Solids

1. Binding types
2. Crystal lattices
3. Lattice vibrations
4. **Electrons in crystal lattices**

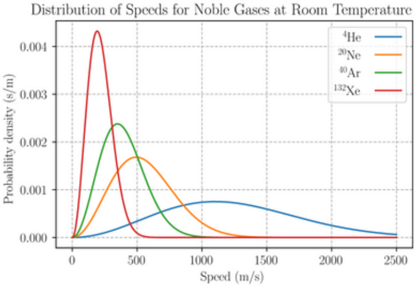
Drude

Electrons in crystal lattices

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

Drude model 1

- Conduction electrons can move freely through a metal and behave like an ideal gas
- the velocities of the conduction electrons follow the Maxwell velocity distribution function



speed in the maximum

$$v_{max} = \sqrt{\frac{2k_B T}{m}}$$

$$m_{^4\mathrm{He}}/m_\mathrm{e} = 7277 \approx 10^4 \rightarrow v_\mathrm{max}(\mathrm{e})/v_\mathrm{max}(^4\mathrm{He}) \approx 100$$

$$\underline{\ell \approx v_\mathrm{max} \cdot \tau \approx 10^{-10}\,\mathrm{m}}$$

Drude model 1

Comment 1

The electron was discovered by J.J. Thomson in 1897.

The study of the Zeeman effect led H. Lorentz in 1899 to the conclusion that the optical properties of atoms are caused by electrons.

Paul Drude published his theory of electric conductivity in 1900.

Drude assumes that there are electrons in metals that are not bound to their atoms.

These quasi-free electrons are called conduction electrons.

Drude also assumes that the conduction electrons behave similarly to an ideal gas.

Drude model 1 Comment 2

This means that the velocity of the conduction electrons follows Maxwell’s velocity distribution function.

The thermal equilibrium between the electron gas and the crystal lattices is established by collisions of the conduction electrons with the atoms of the lattice.

When an electric voltage is applied to a metal, an electric current flows.

The electrons are accelerated by the electric field due to their electric charge q and lose a fraction of the kinetic energy gained when they collide with the atoms of the crystal lattice.

The voltage source does work that increases the temperature of the crystal lattice.

Drude model 1 Comment 3

The mean free path of the electrons can be estimated using the velocity at the maximum of Maxwell's velocity distribution.

The figure shows the velocity distribution of various noble gases.

For helium atoms, the velocity at the maximum of the distribution function is about 1000 m/s at room temperature.

The velocity at the maximum of the distribution function is inversely proportional to the square root of the mass of the gas particles. The formula $\frac{1}{2}mv^2 = k_\mathrm{B}T$ applies.

The ratio of the masses of helium atoms and electrons is about 10000. Therefore a hundred times higher speed can be expected for electrons ($m(^4\mathrm{He}) = 4u$, $m(e^-) = 5.5 \cdot 10^{-4}u$).

Drude model 1 Comment 4

With a mean free flight time of 10^{-15} s and a speed of 10^5 m/s, the mean free path ℓ is 10^{-10} m, which corresponds to the distance between the atoms.

With this estimate one can understand the incredibly high collision rate of the electrons in the context of the Drude model.

By 1900, another of nature's mysteries seemed to have found a plausible explanation.

Unfortunately, the assumption of the Drude model that conduction electrons behave like a classical ideal gas is incorrect.

Although this was not to be expected around 1900, it soon became clear that many experimental results observed for metals cannot be explained in terms of a free electron gas.

Drude model 2

Problems of the Drude model

- a classical ideal gas of quasi free conduction electrons should contribute to the heat capacity of metals

$\rightarrow$ the contribution of each conduction electron to the heat capacity is $\frac{3}{2}k_B$
$\rightarrow$ the contribution of each oscillating atom is at high temperatures $3k_B$
(rule of Dulong-Petit)

this large contribution of a classical conduction electron gas to the heat capacity of metals cannot be observed experimentally.

Drude model 2 Comment

Although the idea of an electron gas is not fundamentally wrong, metals have many properties that cannot be explained with a quasi-classical gas made up of conduction electrons.

Heat capacity measurements are fundamental to understanding solids.

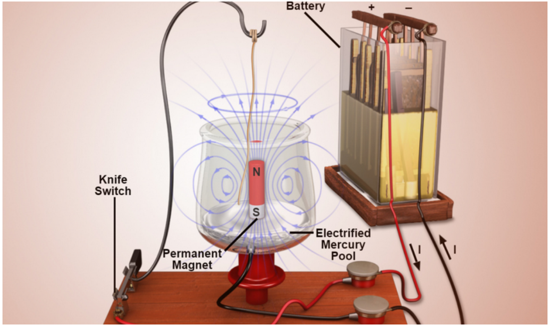
If the conduction electrons behave like a classical ideal gas, the contribution of each conduction electron to the heat capacity should be $\frac{3}{2}k_B$.

This is a very large contribution that can be compared to the maximum contribution of $3k_B$ due to the vibration of an atom at high temperatures.

