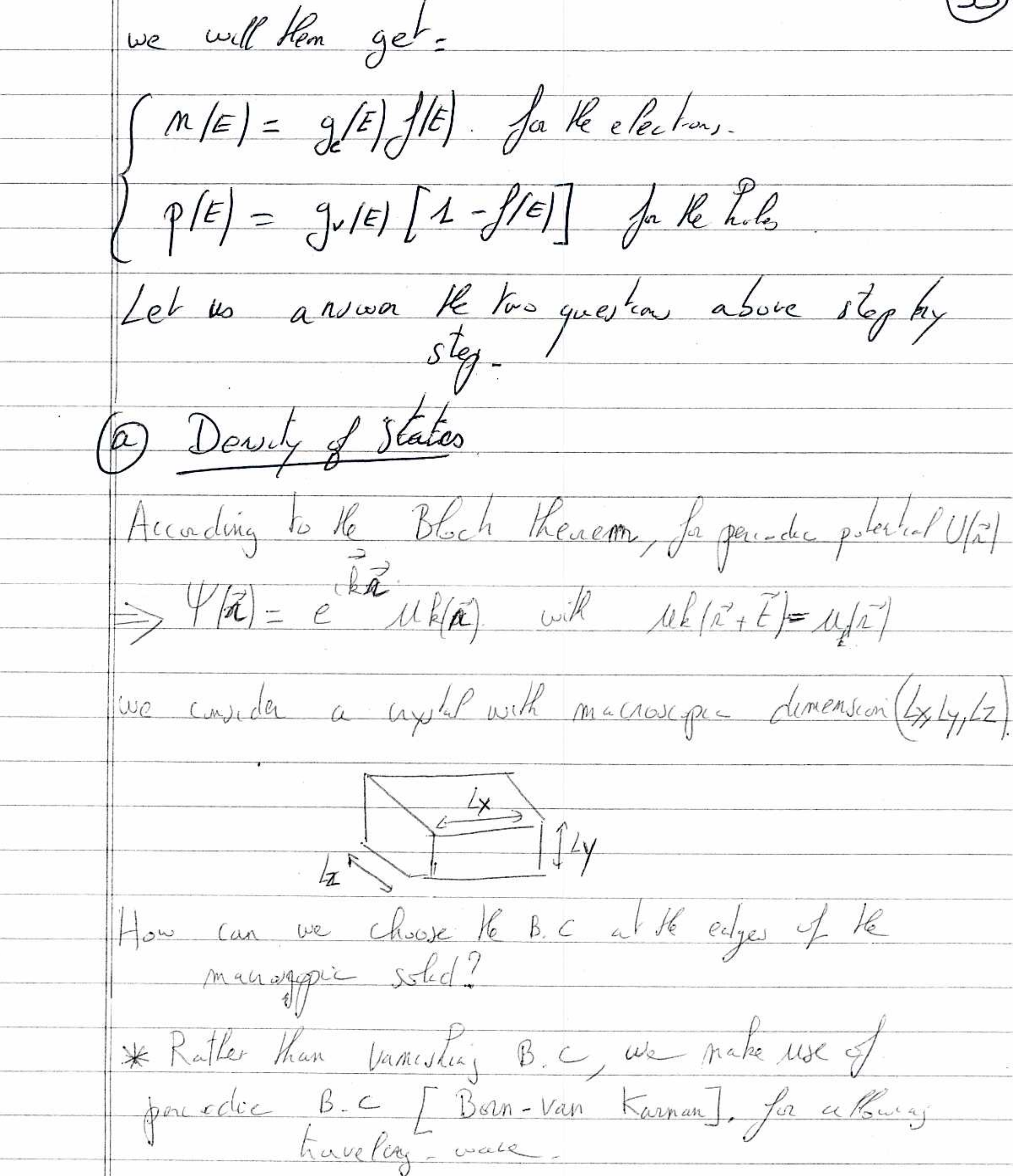


we will then get:

$$\begin{cases} n(E) = g_c(E)\, f(E) & \text{for the electrons.} \\ p(E) = g_v(E)\,[1 - f(E)] & \text{for the holes} \end{cases}$$

Let us answer the two question above step by step.

