Zustandsdichten

effektive Masse, Beweglichkeit

Seniorenseminar 6. 12. 2024

Density of states for electrons $D_e\left(\varepsilon_e\right)$

definition of states from uncertainty principle $\left(\Delta x\right)^3\left(\Delta p\right)^3 \geq h^3$

volume in momentum space for 1 state $\left(\Delta p\right)^3 = \frac{h^3}{\Delta x^3} = \frac{h^3}{V_{state}}$

number of momentum states with $|p'| \leq |p|$ $N\left(|p|\right) = \frac{4\pi/3\,|p|^3}{h^3/V}$

i.e. in a sphere with radius p

We need $N\left(\varepsilon\right)$, because occupation depends on energy, not on momentum

$\varepsilon_e(p) = \varepsilon_C + \alpha p^2 + \;....$ in analogy with free particles $\varepsilon_e - \varepsilon_C = \alpha p^2 = \frac{p^2}{2m_e^*}$

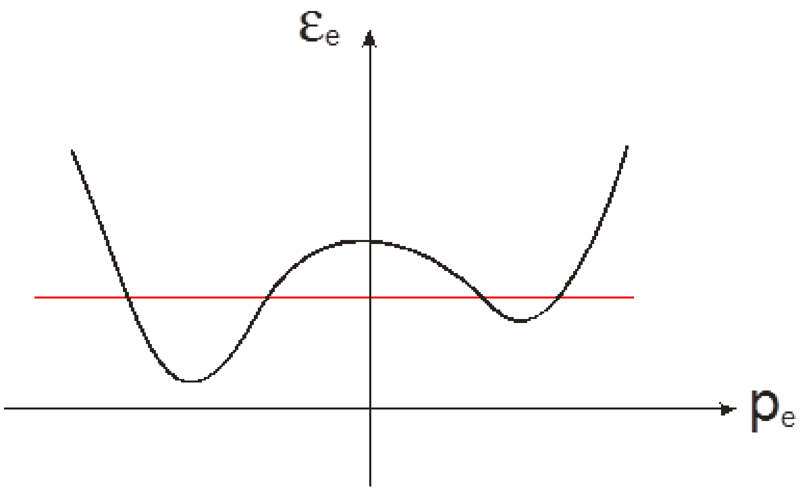
spin

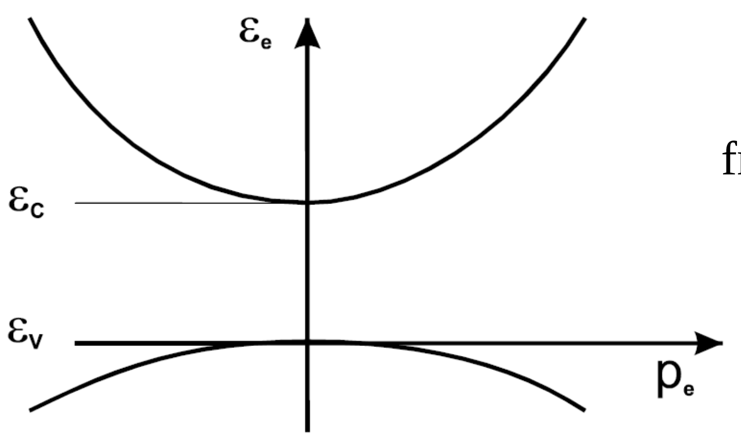
$$N_e(\varepsilon_e) = 2 * \frac{4\pi V\left(2m_e^*\right)^{3/2}}{3h^3}\left(\varepsilon_e - \varepsilon_C\right)^{3/2}$$

$$D_e(\varepsilon_e) = \frac{1}{V}\frac{dN_e(\varepsilon_e)}{d\varepsilon_e} = 4\pi\left(\frac{2m_e^*}{h^2}\right)^{3/2}\left(\varepsilon_e - \varepsilon_C\right)^{1/2}$$

effective mass

can $\varepsilon_e\left(\overrightarrow{p_e}\right)$ be asymmetric?