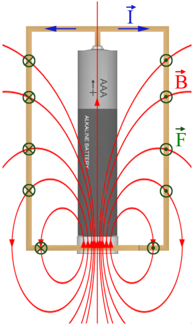
The experiments clearly show that the major contribution of a classical, quasi-free electron gas to the heat capacity of metals is missing. (Compare the 21st lecture: “Heat capacity of the crystal lattice 8”)

Drude model 3

Faraday motor (1821)



(Faradaymotor.mp4)



(Faradaymotorbuegel.mp4)

Drude model 3 Comment

In 1821 Faraday built a first electric motor and presented it to the Royal Society in London.

The video shows the simple electric motor.

The image on the right shows a slightly improved version of the motor.

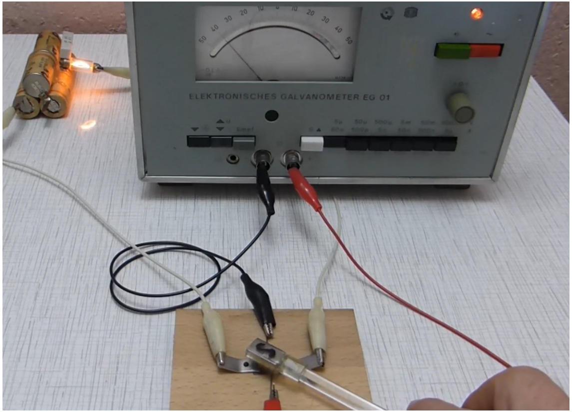
The electric motor is driven by the Lorentz force, which, however, was only theoretically explained by H. Lorentz in 1895.

When Faraday performed his experiment, it was only evident that a force was acting on a conductor carrying an electric current.

The question arose whether the force acts on the conductor as a whole or only on the charge carriers that produce the electric current.

Drude model 4

Hall effect (Edwin Hall 1879)



(Halleffekt.mp4)

Drude model 4 Comment

The question was answered by Edwin Hall in 1879.

The video shows his famous experiment.

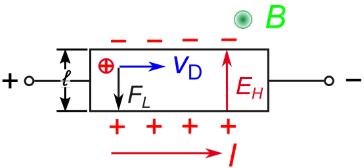
The experiment shows that the force, which was still not properly understood in 1879, acts on the moving charge carriers of the electric current.

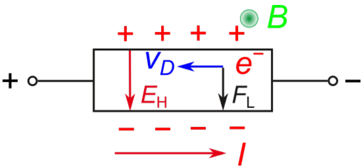
The force deflects the charge carriers and induces an electric potential difference perpendicular to the direction of the current.

The effect depends on the strength and direction of the magnetic field.

Drude model 5

- The Hall effect is due to the Lorentz force $\vec{F} = q\vec{v} \times \vec{B}$
- The sign of the Hall voltage ($E_H \ell$) depends on the sign of the charge carriers.





$U_H = R_H \frac{IB}{d}$ and $R_H^{-1} = q\frac{N}{V}$ (d denotes the thickness of the Hall sensor)

Drude model 5 Comment 1

The Hall effect can easily be understood with the Lorentz force.

The figure on the left shows the Hall effect for positive charge carriers.

The drift speed of the charge carriers points in the direction of the electric current and the Lorentz force points downwards when the magnetic field *B* points out of the projection plane.

This causes the positive charges to accumulate on the lower side of the conductor and the Hall voltage builds up.

Drude model 5 Comment 2

The right figure shows the Hall effect with negative charge carriers.

The drift velocity of the negative charge carriers points in the opposite direction of the electric current.

The Lorentz force also points downwards and the negative charges accumulate on the lower side of the conductor.

The sign of the Hall voltage depends on the sign of the charge of the charge carriers.

Therefore, by measuring the sign of the Hall voltage, the sign of the charge carriers can be determined.

Drude model 6

Cu	$-5.3 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Ag	$-9.0 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Au	$-7.0 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Pt	$-2.0 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Bi	$-5.0 \cdot 10^{-7}\,\mathrm{m^3As^{-1}}$

Mg	$+48.6 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Be	$+24.3 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
In	$+16.0 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Al	$+9.9 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$
Zn	$+6.4 \cdot 10^{-11}\,\mathrm{m^3As^{-1}}$

Hall constants R_H for various elements

Amazingly, the charge of the charge carriers can also be positive in metals

Drude model 6 Comment

The Hall voltage is proportional to the strength of the electric current, the strength of the magnetic field and also depends on the thickness of the conductor along the direction of the magnetic field.

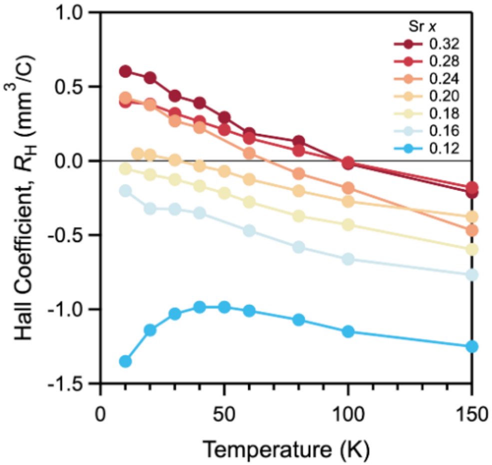
The table gives the constant of proportionality R_H for some metals.

