(2). Scattering rates for Q2D-systems

- Calculation of the scattering rates for confined carriers proceeds in a similar manner as in the 3D case, but the proper wavefunction for 3D carriers must be used. We will illustrate the calculation of the scattering rates for confined carriers on two examples:
  - deformation potential scattering, which will be treated in the elastic and equipartition approximation.
  - surface-roughness scattering, which is dominant scattering mechanism in MOSFETs with high substrate doping or in strong inversion conditions.

- Before we go into the details of the calculation of the above scattering rates, we will first derive some general expressions. Suppose we want to calculate the scattering out of some state $k_{\parallel}$ in a subband n. For that purpose, we will use Fermi's golden rule result:

$$\underbrace{S_{nm}(k_{\parallel}, k_{\parallel}')}_{} = \frac{2\pi}{\hbar} \left| M(k_{\parallel}, K_{\parallel}') \right|^2_{nn'} \delta(E - E' \pm \hbar\omega)$$

transition rate from a state $k_{\parallel}$ in subband 'n' into a state $k_{\parallel}'$ belonging to a subband 'm'.

Assuming plane wave basis for the electronic wavefunctions in the xy-plane, the total wave functions of the initial and final state are of the form:

$$\left.\begin{aligned} \Psi_n(k_{\parallel}) &= \frac{1}{\sqrt{A}} e^{i\vec{k}_{\parallel}\cdot\vec{r}} \varphi_n(z) \\ \Psi_m(k_{\parallel}') &= \frac{1}{\sqrt{A}} e^{i\vec{k}_{\parallel}'\cdot\vec{r}} \varphi_m(z') \end{aligned}\right\}$$

A = area of the sample
$\vec{r}$ = wavevector in the xy-plane
$\vec{R} = (\vec{r}, z)$ → wavevector in 3D

The matrix element for scattering between states $k_{\parallel}$ and $k_{\parallel}'$ in subbands n and m is then equal to:

$$M(k_{\parallel}, k_{\parallel}')_{nm} = \frac{1}{A} \int e^{i(\vec{k}_{\parallel} - \vec{k}_{\parallel}')\cdot r} d^2 r \underbrace{\int dz\, \varphi_m^*(z) H_{qv}(\vec{R}) \varphi_n(z)}_{}$$

the form of this integral depends upon the type of scattering mechanism considered.

(A) ACOUSTIC DEFORMATION POTENTIAL SCATTERING

- In the discussion for deformation potential scattering for bulk materials (3D-case), we showed that the interaction potential is:

$$H_{ep,dp} = C\,\nabla_R \cdot \hat{u} = \Xi_{ac}\,\nabla_R \cdot \hat{u}$$

where $\hat{u}$ is the operator for the lattice displacement and is given by:

$$\hat{u} = \sum_{q\nu} \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\, \vec{e}_{q\nu} \left[\hat{a}_{q\nu}\, e^{i\vec{q}\cdot\vec{R}} + \hat{a}_{q\nu}^{+}\, e^{-i\vec{q}\cdot\vec{R}} \right]$$

This leads to:

$$H_{ep,dp} = \Xi_{ac} \sum_{q\nu} \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}}\, \underbrace{\vec{q}\cdot\vec{e}_{q\nu}}_{\text{restricts to longitudinal modes only}} \left[\hat{a}_{q\nu}\, e^{i\vec{q}\cdot\vec{R}} - \hat{a}_{q\nu}^{+}\, e^{-i\vec{q}\cdot\vec{R}} \right] \quad ; \vec{q}\cdot\vec{R} = \vec{q}_{\parallel}\cdot\vec{r} + q_z z$$

After integrating over the phonon coordinates, the matrix element for scattering between states $\vec{k}_{\parallel}$ and $\vec{k}_{\parallel}'$ in subbands n and m becomes (for either absorption or emission):

$$M(\vec{k}_{\parallel}, \vec{k}_{\parallel}')_{nm} = \sum_{q\nu} \Xi_{ac}\, q \sqrt{\frac{\hbar}{2MN\omega_{q\nu}}} \left(N_{q\nu} + \frac{1}{2} \mp \frac{1}{2}\right)^{1/2} \cdot \underbrace{\frac{1}{A}\int e^{i(\vec{k}_{\parallel} - \vec{k}_{\parallel}' \pm \vec{q}_{\parallel})\cdot\vec{r}}\, d^2r}_{\delta(\vec{k}_{\parallel} - \vec{k}_{\parallel}' \pm \vec{q}_{\parallel})} \cdot \underbrace{\int dz\, \varphi_m^*(z)\, e^{\pm i q_z z}\, \varphi_n(z)}_{I_{nm}(\pm q_z) \,\to\, \text{overlap integral}}$$

i.e.

$$M(\vec{k}_{\parallel}, \vec{k}_{\parallel}')_{nm} = \Xi_{ac} \sqrt{\frac{\hbar}{2\rho V \omega_{q\nu}}}\, q \left(N_{q\nu} + \frac{1}{2} \mp \frac{1}{2}\right)^{1/2} I_{nm}(\pm q_z)\, \delta(\vec{k}_{\parallel} - \vec{k}_{\parallel}' \pm \vec{q}_{\parallel})$$

- The transition rate is, thus, given by:

$$S_{nm}(\vec{k}_{\parallel}, \vec{k}_{\parallel}') = \frac{2\pi}{\hbar}\, \Xi_{ac}^2\, \frac{\hbar q^2}{2\rho V \omega_{q\nu}}\, q \left(N_{q\nu} + \frac{1}{2} \mp \frac{1}{2}\right) |I_{nm}(\pm q_z)|^2\, \delta(\vec{k}_{\parallel} - \vec{k}_{\parallel}' \pm \vec{q}_{\parallel}) \cdot \delta(E_n + E_{k_{\parallel}} - E_m - E_{k_{\parallel}'} \pm \hbar\omega_{q\nu})$$

This rate is different from the one obtained in 3D-case in several aspects:

(1) momentum conservation applies only in the xy-plane

(2) There is an overlap factor $I_{nm}(\pm q_z)$ which depends upon the magnitude of q_z and whether we have inter- or intra-subband transitions.