$$\varepsilon_e - \varepsilon_C = \alpha p_e^2 + \beta p_e^4 \ ......$$

free electrons $\varepsilon = \dfrac{p^2}{2m}$ $\alpha = \dfrac{1}{2m_e^*}$

$$\frac{1}{m_e^*} \approx \frac{d^2\varepsilon_e}{dp_e^2}$$

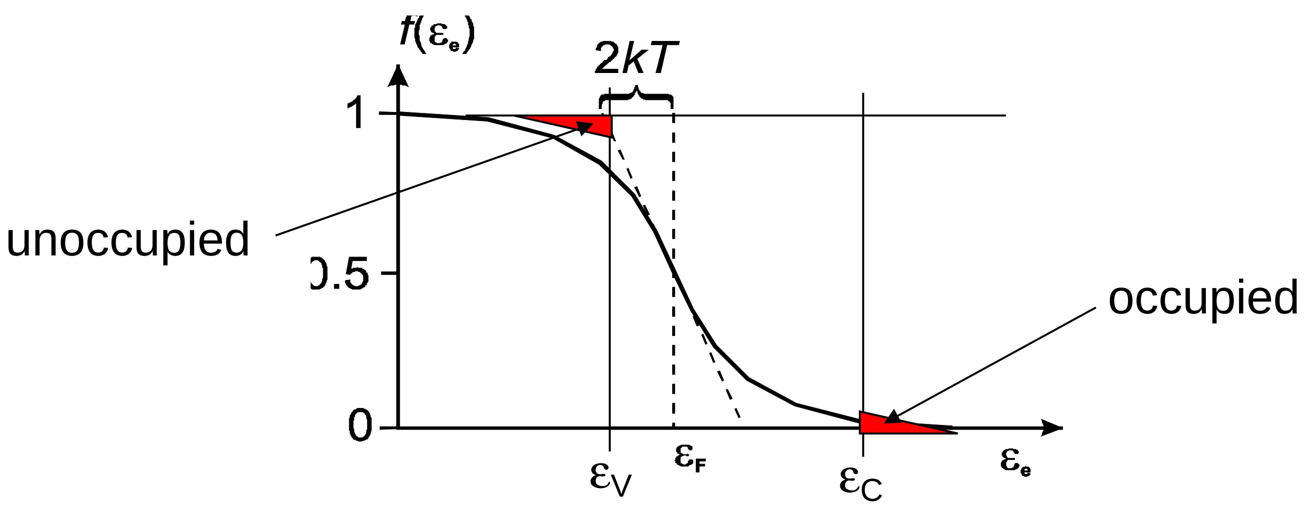
$$\frac{1}{m_e^*} < 0 \quad \text{at} \quad \varepsilon_e \approx \varepsilon_V$$

Energy distribution of electrons n_e

$$dn_e(\varepsilon_e) = D_e(\varepsilon_e)\ f_e(\varepsilon_e)\, d\varepsilon_e$$

density of states $D_e(\varepsilon_e)$ occupation function $f(\varepsilon_e) = \dfrac{1}{\exp\left(\dfrac{\varepsilon_e - \varepsilon_F}{kT}\right) + 1}$