Amazingly, it turns out that the Hall constant can have positive and negative values.

Obviously the charge carriers in some metals are positively charged, which is incomprehensible in view of the negative charge of the electron.

Drude model 7

Hall coefficient as a function of temperature for $Pr_{1-x}Sr_xNiO_2$ thin films
(M Osada et al. · 2020)



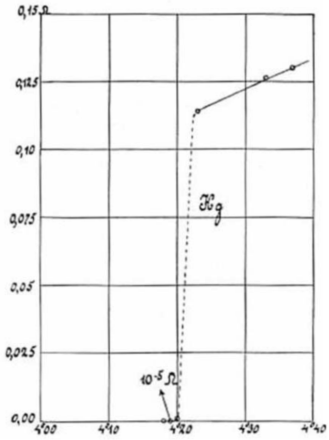
Drude model 7

Comment

The example from current research on a superconductor shows that the Hall coefficient can even change sign with temperature.

Drude model 8

- In 1911 Heike Kamerlingh Onnes discovered superconductivity when he was investigating the electric resistance of mercury



Drude model 8 Comment 1

In 1895 the process for liquefying gases developed by Carl von Linde was patented.

This made it possible to liquefy large quantities of gas and to carry out experiments at low temperatures.

Liquid helium is particularly important for low-temperature experiments, since helium becomes liquid at 4.15 K and remains liquid at ambient pressure down to zero temperature.

Karmeling Onnes investigated the temperature dependence of the conductivity of metals.

The electric resistance of metals decreases with falling temperatures.

Drude model 8 Comment 2

The electric current is hindered by the oscillations of the atoms around their equilibrium positions in the crystal lattice, i.e. by electron-phonon scattering.

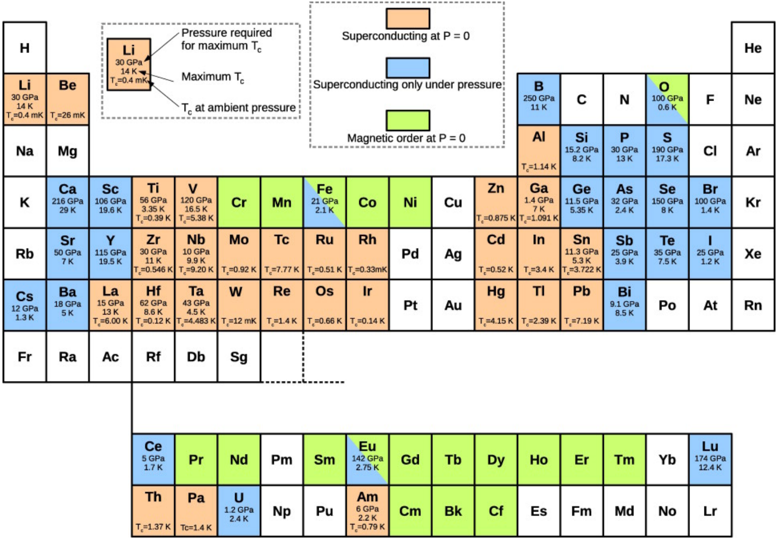
At low temperatures only a few phonons are excited and there is usually a residual resistance left, which is caused by lattice defects (cracks, grain boundaries, impurities, etc.).

Mercury was particularly suitable for such measurements because it is relatively easy to make very perfect crystals when cooling mercury.

The figure shows the famous measurement by Kamerlingh Onnes.

Just above the boiling temperature of helium (i.e. ^{4}He), mercury loses its electrical resistance completely.

Drude model 9



Li 30 GPa 14 K T_c=0.4 mK
Pressure required for maximum T_c
Maximum T_c
T_c at ambient pressure

🟧 Superconducting at P = 0
🟦 Superconducting only under pressure
🟩 Magnetic order at P = 0

