Solids

1. Binding types
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4. **Electrons in crystal lattices**

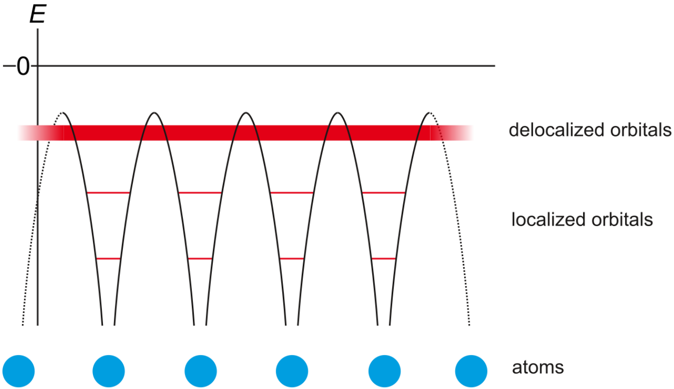
Bloch waves

Electrons in crystal lattices

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

Bloch waves 1

- each electron moves in a cloud of charge that is formed by other electrons in the solid
- the potential energy of each electrons has the periodicity of the crystal lattice



Bloch waves 1 Comment 1

The Sommerfeld model assumes that the potential energy of an electron is completely independent of the position.

The potential energy is a constant that is assigned the value zero.

Only the boundaries of the crystal lattice present a potential barrier, so the electrons need an activation energy to leave the crystal.

The electrons are described by harmonic waves that are limited only by the periodic boundary condition.

The next step in the approximation is therefore to include to periodicity of the potential energy due to the crystal lattice.

Bloch waves 1 Comment 2

It is assumed that each electron can move independently of the other electrons in a charge cloud which is formed by the other electrons. This charge cloud has the periodicity of the crystal lattice.

The independent electron approximation has already been used successfully to determine the orbitals of atoms.

The figure tells the following story:

There are electrons that are tightly bound to their atoms.

The potential barrier between the atoms becomes narrower as the energy of the electrons increases and there is a certain probability that the electrons can tunnel through the barriers.

Bloch waves 1

Comment 3

With increasing energy, the electrons begin to hop from atom to atom.

Finally, the transition probability between the atoms is so large that the atomic orbitals merge into running waves.

Bloch waves 2

time independent Schrödinger equation

$$\boxed{E\varphi(\vec{r}) = \left(-\frac{\hbar^2\nabla^2}{2m} + E_{pot}(\vec{r})\right)\varphi(\vec{r})}$$

and

$$E_{pot}(\vec{r}) = E_{pot}(\vec{r} + \vec{R})$$

with

$$\underline{\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}$$

Bloch waves 2 Comment 1

The equation outlined in red shows the Schrödinger equation for an electron with kinetic and potential energy in a crystal lattice.

The potential energy of the electron is determined by the positive nuclei and the negative charge cloud of the other electrons of the crystal.

The potential energy depends on the electron in question.

The electrons are characterized by the type of atom and the particular orbital in which they reside.

Since samples are considered whose dimensions are much larger than the mean free path of the electrons, the special situation of atoms close to the surface can be neglected when describing the electrical properties of the volume.

Bloch waves 2 Comment 2

In the case of copper, the potential energy for each electron has to be determined from the 1s to the 4s orbital.

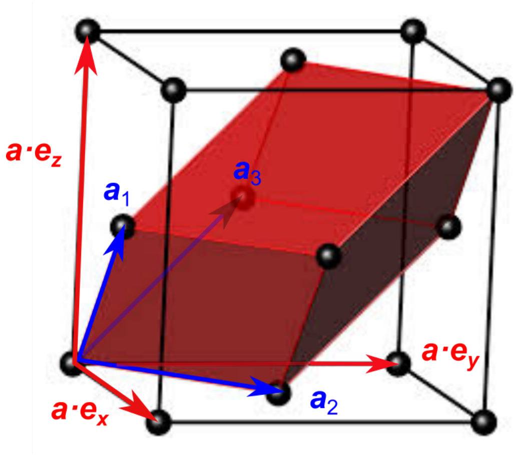
Of course, the potential energy of the 1s electrons is very different from the potential energy of the 4s electrons, which are the conduction electrons in copper.

But regardless of the details, the potential energy for all electrons is a periodic function of the crystal lattice.

As before, the vectors R denote the vectors of the Bravais lattice.

Bloch waves3

cubic unit cell and a primitive unit cell (red rhombohedron) of the fcc lattice



$$\vec{a}_1 = \frac{a}{2}\left(\vec{e}_x + \vec{e}_z\right)$$
$$\vec{a}_2 = \frac{a}{2}\left(\vec{e}_y + \vec{e}_x\right)$$
$$\vec{a}_3 = \frac{a}{2}\left(\vec{e}_z + \vec{e}_y\right)$$

Bloch waves 3 Comment

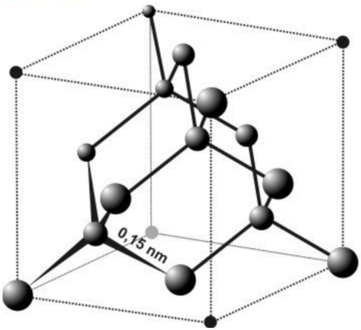
Copper is used as an example below to illustrate the results.