principle: minimum of Free Energy $F = E - TS$



condition: temperature T and volume V must be fixed

Properties of holes

holes = missing electrons in the valence band

$$q_h = +e$$

$$m_h^*\left(\varepsilon_e\right) = -m_e^*\left(\varepsilon_e\right)$$

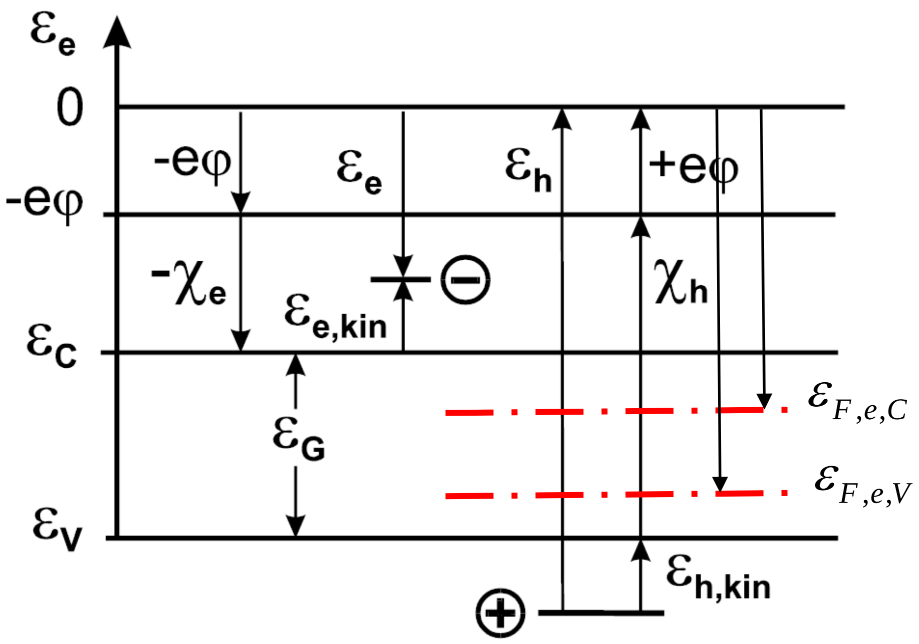
$$\varepsilon_h = -\varepsilon_e$$

$$\varepsilon_{F,h} = -\varepsilon_{F,e}$$

$$f_h = 1 - f_e$$

$$f_h = 1 - \frac{1}{\exp\frac{\varepsilon_e - \varepsilon_{F,e}}{kT} + 1} = \frac{\exp\frac{\varepsilon_e - \varepsilon_{F,e}}{kT}}{\exp\frac{\varepsilon_e - \varepsilon_{F,e}}{kT} + 1}$$

$$f_h = \frac{1}{1 + \exp\left(-\frac{\varepsilon_e - \varepsilon_{F,e}}{kT}\right)} = \frac{1}{\exp\frac{\varepsilon_h - \varepsilon_{F,h}}{kT} + 1}$$



Electron and hole concentrations in the dark

$$f(\varepsilon) \approx \exp\left(-\frac{\varepsilon - \varepsilon_F}{kT}\right) \quad \text{for} \quad \varepsilon - \varepsilon_F \gg kT$$

electrons

$$n_e = \int_{\varepsilon_C}^{\infty} D(\varepsilon) f(\varepsilon) d\varepsilon = N_C \exp\left(-\frac{\varepsilon_C - \varepsilon_F}{kT}\right) \; ; \quad N_C = 2\left(\frac{2\pi m_e^* kT}{h^2}\right)^{3/2}$$

effective density of states

for $m_e^* = m_e$ and $T = 300\text{K}$: $N_C = 2\times 10^{19}\,/\,\text{cm}^3$

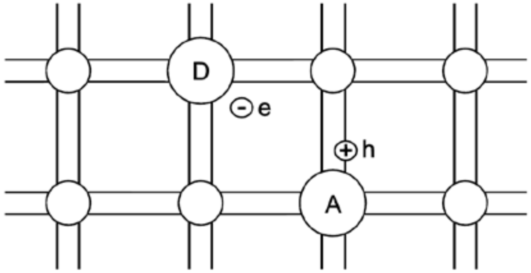
holes

$$n_h = \int_{-\infty}^{\varepsilon_V} D(\varepsilon)\left[1 - f(\varepsilon)\right] d\varepsilon = N_V \exp\left(-\frac{\varepsilon_F - \varepsilon_V}{kT}\right) \quad N_V = 2\left(\frac{2\pi m_h^* kT}{h^2}\right)^{3/2}$$

$$n_e n_h = N_C N_V \exp\left(-\frac{\varepsilon_G}{kT}\right) = n_i^2$$

independent of ε_F
independent of doping

Doping



n – type, donors	p – type, acceptors
1 or more valence electrons more than host	1 or more valence electrons less than host
e.g. P, As in Si Si on Ga site in GaAs	e.g. In, B in Si Si on As site in GaAs

