Electron transport in semiconductor nanodevices using the Monte Carlo method

1. Stochastic solution

2. Boltzmann Transport Equation

3. BTE Inputs: Dispersion and Scattering

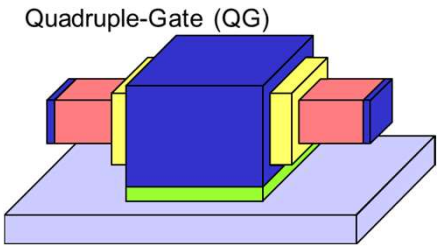
4. BTE Solution: Particle Monte Carlo method
- **Frozen field**
- **Device simulation**

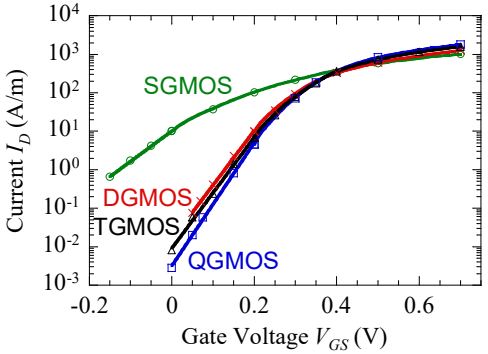
5. BTE Applications and Examples

Context

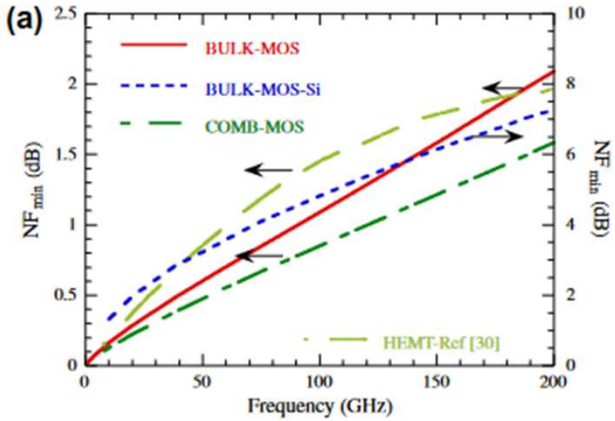
Transport problem: particle, charge, spin, energy, heat…

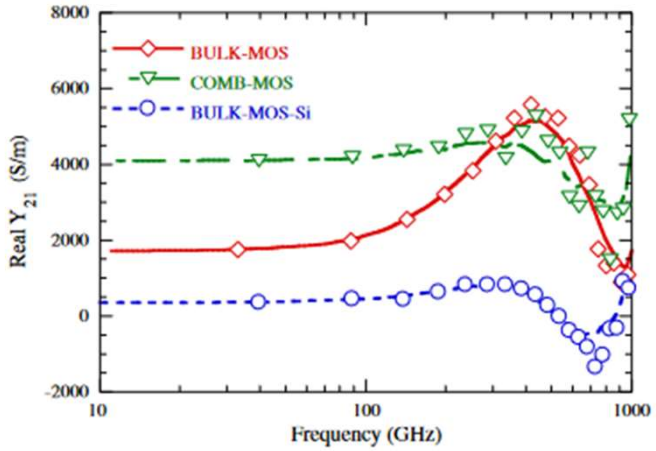
- 1. From material (S.C.) properties to device (transistor…) performance
  Reciprocal space → **Real space (complex geometry)**





- 2. Time evolution
  Frequency response, Noise properties





➢ ***Which formalism is relevant? Deterministic or stochastic solution?***

Stochastic solution: numerical integration

Monte-Carlo integration is the most common application of Monte-Carlo methods

Basic idea: Do not use a fixed grid, but random points, because:

1. Dimensionality: a fixed grid in D dimensions with N meshes requires N^D points
2. The mesh size must be chosen first, with appropriate criteria

