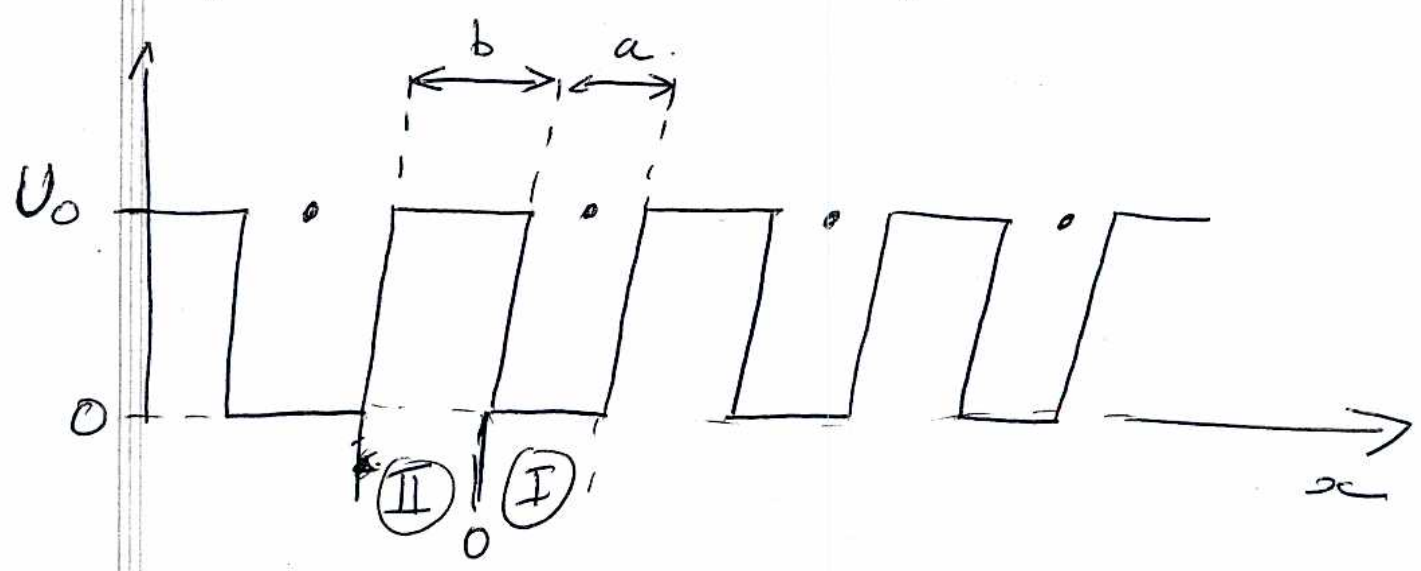


(a) The Krönig-Penney model

1D system where $U(x)$ is replaced by a periodic sequence of rectangular potential.



$$\Psi(x) = \begin{cases} \text{(I)} & A \exp(ik_1 x) + B \exp(-ik_1 x) & k_1 = \sqrt{\frac{2mE}{\hbar^2}} \\ \text{(II)} & C \exp(k_2 x) + D \exp(-k_2 x) & k_2 = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} \text{ if } E < U_0 \end{cases}$$

Boundary conditions =

at $x=0$ continuity $\Psi_{\text{I}}(0) = \Psi_{\text{II}}(0)$
 $\frac{d\Psi_{\text{I}}}{dx}\bigg|_0 = \frac{d\Psi_{\text{II}}}{dx}\bigg|_0$

at $x=a$ or $x=-b$ periodicity. we introduce the vector k via Bloch theorem

$$\Psi_{\text{I}}(a) = e^{ik(a+b)} \Psi_{\text{II}}(-b)$$

$$\frac{d\Psi_{\text{I}}}{dx}\bigg|_a = e^{ik(a+b)} \frac{d\Psi_{\text{II}}}{dx}\bigg|_{-b}$$

A, B, C, D

⇒ 4 unknowns, 4 equations, it comes in the matrix form

$$Mx = 0 \text{ where } x = \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}$$

det(M) = 0 it is a necessary condition to obtain non trivial solution; we get after calculation:

$$\left[\frac{k_2^2 - k_1^2}{2k_1k_2} \sinh(k_2 b) \sin(k_1 a) + \cosh(k_2 b) \cos(k_1 a) \right] = \cos(k(a+b))$$

P(E) since
k₁(E); k₂(E).