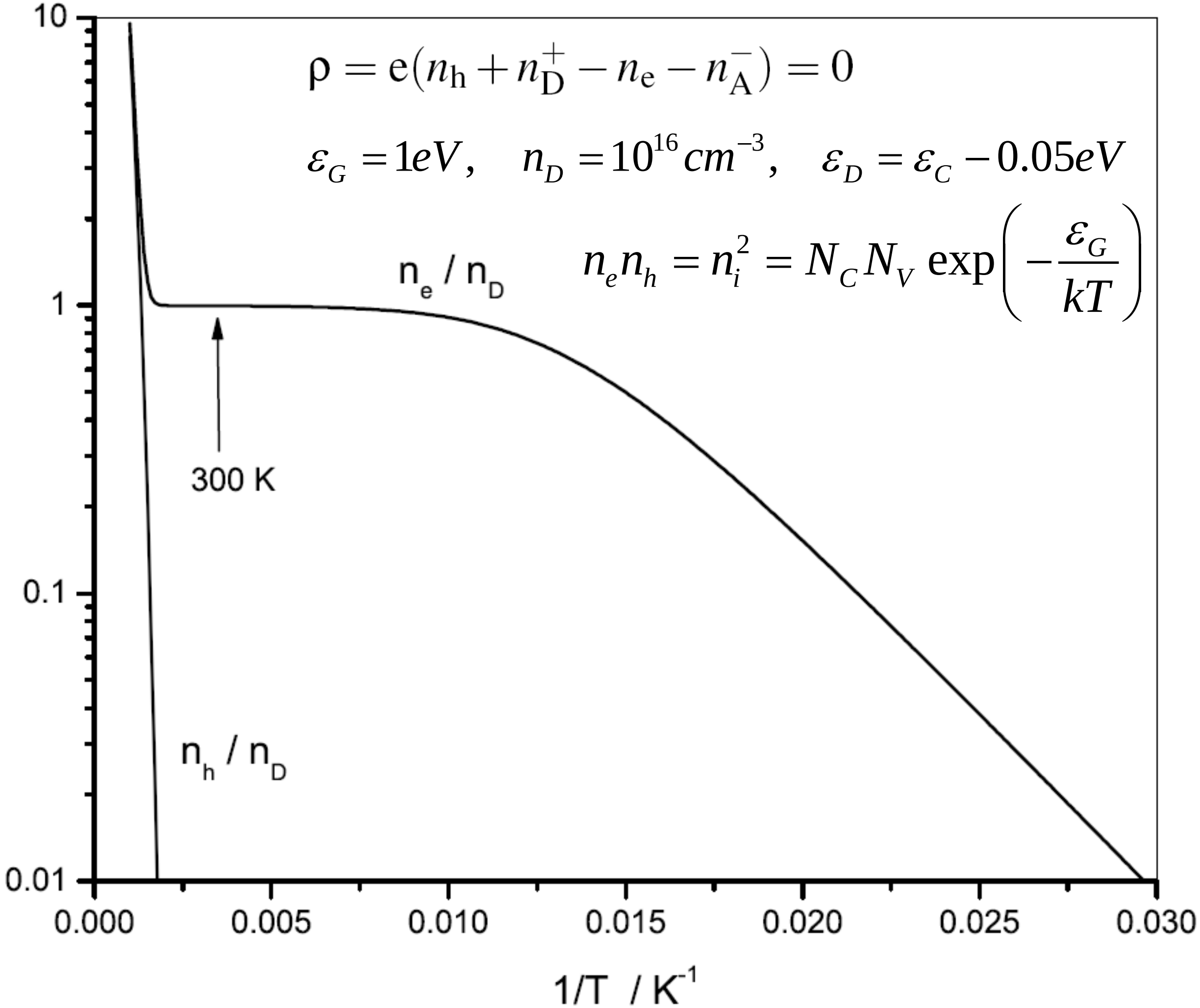
binding energy of electron to donor (hole to acceptor) from hydrogen model

$$\varepsilon_H = \frac{m_e e^4}{2\left(4\pi\varepsilon_0\right)^2 \hbar^2} = 13.6\, eV$$

$$\varepsilon_C - \varepsilon_{e,D} = \varepsilon_H \frac{m_e^*}{m_e \varepsilon^2}$$

order of kT at 300K

Electrons in n-type semiconductor



$$n_h = N_V \exp\left(\frac{\varepsilon_V - \varepsilon_F}{kT}\right)$$

$$n_D^+ = n_D\left[1 - \frac{1}{\exp\left(\frac{\varepsilon_D - \varepsilon_F}{kT}\right) + 1}\right]$$

$$n_e = N_C \exp\left(-\frac{\varepsilon_C - \varepsilon_F}{kT}\right)$$

$$n_A^- = n_A\left[\frac{1}{\exp\left(\frac{\varepsilon_A - \varepsilon_F}{kT}\right) + 1}\right]$$