H																	He
🟧 Li 30 GPa 14 K T_c=0.4 mK	🟧 Be T_c=26 mK											🟦 B 250 GPa 11 K	C	N	🟦🟩 O 100 GPa 0.6 K	F	Ne
Na	Mg											🟧 Al T_c=1.14 K	🟦 Si 15.2 GPa 8.2 K	🟦 P 30 GPa 13 K	🟦 S 190 GPa 17.3 K	Cl	Ar
K	🟦 Ca 216 GPa 29 K	🟦 Sc 106 GPa 19.6 K	🟧 Ti 56 GPa 3.35 K T_c=0.39 K	🟧 V 120 GPa 16.5 K T_c=5.38 K	🟩 Cr	🟩 Mn	🟦🟩 Fe 21 GPa 2.1 K	🟩 Co	🟩 Ni	Cu	🟧 Zn T_c=0.875 K	🟧 Ga 1.4 GPa 7 K T_c=1.091 K	🟦 Ge 11.5 GPa 5.35 K	🟦 As 32 GPa 2.4 K	🟦 Se 150 GPa 8 K	🟦 Br 100 GPa 1.4 K	Kr
Rb	🟦 Sr 50 GPa 7 K	🟦 Y 115 GPa 19.5 K	🟧 Zr 30 GPa 11 K T_c=0.546 K	🟧 Nb 10 GPa 9.9 K T_c=9.20 K	🟧 Mo T_c=0.92 K	🟧 Tc T_c=7.77 K	🟧 Ru T_c=0.51 K	🟧 Rh T_c=0.33mK	Pd	Ag	🟧 Cd T_c=0.52 K	🟧 In T_c=3.4 K	🟧 Sn 11.3 GPa 5.3 K T_c=3.722 K	🟦 Sb 25 GPa 3.9 K	🟦 Te 35 GPa 7.5 K	🟦 I 25 GPa 1.2 K	Xe
🟦 Cs 12 GPa 1.3 K	🟦 Ba 18 GPa 5 K	🟧 La 15 GPa 13 K T_c=6.00 K	🟧 Hf 62 GPa 8.6 K T_c=0.12 K	🟧 Ta 43 GPa 4.5 K T_c=4.483 K	🟧 W T_c=12 mK	🟧 Re T_c=1.4 K	🟧 Os T_c=0.66 K	🟧 Ir T_c=0.14 K	Pt	Au	🟧 Hg T_c=4.15 K	🟧 Tl T_c=2.39 K	🟧 Pb T_c=7.19 K	🟦 Bi 9.1 GPa 8.5 K	Po	At	Rn
Fr	Ra	Ac	Rf	Db	Sg												

🟦 Ce 5 GPa 1.7 K	🟩 Pr	🟩 Nd	Pm	🟩 Sm	🟦🟩 Eu 142 GPa 2.75 K	🟩 Gd	🟩 Tb	🟩 Dy	🟩 Ho	🟩 Er	🟩 Tm	Yb	🟦 Lu 174 GPa 12.4 K
🟧 Th T_c=1.37 K	🟧 Pa Tc=1.4 K	🟦 U 1.2 GPa 2.4 K	Np	Pu	🟧 Am 6 GPa 2.2 K T_c=0.79 K	🟩 Cm	🟩 Bk	🟩 Cf	Es	Fm	Md	No	Lr

Drude model 9 Comment 1

Superconductivity is not an exotic phenomenon.

Most of the elements in the periodic table become superconducting at low temperatures.

There are some elements that do not become superconducting at ambient pressure but become superconducting when pressure is applied.

The periodic table also shows that magnetic order is a rather exotic phenomenon.

It turns out that the magnetism of the transition metals Cr, Mn, Fe, Co and Ni is based exclusively on the conduction electrons.

Drude model 9 Comment 2

In contrast to this, the magnetism of the rare earths is based on an interplay of the localized magnetic moments of the 4f electrons and the conduction electrons of the 5s, 5p and 5d orbitals.

Superconductivity and magnetism of conduction electrons remain completely incomprehensible in the picture of a classical electron gas.

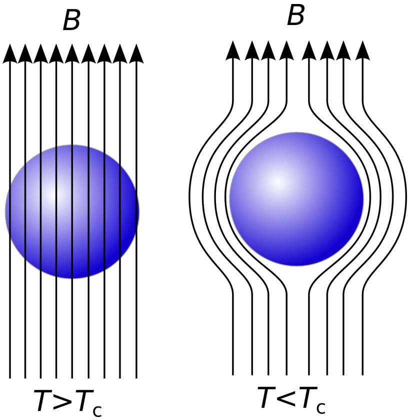
With superconducting coils it can be shown that the electric resistance of superconductors completely disappears below the critical temperature.

Once the superconducting current is established, the magnetic moment of the coil is stable and does not change with time.

This effect is used in the construction of superconducting magnets, e.g. for medical purposes (magnetic resonance imaging).

Drude model 10

Meissner effect



(MeissnerEffekt3.mp4)

Drude model 10 Comment 1

In 1933, Meißner and Ochsenfeld discovered another amazing property of superconductivity.

If a superconductor is cooled below the superconducting transition temperature in a magnetic field *B*, the magnetic field within the superconducting material is eliminated by shielding currents.

The left figure shows the magnetic field that penetrates a superconductor above the transition temperature.

The picture on the right shows the deformation of the magnetic field lines caused by the shielding currents of the superconductor.

The video shows the Meissner effect for tin.

Drude model 10 Comment 2

If a superconductor is cooled below the transition temperature without a magnetic field and a magnetic field is then switched on, shielding currents occur due to Faraday’s law of induction, which prevent the magnetic field from penetrating the superconductor.

If the magnetic field is switched on at a temperature higher than the transition temperature, then the electric resistance dampens the shielding currents to zero and the magnetic field can penetrate the metal.