(a) Density of States

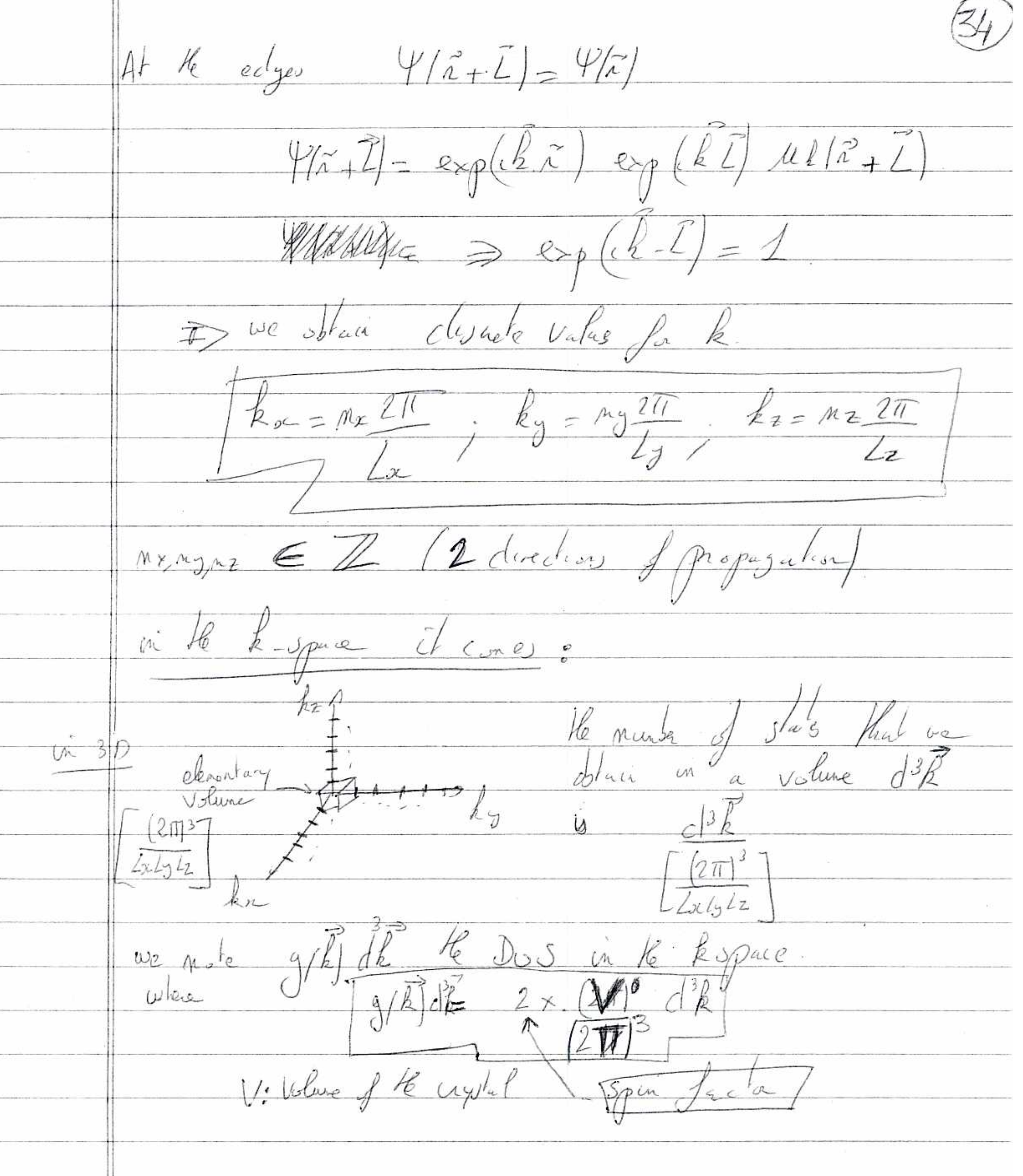
According to the Bloch theorem, for periodic potential $U(\vec{r})$

$\Rightarrow \Psi(\vec{r}) = e^{i\vec{k}\vec{r}}\, u_k(\vec{r})$ with $u_k(\vec{r}+\vec{T}) = u_k(\vec{r})$

we consider a crystal with macroscopic dimension (L_x, L_y, L_z).

How can we choose the B.C at the edges of the macroscopic solid?

* Rather than vanishing B.C, we make use of periodic B.C [Born-van Karman], for allowing traveling wave.



At the edges $\Psi(\vec{r} + \vec{L}) = \Psi(\vec{r})$

$$\Psi(\vec{r} + \vec{L}) = \exp(i\vec{k}\cdot\vec{r})\,\exp(i\vec{k}\cdot\vec{L})\,u_k(\vec{r} + \vec{L})$$

$$\Rightarrow \exp(i\vec{k}\cdot\vec{L}) = 1$$

$\Rightarrow$ we obtain discrete values for k.

$$k_x = n_x \frac{2\pi}{L_x}\ ; \quad k_y = n_y \frac{2\pi}{L_y}\ ; \quad k_z = n_z \frac{2\pi}{L_z}$$

$n_x, n_y, n_z \in \mathbb{Z}$ (2 directions of propagation)

in the k-space it comes:

in 3D

The number of states that we obtain in a volume $d^3\vec{k}$ is $\dfrac{d^3\vec{k}}{\left[\frac{(2\pi)^3}{L_x L_y L_z}\right]}$

we note $g(\vec{k})\,d^3\vec{k}$ the DOS in the k-space

where $g(\vec{k})\,d^3\vec{k} = 2 \times \dfrac{V}{(2\pi)^3}\, d^3\vec{k}$

V: Volume of the crystal

2: spin factor

for dimension $m = 1, 2, 3$, we get

$$g(\vec{k})\, d^m\vec{k}$$

in 3D $\quad d^3\vec{k} = 4\pi k^2 dk$ [elementary volume between two energy sphere]

in 2D $\quad d^2\vec{k} = 2\pi k\, dk$

in 1D $\quad d\vec{k} = 2\, dk$ [2 direction of propagation]

