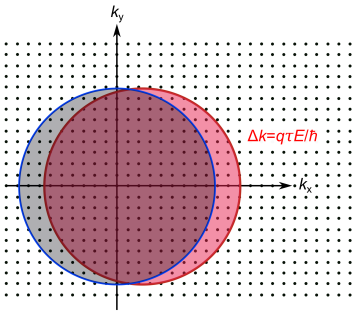
force on a wave packet

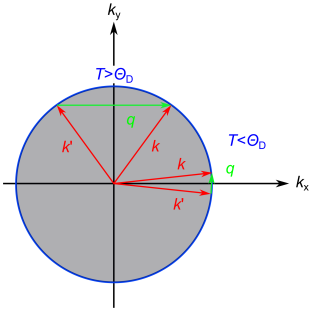
$$\hbar\dot{\vec{k}} = \vec{F} = q\vec{E} + q\vec{v} \times \vec{B} \quad \text{with} \quad q = -e$$

Semi-classical electron dynamics 2

1. Motion in a homogeneous electric field

$$\hbar\dot{\vec{k}} = \vec{F} = q\vec{E} \quad \text{and} \quad \Delta\vec{k} = q\vec{E}\tau$$





Semi-classical electron dynamics 2 — Comment 1

When only a homogeneous electric field is applied, the k-states are shifted.

As in the Drude and Sommerfeld model, there is a mean collision time τ during which the wave packets move freely.

This free evolution of the motion leads to the shift Δk of the k-states.

The figures are the same as in Lecture 24.

However, the interpretation is slightly different.

For the sake of simplicity, a spherical Fermi surface enclosed in the 1st Brillouin zone is assumed.

The dots in the left figure now indicate the wave packets moving with the group velocity $\vec{v} = \hbar^{-1} \partial E(\vec{k}) / \partial \vec{k}$.

Semi-classical electron dynamics 2 Comment 2

The k-states are shifted due to the electric field.

The second figure shows that, as in the Sommerfeld model, electron-phonon scattering limits the shift of the k-states.

However, now a gas made up of wave packets moving in all directions is considered.

As in the Drude model, the drift velocity is added to the motion of the wave packets and as in the Drude model, the drift velocity is determined by the current density $\vec{j} = q\frac{N}{V}\vec{v}_\mathrm{D}$ with known carrier density $n = N/V$.

Semi-classical electron dynamics adds the new insight that there can be negative and positive charge carriers.

Semi-classical electron dynamics 3

2. Motion in a homogeneous magnetic field

$$\hbar\dot{\vec{k}} = \vec{F} = q\vec{v} \times \vec{B} \quad \text{with} \quad q = -e$$

For simplicity: quasi free electron motion

$$E(\vec{k}) = \frac{\hbar^2\vec{k}^2}{2m_{\text{eff}}} \quad \text{and} \quad \vec{v} = \frac{\hbar\vec{k}}{m_{\text{eff}}} \quad \text{and} \quad m_{\text{eff}} \text{ can be positive or negative}$$

and therefore

$$\hbar\dot{\vec{k}} = q\frac{\hbar\vec{k}}{m_{\text{eff}}} \times \vec{B}$$

Semi-classical electron dynamics 3 Comment 1

First, only a homogeneous magnetic field is considered.

The first equation outlined in red gives the semi-classical electron motion in a homogeneous magnetic field.

Since the velocity $\vec{v}$ is proportional to the energy gradient, the Lorentz force cannot change the energy.

The motion of the *k*-states is thus perpendicular to the direction of the magnetic field and within a plane of constant energy.

For the sake of simplicity, the quasi-free movement of electrons is considered.

The second equation gives the kinetic energy with the effective mass, which can be positive or negative.

Semi-classical electron dynamics 3 Comment 2

The second equation outlined in red gives the equation of motion of the *k*-states.

Electrons occupying *k*-states with positive effective mass move in the opposite direction of electrons occupying *k*-states with negative effective mass.

Electrons occupying *k*-states with negative effective mass are usually called electron-hole states although the *k*-states are occupied by electrons.

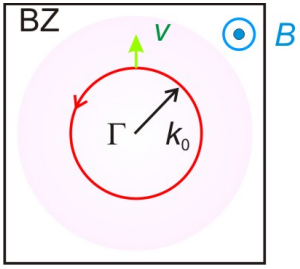
The reason is that the current can either be described by the occupied *k*-states and negative charges or by the unoccupied *k*-states with positive charges.

To avoid confusion, only occupied *k*-states are considered.

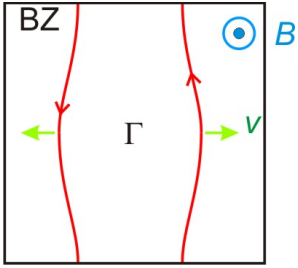
They are called electrons when the effective mass is positive and holes when the effective mass is negative.

Semi-classical electron dynamics 4

closed orbit



open orbit



cyclotron frequency

$$\omega_c = \frac{qB}{m_{\text{eff}}}$$

$$\omega_c(1\,\text{T}) \approx 1.8 \cdot 10^{11}\,\text{s}^{-1}$$

Semi-classical electron dynamics 4 Comment 1

The first figure assumes a Fermi-sphere and quasi-free electron movement with a positive effective mass.

The Fermi-sphere is enclosed by the 1^{st} Brillouin zone and the selected k-state performs a circular motion.

The time required to complete a cycle can be easily calculated (Time for one period $T = 2\pi k \sin\theta/\dot{k}$ and $\dot{k} = qkB\sin\theta/m_{\text{eff}}$). The frequency of rotation is called the cyclotron frequency.

The cyclotron frequency is in a 1 Tesla magnetic field in the range of $10^{11}\ \text{s}^{-1}$, assuming that the effective mass is equal to the mass of the free electron.

If one assumes a mean collision time in the range of 10^{-15} s, one cannot expect that a complete circular motion is possible at room temperature.

Semi-classical electron dynamics 4 Comment 2

The second figure shows a more complicated energy landscape.

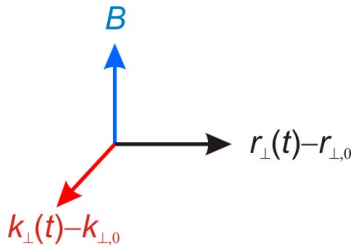
Here, too, a positive effective mass of the *k*-state is considered.

The *k*-states are occupied up to the boundary of the 1st Brillouin zone and the sketch shows the situation of an open orbit.

Semi-classical electron dynamics 5: Spacial motion

Integrating $\hbar\dot{\vec{k}} = q\dot{\vec{r}} \times \vec{B}$ gives

$$\vec{k}_\perp(t) - \vec{k}_{0,\perp} = \frac{q}{\hbar}(\vec{r}_\perp(t) - \vec{r}_{0,\perp}) \times \vec{B}$$



with ($B = 1\,\mathrm{T}$)

$$\frac{qB}{\hbar} := \frac{e \cdot 1\,\mathrm{T}}{\hbar} = 1.5 \cdot 10^{15}\,\mathrm{m}^{-2}$$

$$\vec{k}(t) - \vec{k}_0 = \frac{q}{\hbar}(\vec{r}(t) - \vec{r}_0) \times \vec{B} = \frac{q}{\hbar}(\vec{r}_\perp(t) + \vec{r}_\parallel(t) - \vec{r}_{0,\perp} - \vec{r}_{0,\parallel}) \times \vec{B}$$

$$\vec{k}(t) - \vec{k}_0 = \frac{q}{\hbar}(\vec{r}_\perp(t) - \vec{r}_{0,\perp}) \times \vec{B},$$

Semi-classical electron dynamics 5 Comment

The integration of the semi-classical equation of motion in a magnetic field gives the formula outlined in red.

The component of $\vec{r}$ parallel to the magnetic field does not contribute.

Likewise, the motion in k-space parallel to the magnetic field is not affected by the magnetic field.

The motions in local space and k-space are perpendicular to each other, as indicated in the sketch.

The proportionality factor $qB/\hbar$ is interesting.

At a magnetic field strength of 1 Tesla, it has the value $1.5 \cdot 10^{15}\,\mathrm{m}^{-2}$.

If a $|\vec{k}|$ is assumed in the range of the 1st Brillouin zone e.g. $k \approx 1.5 \cdot 10^{10}\,\mathrm{m}^{-1}$, then one gets im local space an orbit in the range of $10^{-5}\,\mathrm{m}$.