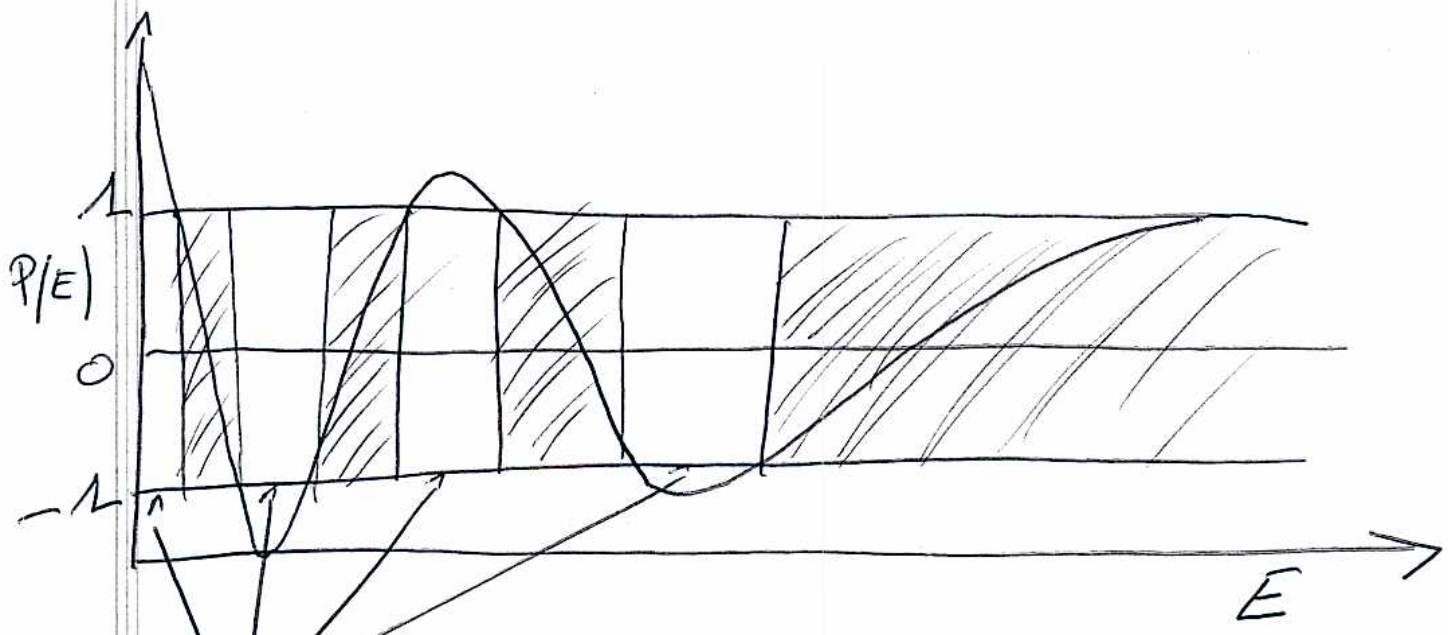
if E > U₀ in region II we rather get with k₂ = $\sqrt{\frac{2m(E-U_0)}{\hbar^2}}$ k₂ → ik₂

$$\left[-\frac{k_2^2 - k_1^2}{2k_1k_2} \sin(k_2 b) \sin k_1 a + \cos k_2 b \cos k_1 a \right] = \cos k(a+b)$$

* $P(E) = \cos[k(a+b)]$

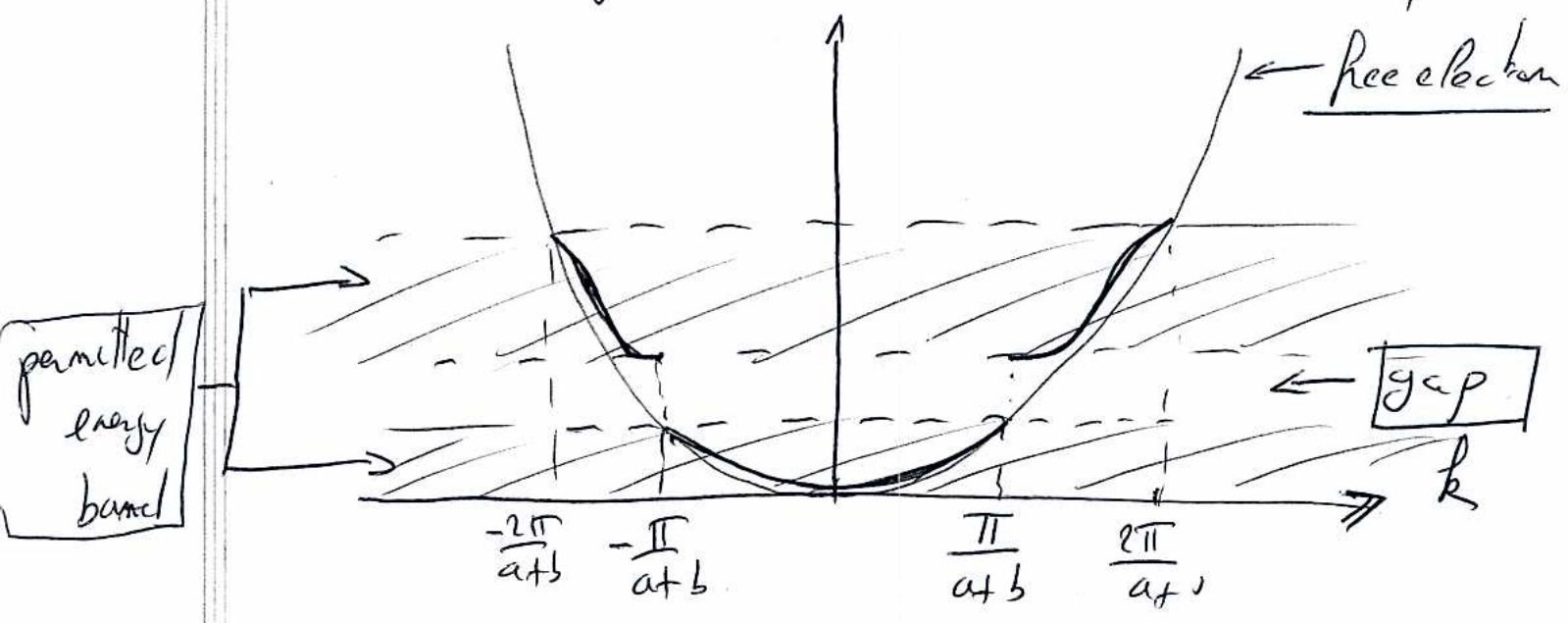
for a specific value of k, we get the allowed values of E
⇒ this provides implicitly the dispersion relation $E(k)$
we are looking at a graphical solution.