The crystal lattice of copper is an fcc lattice.

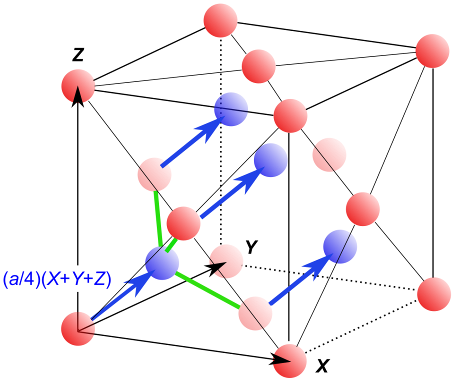
The figure shows the cubic and a primitive unit cell of the fcc lattice.

Bloch waves 4

cubic unit cell of the diamond structure
(fcc lattice with two atoms in the primitive unit cell)



(Diamantstruktur.mp4)



Bloch waves 4 Comment

To illustrate the results, silicon and germanium, which crystallize in the diamond structure, are discussed below.

The sketches show the cubic unit cell of the diamond structure, which is an fcc lattice with a diatomic base.

In the sketch on the right, the two types of atoms are marked in red and blue.

A primitive unit cell of the fcc lattice (e.g. the rhombohedron of the previous slide) contains one atom marked in red and one in blue.

Bloch waves 5

Solution of the Schrödinger equation

$$\underline{E\varphi(\vec{r}) = \left(-\frac{\hbar^2\nabla^2}{2m} + E_{pot}(\vec{r})\right)\varphi(\vec{r})}$$

in principle: sum over plane waves

$$\varphi(\vec{r}) = \sum_{\vec{k}} a_{\vec{k}} \exp(i\vec{k}\vec{r})$$

better idea: Bloch waves (Felix Bloch 1928)

$$\boxed{\varphi_{\vec{k}}(\vec{r}) = u(\vec{r}) \exp(i\vec{k}\vec{r})}$$

with

$$\underline{u(\vec{r}) = u(\vec{r} + \vec{R})}$$

Bloch waves 5

Comment 1

In principle it is possible to develop the solution of the Schrödinger equation in plane waves.

But since the atomic orbitals of the electrons are still important, this is not a good idea.

The first step towards solving the problem of the wave function in a crystal lattice was taken by Felix Bloch in 1928.

He proposed modulated plane waves to solve the Schrödinger equation.

His approach is so fundamental that the waves have been named after him ever since.

The equation outlined in red shows a general Bloch wave.

Bloch waves 5 Comment 2

The Bloch wave is a plane wave that is multiplied by an amplitude function $u(\vec{r})$.

The amplitude function $u(\vec{r})$ has the periodicity of the crystal lattice.

The amplitude function $u(\vec{r})$ makes it possible to establish the relationship between the localized atomic orbitals on the one hand and the propagating wave function of the crystal lattice on the other.

A strategy for determining the function $u(\vec{r})$ was proposed in 1937 by J.C. Slater with the augmented plane wave method.

In the augmented plane wave method, the crystal volume is divided into spherical areas around the atoms.

Bloch waves 5 Comment 3

The localized atomic orbitals are calculated in the spheres, which are then connected by plane waves in the volume between the spheres.

The mathematical problems of the augmented plane wave method are great and have been solved over time by the work of many scientists.

As soon as one has useful wave functions, the same procedure is used to solve the Schrödinger equation that is used for solving a single atom.

The charge densities in the crystal are calculated using the wave functions.

With the charge densities, the potential energy of the selected electron can be calculated.

Bloch waves 5 Comment 4

The wave function of the selected electron is characterized by the quantum numbers of the atomic orbital and by the wave vector of the Bloch wave.

The Schrödinger equation for the selected electron can be solved with the potential energy.

These calculations have to be done for all orbitals occupied by electrons.

E.g. in the case of copper for the electrons of the 1s to 4s orbitals.

These calculations give an improved set of wave functions that reduce the total energy of the electrons.

The process is repeated iteratively with the refined wave functions until the minimum of the total energy is found.

Bloch waves 5 Comment 5

In solid state physics, this is known as the band structure calculation.

The mathematical details are complicated, but fortunately only relevant for real calculations of the wave functions in a crystal lattice.

The theoretical and numerical details of band structure calculations do not need to be known in order to understand the essential electronic properties of solids.

The most important properties are already determined by the symmetry of the Bloch waves.