Semi-classical electron dynamics 6

3. Motion in crossed electric and magnetic fields $\vec{E} \perp \vec{B}$

$$\boxed{\hbar\dot{\vec{k}} = \vec{F} = q\vec{E} + q\vec{v} \times \vec{B}}$$

with

$$\vec{B} \times (\vec{E} \times \vec{B}) = (\vec{B}\vec{B})\vec{E} - (\vec{B}\vec{E})\vec{B} = B^2\vec{E}$$

and

$$\underline{\vec{E} = -\frac{(\vec{E} \times \vec{B}) \times \vec{B}}{B^2}}$$

$$\hbar\dot{\vec{k}} = q\vec{E} + q\vec{v} \times \vec{B} \quad \rightarrow \quad \underline{\hbar\dot{\vec{k}} = q(-\frac{\vec{E} \times \vec{B}}{B^2} + \vec{v}) \times B} \quad \rightarrow \quad \boxed{\hbar\dot{\vec{k}} = q(\vec{v} - \vec{w}) \times \vec{B}}$$

Semi-classical electron dynamics 6 Comment

A little trick is used when considering the electron motion in crossed electric and magnetic fields.

The electric field can be rewritten in the form of the formula underlined in red, yielding the second equation outlined in red.

The drift velocity $\vec{w} = \frac{\vec{E} \times \vec{B}}{B^2}$ is added to the velocity of the k-states.

Semi-classical electron dynamics 7

Drift velocity in crossed electric and magnetic fields

$$\vec{w} = \frac{\vec{E} \times \vec{B}}{B^2}$$

estimate $E = 100\,\mathrm{V/m}$ and $B = 1\,\mathrm{T}$: $w = 100\,\mathrm{ms}^{-1}$

- w is large compared with the drift velocity $v_D \approx \mathrm{cms}^{-1}$
- w is small compared with the Fermi velocity $v_F \approx 10^6\,\mathrm{ms}^{-1}$
- w becomes only effective for closed orbits
- w becomes only effective when $\omega_c \tau >> 1$, i.e. the electrons or holes can perform many circles.

Semi-classical electron dynamics 7 Comment

The estimate shows that the velocity $\vec{w}$ is small compared to the speed of the k-states, i.e. wave packets.

The velocity $\vec{w}$ only becomes effective when the motion of the k-states through the magnetic field averages to zero.

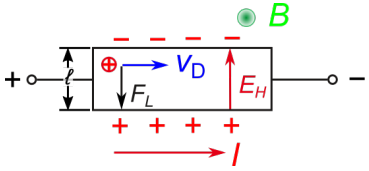
This can only happen on closed orbits and if the condition $\omega_c\tau >> 1$ is fulfilled.

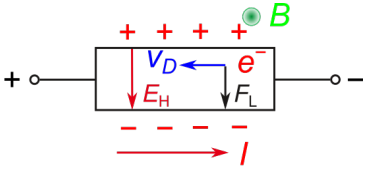
In order to increase the mean collision time τ, low temperatures and very pure crystals are necessary to minimize scattering. A strong magnetic field is also required.

Due to the dependence of $\omega_c\tau$ on temperature and magnetic field, it is obvious that the Hall effect depends on the temperature and the strength of the magnetic field.

Semi-classical electron dynamics 8

lecture 23:





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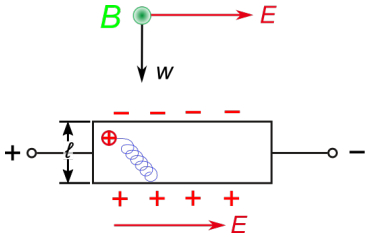
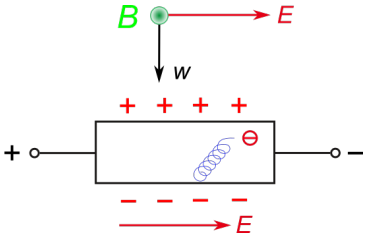




Semi-classical electron dynamics 8 Comment 1

The figures compare interpretation of the Hall effect in the Drude model and with the semi-classical electron dynamics.

The wave packets in semi-classical electron dynamics must move on closed orbits.

Wave packets with effective positive and negative masses move in opposite directions.

The motion is disturbed by scattering events.

The vector $\vec{w}$ gives the direction of the drift if the motion is not disturbed by scattering.

Semi-classical electron dynamics 8 Comment 2

Without scatting in a magnetic field no electric current along the direction of the electric field is expected.

Without scattering no electric current is expected along the direction of the electric field when a magnetic field is present.

This effect is described by the magneto-resistance.

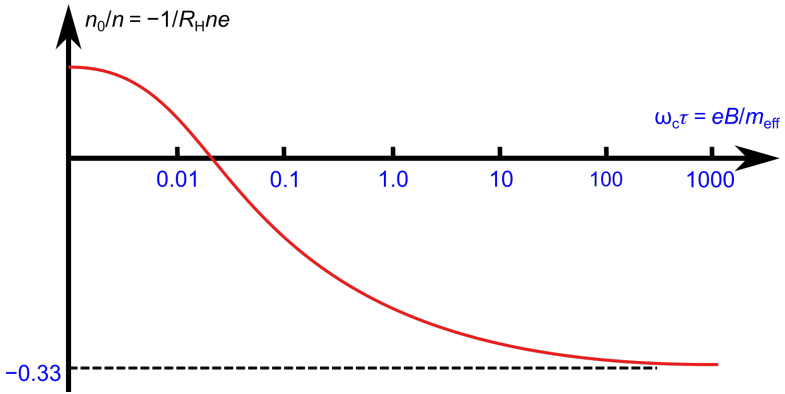
The magneto-resistance become smaller when the scattering becomes more effective.

In fact, Edwin Hall first attempted to measure magnetoresistance.

But in order to observe the effect, very pure samples and high magnetic fields are usually required.

Semi-classical electron dynamics 9

Hall effect of Aluminium



Semi-classical electron dynamics

Comment

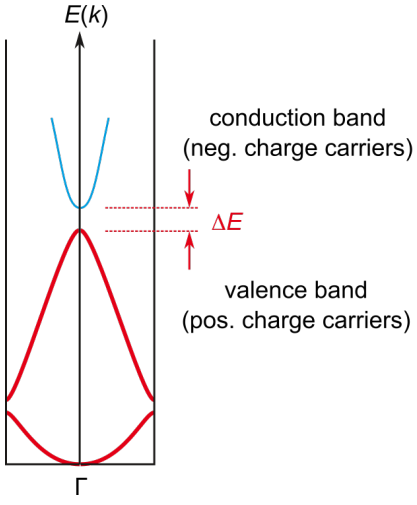
Hall effect of Aluminum as a function of $\omega_c \tau$, i.e. as a function of the magnetic field strength.

Semiconductors

Electrons in crystal lattices

- Electrical conductivity and Ohm's law
- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Electron dynamics and Electron hole bands
- Photoemission Spectroscopy
- Semi-classical electron dynamics
- Semiconductors
- Ferromagnetism
- Superconductivity

Semiconductors 1



Semiconductors 1

Comment 1

The figure shows the energy bands of an insulator or semiconductor for one direction in the reciprocal lattice.

The occupied k states are shown in red.

In the 1st Brillouin zone of an insulator, all k states of an energy band for all directions of the wave vector $\vec{k}$ must be occupied by two electrons.

The solid is a metal if there are regions of an energy band with unoccupied k states in the 1st Brillouin zone.

In a semiconductor, the highest occupied energy band is called the valence band and the lowest unoccupied band is called the conduction band.

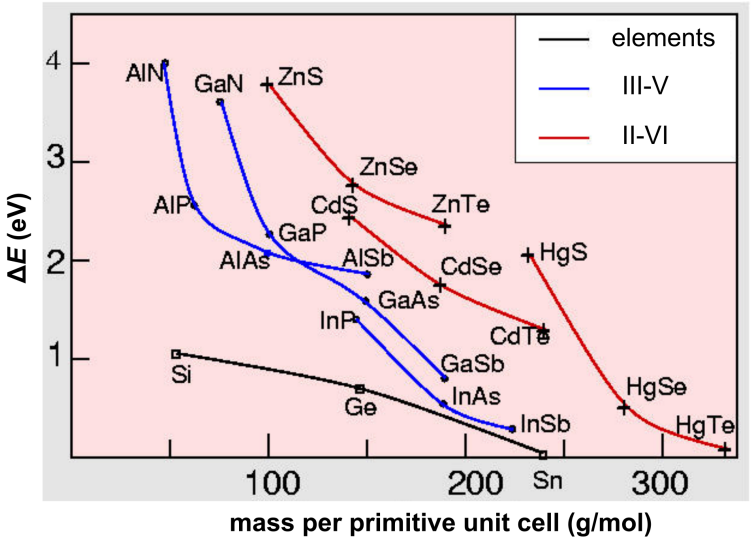
Semiconductors 1

Comment 2

Because of the energy gap between the valence band and the conduction band, the electrical conductivity of a semiconductor approaches zero at zero temperature, i.e. $\sigma \to 0$ for $T \to 0$.

