PH 673
Nano

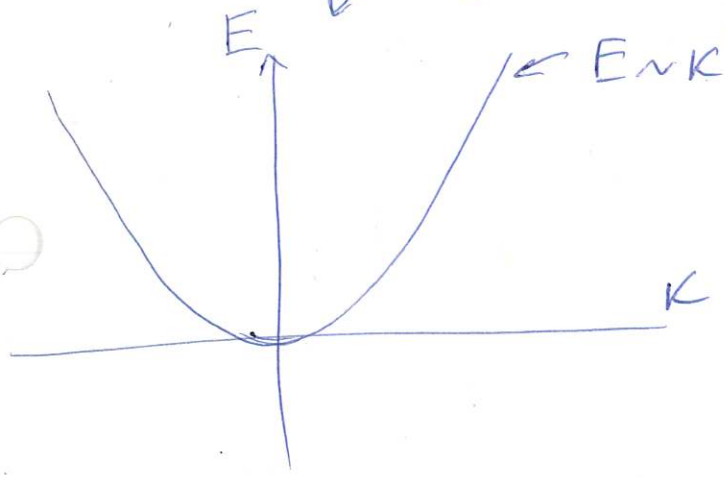
Lecture # 1

Review of Semiconductor Physics

Recall: free electrons ⇒

wave function → $\psi(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$

energy → $E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$



crystalline solid ⇒ periodic potential

$V(\vec{r}) = V(\vec{r} + \vec{R}_n)$

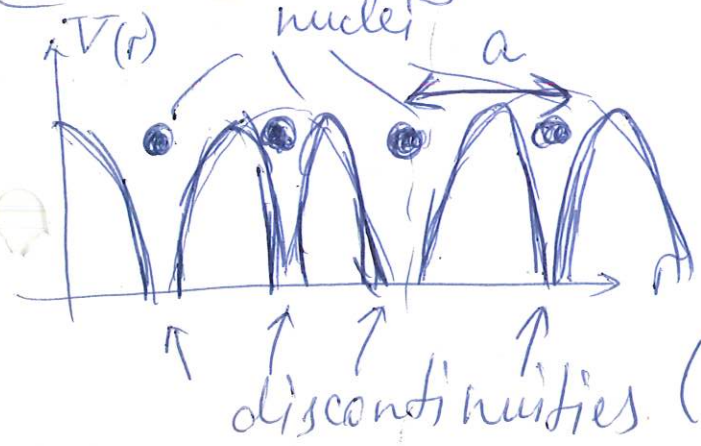
$\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{r})\right]\psi(\vec{r}) = E\psi(\vec{r})$

$\vec{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ (unit lattice vectors)

⇒ Block's theorem

$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})$

$u_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r} + \vec{R}_n)$



↑ Block's functions

In order for $\psi_{\vec{k}}(\vec{r}) = \psi_{\vec{k}}(\vec{r}+\vec{R}_n) \Rightarrow$

$$e^{i\vec{k}\cdot\vec{r}} = e^{i\vec{k}(\vec{r}+\vec{R}_n)} \Rightarrow e^{i\vec{k}\cdot\vec{R}_n} = 1 \Rightarrow$$

$$\vec{k}\cdot\vec{R}_n = 2\pi n \Rightarrow$$

$$k_i = \frac{2\pi}{a_i} n_i \quad \leftarrow \text{integers}$$

$\uparrow$ lattice constant

In 1D: expand periodic function into Fourier series

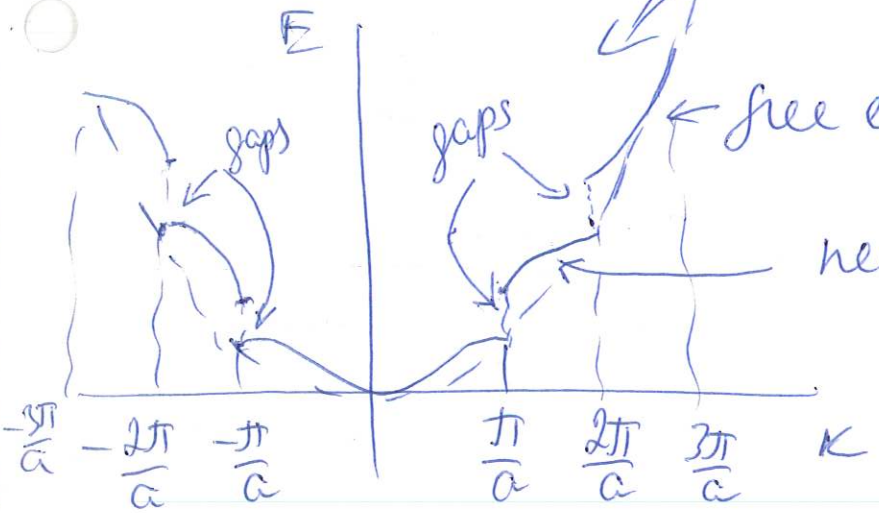
$$V(x) = \sum_{n=-\infty}^{\infty} V_n e^{i\frac{2\pi}{a}nx}$$

