CONFINED CARRIERS – SCATTERING RATES CALCULATION

There are numerous examples of quantum confinement. The most commonly observed ones are:

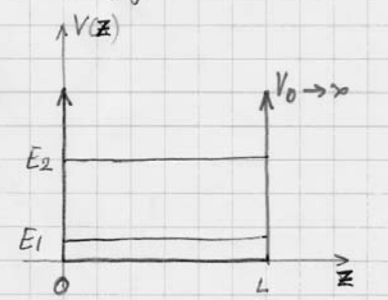
- quantum wells (in modulation-doped heterostructures)
- triangular wells (in MOS capacitors and MOSFETS)

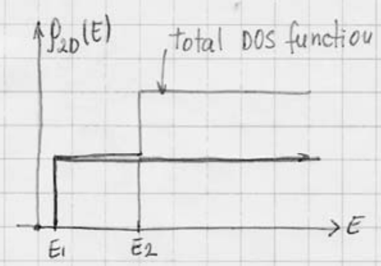
In the rest of this section, an overview of quantum confinement is given first, which is then followed by a description of scattering rates calculation in such systems.

(1.) Review of quantum confinement

(A) Quantum wells

For simplicity, we will only consider now infinite quantum well shown in the figure below.





- The stationary solutions to the TISE in the one-electron approximation are of the form:

$$\varphi_n(z) = \sqrt{\frac{2}{L}}\,\sin(k_n z)\,, \text{ where } k_n = \frac{n\pi}{L}$$

- The carriers are free to move in the xy-plane and for that direction the 2D DOS function is given by:

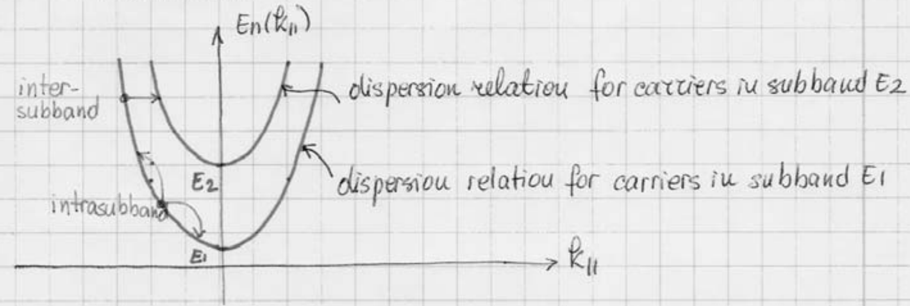
$$\rho_{2D}(E) = \frac{m^*}{\pi\hbar^2}\,\theta(E-E_i)$$

where E_i is the energy level due to the quantization of k_z along the confining direction

- The quantization along the z-direction modifies the carrier dispersion relation

$$E_n(k_{\parallel}) = \frac{\hbar^2 k_{\parallel}^2}{2m^*} + \frac{\hbar^2 k_n^2}{2m^*} = \underbrace{\frac{\hbar^2 k_{\parallel}^2}{2m^*}}_{\text{Kinetic}} + \underbrace{E_n}_{\text{potential energy}}$$

$k_{\parallel} \rightarrow$ crystal momentum in the xy-plane
$E_n \rightarrow$ subband energy due to the space quantization along the z-direction



Even when we have intra-valley scattering, there are two types of scattering events that can occur:

(1) intra-subband scattering
(2) inter-subband scattering

- Using general Fermi-Dirac statistics, the population of various subbands is described by sheet electron density N_n (# carriers per unit area), that is calculated using:

$$N_n = \int_0^{\infty} \rho_{2D}^{n}(E)\, f(E)\, dE = \frac{m^*}{\pi \hbar^2} k_B T \ln\left[1 + \exp\left(\frac{E_F - E_n}{k_B T}\right)\right]$$

- The z-variation of the electron density is calculated using:

$$n(z) = \sum_n N_n \Psi_n^2(z)$$

- Because the uncertainty in particle's position is reduced by confining it in the well region, the uncertainty in particles momentum increases. This directly follows from the uncertainty principle:

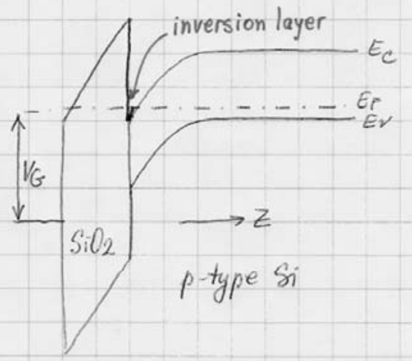
$$\hbar \Delta k_z \cdot \Delta z \geq \hbar/2$$

As we will see later, this is directly reflected on the momentum conservation condition. It holds in the xy-plane where carriers are free to move and have well defined momentum, but it will not hold in the z-direction.

(B) TRIANGULAR WELLS

- In some type of semiconductor devices, electric fields or material properties are used to restrict the motion of the carriers, so that they are confined to a narrow channel, unable to move in the perpendicular direction. One example are quantum wells that were discussed previously, and the second example are the MOS (metal-oxide-semiconductor) structures.

- A schematic diagram of an MOS capacitor is shown below.