we must have $-1 \leq P(E) \leq 1$



it appears regions where there is no solution,
we call these regions - band gaps or forbidden bands.

The $E(k)$ dispersion relation can be also plotted:



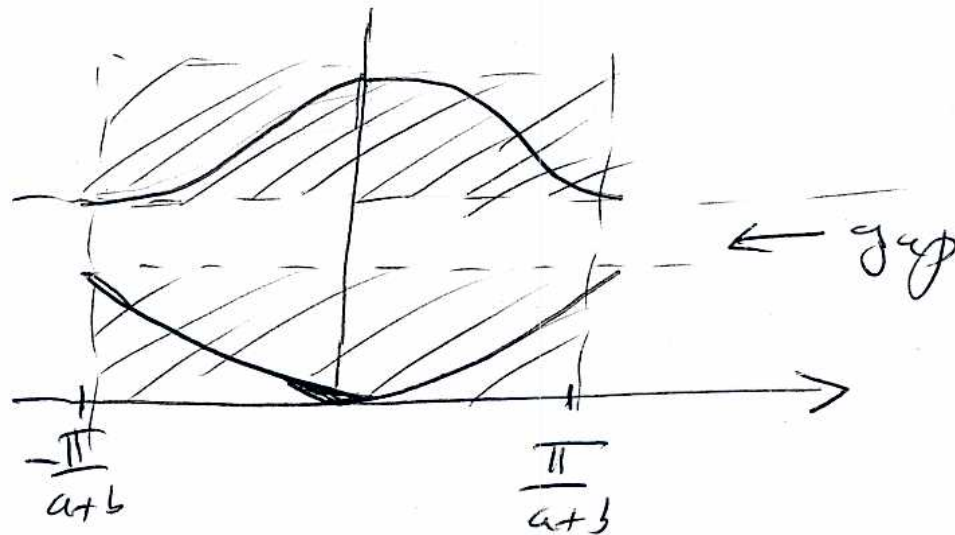
The periodicity of the relation is $\frac{2\pi}{ab}$.

The solution can be limited in the region:

$$-\frac{\pi}{a+b} \leq k \leq \frac{\pi}{a+b} \quad \text{without loss of information.}$$

we call this region the First Brillouin zone.

See
Figure 1.10
Textbook



⑥ General case

we need to solve

$$\left[-\frac{\hbar^2}{2m} \Delta \Psi + U \Psi = E \Psi \right] \text{ in } \Omega.$$

where U is an arbitrary periodic potential, as appropriate for a periodic solid.

