Solids

Sommerfeld model

Electrons in crystal lattices

- Electrical conductivity and Ohm’s law
- Drude model
- Sommerfeld model
- Bloch waves
- Energy bands and Fermi surfaces
- Photoemission Spectroscopy
- Semiclassical Electron Dynamics
- 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 1

- the conduction electrons, like all quantum particles, are subject to the Schrödinger equation
- the potential energy is an effective potential energy and 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 1

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.

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

Introduction 1 Comment 2

The formula outlined in red gives the Schrödinger equation.

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

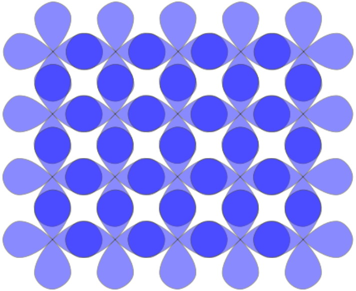
The solutions to this Schrödinger equation are plane waves.

The last underlined formula gives the energy eigenvalues of the Schrödinger equation. This is simply the kinetic energy of a quasi-free electron.

Before delving into the mathematical details in this and subsequent lectures, it is helpful to consider how the properties of electron waves in crystal lattices can be described based on the knowledge of atomic orbitals and waves in crystal lattices already developed in these lectures.

Introduction 2

What do we know and what can we guess?



- The energy of the waves depends on the direction of $\vec{k}$ and the atomic orbitals, i.e. $E_n = E_n(\vec{k})$
- $E_n(\vec{k})$ must be specified in the reciprocal lattice
- Bragg planes will be important
- The energy dispersion of electrons $E_n(\vec{k})$ is similar to the frequency dispersion of phonons (electron band structure)
- The energy bands are periodic in the reciprocal lattice, i.e. $E_n(\vec{k}) = E_n(\vec{k} + \vec{K})$

Introduction 2 Comment 1

The sketch of overlapping d-orbitals shows without calculation that the energy of the electron wave must depend on the direction of propagation $\vec{k}$.

The energy also depends on the atomic orbitals from which the electrons delocalize when the orbitals overlap (e.g. $E_{4s}(\vec{k})$ or $E_{3d}(\vec{k})$).

In the case of copper this is the singly occupied 4s-orbital.

In the case of nickel, the 4s orbital is empty and the conductivity is based on the fully occupied 3d-orbitals.

The more the orbitals overlap, the easier it is for an electron to gain energy.

Assuming that the energy gain can be described by the classical formula for the kinetic energy $E_{\text{kin}} = \hbar^2\vec{k}^2/2m$, one can conclude that the mass of the electrons is not the mass of a free electron, but a parameter - the effective mass - that describes how the electron can gain energy when its momentum increases.

Introduction 2 Comment 2

Since the conduction electrons delocalize from the atomic orbital, they cannot escape the atomic arrangement of the atoms in the crystal lattice.

The assumption of the Sommerfeld model that the electron wave does not depend on the direction of propagation only applies to strongly overlapping s-orbitals (e.g. the alkali metals).

Similar to the lattice vibrations, the electron waves must be specified in the reciprocal lattice and the variation of the electron energy $E_n(\vec{k})$ is expected to resemble the frequency dispersion of the phonons.

For electrons the energy dispersion $E_n(\vec{k})$ is called an energy band.

E.g. there is one band for the 4s electrons and 5 bands for the 3d electrons because the d orbitals point in different directions and the overlap is different for each type of d orbital (e.g. d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$ and d_{3z^2-1}).

Introduction 2 Comment 3

The frequency dispersion of the phonons is periodic in the reciprocal lattice, i.e. $\omega(\vec{q}) = \omega(\vec{q} + \vec{K})$.

The same can be expected for electron waves, since the electron density $\rho(\vec{r}) = \psi_{\vec{k}}(\vec{r}, t)\psi^{*}_{\vec{k}}(\vec{r}, t)$ must be periodic in the crystal lattice.

This periodicity cannot be lost in the reciprocal lattice and one can expect $E_n(\vec{k}) = E_n(\vec{k} + \vec{K})$!

