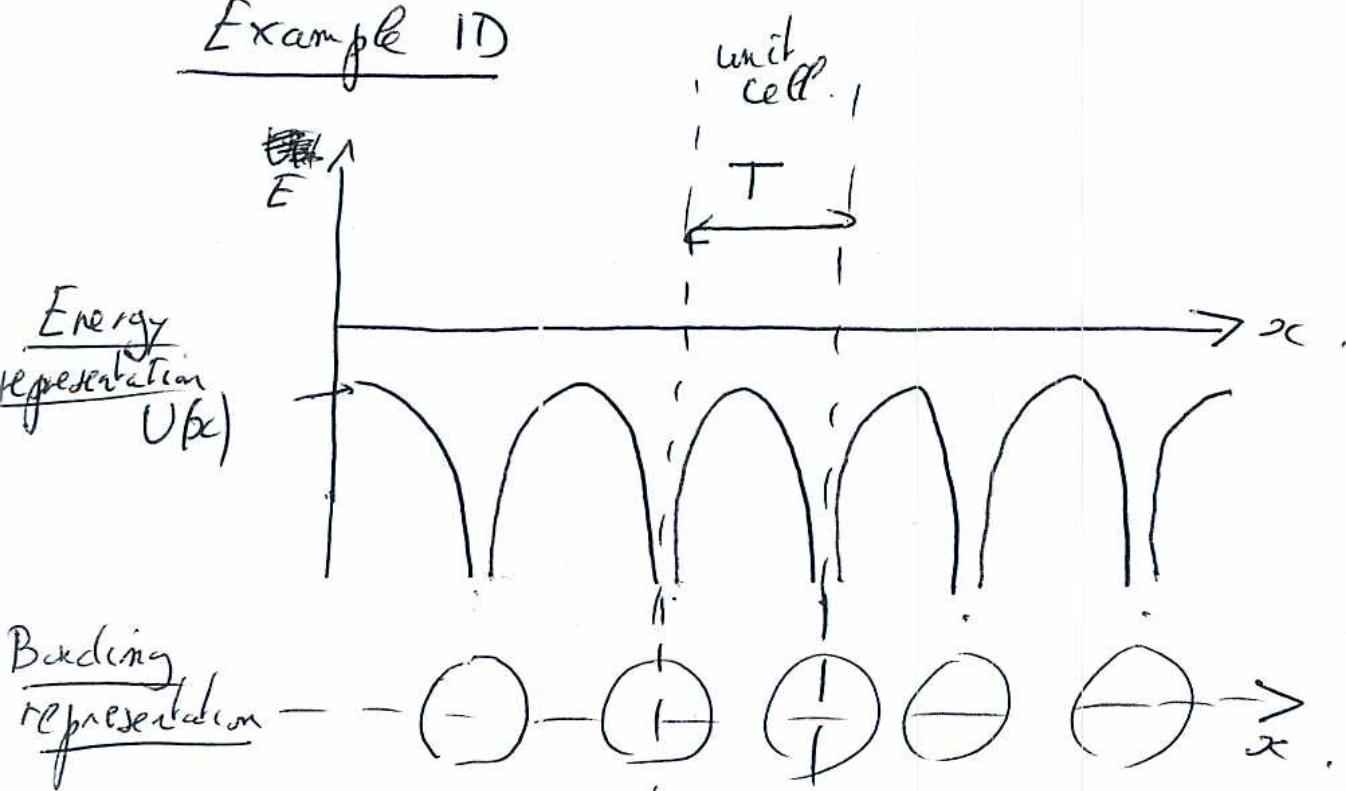


① Bloch Theorem.

In a crystal ("infinite" crystal), the placement of the atoms has a periodic nature.

⇒ if $U(\vec{r})$ is the potential inside a given unit cell then $U(\vec{r}) = U(\vec{r} + \vec{T})$ where \vec{T} is the periodicity.

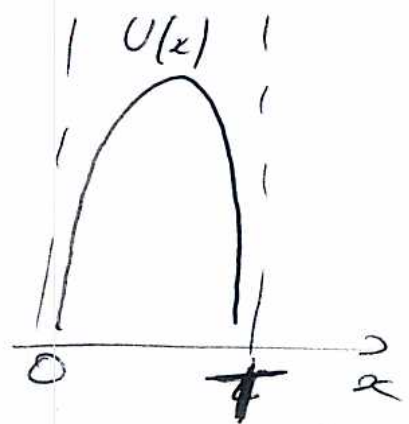
Example 1D



⇒ $U(x) = U(x + t)$

Since the potential is periodic, one can obtain all the properties of the crystal while solving the Schrödinger equation only in one unit cell using the Bloch theorem.