We want to know the density of state in Energy

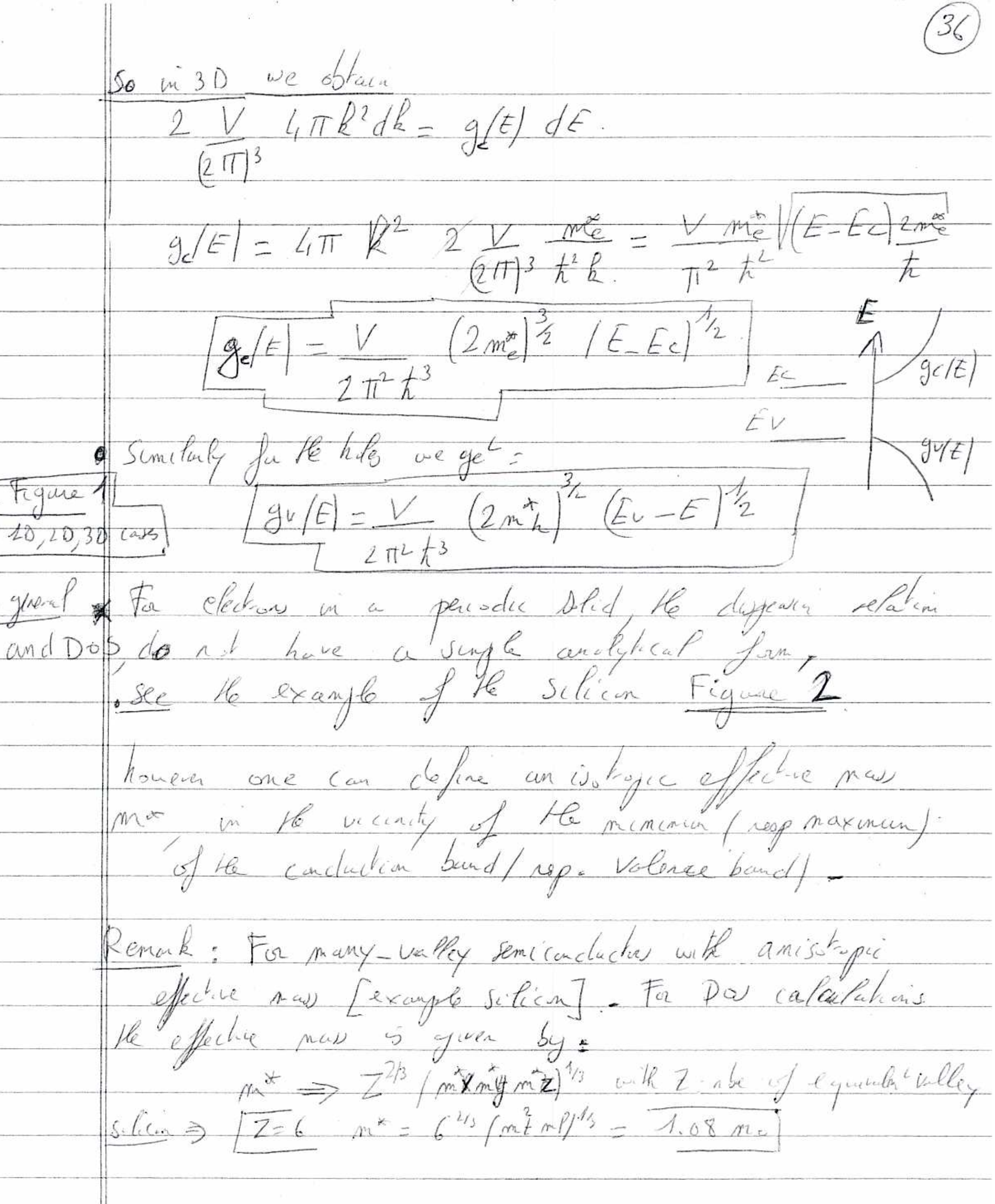
$$g(k)\, dk = g(E)\, dE$$

one needs to know the dispersion relation $E(k)$.