[Bloch theorem]: we are looking ~~for~~ at solutions of this form:

$$\left[\Psi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}) ; u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{L}) \right]$$

we get

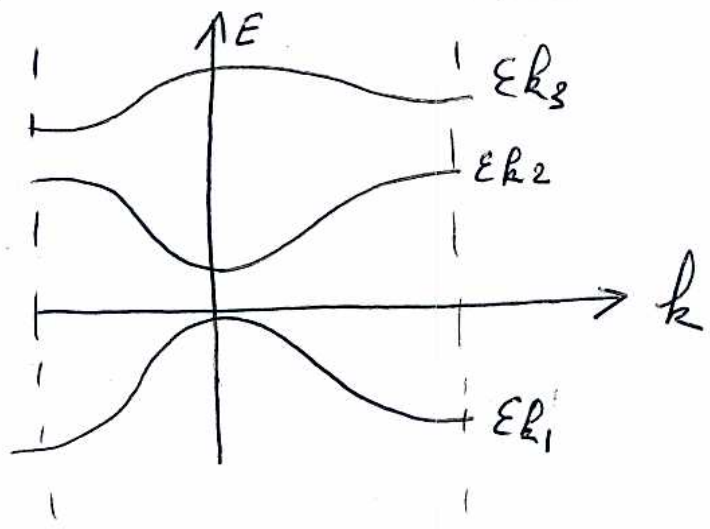
$$\underbrace{\left[\frac{\hbar^2}{2m} (-k^2 + 2ik \vec{\nabla} + \nabla^2) + U(\vec{r}) \right]}_{H_k} \psi_k(\vec{r}) = E_k \psi_k(\vec{r})$$

for a given k we need to solve an eigenvalue problem and we get a set of eigenvalues $\{E_{km}\}$.

$$H_k \psi_{km} = E_{km} \psi_{km} \quad (*)$$

- Numerical techniques are required ~~for~~ ~~to~~
- $\{E_{km}\}$ forms the bandstructure.

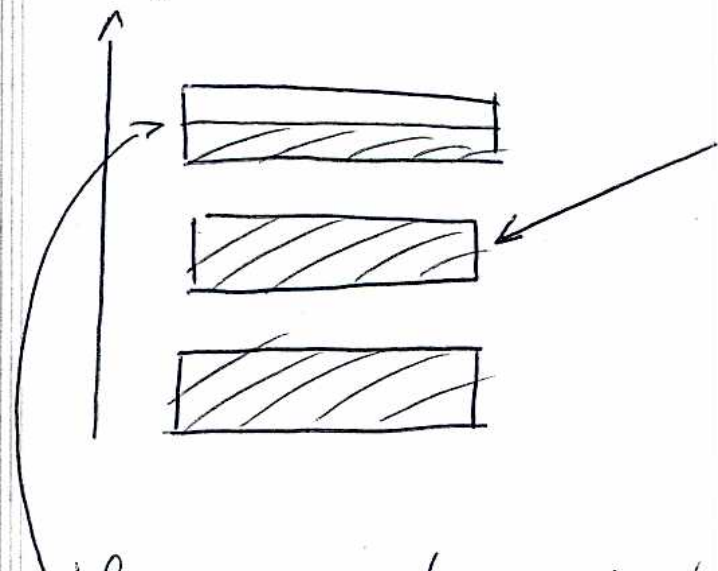
example



- The energy bands of solids are rather complex.

③ Valence band and conduction band

e^- are filling the energy bands by increasing energy order, from the bottom to the top.




the last completely filled band is called the valence band.


The energy band directly above the valence band is called the conduction band.

Remarks

* the energy band diagram can be restricted to the valence and conduction band, since the e^- that are contained in these bands dominate the behavior of the solid.

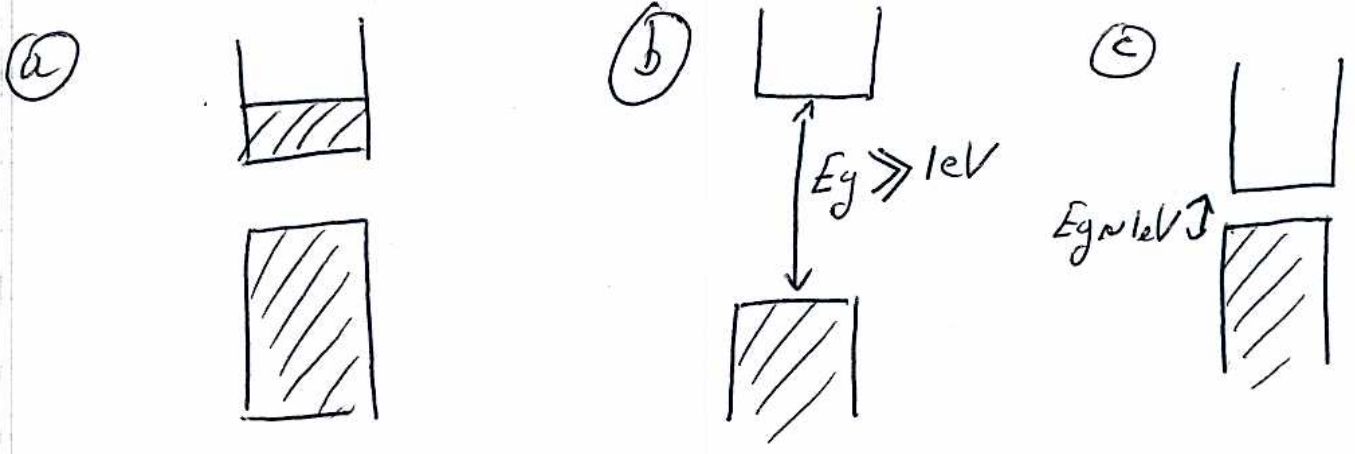
* 2 possibilities

1] The bands are completely filled or empty [conduction band is empty] 
Eg is the energy of the gap between valence and conduction band

2] The conduction band is partially filled; the highest energy level is called the Fermi level 

④ Insulator - Metal or Semiconductor?