Bloch waves 6

the probability density to find an electron is $\varphi^*_{\vec{k}} \cdot \varphi_{\vec{k}}$

with

$$\varphi_{\vec{k}}(\vec{r}) = u(\vec{r})e^{i\vec{k}\vec{r}} \quad \text{and} \quad \boxed{u(\vec{r}) = u(\vec{r}+\vec{R})}$$

is

$$\underline{|\varphi_{\vec{k}}(\vec{r})|^2 = |u(\vec{r})|^2 = |\varphi_{\vec{k}}(\vec{r}+\vec{R})|^2}$$

and the probability density is periodic in the crystal lattice

the solutions of the Schrödinger equation in a crystal lattice have the form of Bloch waves

$$\underline{E(\vec{k})}\varphi_{\vec{k}}(\vec{r}) = \left(-\frac{\hbar^2\nabla^2}{2m} + E_{pot}(\vec{r})\right)\varphi_{\vec{k}}(\vec{r})$$

Bloch waves 6

Comment

The probability of finding an electron is given by the square of the wave function.

Only the amplitude function contributes to the calculation of the probability density, since the exponential functions do not contribute to the square of the absolute value.

Since the probability density has to show the periodicity of the potential energy, the amplitude function has to be a periodic function in the crystal lattice.

The solutions of the Schrödinger equation in a crystal lattice have the form of Bloch waves and the energy eigenvalues depend on the wave vector of the Bloch wave.

There are also other quantum numbers that characterize the energy and the wave function, e.g. the quantum numbers of the atomic orbitals, which are included in the amplitude function.

For the sake of simplicity, I leave out these additional quantum numbers.

Bloch waves 7

definition of the reciprocal lattice

$$\boxed{\vec{K}\vec{R} = 2\pi\, n}$$

vectors of the Bravais lattice $\underline{\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3}$

vectors of the reciprocal lattice $\underline{\vec{K} = h\vec{b}_1 + k\vec{b}_2 + \ell\vec{b}_3}$

$$\boxed{\begin{aligned} \vec{b}_1 &= \frac{2\pi}{V_\text{cell}}(\vec{a}_2 \times \vec{a}_3) \\ \vec{b}_2 &= \frac{2\pi}{V_\text{cell}}(\vec{a}_3 \times \vec{a}_1) \\ \vec{b}_3 &= \frac{2\pi}{V_\text{cell}}(\vec{a}_1 \times \vec{a}_2) \end{aligned}}$$

V_cell denotes the volume of the primitive unit cell $V_\text{cell} = \vec{a}_1(\vec{a}_2 \times \vec{a}_3)$

Bloch waves 7

Comment

Now it is necessary to recall the definition of the reciprocal lattice.

The scalar product of a reciprocal lattice vector with a vector of the Bravais lattice is equal to a multiple of 2π.

The basis vectors of the reciprocal lattice can easily be calculated with the basis vectors of the Bravais lattice and vice versa.

Bloch waves 8

Bloch waves are periodic in the reciprocal lattice

$$\begin{aligned}\varphi_{\vec{k}}(\vec{r}) &= u(\vec{r})e^{i\vec{k}\vec{r}} \\ &= u(\vec{r})e^{-i\vec{K}\vec{r}}e^{i\vec{k}\vec{r}}e^{+i\vec{K}\vec{r}} \\ &= u'(\vec{r})e^{i(\vec{k}+\vec{K})\vec{r}} \quad \text{with} \quad u'(\vec{r}) = u(\vec{r})e^{-i\vec{K}\vec{r}}\end{aligned}$$

small auxiliary calculation

$$\begin{aligned}\underline{u'(\vec{r})} &= u_{\vec{k}}(\vec{r})e^{-i\vec{K}\vec{r}} \qquad \text{with} \quad u(\vec{r}) = u(\vec{r}+\vec{R}) \\ &= u(\vec{r}+\vec{R})e^{-i\vec{K}\vec{r}} \quad \text{with} \quad \vec{K}\vec{R} = 2\pi n \\ &= u(\vec{r}+\vec{R})e^{-i\vec{K}(\vec{r}+\vec{R})} = \underline{u'(\vec{r}+\vec{R})}\end{aligned}$$

therefore

$$\boxed{\varphi_{\vec{k}+\vec{K}}(\vec{r}) = u'(\vec{r})e^{i(\vec{k}+\vec{K})\vec{r}} = \varphi_{\vec{k}}(\vec{r})}$$

Bloch waves 8 Comment 1

A very important property of Bloch waves is that they are periodic in the reciprocal lattice.

It is always possible to add a vector of the reciprocal lattice $\vec{K}$ to the wave vector of a Bloch wave.

This shows a small calculation.

The Bloch wave of the first line is multiplied by one in the second line, i.e. $1 = e^{-i\vec{K}\vec{r}}e^{+i\vec{K}\vec{r}}$.

In the third line the function $u(\vec{r})e^{-i\vec{K}\vec{r}}$ is denoted by $u'(\vec{r})$.

The little auxiliary calculation shows that $u'(\vec{r})$ is also a periodic function in the crystal lattice, i.e. $u'(\vec{r}) = u'(\vec{r} + \vec{R})$.

Bloch waves 8 Comment 2

So the function $\varphi_{\vec{k}+\vec{K}}(\vec{r}) = u'(\vec{r})e^{i(\vec{k}+\vec{K})\vec{r}}$ is also a Bloch wave according to the definition but now for the wave vector $\vec{k}+\vec{K}$.