In contrast to phonons the wave vectors of electrons $\vec{k}$ will not be restricted to the 1st Brillouin zone and one can expect that the Bragg planes are very important for the propagation of electrons waves.

For this reason, higher order Brillouin zones are defined!

For the phonons it was shown that every point in the reciprocal lattice can be examined with a three-axis neutron spectrometer.

Introduction 2

Comment 4

Neutrons are about 2000 times heavier than electrons and are therefore not suitable for studying the energy dispersion of conduction electrons.

Photons, on the other hand, interact strongly with electrons and inelastic photon scattering and in particular the study of photoelectrons are used for the experimental study of the energy bands of conduction electrons.

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 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, are not used in an extended volume because scattering events suppress the formation of standing wave modes.

Fermi sphere 1

Comment 2

For the periodic boundary condition, it is easiest to start with a cubic sample with the edge length L, which repeats itself 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

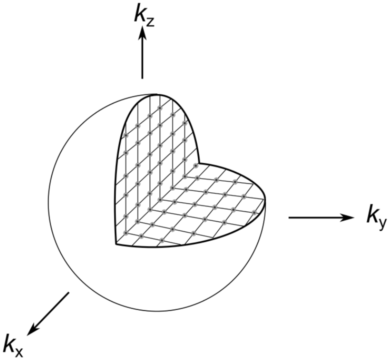
These wave vectors result in periodic wave functions, which have the edge length *L* of the cube-shaped sample as the period length.

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

$$\boxed{E_F = \frac{\hbar^2 k_F^2}{2m} \quad \text{and} \quad T_F = \frac{E_F}{k_B} \quad \text{and} \quad v_F = \sqrt{\frac{2E_F}{m}}} \quad \text{i.e.} \quad E_F = \frac{1}{2} m v_F^2$$

Fermi sphere 3 Comment 1

At the temperature $T = 0$ all occupied k states are enclosed by the surface of 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.

At zero temperature all electrons occupy their k state within the Fermi sphere.

In order for something to happen, electrons must be excited, for example thermally, when the temperature increases.

Fermi sphere 3 Comment 3

However, it is never possible to excite a single k state because other electrons respond to the excitation due to the Coulomb repulsion energy.

Therefore always so called wave packets are excited.

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.

Since the Coulomb interaction between the electrons cannot be completely captured by effective potentials, the electron gas of the Sommerfeld model is not a gas but a liquid.

The Fermi gas of electrons is in reality a Fermi liquid.

Fermi sphere 3

Comment 4

Lew Landau showed in 1956 that any excitation of the Fermi liquid can be traced back to a *k* state of the non-interacting Fermi gas as long as the excitation energy is much smaller than the Fermi energy.

The effect of Coulomb repulsion on the wave packets is that the lifetime of the wave packets is finite.

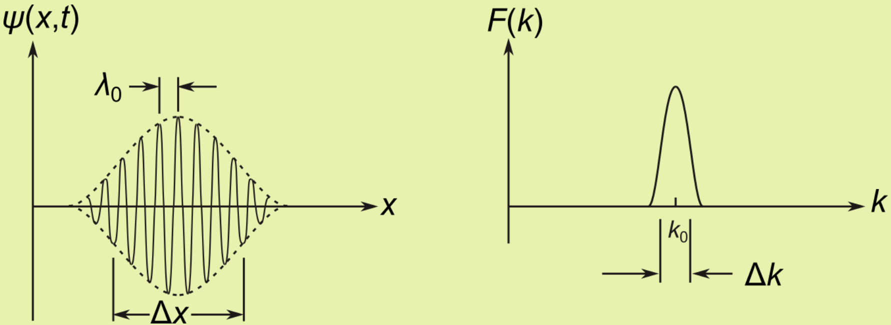
Lew Landau got the Nobel prize 1962 ”for his pioneering theories for condensed matter, especially liquid helium”.

In the following we consider the excitation for *k* states and keep in mind that this involves the excitation of wave packets.