We consider 3 configurations



① There exist unfilled space in the conduction band.

At finite temperature, (thermal excitation) there exist e^- close to the Fermi level, travelling in all directions and many different velocities.

When an electric field is applied, the e^- can be accelerated and it appears an electron flow. The conduction is then possible.

These solids are called Metals (good conductors)

② The energy gap is very large, the valence band is full and cannot carry a current since no empty state is ~~available~~ available.

These solids are Insulators

③ The energy gap is very small. At finite temperature (with thermal excitation) the e^- have enough energy to jump from the valence to the conduction band!

(2)

these solids are very bad insulators and very bad conductors!
we call them semiconductors.

(5) Bandstructure of semiconductors

For a 3D crystal, it is impossible to "represent" the bandstructure (dispersion relation $E(k)$) since $k = k_x, k_y, k_z$ and this involves a 4D plot.

However we can represent $E(k)$ along the main crystal directions in k -space - that allows us to analyse properties of semiconductors
[See figures]

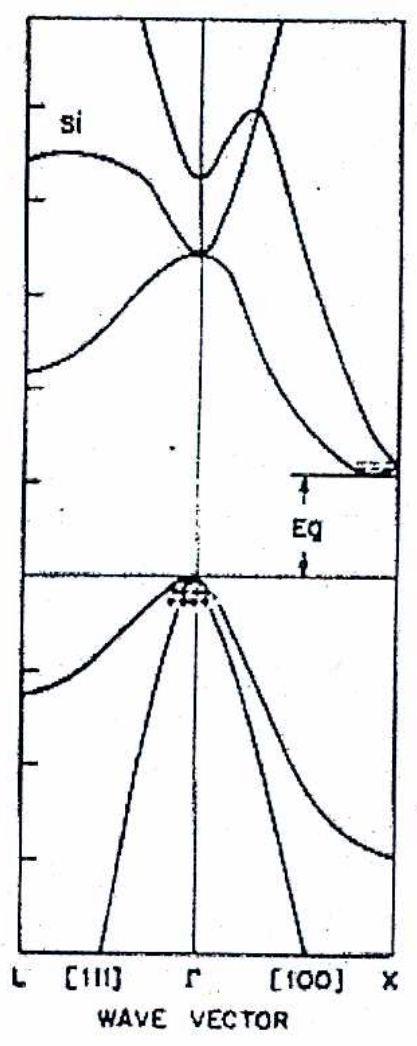
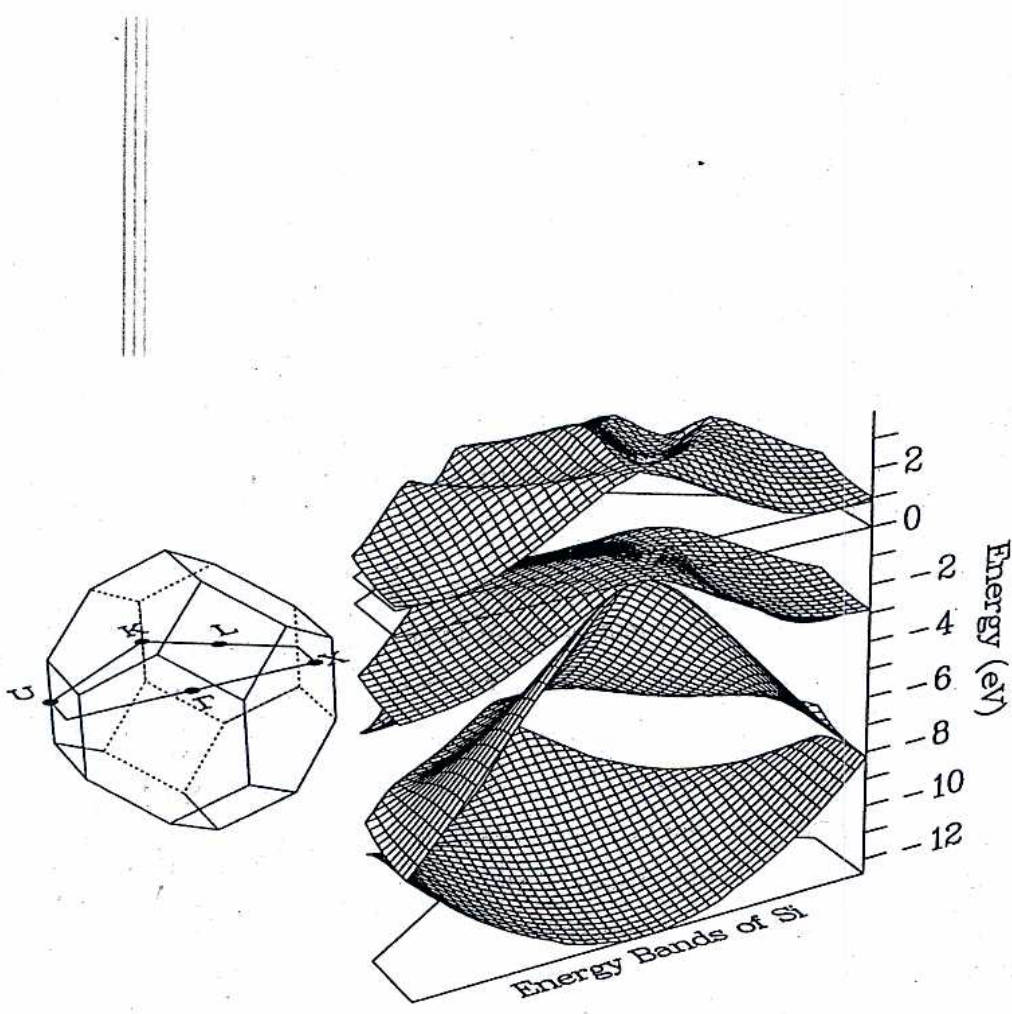
Remark:

semiconductors can exhibit =

- direct band gap (GaAs) = an e^- can fall or jump between the valence band and conduction band without a change in momentum.

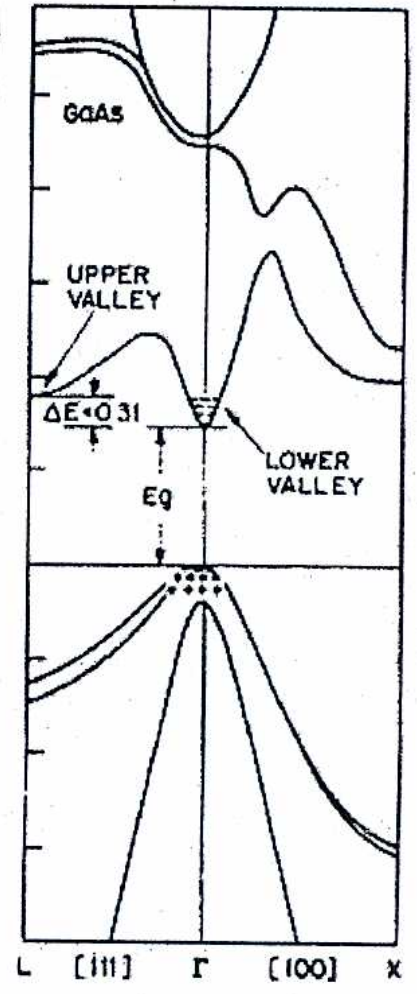
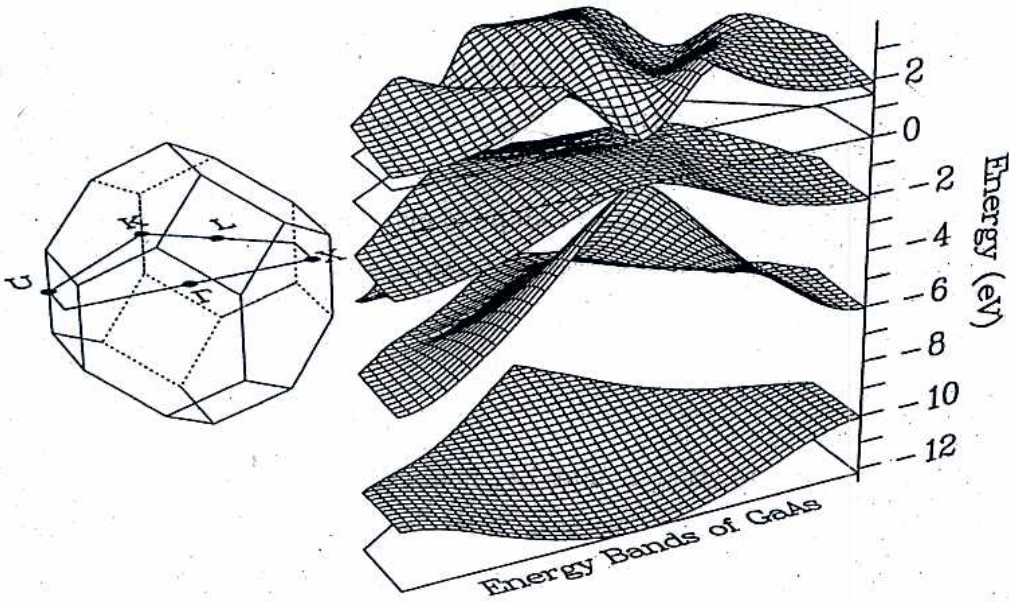
- indirect band gap (Si, Ge) = an e^- cannot fall or jump without a change in momentum.