Transport properties, drift current
caused by electric field E

acceleration $a_i = \frac{z_i e E}{m_i^*}$

$$\langle v_i \rangle = \int_0^\infty a_i \exp(-t/\tau_{c,i})\,\mathrm{d}t = a_i \tau_{c,i}$$

$$\langle v_i \rangle = z_i \frac{\mathrm{e}}{m_i^*} \tau_{c,i} E \;.$$

mobility $b_i = \frac{e\,\tau_{C,i}}{m_i^*}$

drift current

$$j_{Q,f,i} = z_i^2 \mathrm{e} n_i b_i E = \sigma_i E$$

$$j_{Q,f,i} = -\frac{\sigma_i}{z_i \mathrm{e}} \operatorname{grad}(z_i \mathrm{e} \varphi)$$

Diffusion current (looking for a driving force)

diffusion current

$$j_{Q,d,i} = z_i \mathrm{e}(-D_i \,\mathrm{grad}\, n_i)$$

Fick's law of diffusion

$$j_{Q,d,i} = -z_i e n_i D_i \frac{\mathrm{grad}\, n_i}{n_i} = -z_i e n_i D_i \mathrm{grad}\left\{\ln\left(n_i\right)\right\}$$

$$\mu_i = \mu_{i,0} + kT \ln\left(\frac{n_i}{N_i}\right)$$

chemical potential of particles i
= free energy of particles i, if uncharged

Einstein relation $\frac{b_i}{D_i} = \frac{\mathrm{e}}{kT}$

$$j_{Q,d,i} = -\frac{z_i \mathrm{e} n_i b_i}{\mathrm{e}} \,\mathrm{grad}\, \mu_i = -\frac{\sigma_i}{z_i \mathrm{e}} \,\mathrm{grad}\, \mu_i$$

total charge current

$$j_{Q,i} = -\frac{\sigma_i}{z_i e}\{\operatorname{grad}\mu_i + \operatorname{grad}(z_i e\varphi)\}$$

$$j_{Q,i} = -\frac{\sigma_i}{z_i e}\operatorname{grad}(\mu_i + z_i e\varphi) = -\frac{\sigma_i}{z_i e}\operatorname{grad}\eta_i$$

electrochemical potential

$$\eta_i = \mu_i + z_i e\varphi$$

free energy of particles with charge $z_i e$

for electrons (z_i = -1) and holes (z_i = 1)

$$j_Q = \frac{\sigma_e}{e}\operatorname{grad}\eta_e - \frac{\sigma_h}{e}\operatorname{grad}\eta_h$$

$$\eta_e = \mu_e - e\varphi = \varepsilon_{FC}$$

$$\eta_h = \mu_h + e\varphi = -\varepsilon_{FV}$$

$$j_Q = \frac{\sigma_e}{e}\operatorname{grad}\varepsilon_{FC} + \frac{\sigma_h}{e}\operatorname{grad}\varepsilon_{FV}$$

electron current + hole current

Energies of electron-hole pairs

energy

$$\varepsilon_e + \varepsilon_h = \varepsilon_C + 3/2kT \quad + \left(-\varepsilon_V\right) + 3/2kT = \varepsilon_G + 3kT$$