Amazingly, even without Faraday’s law of induction, the shielding currents start up again as soon as the superconductor has been cooled below the transition temperature.

The Meissner effect shows that superconductivity is a thermodynamic phase, comparable to the solid, liquid or gaseous phase of a substance.

Sommerfeld model

Electrons in crystal lattices

- Electric conductivity and Ohm’s law
- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Photoemission Spectroscopy
- Electron dynamics and Electron hole bands
- Semiconductors
- Ferromagnetism
- Superconductivity

Sommerfeld model Comment

This section is divided into six subsections that cover, step by step, the most basic concepts of conduction electrons.

Sommerfeld model

- Introduction
- Fermi sphere
- Fermi distribution function
- Electric conductivity
- Density of states
- Heat capacity of the electron gas

Introduction

- the conduction electrons, like all quantum particles, are subject to the Schrödinger equation
- the potential energy is simply a constant
- the surface is the barrier that encloses the conduction electrons
- the Schrödinger equation only contains the term for the kinetic energy

$$\boxed{E(\vec{k})\psi_{\vec{k}}(\vec{r},t) = -\frac{\hbar^2\nabla^2}{2m}\psi_{\vec{k}}(\vec{r},t)}$$

the wave functions are plane waves

$$\underline{\psi_{\vec{k}}(\vec{r},t) = \psi_0 e^{i(\vec{k}\vec{r}-\omega t)}}$$

the energy is

$$\underline{E(\vec{k}) = \hbar\omega = \frac{\hbar^2\vec{k}^2}{2m}}$$

Introduction Comment 1

It is obvious that the conduction electrons must also be described by wave functions that are determined by the Schrödinger equation.

Based on the Drude model, Arnold Sommerfeld formulated a simple approach in 1927 that already revealed some fundamental properties of electrons in solids.

In his model of the conduction electrons, Sommerfeld assumes that the attractive forces of the positively charged atoms and the repulsive forces between the conduction electrons are averaged so that the potential energy of the conduction electrons is simply constant regardless of the location of the conduction electrons.

The attractive forces of the atoms only dominate on the surface of the solid, so that the conduction electrons are bound to the solid.

Introduction Comment 2

The resulting potential step on the surface corresponds to the work function W_A in the photoelectric effect.

The formula outlined in red gives the Schrödinger equation.

The value zero is assigned to the constant potential energy and $W_A \rightarrow \infty$ is assumed for the sake of simplicity, resulting in the well-known box potential.

The solutions to this Schrödinger equation are plane waves.

The last underlined formula gives the energy eigenvalues of the Schrödinger equation.

This is simply the kinetic energy of a quasi-free electron.

Fermi sphere

Sommerfeld model

- Introduction
- Fermi sphere
- Fermi distribution function
- Electric conductivity
- Density of states
- Heat capacity of the electron gas

Fermi sphere 1

Schrödinger equation

$$\underline{E(\vec{k})\psi_{\vec{k}}(\vec{r},t) = -\frac{\hbar^2\nabla^2}{2m}\psi_{\vec{k}}(\vec{r},t)}$$

plane waves

$$\underline{\psi_{\vec{k}}(\vec{r},t) = \psi_0 e^{i(\vec{k}\vec{r}-\omega t)}}$$

periodic boundary conditions (for a cubic sample with edge length L)

$$\boxed{\begin{aligned}\psi_{\vec{k}}(x,y,z,t) &= \psi_{\vec{k}}(x+L,y,z,t)\\ \psi_{\vec{k}}(x,y,z,t) &= \psi_{\vec{k}}(x,y+L,z,t)\\ \psi_{\vec{k}}(x,y,z,t) &= \psi_{\vec{k}}(x,y,z+L,t)\end{aligned}}$$

$$k_xL = 2\pi n_1 \quad k_yL = 2\pi n_2 \quad k_zL = 2\pi n_3 \quad \text{and} \quad n_{1,2,3} = 0, \pm 1, \pm 2, \ldots$$

Fermi sphere 1

Comment 1

The first underlined equation gives the Schrödinger equation for a conduction electron in the Sommerfeld model.

The solutions of the Schrödinger equation are plane waves and periodic boundary conditions have to be used to adapt the infinite plane waves to the finite dimensions of the sample.

It is the same procedure that has already been used to describe blackbody radiation and lattice vibrations, and the justification for using periodic boundary conditions is always the same.

The standing waves, which were used for exactly the same Schrödinger equation for the box potential, cannot be used in an extended volume because scattering events suppress the formation of standing wave modes.

Fermi sphere 1 Comment 2

The simplest is a cubic sample with the edge length L, which is repeated infinitely often in all spatial directions.

The wave functions in the resulting infinite but periodic structure can be described in the context of a Fourier series expansion using plane waves.

The equations framed in red formulate the periodic boundary condition of the wave functions.

The last line specifies the condition that the components of a wave vector $k_{x,\, y,\, z}$ have to meet within the Fourier series expansion.

