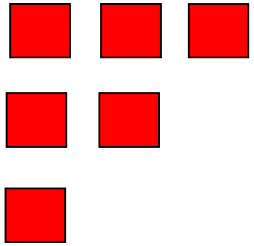
Density of states in the VB and the CB

Density of states in the VB and CB

⇒ number of states of different energies available for carriers

It only depends on the energy

The temperature is responsible for the band filling



Remarks:

- *2 electrons of opposite spin per level at most*
- *at $T = 0$ K, no carriers in the CB*

Density of states

1D: linear chain of N atoms ⇒ N values of k between $-\pi/a$ and $+\pi/a$, separated by $2\pi/Na$

$$k = \frac{2n\pi}{Na}$$

3D: to each k value corresponds a volume in reciprocal space $V_r = (2\pi/Na)^3$, or $V_r = 8\pi^3/V$, with $V=N^3a^3$ the volume of the crystal in real space

Density of states for the electrons in *k*-space:

- density of states in the reciprocal space ⇒ $1/V_r$
- density of states in the reciprocal space per unit volume

  ⇒ $[1/V_r]$ / crystal volume $(V) = (V/8\pi^3)/V = 1/8\pi^3$

The density of states is constant over each *k* interval

However, the density of states over each energy interval increases due to the quadratic relation between E and k

Density of states

Density of states as a function of *E*

$$E = E_0 + \frac{\hbar^2 k^2}{2m^*}$$

Expression valid nearby an energy band extremum only (parabolic band approximation)

$$\Rightarrow k = \sqrt{2m^*\left(E - E_0\right)/\hbar^2}$$

How many states are packed in a sphere of radius *k*?

$N_{3D}(E)$ = V_{sphere} x DOS per unit volume x 2 (spins ±1/2)

= $4/3\ \pi k^3$ x $1/8\pi^3$ x 2

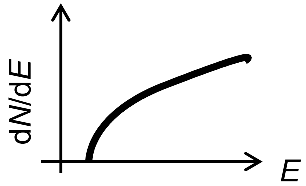
$$= \frac{1}{3\pi^2}\left(\frac{2m^*}{\hbar^2}\left(E - E_0\right)\right)^{3/2}$$

Density of states per energy unit

Density of states per energy unit at energy *E* ⇒ d*N*(*E*)/d*E*

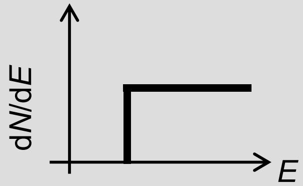
$$N_{3D}(E)=\frac{1}{3\pi^2}\left(\frac{2m^*}{\hbar^2}(E-E_0)\right)^{3/2}$$

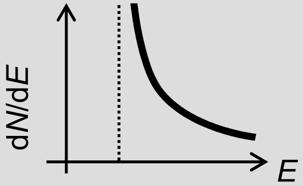
$$\rho_{3D}(E)=\frac{dN_{3D}(E)}{dE}=\frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\sqrt{E-E_0}$$



- **3D density of states (DOS) per energy unit varies as the square root of *E***
- **3D DOS per energy unit varies as the effective mass with the exponent 3/2**

Exercise: calculate the DOS per energy unit for the 2D and 1D cases (series)





Band filling

Electrons and holes obey the Fermi-Dirac distribution (fermions)

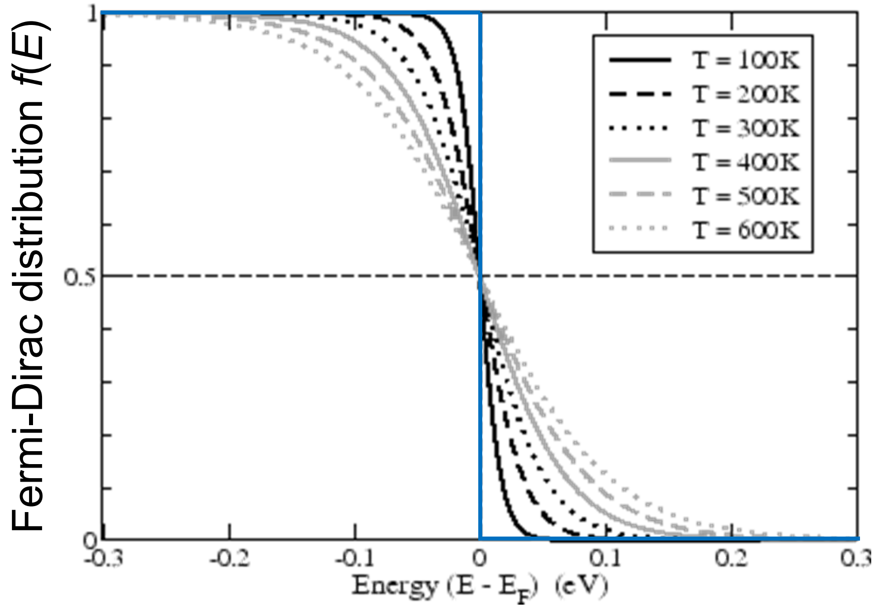
The probability that an energy state E is filled by 1 electron at a temperature T is given by the Fermi-Dirac distribution:

$$f(E) = \frac{1}{1 + e^{(E - E_\mathrm{F})/k_\mathrm{B}T}}$$

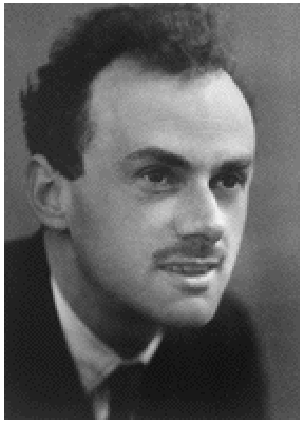
- E_F is the Fermi level ⇒ at $T = 0$ K, this is the highest energy level, which is occupied
- E_F is also the chemical potential
- **E_F corresponds to a certain energy for which $f(E_\mathrm{F}) = ½$ whatever the temperature**

Band filling

Fermi-Dirac distribution



E. Fermi (1901-1954)



P. A. M. Dirac (1902-1984)

Note that $f(E) = 0.5$ when $E = E_F$ whatever T(K)

Named after Fermi and Dirac who derived this distribution independently in 1926!

Illustrative example

At 300 K, for $E - E_F = 0.05$ eV $\Rightarrow f(E) = 0.12$

for $E - E_F = 7.5$ eV $\Rightarrow f(E) = 10^{-129}$

Band filling

In the CB, the density of electrons at an energy E per unit energy is given by the product of the DOS ρ_c(E) by the occupation probability $f_c(E)$

$$n_c(E) = f_c(E)\rho_c(E)$$

In the VB, the density of holes writes similarly considering the occupation probability $f_v(E)$ of an empty state

$$n_v(E) = f_v(E)\rho_v(E) = [1-f_c(E)]\rho_v(E)$$

i.e., $f_c(E)+f_v(E) = 1$

The total concentration of electrons (holes) in the CB (VB) is obtained by integrating the carrier density $n_{c(v)}$ over the bands

$$n_c = \int_{E_c}^{+\infty} \rho_c(E) f_c(E)\,dE$$

$$n_v = \int_{-\infty}^{E_V} \rho_v(E) f_v(E)\,dE = \int_{-\infty}^{E_V} \rho_v(E)[1-f_c(E)]\,dE$$

Band filling

The Fermi level usually lies close to mid-gap for undoped and perfect semiconductors