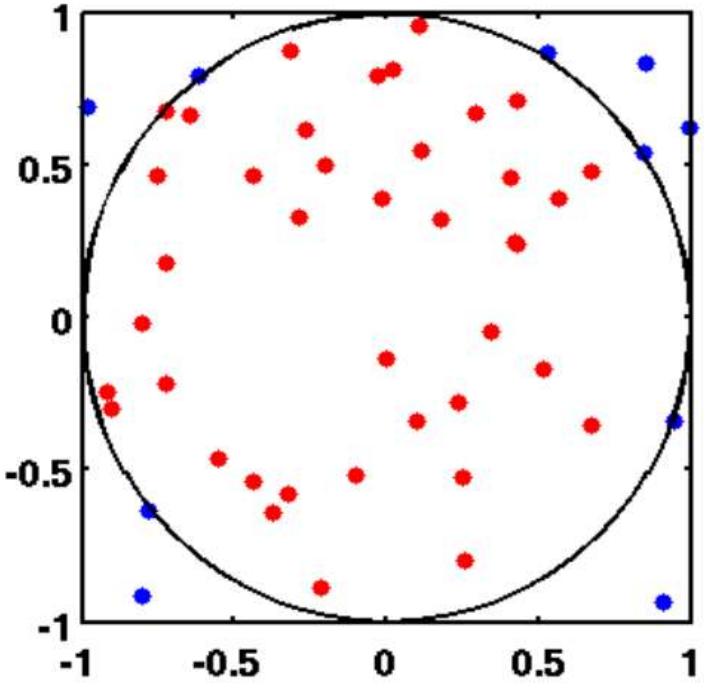
Example of stochastic solution: calculation of π

Consider a circle of radius 1, enclosed by a 2×2 square

The area of the circle is $\pi r^2 = \pi$

The area of the square is 4

Generate a large number of uniformly distributed random points (x,y) with $x,y \in [-1,1]$



N_{inner} is the number of points in the circle

N_{total} is the total number of points

Then (**Law of larges numbers**) $\frac{\pi}{4} \approx \frac{N_{inner}}{N_{total}}$

Random number generators

How to generate many random variables satisfying all randomness properties of the problem?

- Distribution of $\mathrm{R} \in [0,1]$: Uniformity is not sufficient
- Other issues are the period of the generator and the non-correlation between numbers
- **Example of generator** of $R \in [0,1]$

Starting from a seed N_j

Recurrence relation:

$$\left.\begin{aligned} N_{j+1} &= A \times N_j + C \\ I &= \mathrm{mod}\left(N_{j+1}, P\right) \end{aligned}\right\}$$