- For Free electron or effective mass approach

we know that $\quad E(k) = \frac{\hbar^2 k^2}{2m_e^*} + E_c$

it comes $\quad \boxed{dE = \frac{\hbar^2 k}{m_e^*} dk}$



So in 3D we obtain

$$\frac{2V}{(2\pi)^3}\, 4\pi k^2\, dk = g_c(E)\, dE.$$

$$g_c(E) = 4\pi k^2 \, \frac{2V}{(2\pi)^3} \, \frac{m_e^*}{\hbar^2 k} = \frac{V m_e^*}{\pi^2 \hbar^2}\sqrt{(E-E_c)\frac{2m_e^*}{\hbar}}$$

$$\boxed{g_c(E) = \frac{V}{2\pi^2\hbar^3}\,(2m_e^*)^{3/2}\,(E-E_c)^{1/2}}$$

• Similarly for the holes we get:

$$\boxed{g_v(E) = \frac{V}{2\pi^2\hbar^3}\,(2m_h^*)^{3/2}\,(E_v-E)^{1/2}}$$

e Figure 1
1D, 2D, 3D cases

In general * For electrons in a periodic solid, the dispersion relation and DOS do not have a single analytical form, see the example of the silicon Figure 2.

However one can define an isotropic effective mass m^* in the vicinity of the minimum (resp maximum) of the conduction band (resp. valence band).

Remark: For many-valley semiconductors with anisotropic effective mass [example silicon]. For DOS calculations the effective mass is given by:

$$m^* \Rightarrow Z^{2/3}(m_x^* m_y^* m_z^*)^{1/3}$$ with Z: nbe of equivalent valley

silicon ⇒ $\boxed{Z = 6 \quad m^* = 6^{2/3}(m_t^2 m_l)^{1/3} = 1.08\, m_0}$

- For holes which occupy 2 bands, we call these bands light-hole (lh) and heavy-hole (hh) bands, the effective DOS mass equal [1 minima]:

$$m^* \rightarrow \left(m^{*\,3/2}_{hh} + m^{3/2}_{lh}\right)^{2/3}$$

for Silicon = $m^*_{lh} = 0.16\, m_o$, $m^*_{hh} = 0.53\, m_o$

$\Rightarrow m^* = 0.59\, m_o$

for GaAs = $m_{lh} = 0.074\, m_o$, $m_{hh} = 0.62\, m_o$

$\Rightarrow m^* = 0.64\, m_o$

- [The effective mass for conductivity calculation is ≠ than the effective mass for DOS calculations.

here

$$\boxed{\frac{1}{m^*} = \frac{1}{3}\left(\frac{1}{m_x} + \frac{1}{m_y} + \frac{1}{m_z}\right)}$$