Let us consider only $U(x)$ where $x \in [0, \frac{a}{2}]$



in order to obtain Ψ and E we need $U(x)$ (given here) and the Boundary condition at $(x=0; x=\frac{a}{2})$.

1st form of the Bloch theorem

$$2) U(x) = U(x+a) \Rightarrow \boxed{\Psi_k(x+a) = \Psi_k(x) e^{i k a}}$$

(in our case $\Psi_k(a) = \Psi_k(0) e^{i k a}$)

Bloch theorem

if $U(x) = U(x+T)$ (periodic potential),

Then $\psi_k(x) = u_k(x) e^{ikx}$
 with $u_k(x+T) = u_k(x)$

Do $\psi_k(x)$ can be factorized into a Bloch function $u_k(x)$ and a plane wave (e^{ikx}).

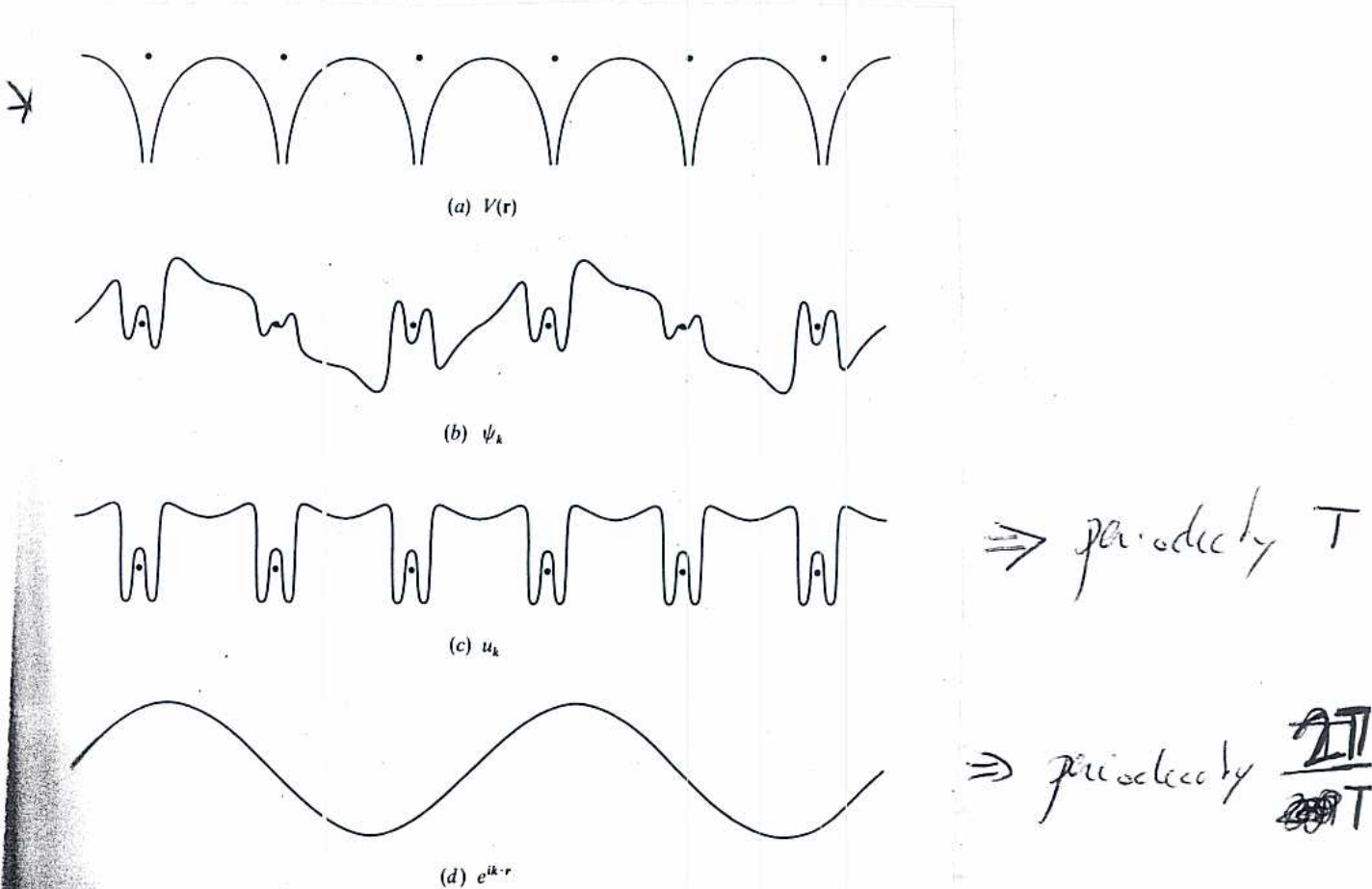


Fig. 2.1 A schematic representation of electronic eigenstates in a crystal. (a) The potential plotted along a row of atoms. (b) A sample eigenstate; the state itself is complex but only the real part is shown. This state can be factored into Bloch function (c), which has the periodicity of the lattice, and (d) a plane wave, the real part of which is shown.