The electrical conductivity increases with increasing temperature, since more and more electrons can be excited from the valence band into the conduction band.

Semiconductors 2



Semiconductors 2

Comment

The figure gives an overview of the energy gaps of various semiconductors.

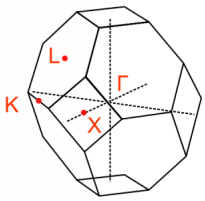
The black line connects the elements silicon, germanium and tin.

The blue line connects the III-V semiconductors and the red line the II-VI semiconductors.

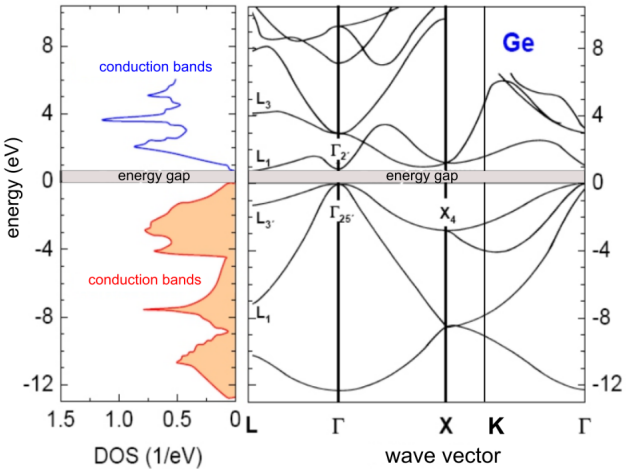
A look at the periodic table of the elements shows what is meant by a III-V or a II-VI semiconductor.

The combination of elements from different groups of the periodic table affects the size of the smallest energy gap between the valence and conduction bands.

Semiconductors 3



band structure of Germanium (electron configuration [Ar] $3d^{10}\ 4s^2\ 4p^2$)



Semiconductors 3

Comment

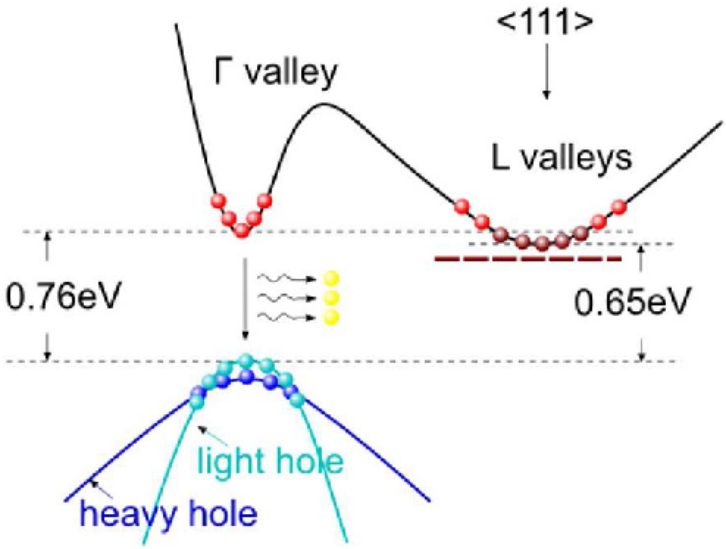
Germanium crystallizes in the fcc lattice of the diamond structure.

The figure on the left shows the 1st Brillouin zone of the fcc lattice.

The first panel shows the density of states and the second panel the energy bands for some selected directions of the wave vector.

The lowest energy of the conduction band is at the L point of 1st Brillouin zone.

Semiconductors 4



Semiconductors 4

Comment

The figure shows the conduction band and the valence band in more detail.

In contrast to the previous figure, the L point is plotted to the right of the Γ point.

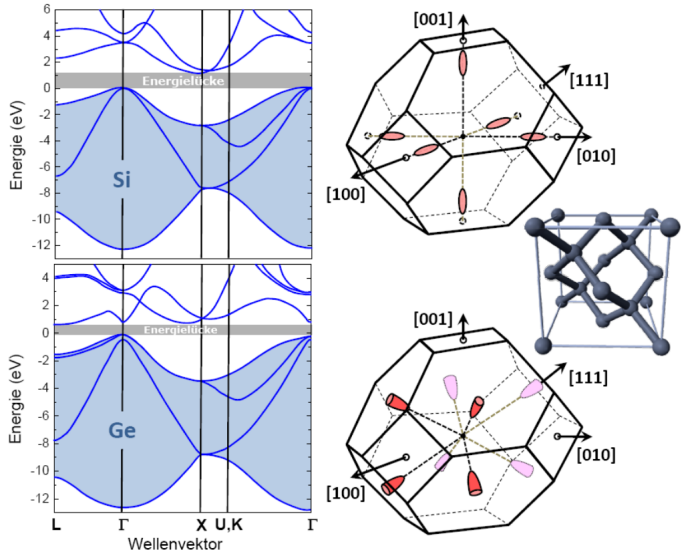
At the Γ point there are three valence bands that have exactly the same energy when the lattice symmetry is the undisturbed diamond structure.

The figure shows the case where the lattice is doped with impurity atoms that act as donor atoms.

The energy of the donor atoms is plotted as a dashed line just below the conduction band minimum.

The energy gap is so small that a large number of electrons can be thermally excited into the conduction band from the donor atoms.

Semiconductors 5



Semiconductors 5

Comment

The figures compare the band structures of silicon and germanium.

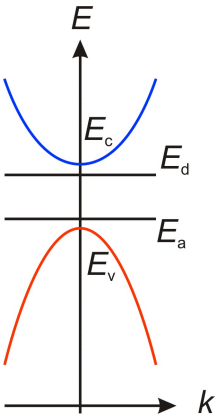
The lowest energy of the silicon conduction band is near the X point of the 1st Brillouin zone.

The areas drawn in red in the 1st Brillouin zone of silicon and germanium show the surfaces of constant energy of the conduction band.

The energy is slightly above the minimum energy of the conduction band.

These regions indicate the occupied *k* states when electrons are excited into the conduction band.

Semiconductors 6



Semiconductors 6 Comment 1

The figure shows schematically the doping of semiconductors.

The horizontal bars show the relevant localized energy levels of the donor and acceptor atoms, E_d and E_a, respectively.

The electrons of the donator and acceptor atoms are localized and the corresponding energy band is simply a horizontal line.

The energy gap between the lowest energy of the conduction band and the relevant energy level of the donor atom is small, so the probability that an electron of the donor atom will be excited into the conduction band is very high.

Semiconductors 6 Comment 2

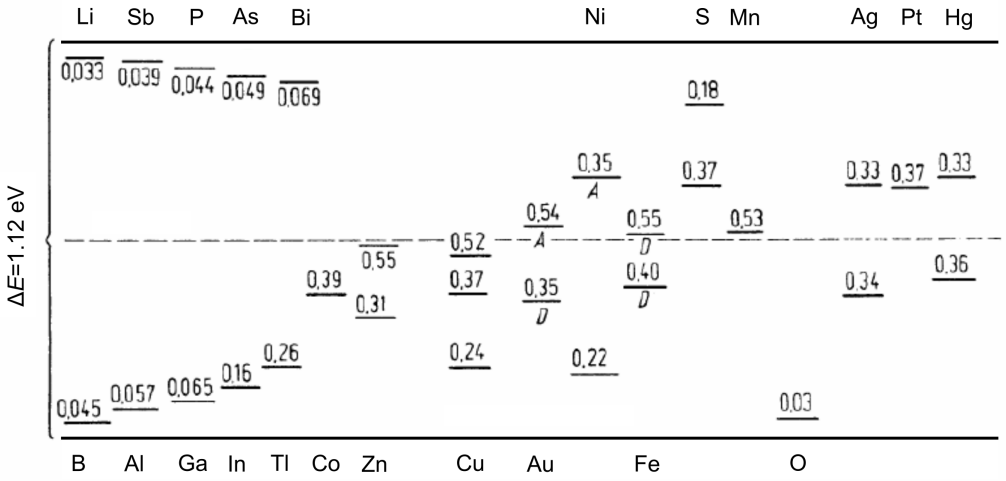
Also, the energy gap between the relevant energy levels of the acceptor atom and the highest energy of the valence band is small, so the probability that an electron of the valence band will be excited to an energy level of an acceptor atom is very large.