The Bloch wave for the wave vector $\vec{k}+\vec{K}$ is identical to the Bloch wave for the wave vector $\vec{k}$, since this Bloch wave was simply multiplied by the number one, i.e. $1 = e^{-i\vec{K}\vec{r}}e^{+i\vec{K}\vec{r}}$.

Bloch waves are periodic functions in the reciprocal lattice.

But neither the vectors $\vec{k}$ nor the functions $u(\vec{r})$ are unique, i.e. $\vec{k} \rightarrow \vec{k}+\vec{K}$ and $u(\vec{r}) \rightarrow u(\vec{r})e^{-i\vec{K}\vec{r}}$.

Bloch waves 9

Bloch waves are periodic functions in the reciprocal lattice

$$\underline{\varphi_{\vec{k}}(\vec{r}) = \varphi_{\vec{k}+\vec{K}}(\vec{r})}$$

the energy eigenvalues of the Schrödinger equation are therefore also periodic in the reciprocal lattice

$$\boxed{E(\vec{k}) = E(\vec{k}+\vec{K})}$$

the functions $E(\vec{k})$ are called energy bands

Bloch waves 9 Comment 1

The first underlined equation formulates the periodicity of the Bloch waves in the reciprocal lattice.

Due to the periodicity of the wave function in the reciprocal lattice, the energy eigenvalues of the Schrödinger equation in the reciprocal lattice are also periodic functions.

The functions of the energy eigenvalues $E(\vec{k})$ are called energy bands.

The $\vec{k}$ vectors that are necessary to describe electron waves in a crystal lattice can be restricted to a primitive unit cell of the reciprocal lattice.

This is pleasant, as one can restrict oneself to a primitive unit cell of the reciprocal lattice when calculating the energy bands.

Bloch waves 9 Comment 2

The wave vector $\vec{k}$ characterize the translation properties of the Bloch wave:

$$\varphi_{\vec{k}}(\vec{r}+\vec{R}) = u(\vec{r}+\vec{R})e^{i\vec{k}(\vec{r}+\vec{R})} = u(\vec{r})e^{i\vec{k}\vec{R}}e^{i\vec{k}\vec{r}} = e^{i\vec{k}\vec{R}}\varphi_{\vec{k}}(\vec{r}).$$

Because of $\vec{K}\vec{R} = n2\pi$ the proportionality factor $e^{i\vec{k}\vec{R}}$ characterizing the translation is the same for all vectors $\vec{k}+\vec{K}$.

Note: In free space $\psi(\vec{r}) = \psi_0 e^{i\vec{k}\vec{r}}$ is an eigenfunction of the momentum operator $\hat{\vec{p}} = -i\hbar\nabla$. With $\psi(\vec{r}+\vec{R}) = \psi_0 e^{i\vec{k}(\vec{r}+\vec{R})} = e^{i\vec{k}\vec{R}}\psi(\vec{r})$ the eigenfunction of the momentum operator behave similar to the Bloch function $\varphi_{\vec{k}}(\vec{r}+\vec{R}) = e^{i\vec{k}\vec{R}}\varphi_{\vec{k}}(\vec{r})$.

Bloch waves 9 Comment 3

The vector $\vec{k}$ of a Bloch wave $\varphi_{\vec{k}}$ describes the properties of the wave function under translation similar to the vector $\vec{k}$ of the eigenfunction of the momentum operator.

However, since $\varphi_{\vec{k}}(\vec{r})$ is not an eigenfunction of the momentum operator, the vector $\vec{k}$ of the Bloch waves does not give the momentum of the particles described by the wave function.

The momentum of a particle described by a Bloch wave is not fixed.

Therefore the vector $\vec{k}$ of a Bloch wave is called crystal- or quasi-momentum.

This is somewhat misleading, since the vector $\vec{k}$ of the Bloch wave only describes the translational properties of the wave function and not the momentum of the particles.

Electrons in crystal lattices

- Drude model
- Sommerfeld model
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- Energy bands and Fermi surfaces
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- Superconductivity

Quasi-free electrons in the sc-lattice

Energy bands and Fermi surfaces 1

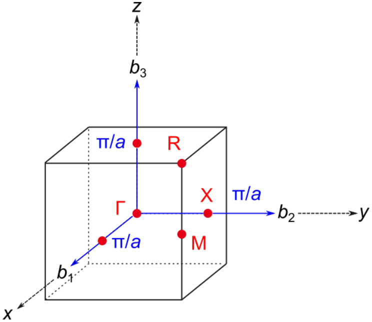
- Quasi-free electrons in the sc-lattice
- Sodium
- Copper
- Silicon

Quasi-free electrons in the sc-lattice 1

Consider an electron in a simple cubic lattice with nearly negligible potential energy