* Let us calculate $\Psi_k(x+T)$

$$\Psi_k(x+T) = \mu_k(x+T) e^{ik(x+T)}$$

$$\Psi_k(x+T) = \underbrace{\mu_k(x)} e^{ikx} e^{ikT}$$

$$\boxed{\Psi_k(x+T) = \Psi_k(x) e^{ikT}}$$

\Rightarrow This expression will be used as Boundary conditions for solving the Schrodinger equation

For our 1D example we get

$$\Rightarrow \Psi_k(T) = \Psi_k(0) e^{ikT}$$

So we need to solve

$$\boxed{-\frac{\hbar^2}{2m} \frac{d^2 \Psi_k(x)}{dx^2} + U(x) \Psi_k(x) = E_k \Psi_k(x) \quad \text{where } x \in [0, T] \\ k \in [-\frac{\pi}{T}, \frac{\pi}{T}]}$$

~~and~~ and $\Psi_k(T) = \Psi_k(0) e^{ikT}$

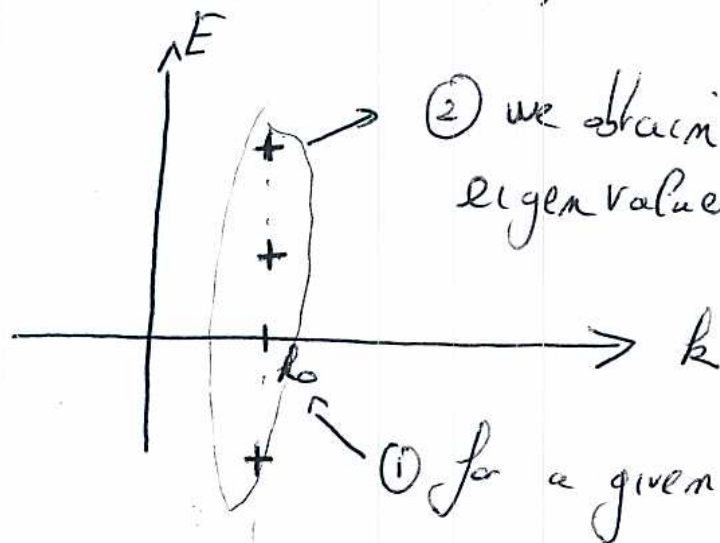
(3)

For a given k , we get to solve an eigenvalue problem to obtain a set of eigenvalues $\{E_{k,m}\}$ and eigenvectors $\{u_{k,m}\}$ $m=1, 2, \dots$

\Rightarrow Numerical techniques are required here.