Since the effective mass of the wave packets at the top of the valence band is negative, the electrical response to an applied electric and/or magnetic field can be described by positive charge carriers.

The positive charge carriers are commonly referred to as “electron holes”.

Semiconductors 7

Energy levels of donor and acceptor atoms in the energy band gap of silicon

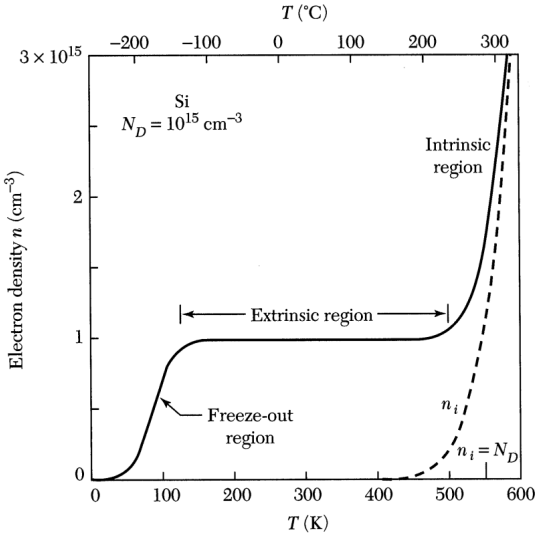


Semiconductors 7

Comment

The figure gives an overview of the energy levels of donor and acceptor atoms in the energy band gap of silicon.

Semiconductors 8



Semiconductors 9 Comment 1

The figure shows the electron density in the conduction band of silicon.

The dashed line shows the intrinsic electron density of pure silicon.

Because of the large energy gap, the electron density is very small for temperatures below 400 K.

The energy gap between the valence and conduction bands of silicon is quite large and a high temperature is necessary to excite electrons from the valence band into the conduction band.

If the semiconductor is doped with donor atoms, the energy gap is much smaller, so that electrons from the donor atom can be excited into the conduction band even at low temperatures.

Semiconductors 8 Comment 2

The electron density in the conduction band is the density of donor atoms over a wide temperature range.

Only when the temperature becomes very high does the electron density increase again, since electrons can be excited from the valence band into the conduction band via the large energy gap.

Ferromagnetism

Electrons in crystal lattices

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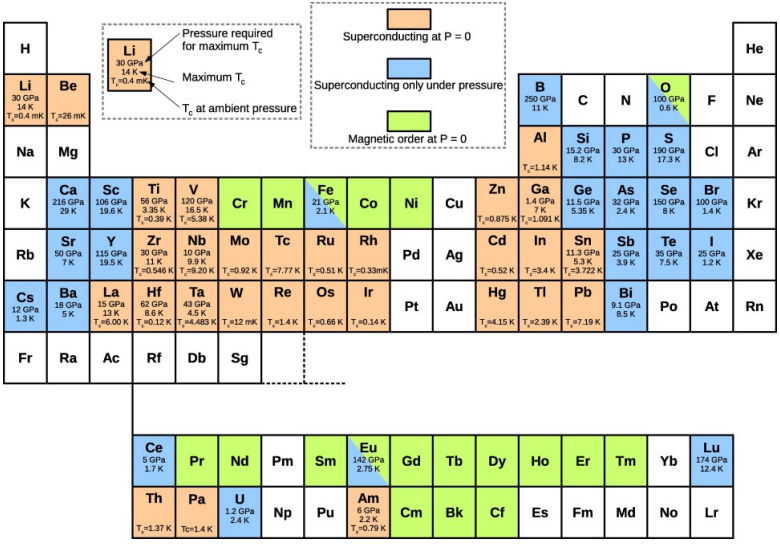
Ferromagnetism 1



Ferromagnetism 1 Comment 1

The periodic table shows that most elements become superconducting at low temperatures.

Many elements spontaneously become superconducting at low temperatures.

For some elements, hydrostatic pressure must be applied before superconductivity can be observed.

Few elements show magnetism.

Chromium is antiferromagnetic below the so-called Néel temperature of 311 K.

Manganese is complicated because it forms four different crystal structures that have very different physical properties, e.g. α-Manganese is antiferromagnetic below the Néel temperature of 100 K.

Ferromagnetism 1

Comment 2

Iron, cobalt and nickel are ferromagnetic below the Curie temperature.

The Curie temperature of iron is 1000 K, of cobalt 1400 K and of nickel 630 K.

Magnetic order is also observed for the rare earth metals.

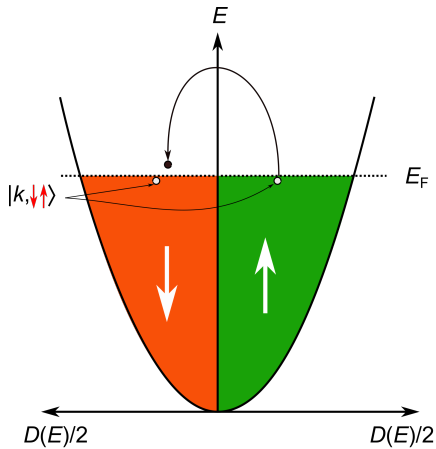
Complicated magnetic spiral structures are caused by the interplay between the localized 4f electrons and the conduction electrons of the 5d and 6s orbitals.

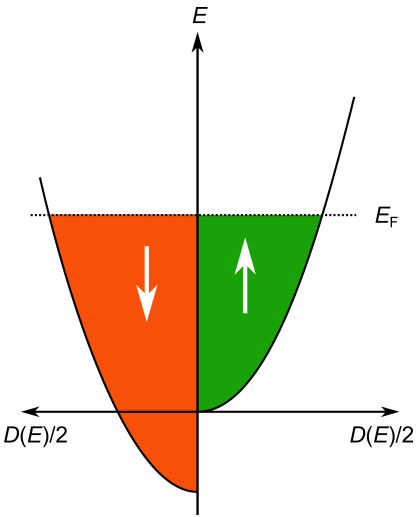
Magnetic order is only observed for a small number of elements.

However, the transition temperatures between the magnetically ordered phase and the paramagnetic phase are comparatively high.

This is in striking contrast to the usually very low transition temperatures of superconductivity.

Ferromagnetism 2





Ferromagnetism 2

Comment 1

The following discussion is limited to the simplest case of ferromagnetism observed in iron, cobalt, and nickel.

The density of states in the Sommerfeld model of quasi-free electrons is proportional to the square root of the energy.

The k states are occupied by electrons up to the Fermi energy.

Each k state can be occupied by two electrons that differ in the spin quantum number $m_s = \pm 1/2$.

The figure on the left shows the densities of states for the spin quantum numbers $m_s = -1/2$ and $m_s = +1/2$ separately for $T = 0$.

Ferromagnetism 2

Comment 2

The areas highlighted in green and red indicate that the *k* states are occupied by spin-up and spin-down electrons, respectively, for these energies.

The two small circles indicate two electrons occupying a *k* state near the Fermi energy.

Because of the uncertainty principle, it is possible for an electron to leave its quantum state and occupies another quantum state for a short time, which the energy-time uncertainty principle allows.

The arrow in the figure on the left indicates that an electron jumps from the green area to a free *k* state in the red area, which is just above the Fermi energy.

Ferromagnetism 2

Comment 3

This electron must change its spin quantum number from $m_s = +1/2$ to $m_s = -1/2$ and additionally increase its kinetic energy if all k states below the Fermi energy are occupied.

On the other hand, it can thereby reduce electron-electron repulsion with the electron with which it previously shared the k state.

This process is the exchange interaction, which favors the parallel alignment of the electron spins in atoms.

In atoms, electrons are confined to atomic orbitals and electron-electron repulsion is comparatively strong.

In solids, the electrons occupy spatially extended k states and the electron-electron repulsion is rather weak.