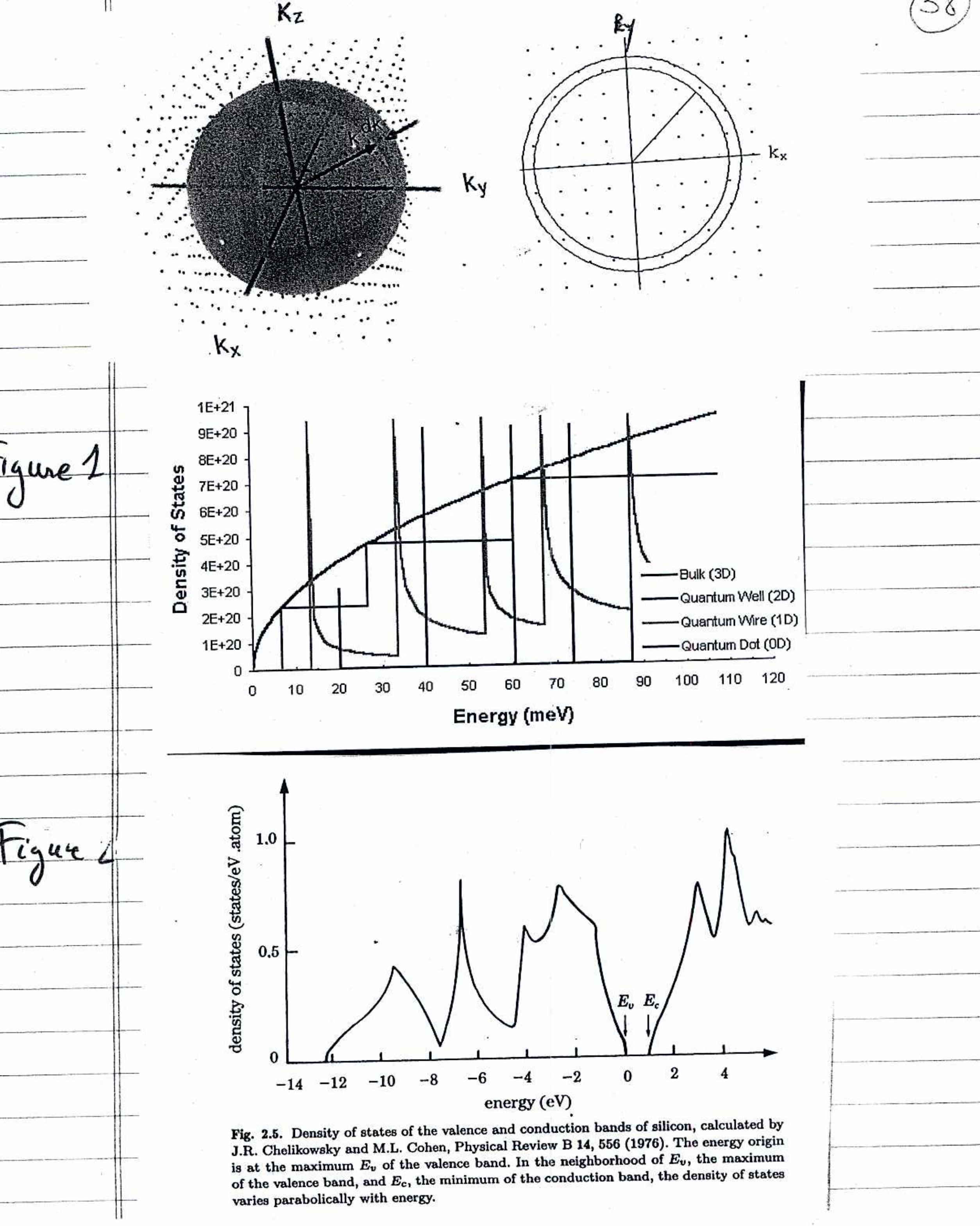


Fig. 2.5. Density of states of the valence and conduction bands of silicon, calculated by J.R. Chelikowsky and M.L. Cohen, Physical Review B 14, 556 (1976). The energy origin is at the maximum E_v of the valence band. In the neighborhood of E_v, the maximum of the valence band, and E_c, the minimum of the conduction band, the density of states varies parabolically with energy.

b) Distribution function

We know from the energy band theory and the definition of the semiconductors, that the probability for a state to be occupied by an e^- should depend on the temperature.

e^- obey the Fermi-Dirac statistics [accounting for the Pauli exclusion principle].

we have:

$$f(E) = \frac{1}{1 + \exp(\beta(E - E_F))}$$

$$\beta = \frac{1}{k_B T}$$

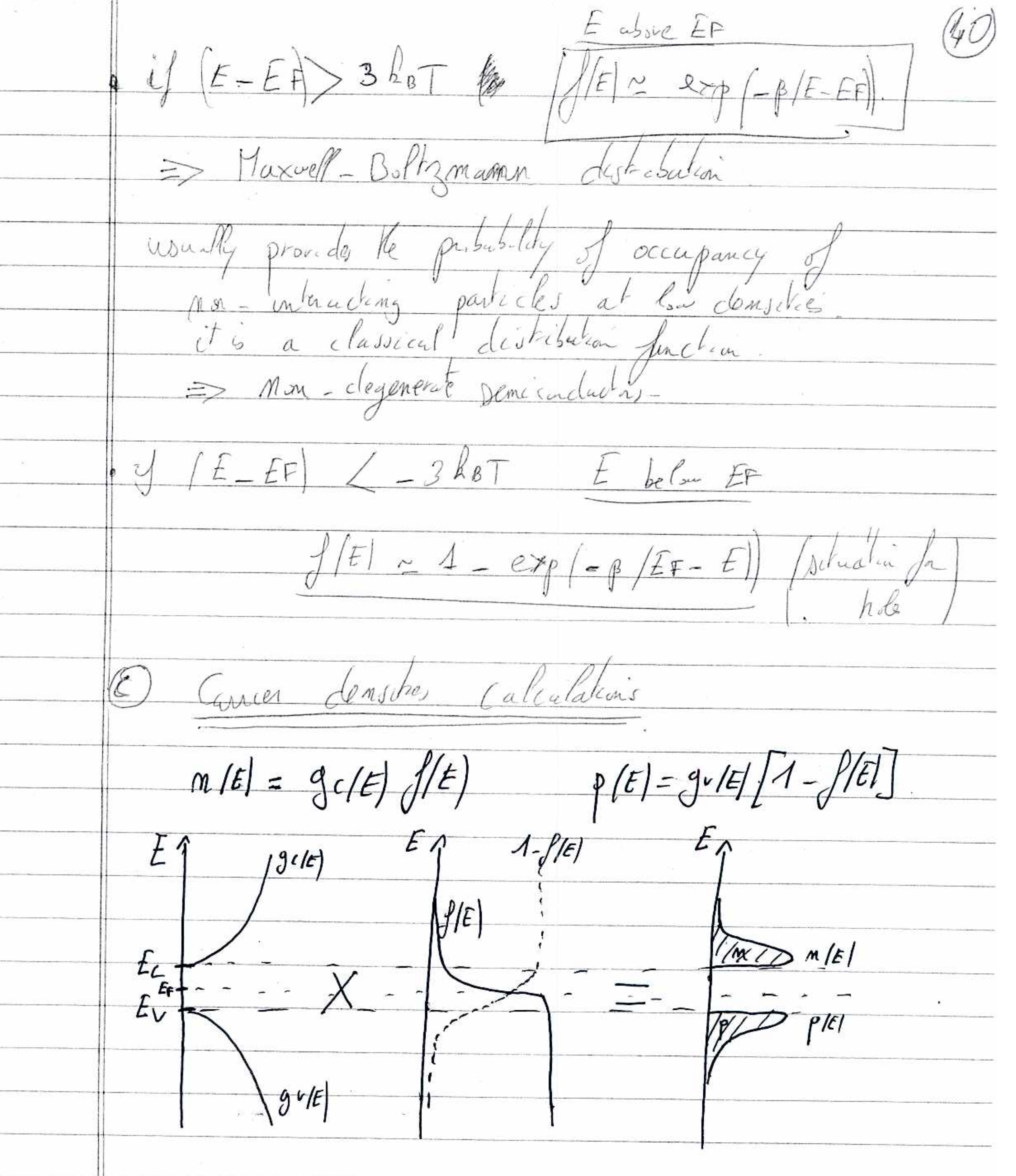
k_B = Boltzmann cte
E_F = Fermi-level

$f(E)$: 1, 1/2, $T = 0$, $T \nearrow$, E_F, E

if $T \neq 0$ $f(E_F) = \frac{1}{2}$

Remark

- For conductors at $T = 0$, we saw ← E_F (maximum of energy for one e^-)
- For Insulators, semiconductors, the fermi level lies between VB and CB
- For semiconductor, with increase of temperature the probability $f(E)$ to find an e^- for $E > E_F$ is different than $\emptyset$.



- if $(E - E_F) > 3 k_B T$ ⇒ $f(E) \simeq \exp(-\beta(E - E_F))$ — E above E_F

⇒ Maxwell-Boltzmann distribution

usually provides the probability of occupancy of non-interacting particles at low densities. it is a classical distribution function.

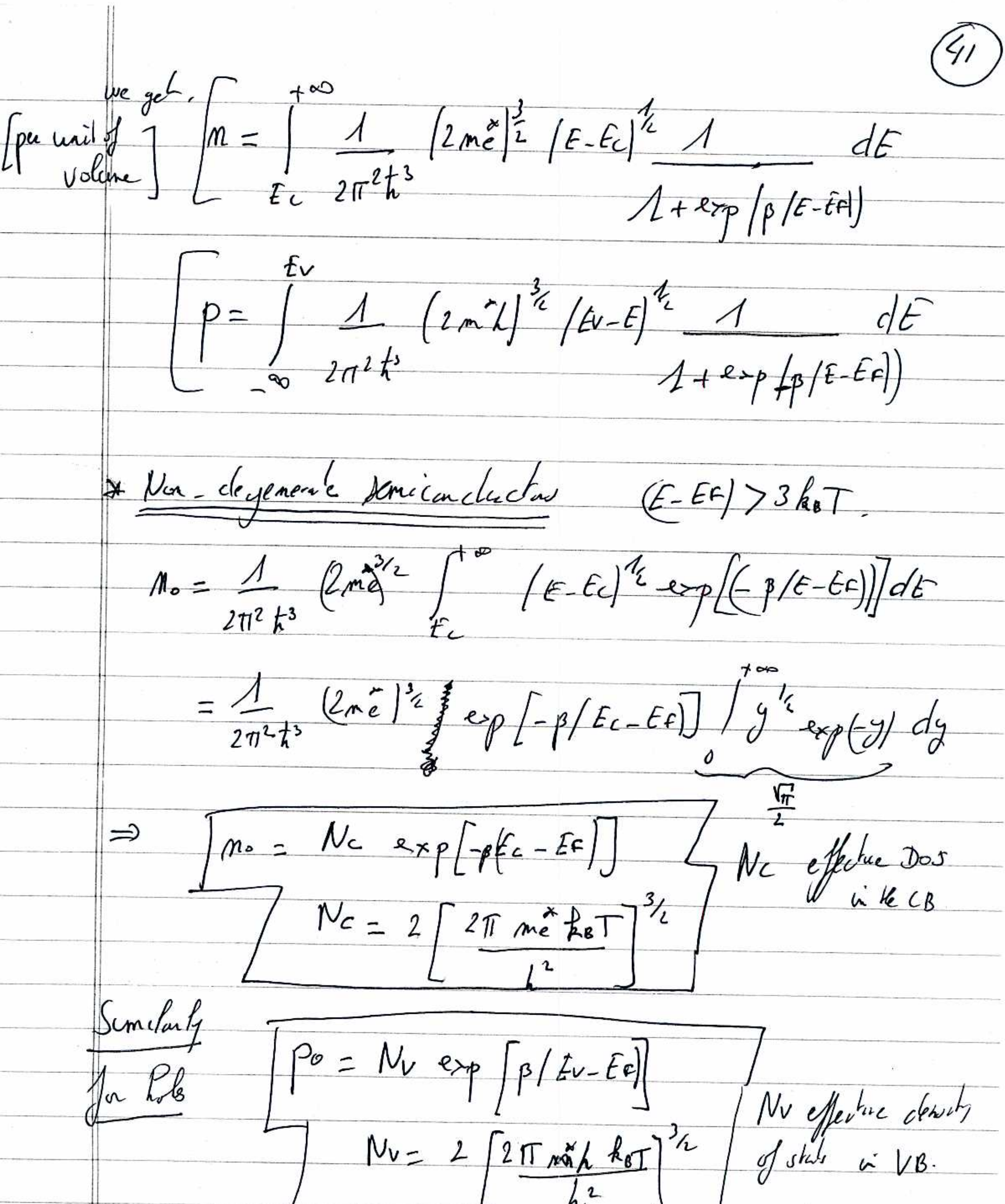
⇒ non-degenerate semiconductors.