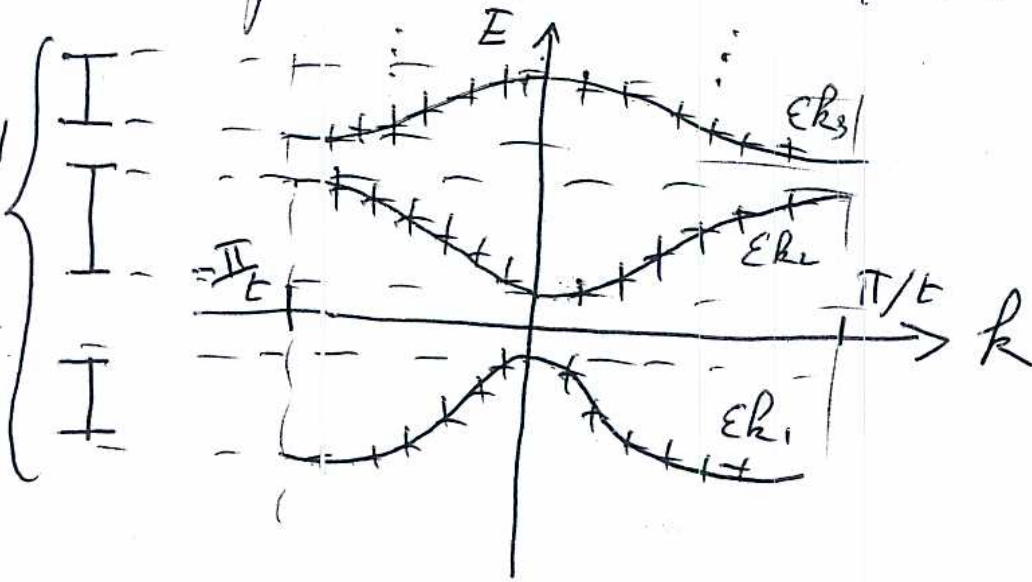
Example

3 steps 1-2-3



(3) we repeat for all k 's and obtain the dispersion relation $E(k)$!

allowed energy band
separated by
energy gaps.



The dispersion can be limited to the region $-\frac{\pi}{t} < k \leq \frac{\pi}{t}$ without loss of information (because of periodicity)

we call this region the first Brillouin zone

(c) Bandstructure of Semiconductors.

The energy band of solids are rather complex.

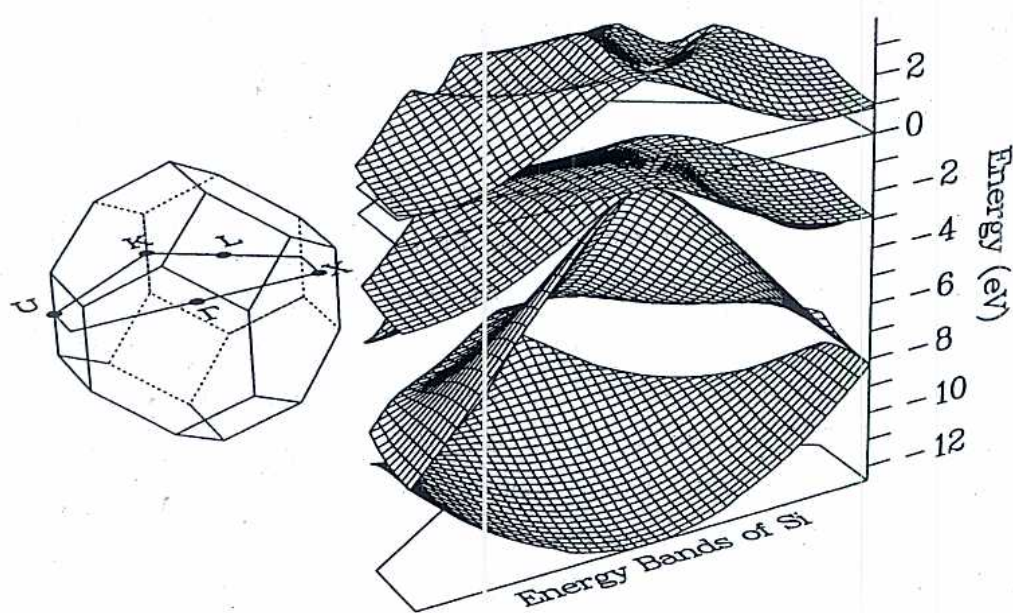
For a 3D crystal, it is impossible to "represent" the bandstructure (dispersion relation $E(k)$,

since $\vec{k} \equiv k_x, k_y, k_z$ and this involve a 4D plot.

However one can represent $E(k)$ along the main crystal direction in k -space that allows us to analyse properties of semiconductors.

⇒ See Figure for GaAs and Si.

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.