Ferromagnetism 2

Comment 4

For most metals, the energy gain from reduced electron-electron repulsion is less than the energy required to adopt a k state above the Fermi energy.

For iron, cobalt, and nickel, the energy gain from reduced electron-electron repulsion is greater than the additional kinetic energy, and a large number of electrons can switch from the green side to the red side.

The figure on the right illustrates this situation.

There are more electrons on the red side than on the green side.

The electrons switch from side to side until an equilibrium is reached between the reduced repulsion energy and the additional kinetic energy.

Ferromagnetism 2

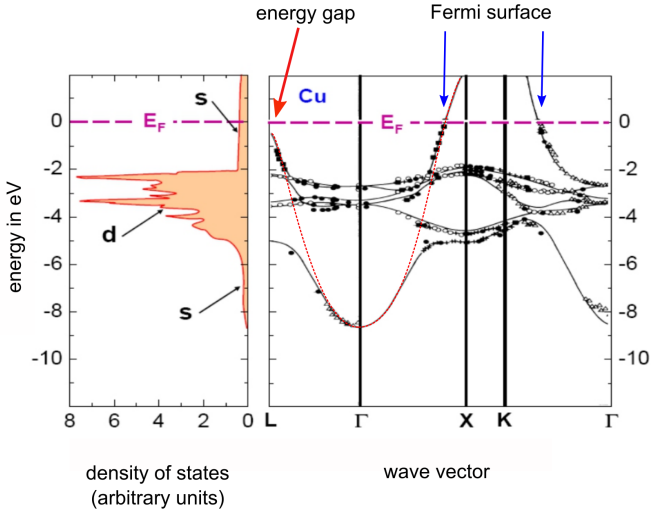
Comment 5

If the exchange interaction favors the parallel alignment of the spins, the electrons can switch from $m_s = +1/2 \rightarrow -1/2$ or just as well from $m_s = -1/2 \rightarrow +1/2$ and magnetic domains begin to form.

Since the spin-orbit coupling for the 3d elements is rather small, the magnetic moment of the domains can point in all directions.

Due to the low spin-orbit coupling, the magnetic domains can easily align in an externally applied magnetic field, resulting in a large magnetic moment of the crystal in a magnetic field.

Ferromagnetism 3



Ferromagnetism 3 Comment 1

The figure shows once again the density of states and the band structure of copper.

The 4s electrons are the conduction electrons, which behave almost like quasi-free electrons.

Unlike the neighboring elements nickel, cobalt and iron, copper is not a magnet.

The main difference between nickel, cobalt, iron on the one hand and copper on the other hand is that the Fermi energy for nickel, cobalt and iron is in the region of the 3d bands, while the Fermi energy for copper is exclusively in the region of the 4s band.

It is therefore interesting to note the differences between the 4s band and the 3d bands shown in the figure.

Ferromagnetism 3

Comment 2

The density of states of the 4s band is small compared to the density of states of the 3d bands.

The 3d bands are narrow and the density of states of the 3d bands is confined to an energy range that is small compared to the energy range of the 4s band.

The 3d electrons are better localized than the 4s electrons and there are five 3d orbitals that make up the 3d bands.

Consequently, the electrical conductivity of copper is greater than that of nickel, cobalt or iron.

Ferromagnetism 3

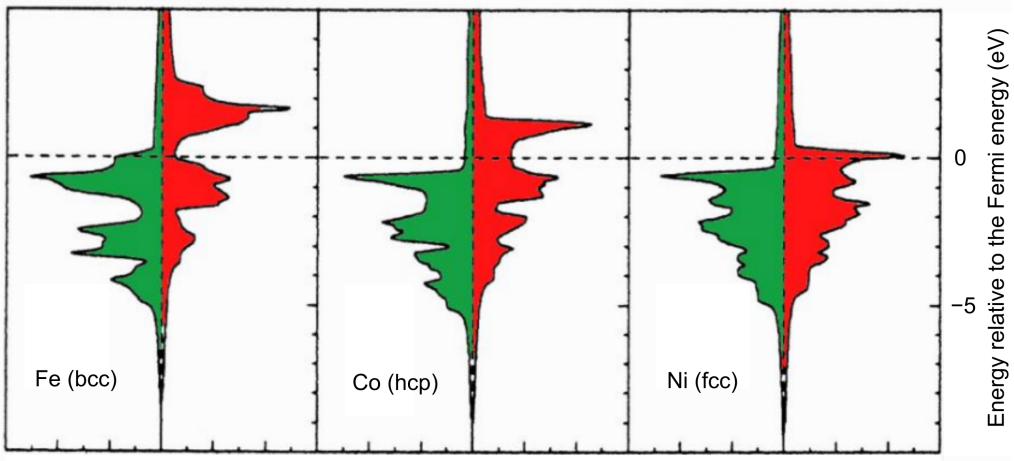
Comment 3

For a 4s electron, the additional kinetic energy is obviously greater than the potential energy gain due to the reduced repulsion force when it jumps to an opposite spin state, since no magnetism is observed for copper.

The opposite is true for nickel, cobalt and iron.

In these elements, there are many states in a narrow energy interval, and the increase in kinetic energy is smaller than the decrease in potential energy due to the reduced repulsive force.

Ferromagnetism 4



Ferromagnetism 4

Comment

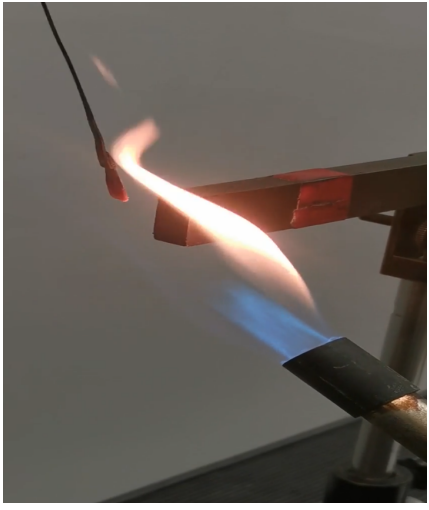
The figure shows the density of states of iron, cobalt and nickel for up and down spin in the ferromagnetic phase.

There is an imbalance between the two spin orientations.

As the temperature increases, more and more electrons are thermally activated and the delicate interplay between kinetic energy and potential energy due to electron-electron repulsion becomes irrelevant above the Curie temperature.

The thermal energy dominates the behavior of the electrons and the k states are equally populated with up and down spins for temperatures above the Curie temperature.

Ferromagnetism 5



(CurieEisen3.mp4)

Ferromagnetism 5 Comment

The video shows a small piece of iron attached to the end of a pendulum.

Since iron is ferromagnetic, the pendulum is attracted to a permanent magnet.

Iron loses its magnetic moment when heated above the Curie temperature of 758° C.

The video shows the alternating heating and cooling of the small piece of iron.

If the temperature of the piece of iron is below the Curie temperature, the pendulum is attracted to the permanent magnet.

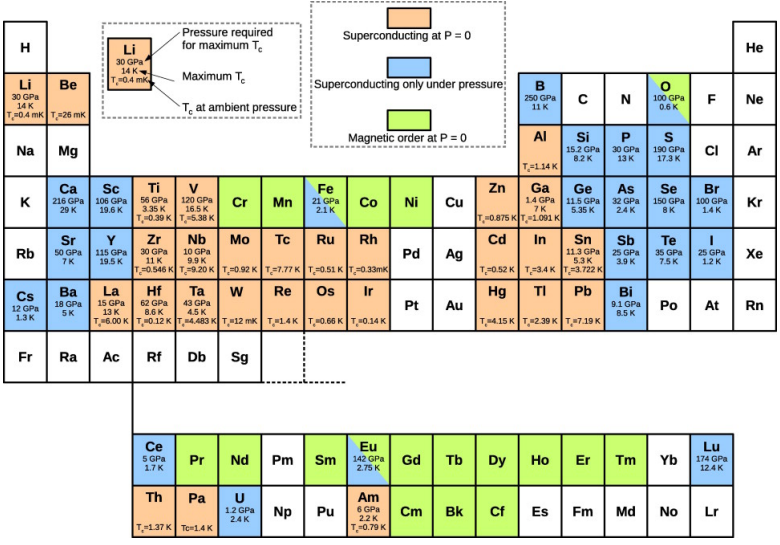
If the temperature of the piece of iron is greater than the Curie temperature, the pendulum can swing freely.