- if $(E - E_F) < -3 k_B T$ — E below E_F

$$f(E) \simeq 1 - \exp(-\beta(E_F - E))$$ (situation for holes)

C) Carrier densities calculations

$$n(E) = g_c(E)\, f(E) \qquad p(E) = g_v(E)\,[1 - f(E)]$$



we get, [per unit of volume]

$$n = \int_{E_c}^{+\infty} \frac{1}{2\pi^2\hbar^3} (2m_e^*)^{3/2} (E-E_c)^{1/2} \frac{1}{1+\exp(\beta(E-E_F))}\, dE$$

$$p = \int_{-\infty}^{E_v} \frac{1}{2\pi^2\hbar^3} (2m_h^*)^{3/2} (E_v-E)^{1/2} \frac{1}{1+\exp(-\beta(E-E_F))}\, dE$$

* **Non-degenerate semiconductor** $(E-E_F) > 3k_BT$.

$$n_0 = \frac{1}{2\pi^2\hbar^3} (2m_e^*)^{3/2} \int_{E_c}^{+\infty} (E-E_c)^{1/2} \exp[(-\beta(E-E_F))]\, dE$$

$$= \frac{1}{2\pi^2\hbar^3} (2m_e^*)^{3/2} \exp[-\beta(E_c-E_F)] \underbrace{\int_0^{+\infty} y^{1/2} \exp(-y)\, dy}_{\frac{\sqrt{\pi}}{2}}$$

$$\Rightarrow \quad n_0 = N_c \exp[-\beta(E_c-E_F)]$$

$$N_c = 2\left[\frac{2\pi m_e^* k_B T}{h^2}\right]^{3/2}$$

N_c effective DOS in the CB

Similarly for holes

$$p_0 = N_v \exp[\beta(E_v-E_F)]$$

$$N_v = 2\left[\frac{2\pi m_h^* k_B T}{h^2}\right]^{3/2}$$

N_v effective density of states in VB.

Typical value for N_C and N_V at $T = 300\,K$.

	$N_C\ (cm^{-3})$	$N_V\ (cm^{-3})$
Si	2.8×10^{19}	1.04×10^{19}
GaAs	1.04×10^{19}	6.0×10^{18}

In general

$$n = N_C\, F_{1/2}\left[-\beta(E_C - E_F)\right]$$

$$p = N_V\, F_{1/2}\left[\beta(E_V - E_F)\right]$$

$F_{1/2}$ is the Fermi-Dirac integral.

$$F_{1/2}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} \frac{\sqrt{\varepsilon}\, d\varepsilon}{1 + \exp(\varepsilon - \eta)}.$$