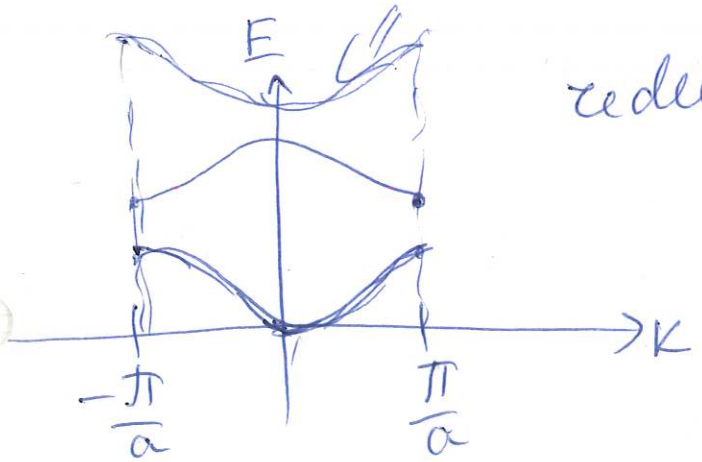
$\uparrow$ consider small compared to $\frac{\hbar^2 k^2}{2m}$

$\Downarrow$ solve Schrödinger's equation

$\Downarrow$

discontinuity in $V \Rightarrow$ discontinuities in energy (energy gaps)





reduced zone representation

Consider equation of motion of the electron:

$$-e\vec{\mathcal{E}} = \hbar\frac{d\vec{k}}{dt}$$

$\vec{\mathcal{E}}$: electric field

⇓ present as a wave packet ⇓

$$\psi(\vec{r},t) \sim \int_{\vec{k}-\frac{\Delta\vec{k}}{2}}^{\vec{k}+\frac{\Delta\vec{k}}{2}} C(\vec{k})\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}\, d\vec{k}$$

⇓ wave packets propagate with group velocity

$$\vec{v}_g = \frac{\partial\omega}{\partial\vec{k}} = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E(\vec{k})$$

In 1D: $v_g = \frac{1}{\hbar}\frac{dE}{dk}$

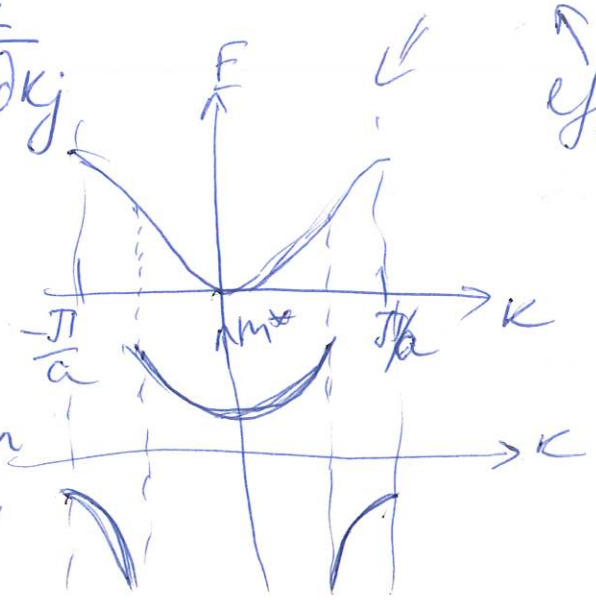
$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\frac{dE}{dk} = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt} = -e\mathcal{E}\,\frac{1}{\hbar^2}\frac{d^2E}{dk^2}$$