(3) In the energy conservation δ-function, the subband energy appears, i.e.

$$E - E' \pm \hbar\omega_{q\nu} = E_n + E_{k_\parallel} - E_m - E_{k_\parallel'} \pm \hbar\omega_{q\nu}$$

$$= E_n - E_m + E_{k_\parallel} - E_{k_\parallel'} \pm \hbar\omega_{q\nu}$$

- After integrating the transition rate over all final states, we can calculate the scattering rate out of some initial state, i.e.

$$\frac{1}{\tau_n(k_\parallel)} = \underbrace{\sum_m}_{\text{sum over all subbands}} \sum_{k_\parallel'} \sum_{k_z'} S_{nm}(\vec{k}_\parallel, \vec{k}_\parallel') =$$

$$= \sum_m \sum_{q_\parallel} \sum_{q_z} \cancel{2} \frac{2\pi}{\hbar} \frac{\cancel{\hbar} q^{\cancel{2}} \Xi_{ac}^2}{\cancel{2}\rho V v_s \cancel{q}} \cdot \frac{k_B T}{\hbar v_s \cancel{q}} |I_{nm}(q_z)|^2 \delta(\vec{k}_\parallel - \vec{k}_\parallel' \pm \vec{q}_\parallel) \delta(E - E' \pm \underbrace{\cancel{\hbar\omega_{q\nu}}}_{0})$$

absorption + emission (elastic and equipartition approximation)

$$= \sum_m \frac{2\pi \Xi_{ac}^2 k_B T}{\hbar \rho v_s^2} \underbrace{\frac{1}{A} \sum_{q_\parallel} \delta(\vec{k}_\parallel - \vec{k}_\parallel' \pm \vec{q}_\parallel) \delta(E - E')}_{\frac{1}{2} g_{2D}(E_n - E_m + E_{k_\parallel})} \underbrace{\frac{L_z}{L_z} \int_{-\infty}^{+\infty} \frac{dq_z}{2\pi} |I_{nm}(q_z)|^2}_{D_{nm}}$$

The function D_{nm} equals to:

$$D_{nm} = \frac{1}{L_z} \int_{-\infty}^{+\infty} L_z \frac{dq_z}{2\pi} \int_{-\infty}^{+\infty} \varphi_m^*(z) e^{\pm i q_z z} \varphi_n(z) dz \int_{-\infty}^{+\infty} \varphi_m(z') e^{\mp i q_z z'} \varphi_n^*(z') dz'$$

$$= \frac{1}{\cancel{L_z}} \int_{-\infty}^{+\infty} dz\, \varphi_m^*(z) \varphi_n(z) \int_{-\infty}^{+\infty} dz'\, \varphi_m(z') \varphi_n^*(z') \cancel{L_z} \underbrace{\int_{-\infty}^{+\infty} \frac{dq_z}{2\pi} e^{\pm i q_z (z - z')}}_{\delta(z - z')}$$

i.e. $$D_{nm} = \int_{-\infty}^{+\infty} dz \int_{-\infty}^{+\infty} dz' \varphi_m^*(z)\varphi_n(z)\varphi_m(z')\varphi_n^*(z')\delta(z-z')$$

$$= \int_{-\infty}^{+\infty} dz\, |\varphi_m(z)|^2 |\varphi_n(z)|^2 = \frac{1}{W_{nm}}$$

The **quantity** $\frac{1}{W_{nm}}$, i.e. W_{nm}, describes the effective extent of the interaction in the z-direction.

- To summarize:

$$\frac{1}{\tau_n(k_\parallel)} = \sum_m \frac{\cancel{2}\bar{\upsilon}\,\Xi_{ac}^2 k_B T}{\hbar \rho v_s^2} \frac{1}{\cancel{2}} g_{2D}(E_n - E_m + E_{k_\parallel}) \frac{1}{W_{nm}}$$

$$= \sum_m \frac{\bar{\upsilon} k_B T\, \Xi_{ac}^2}{\hbar \rho v_s^2 W_{nm}} g_{2D}(E_n - E_m + E_{k_\parallel})$$

From the above result we may conclude that:

(a) The scattering rate is proportional to the 2D DOS-function
(b) For intersubband scattering to occur, the electric field must accelerate the carriers to energies exceeding E_m, i.e. $E_n - E_m + E_{k_\parallel} \geq 0 \Rightarrow E_n + E_{k_\parallel} \geq E_m$. Otherwise, scattering into subband m will not occur.
(c) For infinite well, it is rather straightforward to show that:

$$\frac{1}{W_{nm}} = \frac{2 + \delta_{nm}}{L}$$, where L is the well width, and δ_{nm} is the Kronecker δ-function.