Free Energy: electrochemical energy, electrical energy + chemical energy

$$\eta_e + \eta_h = \mu_e - e\varphi \quad + \mu_h + e\varphi = \mu_e + \mu_h$$

in the dark

$$\varepsilon_{FC} = \varepsilon_{FV} = \varepsilon_F$$

$$\eta_e + \eta_h = \varepsilon_{FC} - \varepsilon_{FV} = \mu_e - e\varphi \quad + \mu_h + e\varphi = \mu_e + \mu_h = 0$$

under illumination

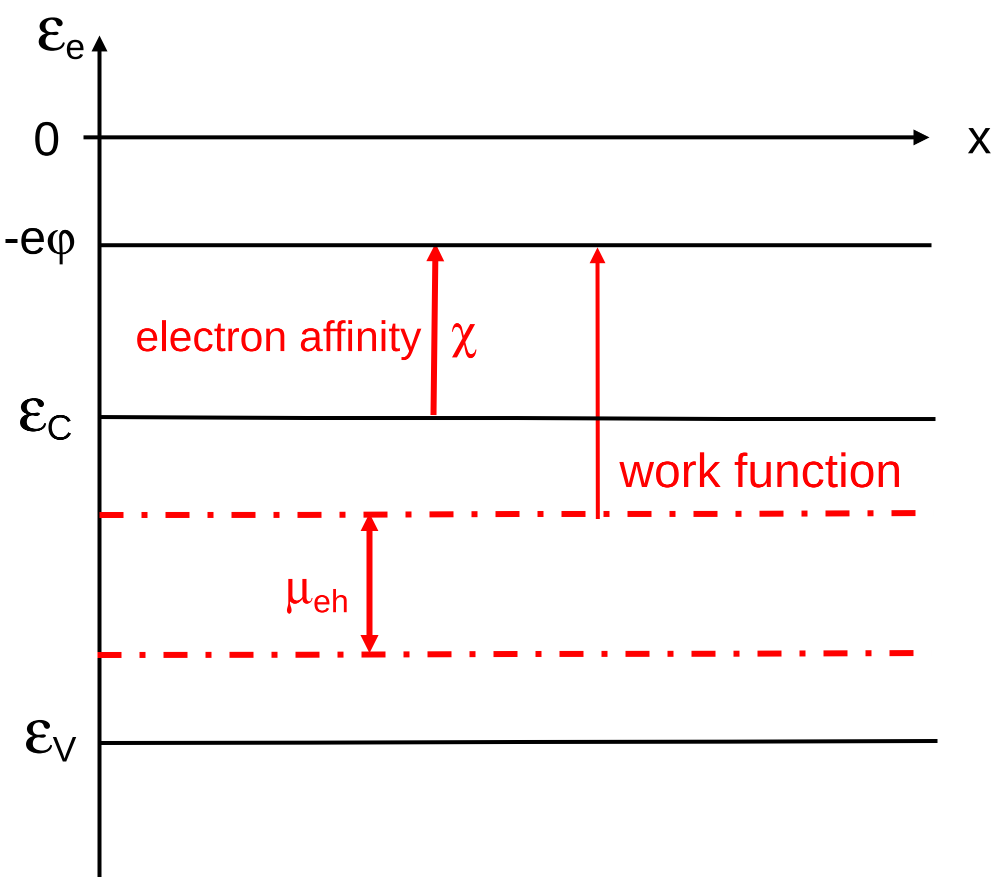
$$\mu_e + \mu_h = \varepsilon_{FC} - \varepsilon_{FV} > 0$$