$\frac{dk}{dt}$ ← from the equation of motion $= -\frac{e\mathcal{E}}{\hbar}$

$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*}$ ← effective mass

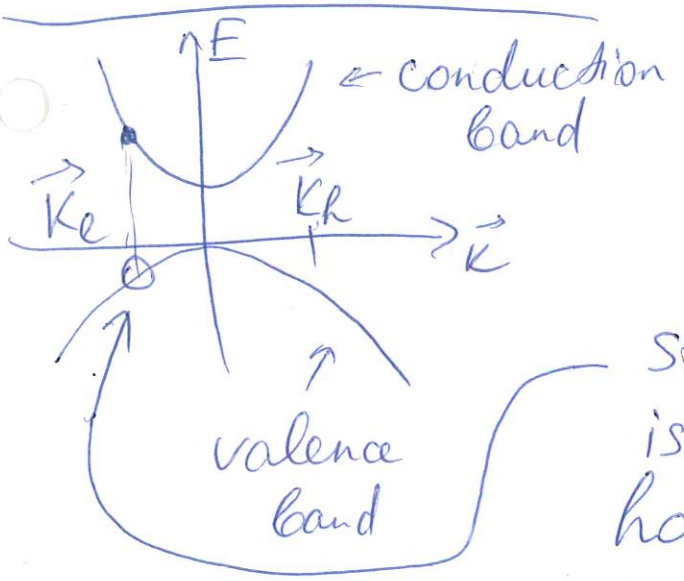
In 3D: $\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$

$\left(\frac{1}{m^*}\right)$: 2nd rank tensor



Note a negative m^* at near $\pm\pi/a$: the electron transfers more momentum than (to the lattice) gains from the applied $\mathcal{E}$-field

Holes & electrons



$$\vec{K}_{total} = \sum_i \vec{K}_i - \vec{K}_e = -\vec{K}_e = \vec{K}_h$$

($=0$ for completely filled band)

state of the missing electron is assigned to a new particle, hole, with $\vec{K}_h = -\vec{K}_e$

and $E_h = \frac{\hbar^2 K^2}{2m_h^*}$

Most technologically important semiconductors

⇓

cubic symmetry

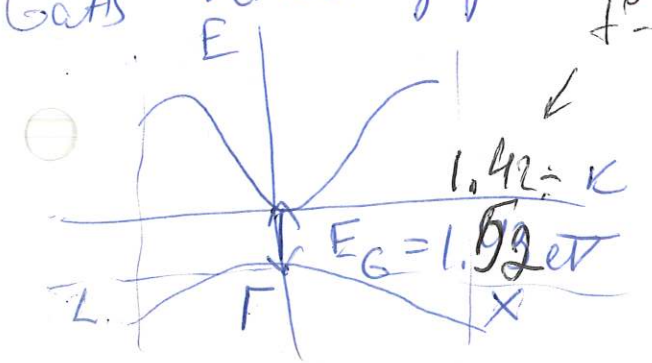
⇓

max of the valence band is at $\vec{K}=0$

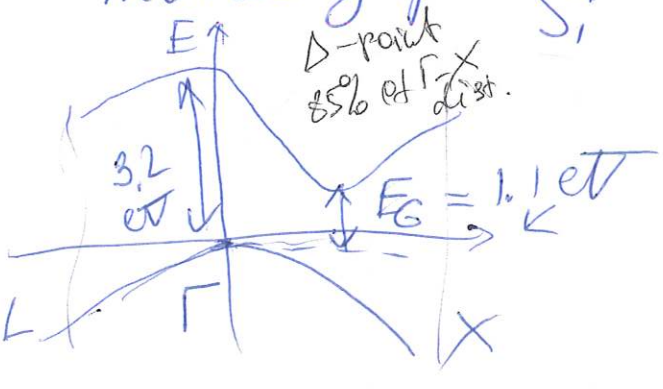
However, min of the conduction band is either at $\vec{K}=0$ (as in GaAs) or not (as in Si, Ge, ...)