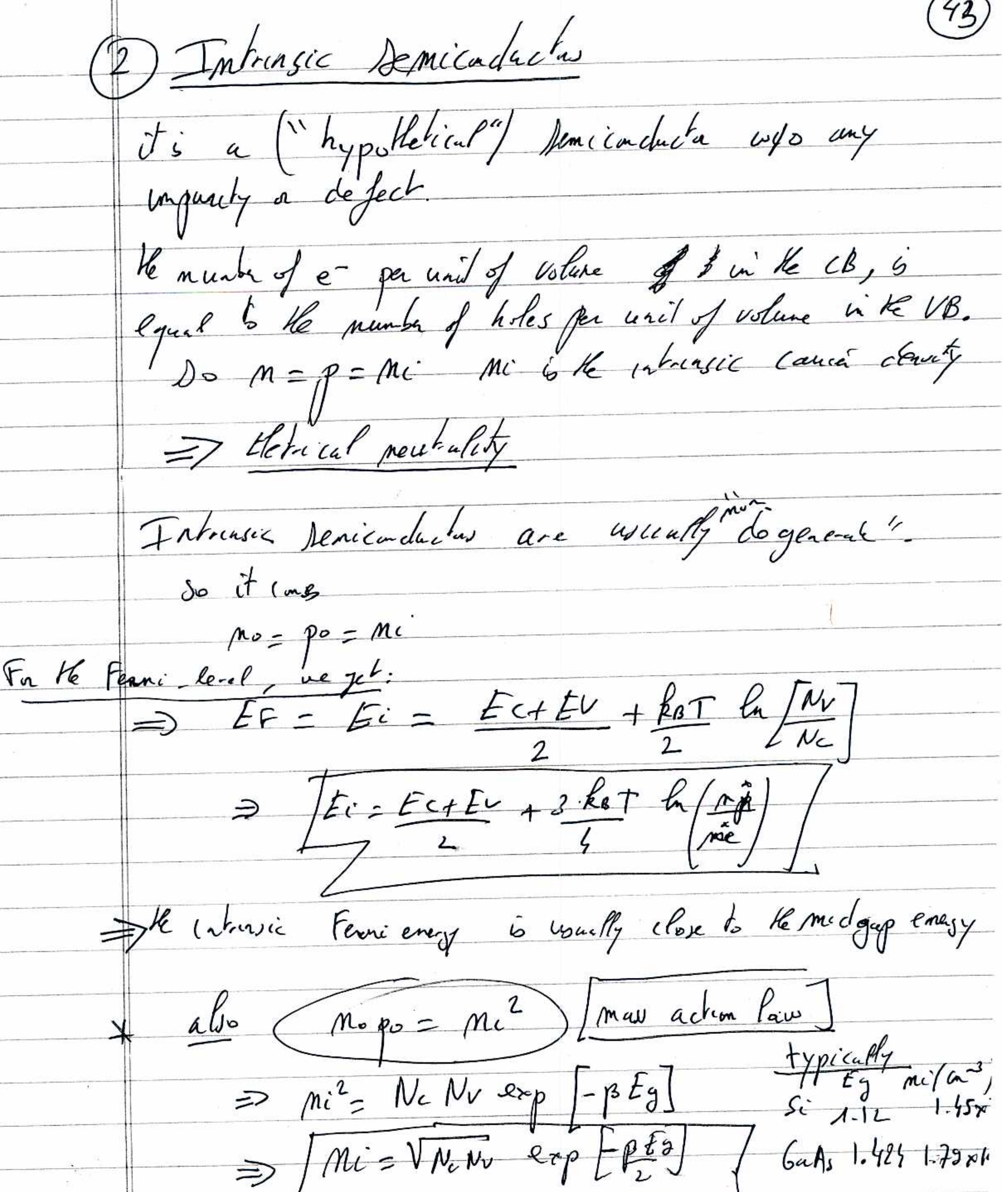
Limiting cases.

(a) $\eta \ll 1 \longrightarrow F_{1/2}(\eta) \simeq e^{\eta}$ [non degenerate]

(b) $\eta \gg 1 \longrightarrow F_{1/2}(\eta) \simeq \frac{4\eta^{3/2}}{3\sqrt{\pi}}.$ [degenerate]

(c) $-4 \ll \eta \ll 4$

$$F_{1/2}(\eta) \simeq \exp\left[-0.32881 + 0.74641\eta - 0.045417\eta^2 - 8.797\times10^{-4}\eta^3 + 1.5117\times10^{-5}\eta^4\right]$$ [cut off]



(2) Intrinsic Semiconductor

it's a ("hypothetical") semiconductor w/o any impurity or defect.

the number of e^- per unit of volume in the CB, is equal to the number of holes per unit of volume in the VB.

So $n = p = n_i$ — n_i is the intrinsic carrier density

⇒ Electrical neutrality

Intrinsic semiconductors are usually "non-degenerate".

so it comes

$$n_0 = p_0 = n_i$$

For the Fermi level, we get:

$$\Rightarrow E_F = E_i = \frac{E_C + E_V}{2} + \frac{k_B T}{2} \ln\left[\frac{N_V}{N_C}\right]$$

$$\Rightarrow \boxed{E_i = \frac{E_C + E_V}{2} + \frac{3 k_B T}{4} \ln\left(\frac{m_h^*}{m_e^*}\right)}$$

⇒ the intrinsic Fermi energy is usually close to the midgap energy

* also $n_0 p_0 = n_i^2$ [mass action law]

$$\Rightarrow n_i^2 = N_c N_v \exp\left[-\beta E_g\right]$$

$$\Rightarrow \boxed{n_i = \sqrt{N_c N_v} \exp\left[-\frac{\beta E_g}{2}\right]}$$

typically

	E_g	n_i (cm^{-3})
Si	1.12	1.45x
GaAs	1.424	1.79x1

The mass action law is valid for non-degenerate semicond and under thermal equilibrium.
It is also valid for extrinsic semiconductors.

(3) Extrinsic semiconductors

Semiconductors that is doped with impurities (foreign atoms incorporated into the crystal).
These impurities:
- can be unintentional, due to the lack of control during the growth of the semiconductor
- can be added on purpose to provide free carriers in the semiconductor.

(a) Donors and acceptors

Donor and acceptor impurities are commonly introduced into semiconductors to increase electron or hole concentrations, which modifies the electrical properties of the material.

example: Si with As donor atoms (5 valence e^-).