Fermi sphere 1 Comment 3

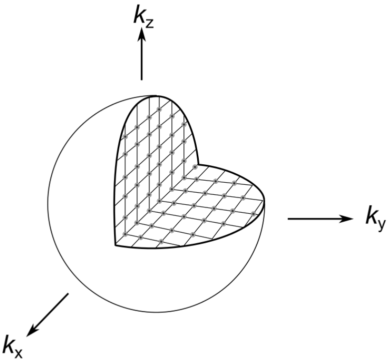
These wave vectors result in periodic wave functions, which have the edge length *L* of the cube-shaped sample as the period length.

With this trick, infinitely plane waves can be used, although only the wave functions of a finite cubic sample are needed.

Fermi sphere 2

allowed wave vectors

$$\boxed{\vec{k}_{n_1,n_2,n_3} = \frac{2\pi}{L}\begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}}$$



volume around the tip of each wave vector

$$\underline{\Delta k^3 = \left(\frac{2\pi}{L}\right)^3 = \frac{(2\pi)^3}{V}}$$

Fermi sphere 2

Comment 1

The formula outlined in red shows the permitted wave vectors.

These wave vectors form a discrete lattice and each of these lattice points, i.e. each of these plane waves can be occupied by two electrons according to the Pauli principle, which differ in their spin quantum number $m_\mathrm{s} = \pm 1/2$.

This lattice of wave vectors fills the reciprocal lattice of the crystal and since the edge length L of the cubic sample is much larger than the lattice parameters of the crystal lattice (e.g. a in the case of a simple cubic lattice), it is obvious that the k -states are very dense compared to the lattice points of the reciprocal lattice.

The figure shows the lattice of k states, with the spacing of the lattice points being exaggerated.

Fermi sphere 2 Comment 2

All k states that are occupied by electrons at zero temperature are surrounded by a sphere called the Fermi sphere.

The largest wave number, i.e. the radius of the Fermi sphere, is called the Fermi wave number.

The underlined formula gives the volume around the tip of each k state.

In the formula L^3 can be replaced by the volume V of the sample.

This is a remarkable detail.

Since scattering events prevent the formation of standing waves, which are caused by the superposition of the waves reflected on the surfaces, the surfaces do not influence the waves in the volume of the sample.

Fermi sphere 2 Comment 3

Therefore, the reference to a cubic shape of the sample is not necessary and L^3 can be replaced by the volume V of an arbitrarily shaped crystal.

Technically, the Fermi sphere is reminiscent of the sphere of the Debye model, although the underlying physics is different.

Fermi sphere 3

radius of the Fermi sphere

$$N = 2 \cdot \frac{\frac{4\pi}{3} k_F^3}{\frac{(2\pi)^3}{V}} = \frac{V k_F^3}{3\pi^2}$$

Fermi wave number k_F

$$\boxed{k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}}}$$

Fermi energy, Fermi temperature and Fermi velocity

$$\boxed{E_F = \frac{\hbar^2 k_F^2}{2m} \quad \text{and} \quad T_F = \frac{E_F}{k_B} \quad \text{and} \quad v_F = \sqrt{\frac{2E_F}{m}}}$$

Fermi sphere 3

Comment 1

At the temperature $T = 0$ all occupied k states are enclosed by the Fermi sphere.

Since all k states can be occupied by two electrons, the condition of the first row results.

The volume of the sphere divided by the volume of a k state is half the number of electrons.

With this condition the radius of the Fermi sphere can be calculated and the first equation outlined in red gives the Fermi wave number.

The Fermi energy can be calculated using the Fermi wave number.

The Fermi energy is the highest kinetic energy of an electron at zero temperature.

Fermi sphere 3

Comment 2

If the Fermi energy is divided by the Boltzmann constant, the Fermi temperature is obtained.

The Fermi temperature is useful to estimate the influence of thermal excitations.

With the formula for the kinetic energy $E_\mathrm{F} = mv_\mathrm{F}^2/2$ the speed of an electron with the Fermi energy can be calculated.

v_F is the Fermi velocity.

The Fermi velocity needs some comments.

The Sommerfeld model assumes infinite electron waves. However, due to the scattering events, the electron waves must be described with finite wave packets.

Fermi sphere 3 Comment 3

Therefore, not the phase velocity of the infinite waves, but the velocity of the wave packets is the relevant velocity to describe electron dynamics.

The speed of wave packets is the group velocity $v_\mathrm{g}(k) = \frac{\mathrm{d}\omega(k)}{\mathrm{d}k}$.

With $E(k) = \hbar\omega(k) = \hbar^2 k^2/2m$ follows that $v_\mathrm{g}(k_\mathrm{F}) = v_\mathrm{F}$, i.e. the wave packets formed with the wave vectors around k_F move with the Fermi velocity.