(The rather cool yellow flame is irrelevant to the experiment. It's just a nasty imperfection of the Bunsen burner.)

Electrons in crystal lattices

- Electrical conductivity and Ohm's law
- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Electron dynamics and Electron hole bands
- Photoemission Spectroscopy
- Semi-classical electron dynamics
- Semiconductors
- Ferromagnetism
- Superconductivity

Superconductivity



Superconductivity

Comment

Superconductivity is not an exotic phenomenon.

Many elements of the periodic table and countless alloys and chemical compounds become superconducting below a critical temperature.

The periodic table shows that superconductivity and magnetism are mutually exclusive.

Only a few elements (oxygen, iron and europium) not only order magnetically, but also become superconducting under pressure.

BCS theory

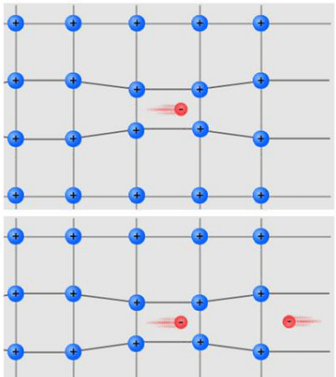
Superconductivity

- BCS theory
- London equations

BCS theory 1

John Bardeen, Leon Cooper, Robert Schriefer 1957 (NP 1972)
Cooper pairs

$$\{+\vec{k}\uparrow, -\vec{k}\downarrow\}$$



spacial extent of the Cooper pairs

$$\xi_0 \approx 2 - 1000\,\mathrm{nm}$$

macroscopic wave function

$$\psi = \psi_0 e^{-iEt/\hbar}$$

BCS theory 1

Comment 1

Superconductivity was discovery by Kamelingh Onnes in 1911.

The first microscopic theory of superconductivity was published in 1957 by Bardeen, Cooper and Schriefer.

The theory is very successful and is called the BCS theory.

The basic idea of the BCS theory is that two counter-propagating electron waves with the same wave number, i.e. $\vec{k}$ and $-\vec{k}$, form a new quantum state with lower energy.

The figure illustrates the idea of the mechanism that couples the two electron waves.

Since atoms are not fixed in their lattice site but can oscillate freely around an equilibrium position, atoms can react to electrical charges flying past them.

BCS theory 1

Comment 2

The figure shows atoms moving in the direction of an electron flying through the crystal lattice.

The speed of the electrons is in the range of the Fermi velocity and therefore very high compared to the movement of the atoms.

The atoms remain in the deflected position on the electron time scale for a very long time, creating a channel that can be used by an electron propagating in the opposite direction to reduce its potential energy.

This gain in energy joins two electrons in a new shared quantum state.

Due to the Pauli principle, this new quantum state can be occupied by two electrons with opposite spin quantum numbers.

BCS theory 1

Comment 3

This coupling mechanism of two electrons with opposite wave vectors $\vec{k}$ and $-\vec{k}$ was discovered by Leon Cooper in 1956.

This new quantum state is called a Cooper pair.

Only electrons whose energy is close to the Fermi energy can form Cooper pairs.

These are also the electrons that contribute to specific heat capacity and electrical conductivity.

Electrons blocked in their *k* states contribute neither to electrical conductivity nor to superconductivity.

Electrons whose energy is close to the Fermi energy also experience scattering processes and therefore move in wave packets that have a certain spatial extent.

BCS theory 1

Comment 4

Cooper pairs can only form when wave packets with opposite wave vectors overlap.

The Cooper pairs therefore have a limited spatial extension, which is given by the correlation length ξ_0.

The correlation length ξ_0 is comparatively large, so that many electrons are in the range of a Cooper pair.

It is therefore not possible to single out two specific electrons that make up the Cooper pair, rather the electrons are constantly falling in and out of a Cooper pair.

The term “pair” in this context means that two electrons form the Cooper pair, which are constantly being exchanged for other electrons.

BCS theory 1

Comment 5

A Cooper pair is therefore stable, although the electrons involved are constantly subject to scattering processes and are exchanged.

Cooper pairs behave similar to bosons, since the electron spins of a Cooper pair add up to the total spin $S = 0$.

Similar to photons ($S = 1$), any number of Cooper pairs can occupy a single quantum state and thus form a macroscopic wave function that extends over the entire solid.

This is similar to the laser where many photons form a macroscopic electromagnetic wave.

It is therefore possible to carry out interference experiments with these macroscopic wave functions.

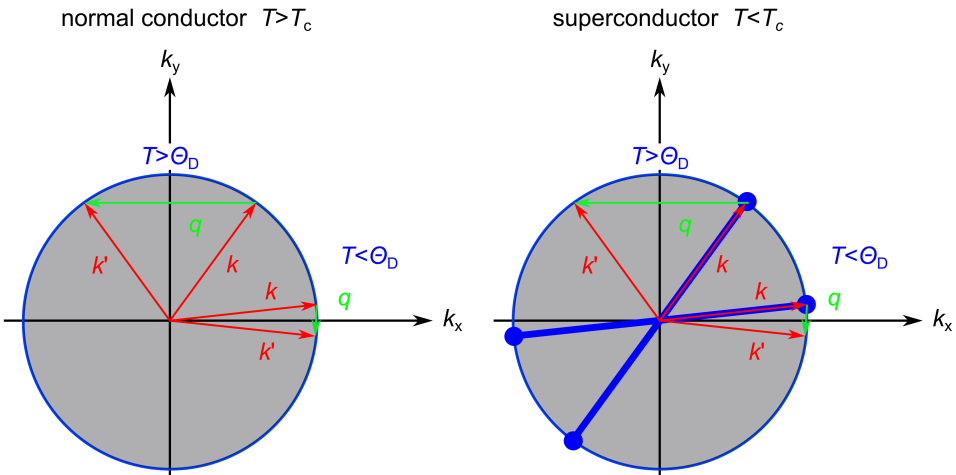
BCS theory 1

Comment 6

Electrical circuits based on the interference of the macroscopic wave functions of a superconductor are called SQUIDs (Superconducting Quantum Interference Device).

BCS theory 2

Cooper pairs cannot lose energy due to scattering



BCS theory 2

Comment 1

The figure on the left shows the electron-phonon scattering that leads to electrical resistance in metals.

An electron absorbs a phonon and is thereby deflected in a different direction.

At low temperatures well below the Debye temperature, only acoustic phonons are excited, which can only slightly deflect electrons.

At temperatures above the Debye temperature, all phonon modes within the 1st Brillouin zone are excited and electrons can be strongly deflected by electron-phonon scattering.

Strong deflections also occur when an electron is scattered off an impurity atom or a crystal defect.

BCS theory 2

Comment 2

The figure on the right shows the case that electrons form Cooper pairs.

These are represented in the figure by the blue dots connected by the blue line.

The scattering can only take place if the binding energy of the Cooper pair can be overcome by the scattering.

If the energy of a phonon is less than the binding energy, the Cooper pair cannot be broken by a phonon.

Cooper pairs move through the crystal lattice without being able to gain or lose energy from the crystal.

The superconducting current flows without resistance.

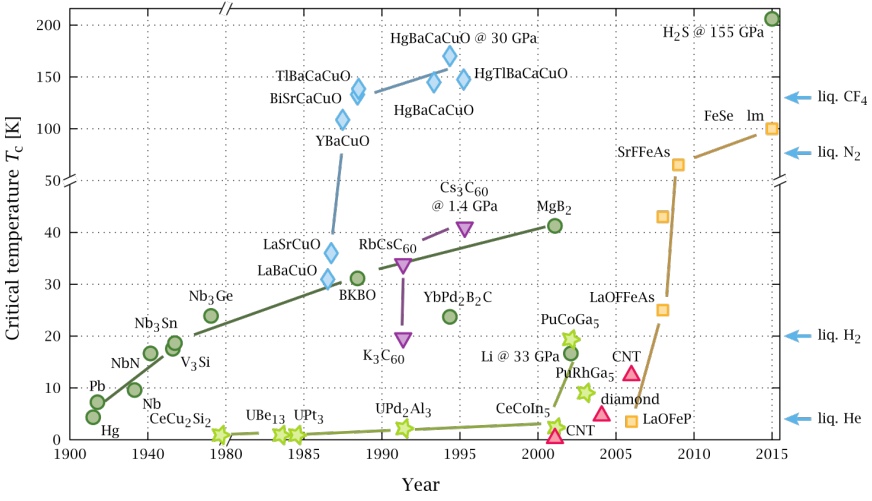
BCS theory 2

Comment 3

The binding energy of the Cooper pairs is usually very small, so that the transition temperatures T_c of superconductors are often very low.