⇓ ⇓

GaAs direct gap



indirect gap Si



GaAs:

$E_{\Gamma} = \frac{\hbar^2 k^2}{2m_e^*}$

$m_e^* = 0.066\, m_0$

Si:

$E = \frac{\hbar^2}{2}\left(\frac{k_l^2}{m_l^*} + \frac{k_t^2}{m_t^*}\right)$

Δ (X) (along min. of cond. band)

longitudinal & transverse masses

$\parallel X$ ↓ $m_l^* = 0.98\, m_0$, $m_t^* = 0.19\, m_0$ ← $\perp X$

(electrons)

Points: $\Gamma \Rightarrow k_x = k_y = k_z = 0$

$X \Rightarrow k_i = \pm \frac{2\pi}{a}$, $k_j = k_k = 0$ → Δ: $k_x = \frac{\pi}{a} b$, $k_y = 0$, $k_z = 0$ $(b < a)$

$L \Rightarrow k_x = k_y = k_z = \pm \frac{\pi}{a}$ Λ: $k_{x,y,z} = \frac{\pi}{a} b$ $(b < a)$

$E_G \sim 0.2 - 3\ eV$; if $> 4\ eV \Rightarrow$ insulator

↑ bandgap

if $2 - 3\ eV \Rightarrow$ wide bandgap semiconductor

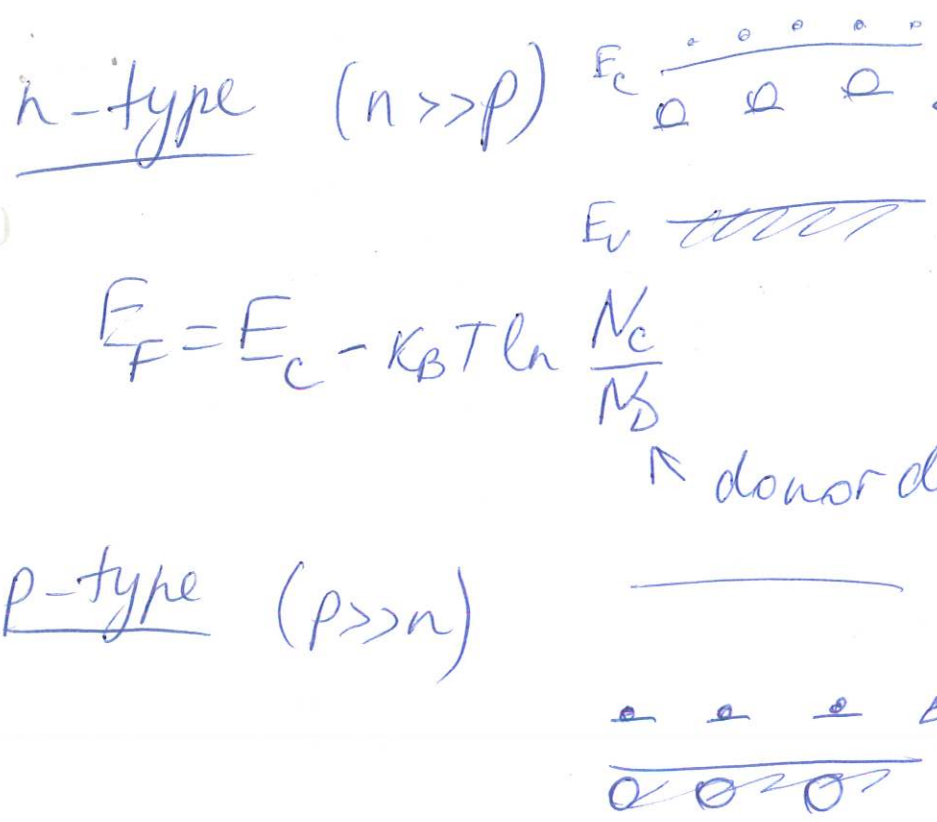
Intrinsic semiconductor: $n = p = \sqrt{N_c N_v}\, e^{-\frac{E_G}{2k_BT}}$

n ↑ electron density, p ↑ hole density; N_c, N_v — DOS in the conduction (c) or valence (v) band