$E_g = 1.12 \text{ eV}$

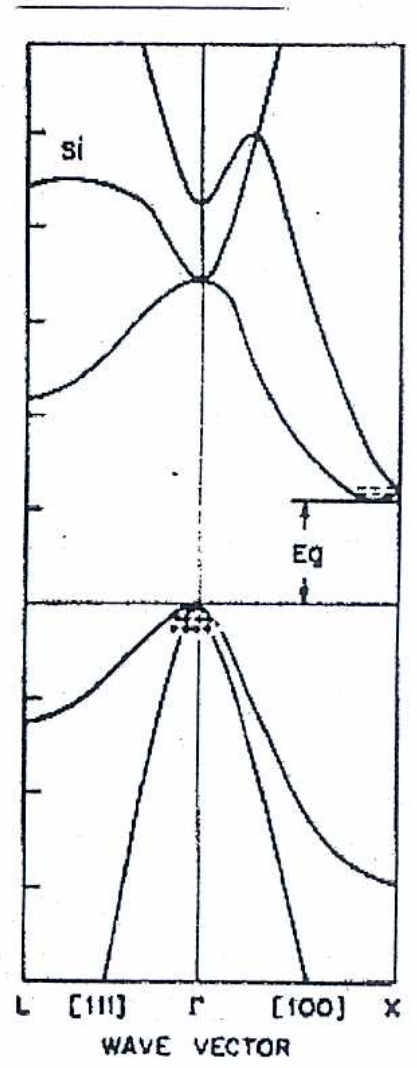
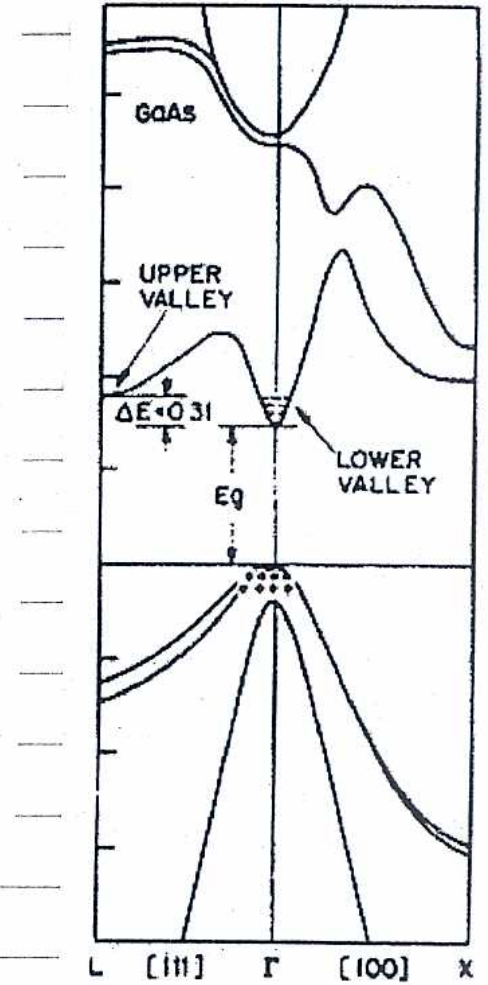
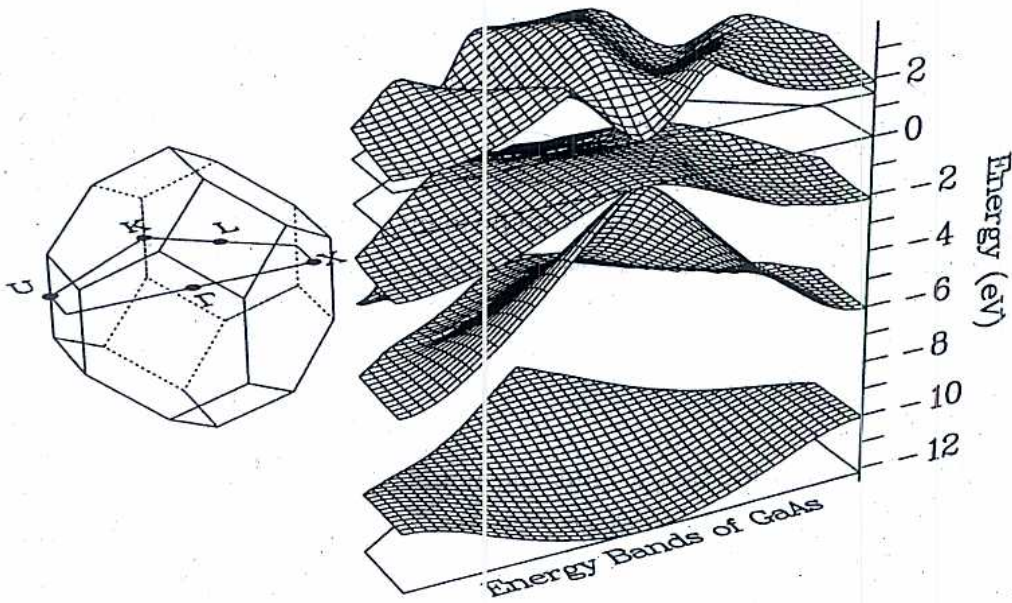


Figure 2: Perspective plot of the energy band structure of gallium arsenide. The conventions of the figure are the same as those of Fig. 1. The conduction-band minimum of GaAs occurs at $k = 0$, and thus GaAs has a direct-gap band structure.