1st Brillouin zone of the sc lattice: $\vec{a}_1 = a\vec{e}_x$, $\vec{a}_2 = a\vec{e}_y$, $\vec{a}_3 = a\vec{e}_z$

and $\vec{b}_1 = \frac{2\pi}{V_\text{cell}}(\vec{a}_2 \times \vec{a}_3)$, $\quad \vec{b}_2 = \frac{2\pi}{V_\text{cell}}(\vec{a}_3 \times \vec{a}_1)$, $\quad \vec{b}_3 = \frac{2\pi}{V_\text{cell}}(\vec{a}_1 \times \vec{a}_2)$



$$\vec{b}_1 = \frac{2\pi}{a^3}(a\vec{e}_y \times a\vec{e}_z) = \frac{2\pi}{a}\vec{e}_x$$

$$\vec{b}_2 = \frac{2\pi}{a}\vec{e}_y$$

$$\vec{b}_3 = \frac{2\pi}{a}\vec{e}_z$$

Quasi-free electrons in the sc-lattice 1 Comment

As an example, consider an electron in a simple cubic lattice.

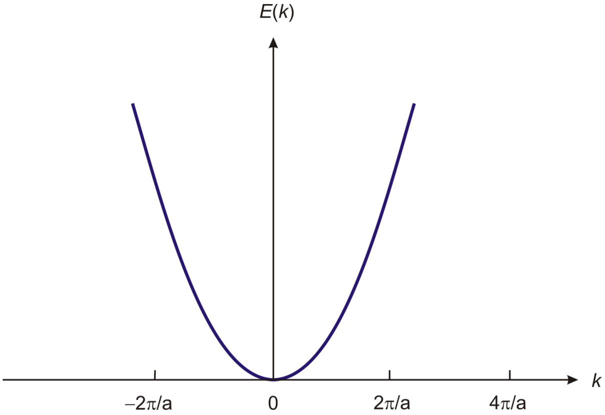
The figure shows the 1st Brillouin zone of a simple cubic lattice.

The basis vectors $\vec{b}_i$ of the reciprocal lattice are parallel to the basis vectors of the Bravais lattice $\vec{a}_i$.

The Bragg planes which enclose the 1st Brillouin zone intersect the basis vectors of the reciprocal lattice in the middle over a length of π/a away from the Γ point

Quasi-free electrons in the sc-lattice 2

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

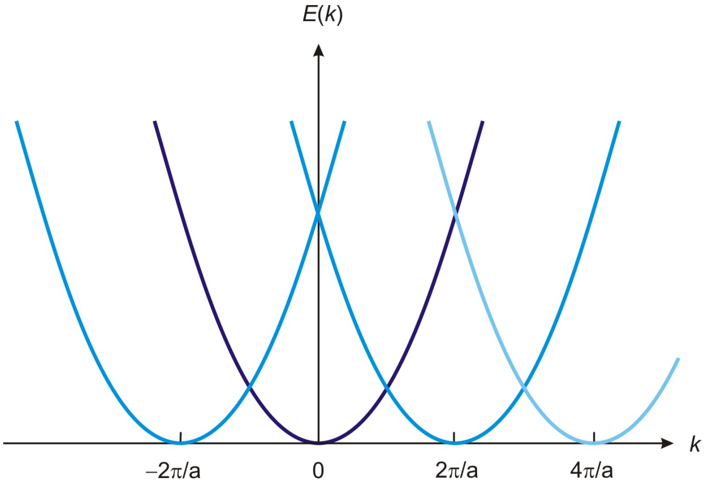


Quasi-free electrons in the sc-lattice 2 Comment

The figure shows the parabola of the kinetic energy of the free electrons e.g. along the *x*, *y*, or *z*-axis of the simple cubic lattice, when the influence of the crystal lattice can be completely neglected.

This is the situation of the Sommerfeld model.

Quasi-free electrons in the sc-lattice 3: periodic zone scheme



$$\vec{k} \parallel \vec{b}_{1,2,\text{ or } 3}$$

Quasi-free electrons in the sc-lattice 3

Comment

If the modulation of the potential energy is still small, but no longer completely negligible, the solution of the Schrödinger equation in a periodic potential must be considered.

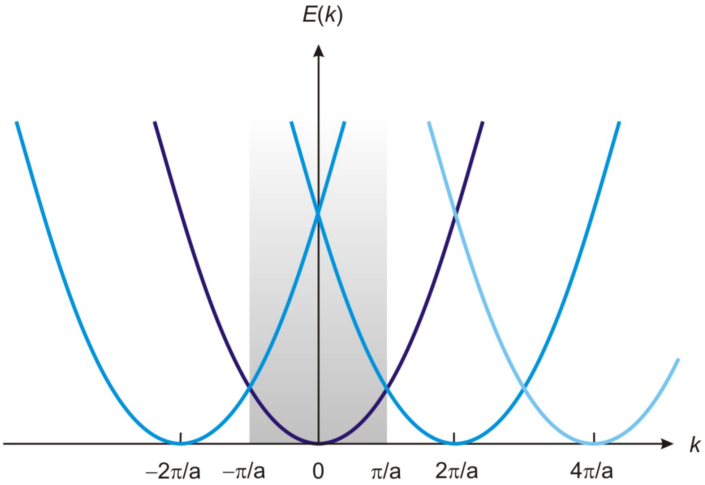
The energy is periodic in the reciprocal lattice, i.e. $E(\vec{k}) = E(\vec{k} + \vec{K})$.