Fermi sphere 3

Comment 5

Velocity of a wave packet (compare the 2nd lecture)



A one-dimensional wave packet

$$\psi(x,t) = \int dk F(k) e^{i(kx-\omega(k)t)}.$$

Fermi sphere 3

Comment 6

with

$$\omega(k) = \omega(k_0) + \left.\frac{d\omega(k)}{dk}\right|_{k=k_0} (k - k_0) + \dots$$

follows

$$\psi(x,t) = \int dkF(k)e^{i(kx-\omega(k)t)} = \int dkF(k)e^{i((k-k_0)x+k_0x-\omega(k_0)t-\left.\frac{d\omega(k)}{dk}\right|_{k=k_0}(k-k_0)t)}$$
$$= \left\{\int dkF(k)e^{i(k-k_0)\left[x-t\left.\frac{d\omega(k)}{dk}\right|_{k=k_0}\right]}\right\} e^{i(k_0x-\omega(k_0)t)}$$

This is a wave $e^{i(k_0x-\omega(k_0)t)}$ whose amplitude function (curly bracket) moves with the group 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.

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 calculated using the formula

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

For the calculation, the mass of a free electron $mc^2 = 500$ keV 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.

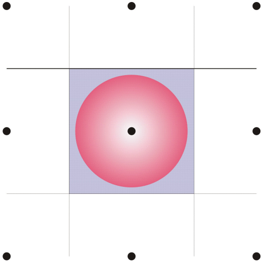
Fermi sphere 6

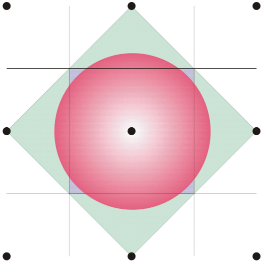
one electron per primitive unit cell
of a simple cubic lattice

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

two electrons per primitive unit cell
of a simple cubic lattice

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





Fermi sphere 6

Comment 1

Since the crystal lattice cannot be ignored, it is helpful to get an idea of how the Fermi sphere is embedded in the reciprocal lattice.

For the sake of simplicity, a simple cubic lattice with the lattice parameter a is considered as the 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

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- **Fermi distribution function**
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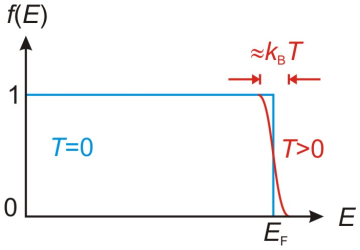
Fermi distribution function



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 describes 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.

For an electron gas, the chemical potential is almost equal to the Fermi energy because when another electron is added, the energy increases by 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.

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 surface of the Fermi sphere is the Fermi surface.

Fermi distribution function Comment 6

In general, the Fermi surface separates the occupied k states from the unoccupied k states at $T = 0$.

However, a spherical Fermi surface is an idealization that approximately occurs, for example, in the alkali metals.

Electric conductivity

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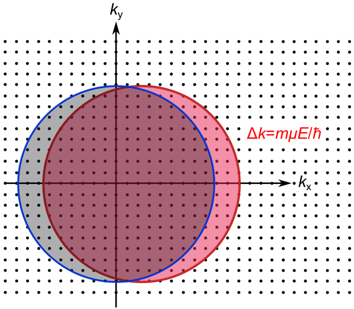
Electric conductivity 1

drift velocity: $\vec{v} = \mu \vec{E}$ → shift of the Fermi sphere $\Delta \vec{k} = \frac{m\vec{v}}{\hbar} = \frac{m\mu}{\hbar}\vec{E}$



estimate of the shift:

$\mu = 4.4 \cdot 10^{-3}\,\mathrm{m^2V^{-1}s^{-1}}$ for copper and
$E = 100\,\mathrm{V/m}$

$$\Delta k = \frac{2\pi\, 500 \cdot 10^3\,\mathrm{eV}\, 4.4 \cdot 10^{-3}\,\mathrm{m^2V^{-1}s^{-1}}}{4.14 \cdot 10^{-15}\,\mathrm{eVs}\,(3 \cdot 10^8\,\mathrm{ms^{-1}})^2} 100\,\mathrm{V/m}$$
$$= 3710\,\mathrm{m^{-1}} <<<< k_\mathrm{F} \approx 10^{10}\,\mathrm{m^{-1}}$$

(electron mass $m \approx 500\,\mathrm{keV}/c^2$)

Electric conductivity 1 Comment 1

When an electric field is applied to a conductor, the charge carriers begin to drift along the direction of the electric field.