Fermi sphere 4

	valency	N/V [cm^{-3}]	k_F [10^{10} m^{-1}]	E_F [eV]	T_F [K]	v_F [10^6 m/s]
Li	1	$4.70 \cdot 10^{22}$	1.11	4.72	54800	1.29
Rb	1	$1.15 \cdot 10^{22}$	0.70	1.85	21500	0.81
Cu	1	$8.45 \cdot 10^{22}$	1.36	7.00	81200	1.57
Au	1	$5.90 \cdot 10^{22}$	1.20	5.51	63900	1.4
Be	2	$24.20 \cdot 10^{22}$	1.93	14.14	164100	2.25
Zn	2	$13.10 \cdot 10^{22}$	1.57	9.39	109000	1.83
Al	3	$18.06 \cdot 10^{22}$	1.75	11.63	134900	2.03
Pb	4	$13.20 \cdot 10^{22}$	1.58	9.37	108700	1.83

Fermi sphere 4 Comment

The table shows the valency, i.e. the number of conduction electrons per atom, the density of conduction electrons and the Fermi wave number, energy, temperature and velocity.

The Fermi wave number is comparable to the dimensions of the 1st Brillouin zone.

The Fermi temperature is very high compared to the melting temperatures of the metals.

Therefore, the thermal energy has only a very small influence on conduction electrons at ambient temperatures.

The Fermi speed is about a factor of 100 smaller than the speed of light.

Therefore, using the classical formula $E_\mathrm{F} = \hbar^2 k_\mathrm{F}^2/2\mathrm{m} = m v_\mathrm{F}^2/2$ for the kinetic energy is justified.

Fermi sphere 5

	valency	N/V [cm^{-3}]	E_F [eV]	v_F [10^6 m/s]	ρ [n$\Omega\cdot$ m]	ℓ [10^{-10} m]
Li	1	$4.70 \cdot 10^{22}$	4.72	1.29	92.8	100
Rb	1	$1.15 \cdot 10^{22}$	1.85	0.81	128.0	190
Cu	1	$8.45 \cdot 10^{22}$	7.00	1.57	16.8	171
Au	1	$5.90 \cdot 10^{22}$	5.51	1.4	22.1	147
Be	2	$24.20 \cdot 10^{22}$	14.14	2.25	36.0	90
Zn	2	$13.10 \cdot 10^{22}$	9.39	1.83	59.0	82
Al	3	$18.06 \cdot 10^{22}$	11.63	2.03	26.5	147
Pb	4	$13.20 \cdot 10^{22}$	9.37	1.83	208.0	23

Fermi sphere 5

Comment 1

The table shows in the 6th column the electric resistivity $\rho = \sigma^{-1}$ at 20 °C and in the last column an estimate of the mean free path $\ell = v_\mathrm{F} \cdot \tau$ when the electrons move with the Fermi velocity.

For this purpose, the mean free time τ is estimated using the formula

$$\sigma = \frac{e^2}{m}\frac{N}{V}\tau.$$

For the estimation, the mass of a free electron $mc^2 = 500$ eV is assumed for the mass of the electrons.

Fermi sphere 5 Comment 2

The estimate of the mean free path shows that an electron wave packet on the surface of the Fermi sphere can fly past many atoms before a scattering event occurs.

Since waves can propagate through a perfect crystal lattice without scattering, the long free paths of the conduction electrons are to be understood in the wave image.

On the other hand, the estimate of the mean free path shows that the assumption of periodic boundary conditions is no longer applicable in the context of nanophysics.

This lecture deals exclusively with macroscopic samples, i.e. samples whose dimensions are much larger than the mean free path of the electrons and the influence of the surfaces can safely be neglected.

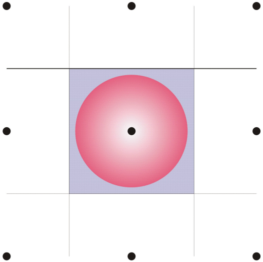
Fermi sphere 6

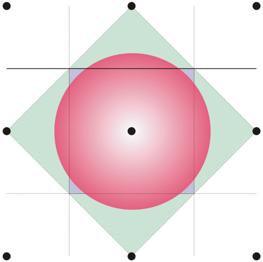
one electron per primitive unit cell
of a simple cubic lattice

$$\boxed{k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} = \frac{(3\pi^2)^{\frac{1}{3}}}{a} = \frac{3.09}{a} < \frac{\pi}{a}}$$

two electrons per primitive unit cell
of a simple cubic lattice

$$\boxed{k_F = \left(3\pi^2 \frac{N}{V}\right)^{\frac{1}{3}} = \frac{(3\pi^2 \cdot 2)^{\frac{1}{3}}}{a} = \frac{3.9}{a} > \frac{\pi}{a}}$$





Fermi sphere 6 Comment 1

It is helpful to get an idea of how the Fermi sphere is embedded in the reciprocal lattice.

Since the situation is somewhat complicated for real substances, a simple cubic lattice with the lattice parameter a is considered as a model. (Examples of real substances are discussed later.)

The lattice parameter of the cubic cell of the reciprocal lattice is $2\pi/a$.

The figure on the left shows the case that there is one conduction electron in the primitive unit cell of the lattice.