If the band-bending is sufficient to bring the conduction band minimum slightly below the Fermi level, electrons will accumulate in the surface region. These electrons are confined in the z-direction in a surface layer of a thickness of approximately 100 Å by a potential barrier associated with the ionized acceptors and SiO_2. The surface electrons are present in a region that would be p-type in the absence of bias, hence the term 'INVERSION LAYER'. Many interesting properties of this system result from the fact that the electron density in the inversion layer can be controlled by varying the bias between gate and substrate.

- Because the electron motion is restricted in the z-direction, as in quantum wells, a set of discrete energy levers arise. However, there is an immediate complication when considering Si or Ge, which arises from the many-valley nature of the conduction bands. The energy levels will depend upon the surface orientation. Since the kinetic energy term in the 1D TISE depends inversely on m^*, the lowest levels will be associated with the largest mass. Let us consider for this purpose Si and {100} orientation of the surface. The conduction band minima in Si are a set of six ellipsoids of revolution lying along <100> direction in $\vec{k}$-space, with the centers being about 85% of the distance from the zone center to the face of the Brillouin zone (X-point). Long axis has $m_l^* = 0.916\ m_0$ and short axes have $m_t^* = 0.190\ m_0$.

- For such system, the effective mass Schrödinger equation is:

$$\left[-\frac{\hbar^2}{2m_x^*}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y^*}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2} + V(z)\right]\Psi(x,y,z) = E\,\Psi(x,y,z)$$

where it is convenient to measure the energy from the bottom of the conduction band. If carriers are free to move in the xy-plane then:

$$\Psi(x,y,z) = \frac{1}{\sqrt{A}}\, e^{i(xk_x + yk_y)}\, \varphi(z)$$

which, when substituted into the 3D Schrödinger equation gives:

$$\left[\frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*} - \frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2} + V(z)\right]\frac{1}{\sqrt{A}}\, e^{i(xk_x + yk_y)}\varphi(z) =$$

$$= E\,\frac{1}{\sqrt{A}}\, e^{i(xk_x + yk_y)}\varphi(z)$$

i.e.

$$\left[-\frac{\hbar^2}{2m_z^*}\frac{\partial^2}{\partial z^2} + V(z)\right]\underbrace{\varphi(z)}_{\varphi_n(z)} = \underbrace{\left[E - \frac{\hbar^2 k_x^2}{2m_x^*} - \frac{\hbar^2 k_y^2}{2m_y^*}\right]}_{E_n}\underbrace{\varphi(z)}_{\varphi_n(z)}$$

The above equation is the 1D TISE for the triangular well confinement (for the case we are considering) in which:

$$E_n = E - \frac{\hbar^2 k_x^2}{2m_x^*} - \frac{\hbar^2 k_y^2}{2m_y^*} \Rightarrow E_n(k_x, k_y) = E_n + \frac{\hbar^2 k_x^2}{2m_x^*} + \frac{\hbar^2 k_y^2}{2m_y^*}$$

To solve this equation, one needs to calculate the potential energy term $V(z)$. Here we can consider two cases:

(a) Airy function solutions for $\varphi_n(z)$ when $V(z) = eE_z z$, i.e. this is valid only when the electrons do not make significant solution to the band-bending.
(see notes in EEE 434 for this case)

(b) One must self-consistently solve the 1D TISE:

$$-\frac{\hbar^2}{2m_z^*}\frac{\partial^2\varphi_n(z)}{\partial z^2} + V(z)\varphi_n(z) = E_n\varphi_n(z)$$

with the 1D Poisson equation:

$$-\frac{1}{e}\frac{d^2V}{dz^2} = -\frac{e}{K_s\varepsilon_0}\left[N_D^+ - N_A^- + p(z) - n(z)\right]$$

i.e. $$\frac{d^2V}{dz^2} = \frac{e^2}{K_s\varepsilon_0}\left[N_D^+ - N_A^- + p(z) - n(z)\right]$$

where the electron density is given by:

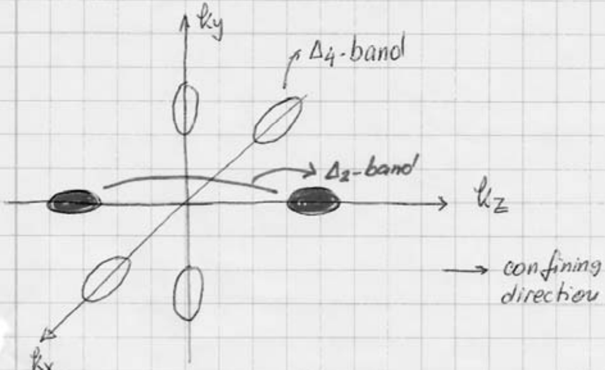
$$n(z) = \sum_n N_n\varphi_n^2(z)$$ (sum over n includes sum over all subbands from all valleys)

The sheet electron density N_n is calculated using:

$$N_n = g_v\frac{m_{xy}^*}{\pi\hbar^2}k_BT\ln\left[1+\exp\left(\frac{E_F-E_n}{k_BT}\right)\right]$$

valley degeneracy

$m_{xy}^* = \sqrt{m_x^* m_y^*}$ → effective DOS mass in the xy-plane.



Δ_2-band:

$m_z^* = m_l^* = 0.916 m_0$
$m_{xy}^* = m_t^* = 0.19 m_0$
$g_v = 2$

lowest level belongs to Δ_2-band

Δ_4-band:

$m_z^* = m_t^* = 0.19 m_0$
$m_{xy}^* = \sqrt{m_l^* m_t^*}$

$g_v = 4$