The drift velocity shifts the Fermi sphere somewhat along the direction of the electric field.

The sketch shows, greatly exaggerated, the displacement of the Fermi sphere when the electric field is applied in the x direction.

In the figure, the black dots denote the *k* states.

The blue circle indicates the Fermi sphere when no electric field is applied.

The red circle indicates the Fermi sphere when an electric field is applied.

Electric conductivity 1

Comment 2

Most electron waves have a counter wave and only a small part of the occupied *k* states near the Fermi surface on the right side of the Fermi sphere can contribute to the transport of the electric charge.

The drift velocity can be calculated from the electrical mobility μ and the electric field strength E.

The displacement of the Fermi sphere in *k* space can be calculated with the momentum mv.

The calculation shows the estimate based on the mobility μ of copper and a field strength of 100 V/m.

For the calculation it is assumed that the mass of the charge carriers corresponds to the mass of a free electron, i.e. $500\,\mathrm{eV}/\mathrm{c}^2$.

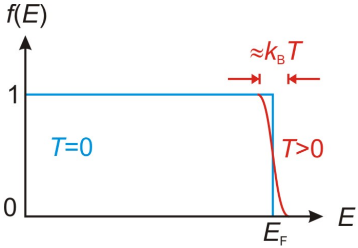
Electric conductivity 1

Comment 3

This assumption is only approximately fulfilled for copper, but this has no influence on the result of the estimate.

The displacement of the Fermi sphere due to the drift speed of the electrons in an electric field is about 6 orders of magnitude smaller than the Fermi wave number k_F.

Electric conductivity 2



Thermal softening of the Fermi surface

$$E = \hbar^2 k^2/2m \quad \rightarrow \quad \frac{\Delta E}{E} = 2\frac{\Delta k}{k}$$

with $\Delta E = k_B T$, $T = 300\,\mathrm{K}$, $E = E_\mathrm{F} = 7\,\mathrm{eV}$ (copper) and $k = k_F$

$$\begin{aligned}\Delta k_F =& k_F \frac{1}{2}\frac{k_B T}{E_F}\\ =& k_F \frac{8.62 \cdot 10^{-5}\,\mathrm{eVK}^{-1} \cdot 300\,\mathrm{K}}{2 \cdot 7\,\mathrm{eV}}\\ =& k_F \cdot 1.85 \cdot 10^{-3}\end{aligned}$$

$$\Delta k_F = 1.36 \cdot 10^{10}\,\mathrm{m}^{-1} \cdot 1.85 \cdot 10^{-3} \approx 2.5 \cdot 10^{7}\,\mathrm{m}^{-1} >> \Delta k \approx 3.7 \cdot 10^{3}\,\mathrm{m}^{-1}$$

Electric conductivity 2 Comment 1

The figure shows once again the influence of temperature on the Fermi distribution function, greatly exaggerated.

In the case of Fermi energy, the step of the distribution function softens in an energy range that corresponds to thermal energy.

In this way, the softening of the Fermi surface in the wavenumber space can also be estimated.

Since the thermal energy at room temperature is about a thousandth of the Fermi energy, the surface of the Fermi sphere is also smeared in this order of magnitude in the wavenumber space.

The estimate for copper shows that the displacement of the Fermi sphere by an electric field is generally much smaller than the thermal smearing of the Fermi surface.