$E_F = \frac{E_G}{2} + \frac{3}{4} k_B T \ln \frac{m_h^*}{m_e^*}$

↑ Fermi energy ← uppermost occupied energy level in a solid

$N_{c,v} = 2\left(\frac{m_{e,h}^* k_B T}{2\pi \hbar^2}\right)^{3/2}$



$$E_F = E_c - k_B T \ln \frac{N_c}{N_D}$$

N_D ← donor density

(n-type Si:
$N_D \sim 10^{17}\ cm^{-3}$
$N_c \sim 2.8 \cdot 10^{19}\ cm^{-3}$
$k_B T \ln \frac{N_c}{N_D} \sim 3.6 k_B T$
90 meV @ RT)

$$E_F = E_v + k_B T \ln \frac{N_v}{N_A}$$

N_A ← acceptor density

Carrier transport

$n \sim 10^{14 \div 17}\ cm^{-3}$ ($\ll 10^{22}\ cm^{-3}$ in metals)

↑ carrier concentration

$$\mu_{e,h} = \frac{q\,\tau_{e,h}}{m^*_{e,h}}$$

Charge ← q; $\tau_{e,h}$ ← relaxation time; $m^*_{e,h}$ ← effective mass

↑ mobility $= \frac{v_{e,h}}{\mathcal{E}}$ ← drift velocity

↑ $\left[\frac{cm^2}{Vs}\right]$

int. Si:
$\mu_e \sim 1400 \frac{cm^2}{Vs}$
$\mu_h \sim 450 \frac{cm^2}{Vs}$
GaAs: $\mu_e \sim 8500 \frac{cm^2}{Vs}$, $\mu_h \sim 400 \frac{cm^2}{Vs}$

$v_e = v_e(t=0)\, e^{-t/\tau_e}$

↑ relaxation upon disconnecting $\mathcal{E}$-field

$\sigma = q(n\mu_e + p\mu_h)$; $J = \sigma \mathcal{E}$

↑ electrical conductivity

J ↑ (e+h) current density (drift)

diffusion currents (in 1D): $J_e = q D_e \frac{dn}{dx}$; $J_h = -q D_h \frac{dp}{dx}$

↑ diffusion coeff.

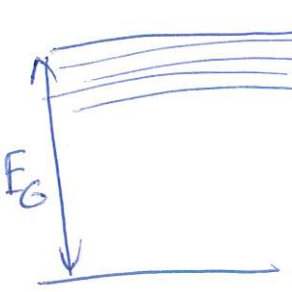
Einstein relations:

$$\frac{D_e}{\mu_e} = \frac{k_B T}{q} = \frac{D_h}{\mu_h} = 0{,}026\ V$$

at room temperature

Optical properties

optical absorption ⇒ $I_0 \rightarrow$ [ ] $\rightarrow I(z) = I_0 e^{-\alpha z}$ (z →)



$$\alpha(h\nu) = \frac{1}{2\pi^2}\left(\frac{2\mu}{\hbar^2}\right)^{3/2}(h\nu - E_G)^{1/2}$$

↑ abs. coeff.

$\mu = \frac{m_e^* m_h^*}{m_e^* + m_h^*}$ ↑ reduced mass

(13,6eV) ← Rydberg const for (H)-atom

$$E_n = -\frac{\mu R_H}{m_e \mathcal{E}^2}\frac{1}{n^2} = -\frac{R_{ex}}{n^2}$$

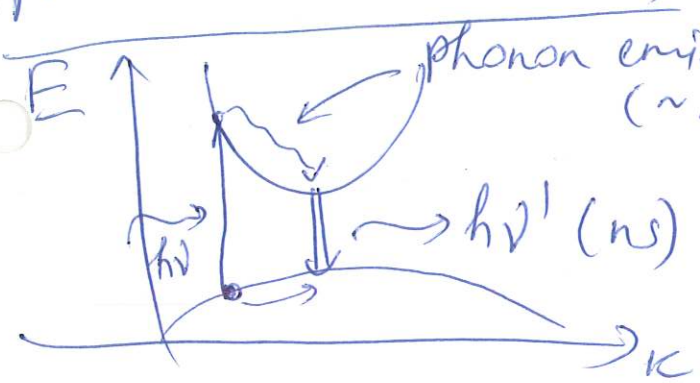
↑ diel. const. ← exciton Rydberg const

GaAs: $R_{ex} = 4{,}2\ meV$ ← can resolve at low T

$\varepsilon_{Si} \approx 11{,}7$ @ RT

$\varepsilon_{GaAs} \sim 13$

photoluminescence (PL)



PL yields $\sim 0.1 - 10^{-3}$
(the rest of excitation goes into non-radiative recombination)