The figure shows the resulting band structure if the k-vector is parallel to one of the basis vectors of the reciprocal lattice $\vec{b}_{1,2,3}$.

By adding reciprocal lattice vectors, the parabola of the kinetic energy is shifted.

This representation of the band structure is called the periodic zone scheme.

Quasi-free electrons in the sc-lattice 4: reduced zone scheme



Quasi-free electrons in the sc-lattice 4 Comment

The shaded area in the picture shows the band structure within the 1st Brillouin zone.

This section of the band structure is sufficient because the entire band structure results from the translation of the 1st Brillouin zone.

The representation of the band structure within the 1st Brillouin zone is called the reduced zone scheme.

Quasi-free electrons in the sc-lattice 5

periodic boundary conditions:

volume of a single *k* state

$$\frac{(2\pi)^3}{V}$$

volume of the 1st Brillouin zone is

$$\frac{(2\pi)^3}{V_{\text{Cell}}}$$

V_{Cell} volume of the primitive elementary cell of the Bravais lattice

- The number of *k* states in the 1st Brillouin zone equals the number of primitive unit cells of the crystal lattice

$$\frac{(2\pi)^3/V_{\text{Cell}}}{(2\pi^3)/V} = V/V_{\text{Cell}} = N$$

Quasi-free electrons in the sc-lattice 5 Comment 1

Since finite crystal lattices are always considered, periodic boundary conditions must also be used for the Bloch waves.

The wave vectors do not change continuously, but in discrete steps.

The first formula underlined in red indicates the volume in k space that a wave vector can occupy.

V denotes the volume of the crystal.

The second formula underlined in red gives the volume of the 1st Brillouin zone.

For a simple cubic lattice, the formula $(2\pi)^3/a^3$ results.

Quasi-free electrons in the sc-lattice 5 Comment 2

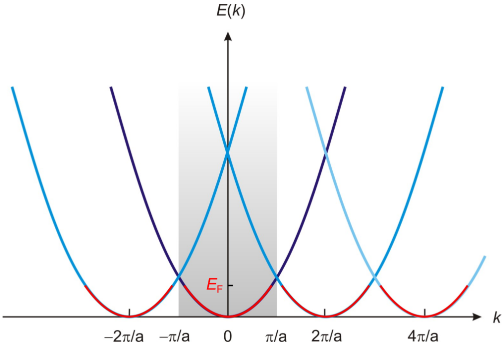
Similar to the lattice vibrations, with the Bloch waves the total number of different wave vectors in the 1st Brillouin zone is equal to the number of primitive unit cells in the crystal lattice.

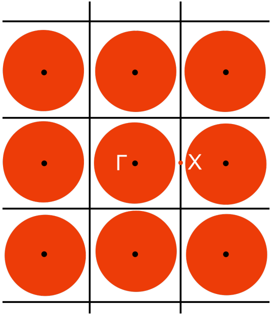
Due to the Pauli principle, each Bloch wave can be occupied with a maximum of two electrons.

Quasi-free electrons in the sc-lattice 6

one quasi-free electron per primitive unit cell of a simple cubic lattice

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





Quasi-free electrons in the sc-lattice 6 Comment 1

If the influence of the periodicity of the potential energy is very small, the kinetic energy of the electrons $E(\vec{k}) = \hbar^2\vec{k}^2/2m$ remains almost unchanged.

As in the Sommerfeld model, the occupied k states at $T = 0$ are enclosed by the Fermi sphere.

The formula calculates the radius of the Fermi sphere for the case that there is one electron in a primitive cubic unit cell with the lattice parameter a.

The left figure shows the band structure of the Bloch waves for quasi-free electrons in the periodic zone scheme.

The wave vector $\vec{k}$ lies parallel to the connecting line between the Γ point and the X point of the 1st Brillouin zone.

Quasi-free electrons in the sc-lattice 6 Comment 2

The red marked area of the parabolas shows the occupied k states at $T = 0$.

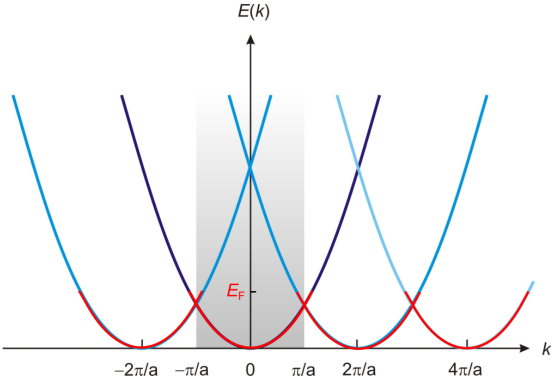
The figure on the right shows the Fermi sphere in the periodic zone scheme.