The transition temperature of a superconductor is called the critical temperature.

BCS theory 3


Critical temperature T_c [K]
Year
HgBaCaCuO @ 30 GPa
H_2S @ 155 GPa
TlBaCaCuO
HgTlBaCaCuO
BiSrCaCuO
HgBaCaCuO
YBaCuO
liq. CF_4
FeSe lm
SrFFeAs
liq. N_2
Cs_3C_{60} @ 1.4 GPa
MgB_2
LaSrCuO
$RbCsC_{60}$
LaBaCuO
BKBO
Nb_3Ge
$YbPd_2B_2C$
LaOFFeAs
Nb_3Sn
$PuCoGa_5$
liq. H_2
K_3C_{60}
Li @ 33 GPa
CNT
NbN
V_3Si
$PuRhGa_5$
Pb
diamond
Nb
$CeCu_2Si_2$
UBe_{13}
UPt_3
UPd_2Al_3
$CeCoIn_5$
LaOFeP
liq. He
Hg
CNT

BCS theory 3

Comment 1

Since the discovery of superconductivity in 1911, physicists and chemists have tried to find substances with higher transition temperatures.

The figure shows how substances with higher transition temperatures have been discovered over the years.

In the search for substances with higher transition temperatures, chance played a major role.

The BCS theory of superconductivity did not bring a breakthrough in 1957 either.

The dark green dots show superconductors that can be well understood with the BCS theory.

The green stars show so-called heavy fermion superconductors.

BCS theory 3

Comment 2

The Cooper pairs are bound by magnetic interactions.

Therefore, this class of superconductors is used as model systems to study unconventional superconductivity, although the critical temperatures are usually very small.

The light blue diamonds show the cuprate superconductors.

The discovery of cuprate superconductors in 1986 was a breakthrough because it made it possible to use liquid nitrogen as a coolant instead of expensive helium.

The cuprate superconductors are based on copper-oxygen planes and the Cooper pairs are believed to form due to the interaction of the electrons with strong two-dimensional magnetic correlations.

BCS theory 3

Comment 3

Another class of high-temperature superconductors are the iron pnictide superconductors discovered in 2006.

These superconductors are based on iron planes separated by pnictides.

Pnictides are the elements of the periodic table that are in the column below nitrogen, e.g. phosphorus or arsenic.

The phase diagrams of the iron pnictides are very similar to the phase diagrams of the heavy fermion and cuprate superconductors.

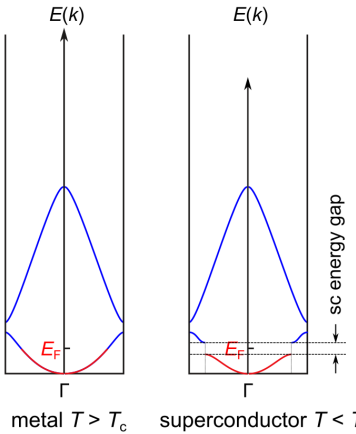
Finally, the figure also shows some carbon-based superconductors (red triangles).

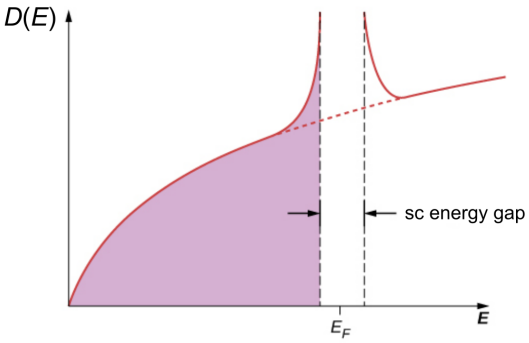
They are based on buckminsterfullerenes (C_{60}) or carbon nanotubes (CNT).

Even heavily doped diamond becomes superconducting at a critical temperature in the range of 3K.

BCS theory 4

energy gap at the Fermi energy





BCS theory 4

Comment 1

The figure on the left shows the schematic band structure in the quasi-free-electron approximation.

The occupied k states are marked in red.

The Fermi energy of a metal is somewhere in the energy band and electrons can be excited with a minimal amount of energy.

An energy gap opens at the Fermi energy when the metal becomes superconducting below the critical temperature T_c.

The electrons occupying k states near the Fermi surface couple to form Cooper pairs.

BCS theory 4

Comment 2

At least the energy of the superconducting energy gap is necessary to break the Cooper pairs.

The second figure shows the deformation of the energy band due to the opening of the superconducting energy gap.

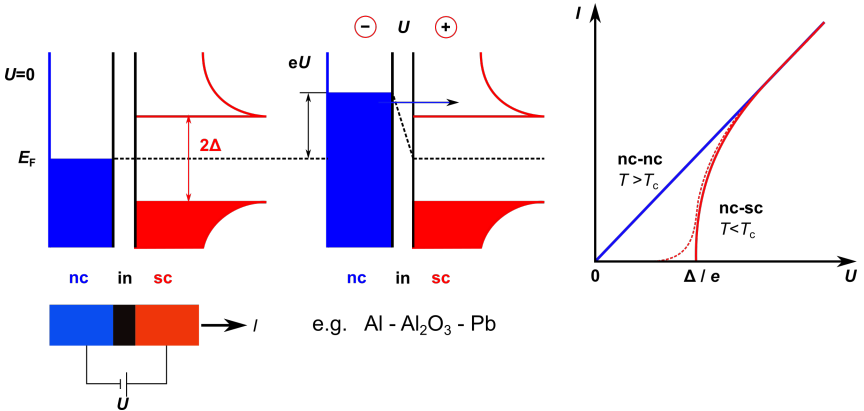
The figure on the right shows the density of states for quasi-free electrons, which is proportional to the square root of the energy.

The *k* states in the energy gap region are shifted to higher and lower energies as the energy gap opens.

Therefore, the density of states is increased just below and just above the superconducting energy gap.

BCS theory 5

Measurement of the energy gap with a tunnel junction between a normal conductor (e.g. Al $T_c = 1.2\,\mathrm{K}$) and a superconductor (e.g. Pb: $T_c = 7.2\,\mathrm{K}$)



BCS theory 5

Comment 1

The superconducting energy gap can be measured with a tunnel junction between a normal conductor and a superconductor.

A nice example is the tunnel contact between aluminum and lead.

Both metals are separated by a thin layer of aluminum oxide.

Electrons can tunnel through this barrier.

The figure below left shows the tunnel junction with the current and the applied voltage.

The figure on the right shows the current-voltage curve of the tunnel junction.

BCS theory 5

Comment 2

If the current-voltage characteristic is measured at a temperature above the critical temperature of lead, the linear current-voltage characteristic of an ohmic resistor is obtained.

The resistance is mainly determined by the oxide barrier.

The figures on the left show the density of states at the Fermi energy when the temperature is below the critical temperature of lead but above the critical temperature of aluminum.

The figure on the left shows the case that no voltage is applied.

Because of the energy gap of lead, no electrons can tunnel from aluminum to lead, since there are no k states in the energy gap of lead.

BCS theory 5

Comment 3

If the potential energy of the electrons in aluminum is increased by an applied voltage, an electric current can flow as soon as the Fermi energy of aluminum is above the energy gap of lead.

Once this occurs, electrons can tunnel from the aluminum into the free k-states of lead and an electric current begins to flow.

If the current-voltage characteristic of the tunnel junction is measured at a temperature below the critical temperature of lead but above the critical temperature of aluminum, the current-voltage characteristic shown in red is obtained.

The current begins to flow when the applied voltage satisfies the condition $eU = \Delta$.

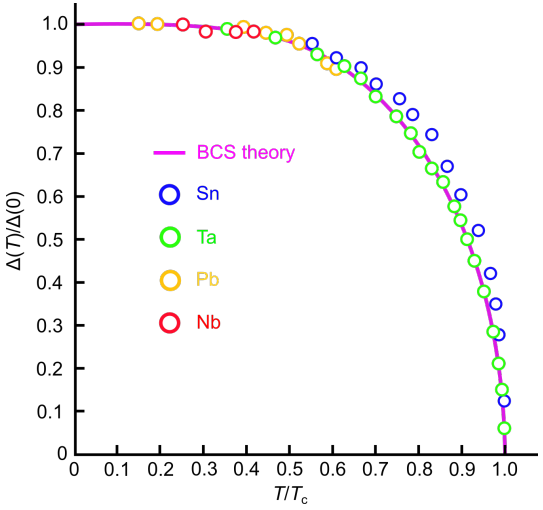
BCS theory 5

Comment 4

The solid red line shows the ideal case when thermal excitations of electrons across the tunnel junction can be neglected.