The right figure shows the case that there are two conduction electrons in the primitive unit cell of the lattice.

Fermi sphere 6

Comment 2

The Fermi wave number can be calculated with the density of the conduction electrons.

If there is one conduction electron per primitive unit cell, the Fermi sphere lies within the 1st Brillouin zone.

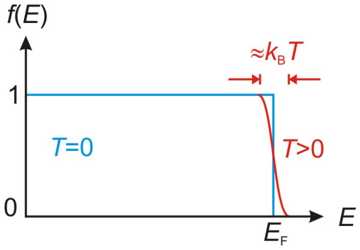
With two conduction electrons per primitive unit cell, the Fermi sphere is slightly larger than the 1st Brillouin zone and there are wave vectors ending on the Bragg planes that enclose the 1st Brillouin zone.

Fermi distribution function

Sommerfeld model

- Introduction
- Fermi sphere
- Fermi distribution function
- Electric conductivity
- Density of states
- Heat capacity of the electron gas

Fermi distribution function



Fermi distribution function

$$\boxed{f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}}$$

the chemical potential μ equals nearly the Fermi energy E_{F}

$$\lim_{T \to 0} \mu(T) = E_F$$

Fermi distribution function Comment 1

The Fermi distribution function indicates the probability that a k state with the energy E is occupied by an electron.

If the temperature approaches zero, the Fermi distribution function changes into a step function.

The step function is marked in the figure by the blue line.

For $T \to 0$ all k states below the Fermi energy are occupied with probability 1, and the probability for the occupation of a k state with a higher energy than the Fermi energy is zero.

Since a k state can be occupied by two electrons, the probability below the Fermi energy is 1 for $m_s = +1/2$ and 1 for $m_s = -1/2$, i.e. the spin quantum number does not matter.

Fermi distribution function Comment 2

The step will soften as the temperature rises. This is indicated by the red line in the figure.

Since the Fermi energy is much greater than the thermal energy at normal temperatures, only electrons in k states just below the Fermi energy can be excited in k states just above the Fermi energy.

The energy range around the Fermi energy in which electrons can be thermally excited is extremely small and exaggerated in the figure, e.g. for $T \approx 300\,\mathrm{K}$ one has $k_{\mathrm{B}}\mathrm{T} \approx 26\,\mathrm{meV} << E_{\mathrm{F}}$.

In the case of k states that lie within the Fermi sphere, the Pauli principle prevents electrons from being excited by thermal energies.

Fermi distribution function Comment 3

The formula outlined in red gives the mathematical expression of the Fermi distribution function.

The derivation of this formula can be looked up in textbooks on solid state physics.

The formula is somewhat similar to the formula of Planck's law of radiation and the formula of the heat capacity of phonons.

Since photons and phonons are bosons and electrons are fermions, there are two important differences.

The first difference is that $+1$ is added to the exponential function in the denominator instead of the -1 of Planck's radiation law and the heat capacity of phonons.

This $+1$ is the reason why the Fermi distribution function is almost a step function.

Fermi distribution function Comment 4

The second difference is that in the exponent of the exponential function the chemical potential μ is subtracted from the energy E.

In thermodynamics, the chemical potential μ describes the change in energy when the number of particles dN changes, i.e. $dE = \mu \mathrm{d}N$ (dE is usually the free energy F).

In the case of photons or phonons, the chemical potential is zero, since photons or phonons only interact very weakly with one another.

In the case of an electron gas, the chemical potential corresponds almost to the Fermi energy.

Fermi distribution function

Comment 5

Since the step of the Fermi distribution function softens somewhat with increasing temperature, the chemical potential decreases somewhat with increasing temperature.

The influence of temperature on the chemical potential is very small, so that the temperature dependence of the chemical potential can be neglected in most cases.

Fermi distribution function Comment 6

The Fermi distribution function is the mathematical expression for the fact that most electrons are blocked in their k states due to the Pauli principle.

Only those electrons that occupy k states very close to the surface of the Fermi sphere can be thermally excited.

The Fermi sphere is an idealization that is only approximately realized in nature.

The generalization of the spherical surface of the Fermi sphere is the Fermi surface.

The Fermi surface separates the occupied k states from the unoccupied k states at $T = 0$.

The surface of the Fermi sphere is a special Fermi surface.

Revision

Summary in Questions

1. What is the basic idea of the Drude model of metallic conductivity?
2. How does the Sommerfeld model differ from the Drude model of electric conductivity?
3. Write down the Schrödinger equation of the Sommerfeld model.
4. How does the Schrödinger equation of the Sommerfeld model differ from the Schrödinger equation of the box potential?
5. Which volume can be assigned to a k state in the Sommerfeld model?
6. What is meant by the Fermi sphere?
7. Calculate the radius of the Fermi sphere.
8. Calculate the Fermi wave number of copper.
9. Compare the Fermi number of copper with the 1st Brillouin zone of copper. (The lattice parameter of the cubic unit cell of copper is $a = 3.61 \cdot 10^{-10}$ m)
10. What is meant by a Fermi surface?