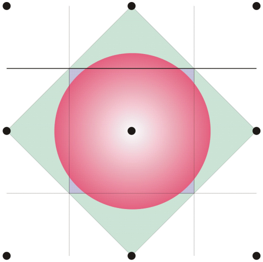
The red circular areas indicate the k states that are occupied at $T = 0$.

Quasi-free electrons in the sc-lattice 7

two electrons per primitive unit cell of a simple cubic lattice

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





Quasi-free electrons in the sc-lattice 7 Comment

Now consider the case where there are two conduction electrons in the primitive unit cell of a simple cubic crystal lattice.

The formula calculates the radius of the Fermi sphere.

The left figure shows the band structure for quasi-free electrons in the periodic zone scheme.

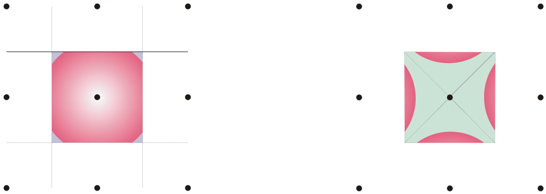
The wave vector $\vec{k}$ lies parallel to the connecting line between the Γ point and the X point of the 1st Brillouin zone.

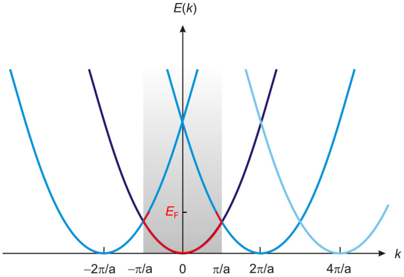
The parabolas drawn in red denote the occupied k states at $T = 0$.

The right figure now shows the Fermi sphere, which is partly in the 1st Brillouin zone and partly in the 2nd Brillouin zone.

Quasi-free electrons in the sc-lattice 8

the reduced zone scheme for two electrons per primitive unit cell of a simple cubic lattice





Quasi-free electrons in the sc-lattice 8 Comment 1

In the reduced zone scheme, only the 1^{st} Brillouin zone is taken into account.

The left figure shows the part of the Fermi sphere that lies in the 1^{st} Brillouin zone.

The middle figure shows the part of the Fermi sphere that lies in the 2^{nd} Brillouin zone.

By adding a vector of the reciprocal lattice, the spherical segments are shifted into the 1^{st} Brillouin zone.

The right figure shows the energy bands when the k vector points from the Γ point of the 1^{st} Brillouin zone to the X point.

In the reduced zone scheme, only the area highlighted in gray is considered.

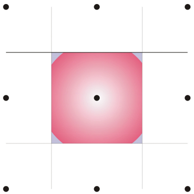
Quasi-free electrons in the sc-lattice 8 Comment 2

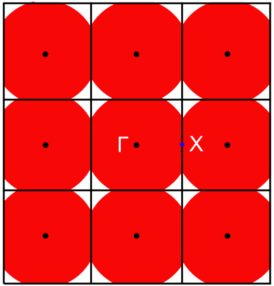
The occupied states are marked in red.

There is an energy band for the *k* states originally located in 1st Brillouin zone and a second energy band for the *k* states shifted in 1st Brillouin zone.

Quasi-free electrons in the sc-lattice 9

Fermi surfaces for two electrons per primitive unit cell of a simple cubic lattice





The occupied *k* states of the 1^{st} energy band in the reduced zone scheme (left) and the periodic zone scheme (right)

Quasi-free electrons in the sc-lattice 9 Comment

The left figure shows in the reduced zone scheme the occupied *k* states of the lowest energy band.

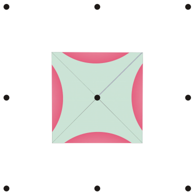
The right figure shows in the periodic zone scheme the occupied *k* states of the lowest energy band.

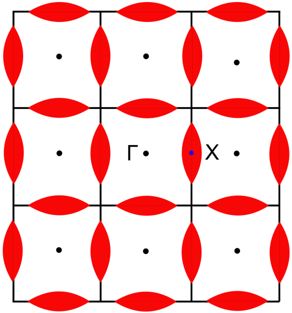
In the periodic zone scheme, the Fermi surface of the lowest energy band becomes visible.

The Fermi surface encloses the almost square white areas.

Quasi-free electrons in the sc-lattice 10

Fermi surfaces for two electrons per primitive unit cell of a simple cubic lattice





The occupied *k* states of the 2nd electron band in the reduced zone scheme (left) and the periodic zone scheme (right)

Quasi-free electrons in the sc-lattice 10 Comment

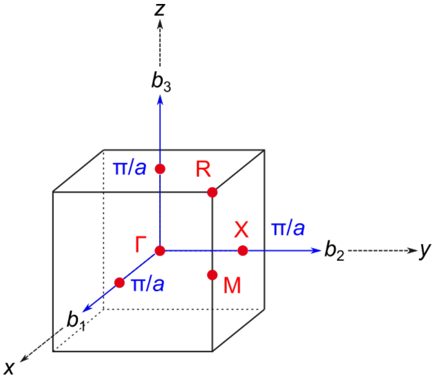
The left figure shows the occupied *k* states of the second energy band in the reduced zone scheme.