Electric conductivity 2

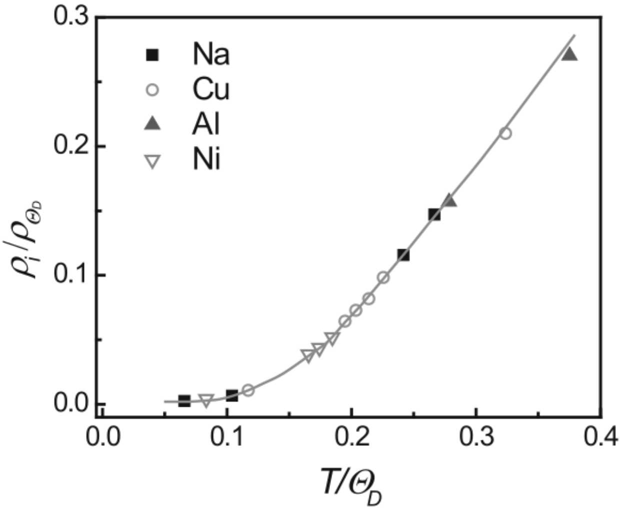
Comment 2

E.g. the energy gain per electron in copper for an electric field of 100 V/m is only

$$\Delta E = E_F 2\Delta k / k_F = 2 \cdot 7\text{eV} \cdot 3700/1.36 \cdot 10^{+10} = 3.8\,\mu\text{eV}$$

and therefore very much smaller than the thermal energy at room temperature.

Electric conductivity 3



Electric conductivity 3

Comment

The temperature dependence of the specific resistance of the metals follows a universal curve if the temperature is normalized to the Debye temperature Θ_D and the specific resistance to a suitable value.

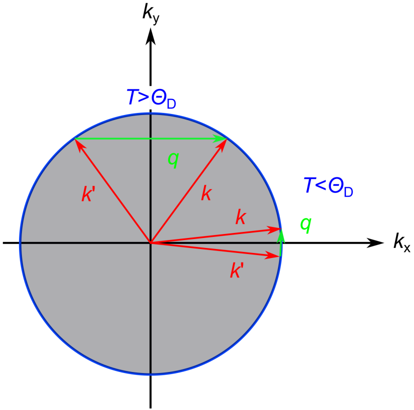
The temperature dependence is essentially determined by the fact that the conduction electrons can absorb and emit phonons.

In addition, there is a temperature-independent component that arises from the scattering of the conduction electrons at imperfections, i.e. impurity atoms and other lattice defects.

This contribution determines the temperature-independent resistance at low temperatures, which is subtracted in the figure.

Electric conductivity 4

electron-phonon scattering $\vec{k} = \vec{k}' \pm \vec{q}$ and $E(\vec{k}) = E(\vec{k}') \pm \hbar\omega(\vec{q})$



- Only electrons in the range of the Fermi surface participate in the scattering
- $E(\vec{k}), E(\vec{k}') >>> \hbar\omega(\vec{q})$, i.e. quasi elastic scattering
- the scattering rate is proportional to the phonon number

$$\bar{n} = \frac{1}{\exp(\hbar\omega(\vec{q})/k_B T) - 1}$$

Electric conductivity 4 Comment 1

The temperature dependence of the electric resistance is due to electron-phonon scattering

In the first line the law of momentum and energy conservation for the emission (+) and absorption (-) of a phonon by a conduction electron is formulated.

Only electrons can take part in the scattering processes whose wave vectors $\vec{k}$ lie in the thermally softened area around the Fermi surface.

The energy of the phonon is always very much smaller than the Fermi energy of the electrons.

Therefore, the electron-phonon scattering is quasi-elastic.

The influence of electron-phonon scattering on the electrical resistance depends on the number of phonons.

Electric conductivity 4

Comment 2

Therefore, it can be expected that the electrical resistance decreases with decreasing temperature.

The figure outlines two scattering processes.

In one scattering process there is a large angle between the wave vectors of the electrons, in the other scattering process the angle is small.

If the temperature is higher than the Debye temperature, then all phonon modes within the 1st Brillouin zone are excited.

Since the dimensions of the Fermi sphere roughly correspond to the dimensions of the 1st Brillouin zone, the scattering with phonons at the edge of the 1st Brillouin zone can lead to large scattering angles.