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

Semiconductors can exhibit:

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

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

(d) Effective mass approximation

For a free electron in the vacuum, the dispersion relation is quadratic parabola.

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

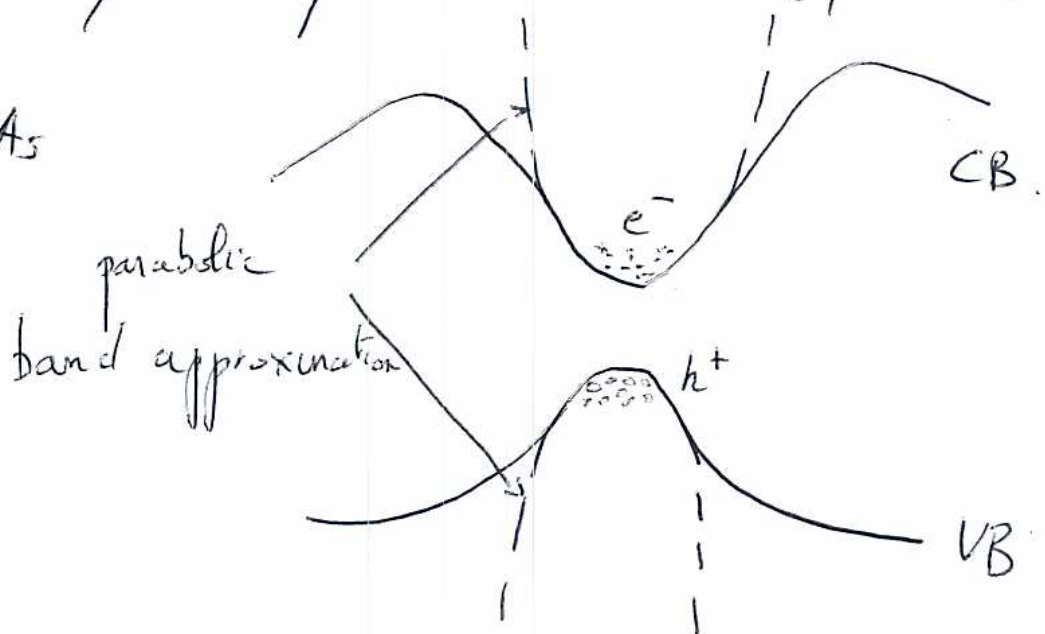
in 1D



In a crystal, the situation is far more complex. However, physics of semiconductors usually deals with e^- situated near the minimum of the CB, and holes near the maximum of the VB.

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

Example GaAs



\Rightarrow within the parabolic band approximation, the e^- (h^+) behaves like free e^- (h^+) in the vacuum. However they have now an effective mass m^* that accounts for the crystal structure.

e^- in free space

e^- in crystal

$$E = \frac{\hbar^2 p^2}{2m_0} + U$$

kinetic energy \nearrow $2m_0$ \nearrow e^- mass
 potential energy \nwarrow U \nwarrow a given potential energy