The dashed red line shows the more realistic current-voltage characteristic when thermal excitations cannot be neglected.

BCS theory 6



BCS energy gap

$$2\Delta(0) = 3.52\, k_B T_c$$

and

$$\Delta(T \to T_c) = \Delta(0)\sqrt{1 - \frac{T}{T_c}}$$

BCS theory 6

Comment

The figure shows the temperature dependence of the energy gap that occurs below the critical temperature.

The prediction of the BCS theory is confirmed by the experimental results.

The first formula on the right shows BCS theory's prediction for the maximum energy gap at low temperatures.

The second formula gives the temperature dependence of the energy gap just below the critical temperature.

BCS theory 7

BCS energy gap

$$2\Delta(0) = 3.52\, k_B T_c$$

element	T_c [K]	$2\Delta(0)/k_B T_c$
Cd	0.56	3.2
Al	1.196	3.4
In	3.4	3.6
Sn	3.72	3.5
Ta	4.48	3.6
V	5.3	3.4
Pb	7.19	4.3
Nb	9.26	3.8

BCS theory 7

Comment

The boxed equation gives the relation between the superconducting energy gap and the critical temperature according to the BCS theory.

The table shows the experimental results for some elements which confirm the BCS theory.

London equations

Superconductivity

- BCS theory
- London equations

London equations 1

Fritz and Heinz London (1935): equation of motion of superconducting charge carriers

$$m\frac{\partial \vec{v}}{\partial t} = q\vec{E}$$

with the superconducting current density

$$\vec{j}_s = qn_s\vec{v}$$

follows

$$\frac{m}{q^2 n_s}\frac{\partial \vec{j}_s}{\partial t} = \vec{E}$$

definition of the London penetration depth

$$\lambda_L^2 = \frac{m}{\mu_0 q^2 n_s}$$

London equations 1 Comment 1

The first theoretical approach to superconductivity was formulated by Fritz and Heinz London in 1935.

Their theory is known as the London theory of superconductivity.

The London theory assumes that there are superconducting charge carriers that react to an applied external electric field according to Peierl's equations of motion with an effective mass.

This assumption is formulated by the first equation.

The superconducting charge carriers are the Cooper pairs, i.e. $q = -2e$.

The main difference between electron dynamics and Cooper pair dynamics is that they are unaffected by the scattering processes.

London equations 1

Comment 2

The second equation is the superconducting current density j_s, which results from the density n_s of the superconducting charge carriers, their charge $q = -2e$ and the drift velocity.

The underlined equation results from inserting the current density into the equation of motion.

Dividing the prefactor on the left side of the equation by the magnetic field constant $\mu_0 \approx 4\pi \cdot 10^{-7}\,\mathrm{Vs/Am}$ gives a quantity that is measured in square meters.

It turns out that this quantity is the square of the penetration depth of an external magnetic field into the superconductor.

The equation outlined in red gives the definition of the London penetration depth.

London equations 2

1st London equation

$$\vec{E} = \mu_0 \lambda_L^2 \frac{\partial \vec{j}_s}{\partial t}$$

with the 1st London equation and the 3rd Maxwell equation (induction law)

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} = \mu_0 \lambda_L^2 \frac{\partial}{\partial t} \nabla \times \vec{j}_s$$

results the

2nd London equation

$$\vec{B} = -\mu_0 \lambda_L^2 \nabla \times \vec{j}_s$$

London equations 2

Comment

The formula outlined in red now gives the first London equation with the London penetration depth.

If the first London equation is inserted into Faraday's law of induction, then the second London equation can be read from it.

The second formula outlined in red shows the second London equation.

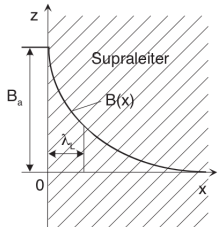
London equations 3

With the 2nd London equation and Ampere's law $\nabla \times \vec{B} = \mu_0 \vec{j}_s$ results

$$\vec{B} = \lambda_L^2 \nabla^2 \vec{B}$$

use $\nabla \vec{B} = 0$ (2nd Maxwell law) and $\nabla \times (\nabla \times \vec{B}) = \nabla(\nabla \vec{B}) - \nabla^2 \vec{B}$

in one dimension one gets $B(x) = \lambda_L^2 \frac{\partial^2 B(x)}{\partial x^2} \quad \rightarrow \quad B(x) = B_a e^{-x/\lambda_L}$



a magnetic field cannot penetrate a superconductor $\rightarrow$ Meissner effect

London equations 3

Comment 1

Substituting the 2nd London equation into Ampere's law gives the underlined equation.

The figure illustrates the meaning of this equation.

The magnetic field B_a is applied along the z-direction parallel to the surface of a superconductor.

The drop in the magnetic field within the superconductor perpendicular to the surface can be calculated using the differential equation.

The solution is a simple exponential decay and the decay length is the London penetration depth.

London equations 3

Comment 2

The magnetic field can only penetrate the superconductor in a thin surface layer.

There is no magnetic field in the bulk of the superconductor.

This is the Meissner effect.

Shield currents begin to circulate when a superconducting material is cooled below the critical temperature in a magnetic field.

If the temperature is above the critical temperature, the magnetic field can penetrate the material, since the shielding currents that occur due to Lenz's law are quickly reduced to zero by the ohmic resistance.

Screen currents always suppress the magnetic field within the superconducting material when the temperature is below the critical temperature.

London equations 3

Comment 3

The shielding currents lead to a strong magnetic moment in the superconducting material, which reacts very quickly to any change in the external magnetic field.

London equations 4

(Moebiusband.mp4)

London equations 4

Comment

The video shows a superconductor located at a certain distance above a magnetic rail.

Any change in distance changes the magnetic field strength, which leads to an immediate reaction of the shielding currents.

The magnetic moment of the superconductor is always set in such a way that the distance to the magnetic rail does not change.

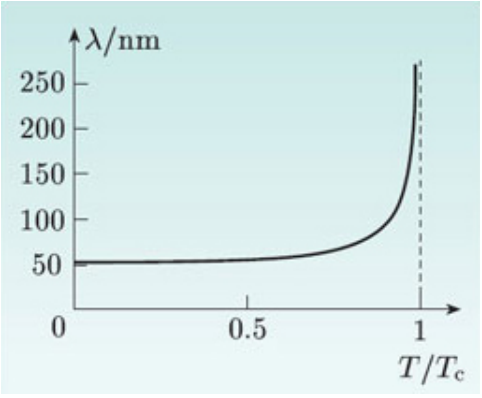
The video shows a small piece of an high temperature superconductor.

Liquid nitrogen is used to cool the superconductor below the critical temperatures.

The superconductor is placed in a small container made of foamed plastic for thermal insulation.

London equations 5

London penetration depth of various elements



element	T_c [K]	$\lambda_L(T \to 0)$ [nm]
Cd	0.56	110
Al	1.196	16
Sn	3.72	34
Pb	7.19	37
Nb	9.26	39

London equations 5

Comment

The London penetration depth is temperature dependent.

It is minimal for $T \to 0$ and diverges for $T \to T_c$.

$$\lambda_L(T) = \lambda_L(0)/\sqrt{1-(T/T_c)^4}$$

The table shows the critical temperatures and the London penetration depth of some elements.

The London penetration depth is in the range of a few 10 nm.

Revision

Summary in Questions 1

1. Sketch the conductivity as a function of temperature for a metal and for a semiconductor.
2. Why do impurities affect the electrical conductivity of semiconductors so much?
3. How do donor atoms differ from acceptor atoms?
4. Sketch the conduction electron density of a semiconductor doped with donor atoms as a function of temperature.
5. There are three different temperature ranges. How do these temperature ranges differ?
6. Explain the exchange interaction for conduction electrons.
7. Which conditions must be fulfilled for conduction electrons to order ferromagnetically?

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Modern Physics (Winter Semester 2022/23)

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Atoms

Atoms

3 Quantum mechanics

Atoms

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Solids

Solids

Solids

Solids