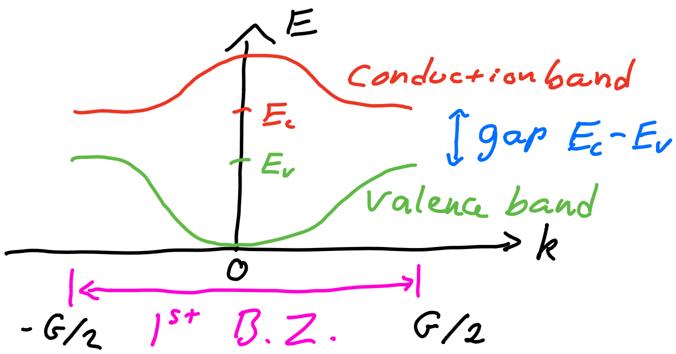
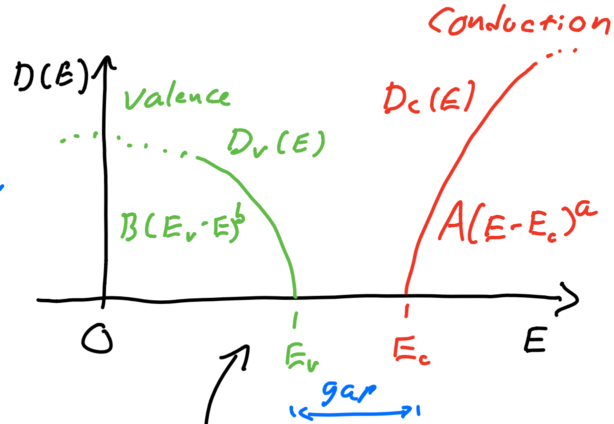
Fermi energy in gap (Semiconductor or insulator)

Model band structure:

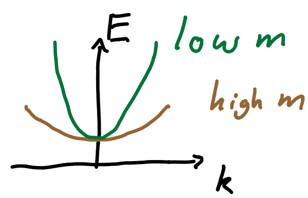




Recall effective mass:

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

curvature ~ 1/mass



Usually in 3D $a = b = \frac{1}{2}$

Also A and $B \sim m^{3/2}$

1. $N = \int_{-\infty}^{\infty} dE\, D(E) f_{T\mu}(E) = \int_{-\infty}^{E_v} dE\, D(E) f_{T\mu}(E) + \int_{E_c}^{\infty} dE\, D(E) f_{T\mu}(E)$ Count all electrons, $T>0$

2. $N = \int_{-\infty}^{E_v} dE\, D(E)$ Count all electrons. $T=0$

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1. - 2. (subtract)

$$0 = \int_{-\infty}^{E_v} dE\, D(E) \underbrace{\left(f_{T\mu}(E) - 1\right)}_{\text{− Occupation of "holes" in Valence band}} + \int_{E_c}^{\infty} dE\, D(E) \underbrace{f_{T\mu}(E)}_{\text{Occupation of electrons in conduction band}}$$

∴ # electrons in conduction band = # holes in valence band

Recall $(x+1)^{-1} = 1 - (\frac{1}{x}+1)^{-1} \Rightarrow f_{T\mu}(E) = 1 - f_{T-\mu}(-E)$

$$\therefore \int_{E_c}^{\infty} dE\, D(E)\left(e^{\beta(E-\mu)}+1\right)^{-1} = \int_{-\infty}^{E_v} dE\, D(E)\left(e^{-\beta(E-\mu)}+1\right)^{-1} \quad ☆$$

Note: $E_v < \mu < E_c$

$(e^{\beta(E-\mu)}+1)^{-1} \ll 1$ $\quad E_c < E$ conduction band

$(e^{-\beta(E-\mu)}+1)^{-1} \ll 1$ $\quad E < E_v$ valence band

} Classical Boltzmann limit

Model DOS $\begin{cases} D_c(E) = A(E-E_c)^a & x \equiv \beta(E-E_c) \quad \text{C.B.} \\ D_v(E) = B(E_v - E)^b & y \equiv \beta(E_v - E) \quad \text{V.B.} \end{cases}$

$$A \Rightarrow A e^{\beta(\mu - E_c)} \beta^{-1-a} \underbrace{\int_0^\infty x^a e^{-x} dx}_{=\,a!} = B e^{\beta(E_v - \mu)} \beta^{-1-b} \underbrace{\int_0^\infty x^b e^{-x} dx}_{=\,b!}$$

Usual case: $a = b = 1/2$ $\quad A e^{\beta(\mu - E_c)} = B e^{\beta(E_v - \mu)} \Rightarrow \mu = \frac{E_v + E_c}{2} + \frac{kT}{2} \ln(B/A)$

mid-gap at $T=0$, shifts towards lower DOS at high T

General case: a, b differ $\quad \mu = \frac{E_v + E_c}{2} + \frac{kT}{2}(b-a)\ln(kT) + \frac{kT}{2}\ln\left(\frac{b!\,B}{a!\,A}\right)$

Electron concentration $\quad$ # electrons in CB = # holes in VB (both conduct!)

$$N_e = \int_{E_c}^\infty dE\, D(E) \left(e^{\beta(E-\mu)}+1\right)^{-1}$$

Set $\mu \approx \frac{E_v + E_c}{2}$, $\quad$ Define $E_g \equiv E_c - E_v$, $\quad$ Note $e^{\beta(E-\mu)} \gg 1$

Let $D(E) = A\sqrt{E - E_c}$, $\quad$ Substitute $x \equiv \beta(E - E_c)$, $\quad$ Note $\int_0^\infty dx \sqrt{x}\, e^{-x} = \frac{\sqrt{\pi}}{2}$

$$\therefore N_e = \frac{\sqrt{\pi}}{2} A (k_B T)^{3/2} e^{-\beta E_g/2}$$

Typical gaps and N_e

$T = 300K \quad k_B T = 0.026$ eV

$\beta = 39/\text{eV}$

	E_g (eV)	$e^{-\beta E_g/2}$
Ge	0.67	2×10^{-6}
Si	1.11	5×10^{-10}
GaAs	1.43	1×10^{-12}
C (diamond)	5.47	$\sim 10^{-46}$

$\ll 1$ electron in sample $\longrightarrow$ C (diamond)