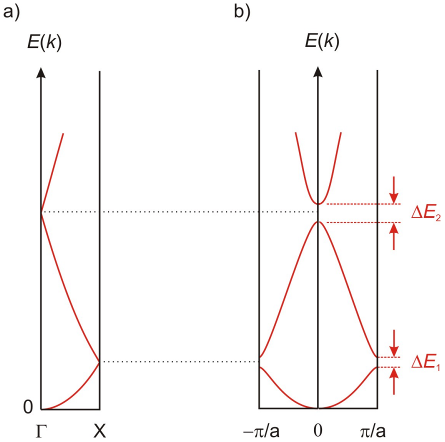
The right figure shows the occupied *k* states for this band in the periodic zone scheme.

The Fermi surface for this band encloses the surfaces drawn in red, which in three-dimensional space have the shape of a discus.

Quasi-free electrons in the sc-lattice 11

- energy gaps open at the intersection points of the energy bands
  → “avoided level crossing”





Quasi-free electrons in the sc-lattice 11 Comment 1

Energy gaps open when the periodicity of the potential energy is no longer negligibly small.

The figure on the left side shows the 1st Brillouin zone of the simple cubic lattice.

Figure a) on the right shows the band structure between the Γ point and X when the periodicity of the potential energy is negligibly small.

Figure b) shows what happens when the periodicity of the potential energy can no longer be neglected.

Energy gaps open at the intersection of the energy bands.

Energy bands and Fermi surfaces 11 Comment 2

It is a common feature of quantum mechanics that energy levels avoid crossing points.

The energy gaps increase with increasing periodic variation of the potential energy.

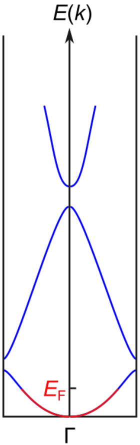
The energy gaps get bigger and the energy bands get narrower.

The stronger the periodic variation of the potential energy, the better the electrons are localized on their atoms and the narrower the energy bands are.

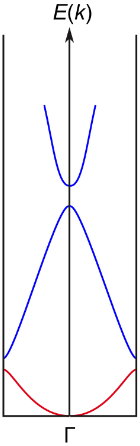
The width of an energy band indicates the mobility of the electrons.

The narrower a band, the better the electrons are localized on their atoms.

Quasi-free electrons in the sc-lattice 12



metal



insulator or semiconductor

Quasi-free electrons in the sc-lattice 12 Comment 1

The left figure illustrates the situation of a metal.

Not all k states of an energy band are occupied by two electrons.

Only a small amount of energy is required to excite electrons.

When an electric field is applied to the solid, an electric current flows and the solid is a metal.

The figure on the right shows the situation of an insulator.

If all k states of an energy band are occupied by two electrons, the excitation energy is determined by the smallest energy gap to the next higher energy band.

Quasi-free electrons in the sc-lattice 12 Comment 2

If this energy gap is much larger than the thermal energy at room temperature, no electric current can be induced by an applied electric field.

All electrons are blocked in their *k* states and the solid is an insulator.

The transition between an insulator and a semiconductor is gradual.

If the energy gap is small enough that electrons can be thermally excited at room temperature via the energy gap, one speaks of a semiconductor or semi-metal if the energy gap is even smaller.

When the temperature is lowered, the conductivity of these materials becomes lower because the number of excited electrons also becomes smaller.

Quasi-free electrons in the sc-lattice 12 Comment 3

This is in contrast to metals, where the electrical resistance is determined by electron-phonon scattering.

The conductivity of metals increases with decreasing temperature, as electron-phonon scattering freezes out.

The requirement that all *k* states of an energy band must be occupied for an insulator, however, applies to the entire reciprocal lattice.

In the cubic model system considered at the beginning, the lowest band is metallic, since there are unoccupied states for this band in the reciprocal lattice.

Usually there is an energy gap between the bands, which can cause the electrons of the 2nd band to migrate to the lowest band and fill the free *k* states.

Quasi-free electrons in the sc-lattice 12 Comment 4

If the number of electrons in the primitive unit cell is even, all k states of the occupied energy bands can be completely occupied by electrons and there is a good chance that the solid is an insulator.

Revision

Summary in Questions

1. Give the definition of a Bloch wave.
2. The *k*-vector is a quantum number which characterizes the translation symmetry of the Bloch waves. How?
3. The *k*-vector of a Bloch wave is sometimes called a crystal- or quasi-momentum. Why?
4. How many different wave *k*-vectors are there within the 1st Brillouin zone.
5. Sketch the band structure of quasi-free electrons in a simple cubic crystal lattice for the path Γ-X-M-Γ for the 1st and 2nd energy bands.
6. Calculate the Fermi wave number k_F when 3 electrons are in the primitive unit cell of the simple cubic lattice.
7. Sketch the Fermi surfaces for the 2nd and 3rd energy band in the reduced and periodic zone scheme.