$$E = \frac{\hbar^2 p^2}{2m_m^*} + E_c$$

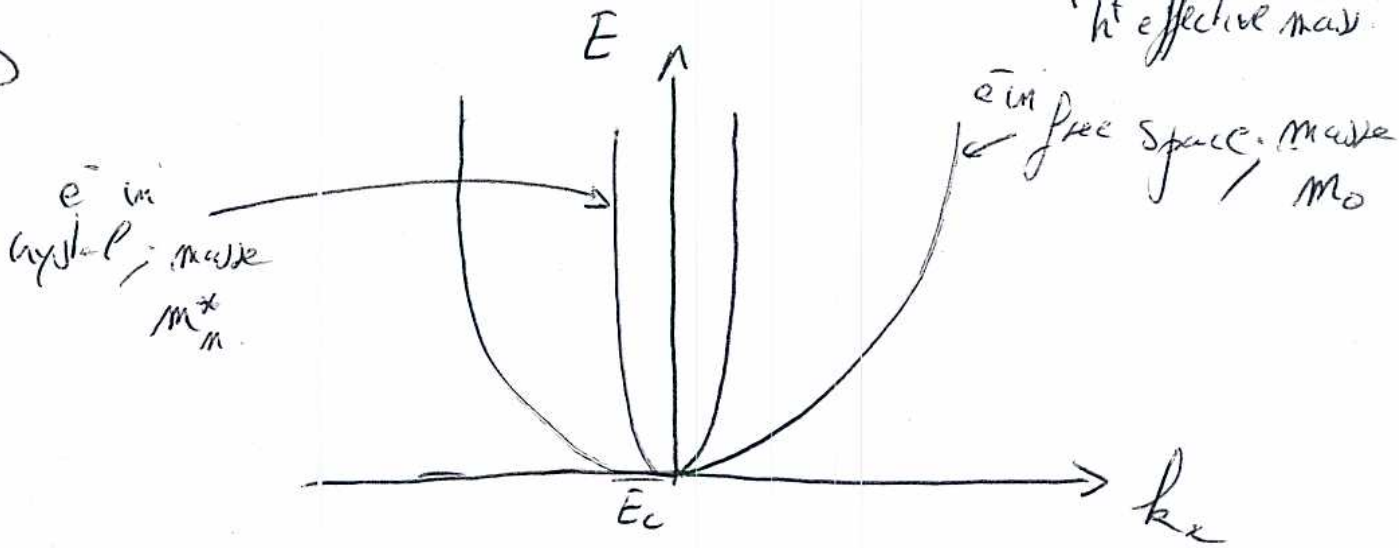
e^- effective mass

h^+ in crystal

$$E = -\frac{\hbar^2 p^2}{2m_p^*} + E_c$$

h^+ effective mass

in 1D



$$m^* = \frac{\hbar^2}{\left(\frac{\partial^2 E}{\partial k^2}\right)}$$

if material is isotropic
 ($E(k)$ curvature is the same in all directions)

* For GaAs.

$$m_{\text{Al}}^* = 0.067 m_0$$

$$m_p^* = 0.64 m_0 \text{ (average)}$$

* For Si

$$m_n^* = 1.08 m_0$$

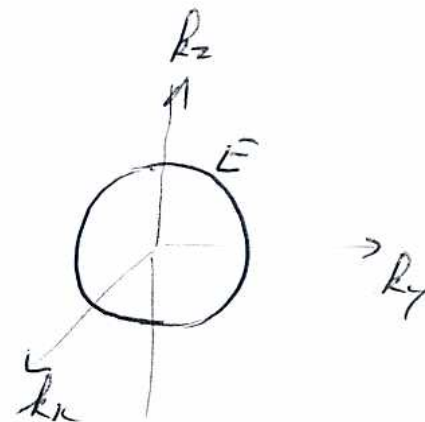
$$m_p^* = 0.59 m_0$$

} average.

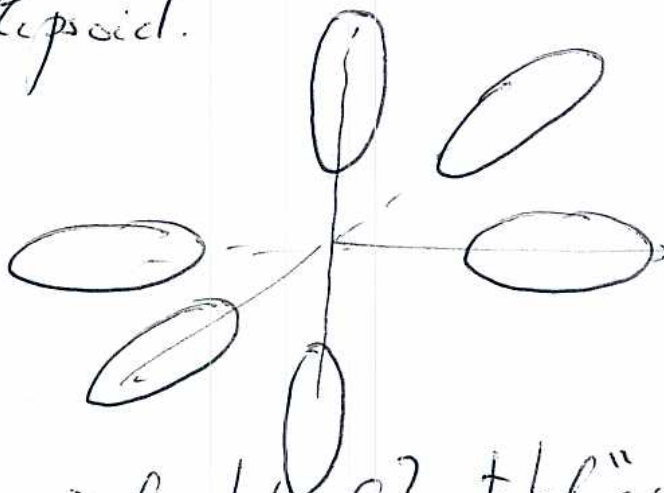
Remark in 3D (C.B)

constant energy surface for GaAs

⇒ sphere



for Si ⇒ Ellipsoid.



⇒ 2 masses

$$m_p^* = 0.58 m_0 \Rightarrow \text{longitudinal}$$

$$m_t^* = 0.19 m_0 \Rightarrow \text{transverse}$$

} total "average"

$$1.08 m_0$$