Figure 1: Perspective plot of the energy band structure of silicon. The figure to the left shows the Brillouin zone, and the two-dimensional section over which the energy bands are displayed. The energy bands are plotted to the right. The four surfaces lying below 0 eV are the valence bands, and the upper surface is the lowest conduction band. The maximum valence band energy occurs at $k = 0$, which on this figure is the center of the front boundary of the Brillouin-zone section. The minimum conduction-band energy occurs along the front boundary of the section, near the left and right ends. Thus, Si has an indirect-gap band structure.



$$E_g = 1.12 \text{ eV}$$

Figure 2: Perspective plot of the energy band structure of gallium arsenide. The conventions of the figure are the same as those of Fig. 1. The conduction-band minimum of GaAs occurs at $k = 0$, and thus GaAs has a direct-gap band structure.

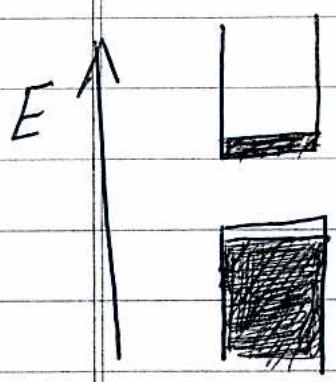


$$E_g = 1.42 \text{ eV}$$

⑥ Electrons and holes in semiconductor

We know that with thermal excitation, e^- can jump from the valence band to the conduction band.

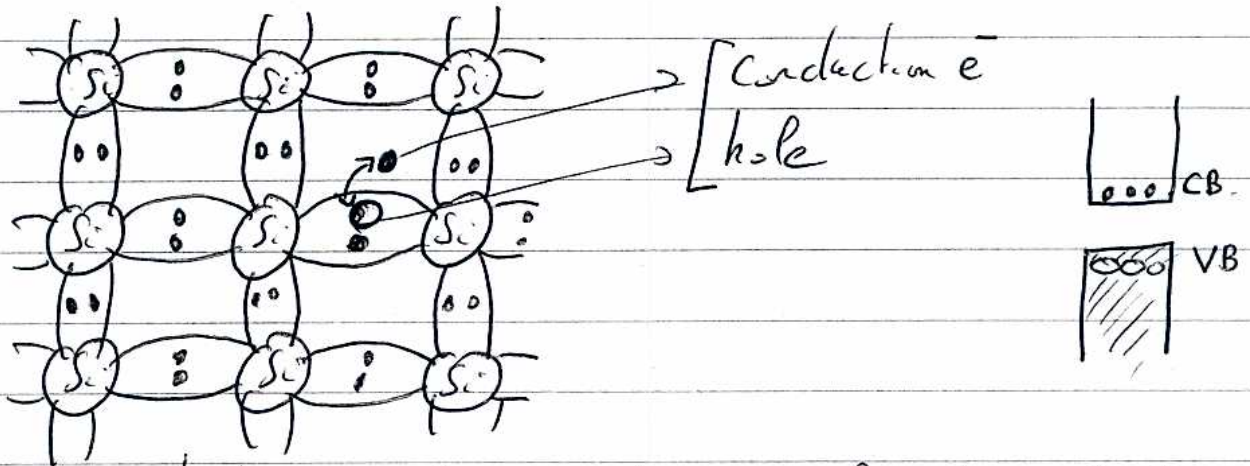
- The conduction band is then an "almost empty" band
- The valence band is an "almost full" band.



the concept of holes is introduced to keep track of the missing e^- in the valence band.

Holes are missing electrons

Example Si



* holes behave like positively charged particles, they can move inside the valence band.

* However holes are not real particles! they rather account for the combined behavior of all the electrons.

⇒ this means that we have to deal with the transport of carriers in both bands

⑦ Effective mass approximation

→ For a free electron, the dispersion relation is quadratic (parabola) $E = \frac{\hbar^2 k^2}{2m}$.