Density of states

Recall: Fermi energy $E_F = \frac{\hbar^2 K_F^2}{2m_e}$ $V_{tot} = \frac{4}{3}\pi K^3$ $V_K = \frac{(2\pi)^3}{V}$

3D space: volume of $\vec{K}$-space per state:

$K_i = \frac{2\pi}{a_i}$ (p. 2)

$\frac{(2\pi)^3}{V}$ ← $a_1 a_2 a_3 = V$ (volume; lattice const)

Volume of $\vec{K}$-space filled by N electrons $= \frac{N}{2} \cdot \frac{(2\pi)^3}{V} = \frac{4N\pi^3}{V}$

2 electrons of opposite spins can occupy each state

$\frac{4N\pi^3}{V} = \frac{4\pi}{3} K_F^3 \Rightarrow K_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = (3\pi^2 n_e)^{1/3}$

n_e: electron density

$$E_F = \frac{\hbar^2}{2m_e}(3\pi^2 n_e)^{2/3}$$

Density of states $\Rightarrow N_{3D}(E) \Rightarrow$

$$N_s = \int N_{3D}(E)\,dE = \frac{1}{V}\cdot 2 \cdot \frac{1}{\frac{(2\pi)^3}{V}} \int 4\pi k^2\,dk =$$

N_s: total # of states per unit volume in energy band

2: 2 spin states per $\vec{k}$

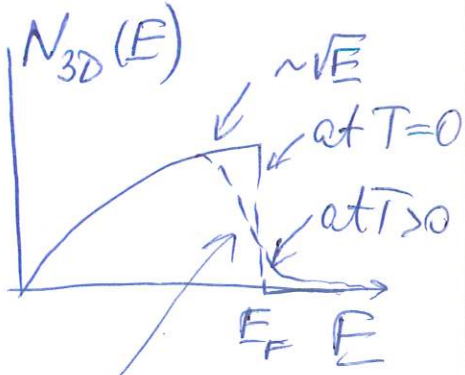
$\frac{(2\pi)^3}{V}$: volume of $\vec{k}$-space per state

$$= \frac{1}{4\pi^3}\int 4\pi k^2 \underbrace{\frac{dk}{dE}}\,dE = \frac{1}{\pi^2}\frac{m_e^*}{\hbar^2}\int k\,dE \Rightarrow$$

$$E = \frac{\hbar^2 k^2}{2m_e^*} \Rightarrow \frac{dE}{dk} = \frac{\hbar^2 k}{m_e^*}$$

$k = \sqrt{\frac{2m_e^* E}{\hbar^2}}$

$$N_{3D}(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{3/2}\sqrt{E} \Rightarrow$$



$$N_{electrons} = \int N_{3D}(E)\,f(E)\,dE$$

Fermi-Dirac function $\rightarrow f(E) = \frac{1}{e^{\frac{E-E_F}{k_B T}}+1}$

$$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{\hbar k}{m_e^*} = \frac{\hbar}{m_e^*}\frac{\pi^2\hbar^2}{m_e^*}N_{3D}(E) = \frac{\pi^2\hbar^3}{m_e^{*2}}N_{3D}(E)$$

Characteristic lengths

(i) de Broglie wavelength $\lambda_B = \frac{h}{m_e^* v}$

easier to observe quantum effects for smaller m^* in nanostructures of a given size ⇐

↑ $0.067 m_e$ in GaAs
$0.014 m_e$ in InSb

(ii) mean free path $l_e = v \tau_e$ ← relaxation time

↑ distance between two inelastic collisions

(iii) diffusion length $L_e = \sqrt{D \tau_e}$

↑ diffusion coeff.

if $l_e \gg L_e \Rightarrow$ ballistic transport

$l_e \ll L_e \Rightarrow$ diffusion

(iv) screening length $\lambda_s = \sqrt{\frac{\varepsilon K_B T}{e^2 n}}$

↑ (Debye) of free carriers by charges of opposite polarity

↑ ~10–100nm in semiconductors; smaller in metals

↖ mean background carrier concentration

large λ_s ← bad for devices = poor electrostatic screening (E-fields penetrate)

(v) localization length $\psi \sim e^{-r/\lambda_{loc}}$

↑ electron wave function

important ⇐ for quantum Hall effect, Anderson localization ⇒ metal-insulator transition