Free energy of electron-hole pair at one location is chemical energy

Energy scale for electrons

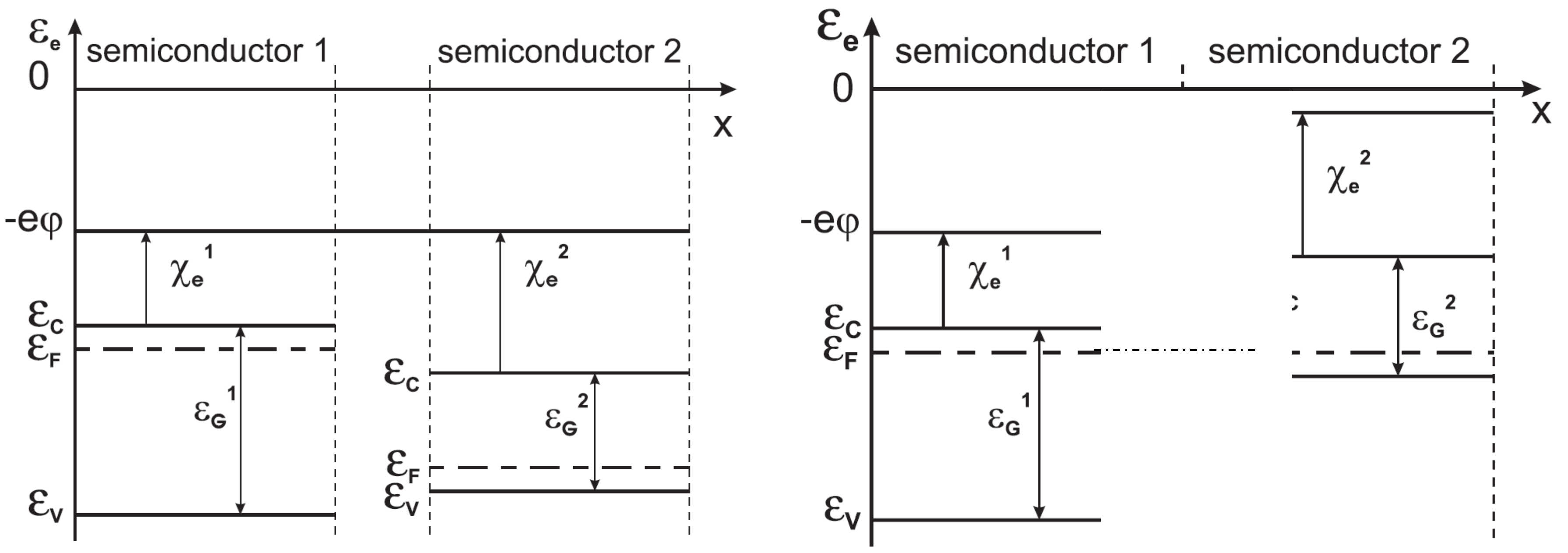
$\varepsilon_e = 0$ for a free electron

1. in vacuum
2. in el. potential $\varphi = 0$
3. with $\varepsilon_{e,kin} = 0$



energy scale for holes ?

Contact between different materials



Density of states for photons $D_\gamma(\hbar\omega)$

energy distribution of states from uncertainty principle $(\Delta x)^3(\Delta p)^3 \geq h^3$

volume in momentum space for 1 state $(\Delta p)^3 = \dfrac{h^3}{V}$

number of momentum states with $|p'| \leq |p|$
i.e. in a sphere with radius $|p|$

$$N(|p|) = \frac{4\pi/3\,|p|^3}{h^3/V}$$

$$\varepsilon_\gamma(p) = \hbar\omega = c|p|$$

2 polarisation directions

$$N_\gamma(\hbar\omega) = 2 \times \frac{4\pi V}{3h^3c^3}(\hbar\omega)^3$$

$$D_\gamma(\hbar\omega) = \frac{1}{V}\frac{dN_\gamma(\hbar\omega)}{d\hbar\omega} = \frac{8\pi}{h^3c^3}(\hbar\omega)^2$$

in solid angle Ω : $D_{\gamma,\Omega}(\hbar\omega) = \dfrac{2\,\Omega}{h^3c^3}(\hbar\omega)^2 = \dfrac{\Omega}{4\pi^3\hbar^3c^3}(\hbar\omega)^2$

in matter: $c = c_0 / n$

Planck`s law

photon current density per solid angle

$$dj_{\gamma,\Omega}\left(\hbar\omega\right) = cD_{\gamma,\Omega}\left(\hbar\omega\right) f_{\gamma}\left(\hbar\omega\right) d\hbar\omega$$

$$D_{\gamma,\Omega}(\hbar\omega) = \frac{2}{h^3c^3}\left(\hbar\omega\right)^2 = \frac{\left(\hbar\omega\right)^2}{4\pi^3\hbar^3c^3}$$

$$f_{\gamma}\left(\hbar\omega\right) = \frac{1}{\exp\left(\frac{\hbar\omega}{kT}\right)-1}$$