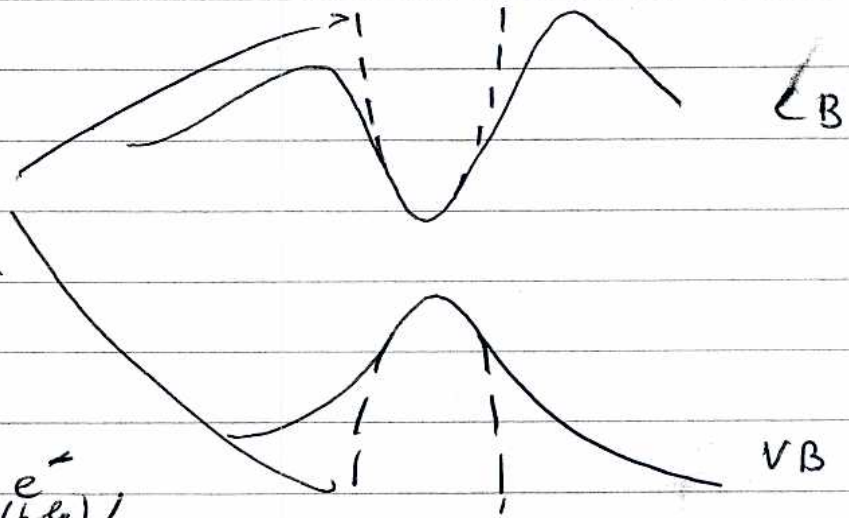
→ ~~in a crystal~~ In a crystal, the situation is far more complex.

However, physics of semiconductors usually deals with electrons situated near the minimum of the conduction band, or holes near the maximum of the valence band.

These extrema in the dispersion relation can be approximated by a quadratic curve (parabola)

example GaAs

parabolic band approximation



→ the e^- (holes) behave like free e^- (holes)

however they have now an effective mass m^* that accounts for the crystal structure

it comes

$$E = \frac{\hbar^2 k^2}{2m^*}$$

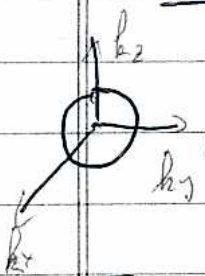
m^* contains all the details of the bandstructure around the extrema.

in general for 3D crystal, we get an effective mass tensor

$$m^* = \begin{bmatrix} m_{xx}^* & m_{xy}^* & m_{xz}^* \\ m_{yx}^* & m_{yy}^* & m_{yz}^* \\ m_{zx}^* & m_{zy}^* & m_{zz}^* \end{bmatrix} \quad \text{with} \quad m_{ij}^* = \frac{\hbar^2}{\partial^2 E / \partial k_i \partial k_j}$$

in particular =

For GaAs = m^* is isotropic, tensor is diagonal [all



constant energy surface are spheres) and elements are equal

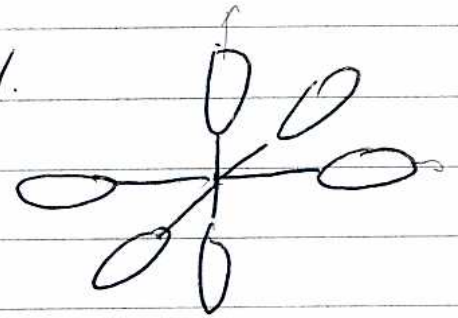
$$\left[\begin{array}{l} \frac{m^*}{m_0} = 0.067 \text{ for } e^- \\ \text{m. mass of electron} \\ \frac{m^*}{m_0} = 0.52 \text{ for holes} \end{array} \right]$$

For Si = tensor is diagonal, one longitudinal, two transverse effective mass (m_l^* , m_t^* , m_t^*).

$$\left[\frac{m_l^*}{m_0} = 0.98 \right], \left[\frac{m_t^*}{m_0} = 0.19 \right] \text{ for } e^-$$

constant energy surface are ellipsoid.

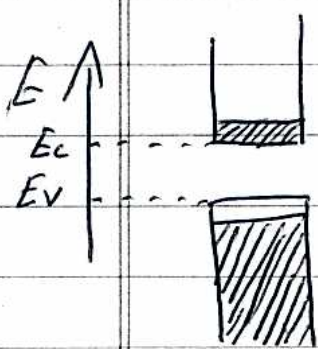
6 valleys



III Semiconductor Fundamentals

I Carrier densities

We want to know the population of e^- (resp. h^+) inside the CB (resp. VB).



electron density

$$n = \int_{E_c}^{+\infty} n(E) dE$$

hole density

$$p = \int_{-\infty}^{E_v} p(E) dE$$

$n(E), p(E)$ density of occupied states per unit volume and energy.

One needs to answer two questions:

(a) How many states are available at each energy?
 we call $g(E)dE$ the density of states (DOS) — number of states that are available between E and $E+dE$.

(b) What is the probability that a state is occupied by an electron?

we call $f(E)$ the distribution function for the electron.
 The derivation of $f(E)$ belongs to a statistical physics course.