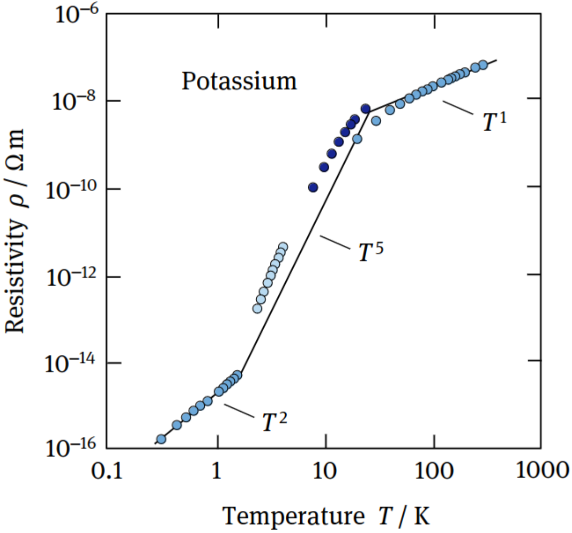
Electric conductivity 4

Comment 3

Such scattering processes hinder effectively the charge transport and increase the electrical resistance.

For $k_B T >> \hbar\omega_{\text{max}}$, i.e. $T > \Theta_D$, $\bar{n}$ is proportional to temperature, which explains the linear increase in electrical resistance with temperature, i.e. $\rho \propto T$.

Electric conductivity 5



Electric conductivity 5 Comment 1

The figure shows the temperature dependence of the electrical resistance of potassium.

The Debye temperature of potassium is $\Theta_D = 100\,\mathrm{K}$ and the resistance varies proportionally to T for $T > \Theta_D$.

For $T < \Theta_D$ the resistance varies proportionally to T^5.

The quadratic temperature dependence below $\approx$2 K is attributed to electron-electron scattering.

The variation of T^5 is due to the scattering of electrons from acoustic phonons.

Electric conductivity 5

Comment 2

These phonons have a small momentum and cannot change the direction of propagation of the electron wave significantly (compare the figure on page 4).

For this reason, the influence of the electron-phonon scattering on the electrical resistance becomes very small at low temperatures.

The reason for the T^5 dependency is as follows:

First, the energy of the acoustic phonons is very small $\hbar q_{\text{max}} c_S \approx k_B T$.

Electron scattering is therefore almost elastic and only phonons in a disk with radius q_{max} at the tip of $\vec{k}$ can contribute.

This geometric effect contributes to the scattering according to $q_{\text{max}}^2 \propto T^2$.

Second, the total number of acoustic phonons varies proportionally to T^3 at low temperatures.

Electric conductivity 5

Comment 3

Due to these two effects, the electrical resistance at low temperatures varies according to T^5.

The total number of acoustic phonons is $N = 3\sum_{\vec{q}} \frac{1}{\exp(\hbar c_S q/k_B T)-1}$.

Since at low temperatures only acoustic phonons around the Γ point are excited, the sum can be replaced by an integral over a sphere, i.e.

$$N = 3\frac{1}{(2\pi)^3/V}\int_{q=0}^{q_{\text{max}}} q^2 dq\, \frac{1}{\exp(\hbar c_S q/k_B T) - 1}.$$

With the substitution $x = \hbar c_S q/k_B T \rightarrow q = x k_B T/\hbar c_S$ and $x_{\text{max}} \rightarrow \infty$ for $T \rightarrow 0$ one gets $N \propto T^3$. (By the way: With the energy $E(q) = \hbar c_S q$ of the acoustic phonons you get $E \propto T^4$ for the total energy of all phonons at low temperatures.)

Revision

Summary in Questions 1

1. How does the Sommerfeld model differ from the Drude model of electric conductivity?
2. Write down the Schrödinger equation of the Sommerfeld model.
3. How does the Schrödinger equation of the Sommerfeld model differ from the Schrödinger equation of the box potential?
4. Which volume can be assigned to a k state in the Sommerfeld model?
5. What is meant by the Fermi sphere?
6. Calculate the radius of the Fermi sphere.
7. Calculate the Fermi wave number of copper.
8. 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)
9. What is meant by a Fermi surface?

Summary in Questions 2

10. Why is the Debye temperature a characteristic temperature for the electrical resistance of a metal?
11. What is the displacement of the Fermi sphere when an electric field strength of 1000 V/m is applied to a metal?