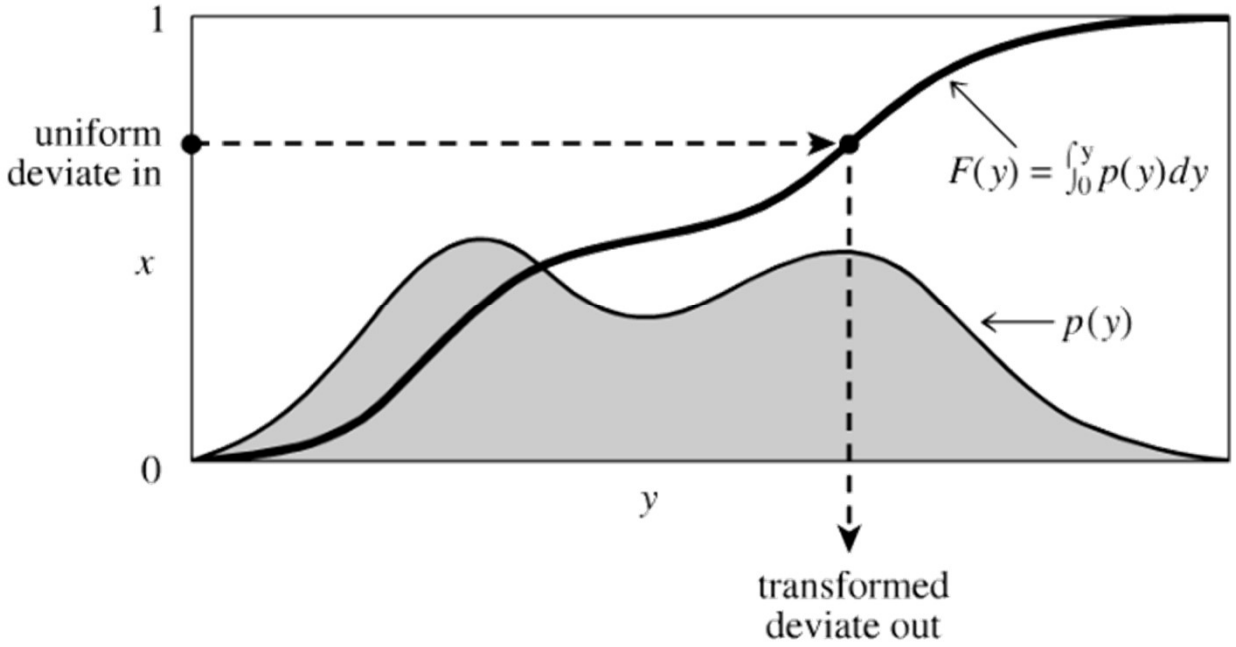
$$N_{j+1} = I$$

With e.g. $A = 5^5$, $C = 7$, $P = 2^{19}$

$$\boxed{R = \frac{I}{P}}$$

P is the period of the generator

Random number from any distribution



The transformation method:

1. Given a normalized distribution p(y), the cumulative distribution function (CDF) of p(y) is

$$F(y) = \int_0^y p(w)\,dw$$

2. Drawing a number y according to $p(y)$ (shaded area) amounts to draw uniformly $F(y)$

   by construction: $0 \le F(y) \le 1$

3. We draw $x = R \in [0,1]$ and determine y so that $x = F(y)$

4. Therefore: $y = F^{-1}(x)$

- ***Using a uniform distribution for x and the inverse of the cumulative (relevant) distribution function F***

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Distribution Function

Classical approach (quantum properties are neglected)

One can specify at each time t their position $\vec{r}$ and their wave vector $\vec{k}$ (or their momentum $\vec{p} = \hbar\vec{k}$)

The system is fully described by the distribution function $f\left(\vec{r},\vec{k},t\right)$ which is the « probability » to have an electron in state $\vec{k}$ at position $\vec{r}$ at time t

→ All physical quantities A and fluxes related to the electron gas are deduced from this function:

⇒ *e.g.*

$$\begin{cases} n(\vec{r},t) = \sum_k f\left(\vec{r},\vec{k},t\right) = \int \rho(k)\, f\left(\vec{r},\vec{k},t\right) d\vec{k} \\ v_x(\vec{r},t) = \sum_k v_x\left(\vec{k}\right) f\left(\vec{r},\vec{k},t\right) = \int v_x\left(\vec{k}\right) \rho(k)\, f\left(\vec{r},\vec{k},t\right) d\vec{k} \\ A(\vec{r},t) = \sum_k A\left(\vec{k}\right) f\left(\vec{r},\vec{k},t\right) = \int A\left(\vec{k}\right) \rho(k)\, f\left(\vec{r},\vec{k},t\right) d\vec{k} \\ \vec{J}_A(\vec{r},t) = \sum_k \vec{v}\left(\vec{k}\right) A\left(\vec{k}\right) f\left(\vec{r},\vec{k},t\right) = \int \vec{v}\left(\vec{k}\right) A\left(\vec{k}\right) \rho(k)\, f\left(\vec{r},\vec{k},t\right) d\vec{k} \end{cases}$$

- ***Violatation of uncertainty principle ? Eulerian description ?***

Distribution Function and density operator

Classical approach : Distribution Function

e.g.

$$\begin{cases} n(\vec{r},t) = \sum_k f(\vec{r},\vec{k},t) = \int \rho(k)\, f(\vec{r},\vec{k},t)\, d\vec{k} \\ v_x(\vec{r},t) = \sum_k v_x(\vec{k})\, f(\vec{r},\vec{k},t) = \int v_x(\vec{k})\, \rho(k)\, f(\vec{r},\vec{k},t)\, d\vec{k} \\ \vec{J}_E(\vec{r},t) = \sum_k \vec{v}(\vec{k}) E(\vec{k})\, f(\vec{r},\vec{k},t) = \int \vec{v}(\vec{k}) E(\vec{k})\, \rho(k)\, f(\vec{r},\vec{k},t)\, d\vec{k} \end{cases}$$

Quantum approach : density matrix

→ All physical quantities are deduced from this density matrix:

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i| \qquad \rho(\mathbf{r},\mathbf{r}',t) = \langle \mathbf{r}|\hat{\rho}(t)|\mathbf{r}'\rangle = \sum_i p_i(t)\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')$$

$$\begin{cases} n(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r}) = \sum_i p_i(t)\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}) \\ \langle \hat{A} \rangle = \langle \Psi|\hat{A}|\Psi\rangle = Tr(\hat{A}\hat{\rho}) = Tr(\hat{\rho}\hat{A}) \end{cases}$$

Boltzmann Transport Equation (BTE)

Problem: Time-evolution of the distribution function $f(x,k,t)$

$$f(x,k,t) = f\left(x - \left(\frac{dx}{dt}\right)dt, k - \left(\frac{dk}{dt}\right)dt, t - dt\right) + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

$$\frac{\partial f}{\partial t} + \frac{dx}{dt}\frac{\partial f}{\partial x} + \frac{dk}{dt}\frac{\partial f}{\partial k} = \left.\frac{\partial f}{\partial t}\right|_{coll}$$

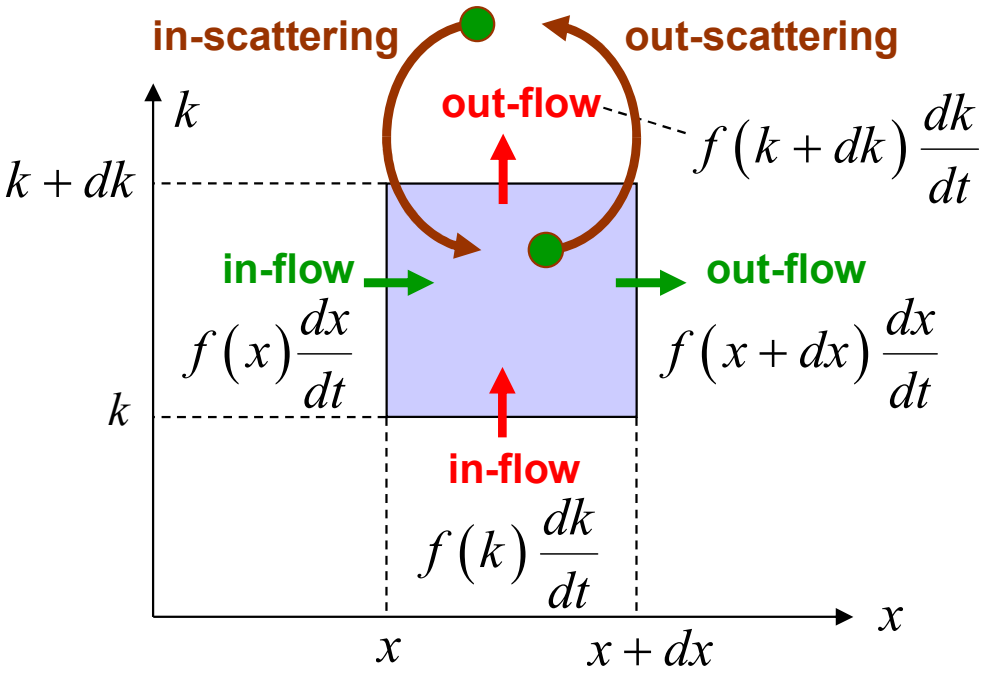
$$\frac{\partial f}{\partial t} = -v\frac{\partial f}{\partial x} - \frac{F}{\hbar}\frac{\partial f}{\partial k} + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

Generalization in 3D space:

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

BTE in 6-dimensional phase space

Boltzmann Transport Equation (BTE)



$$\begin{cases} \dfrac{dx}{dt} = v \\ \dfrac{dk}{dt} = \dfrac{F}{\hbar} \end{cases} \qquad (p = \hbar k)$$

During δt, f increases by δf

→ **Conservation** of the number of particles in the small volume $dx\,dk$:

in and out scatterings

$$\delta f\ dx\,dk = \left[f(x) - f(x+dx)\right] v\,\delta t\ dk + \left[f(k) - f(k+dk)\right] \frac{F}{\hbar}\,\delta t\ dx + \left.\frac{\partial f(x,k,t)}{\partial t}\right|_{coll} \delta t\ dk\ dx$$

$$\frac{\delta f}{\delta t} = \frac{\left[f(x) - f(x+dx)\right]}{dx}\ v + \frac{\left[f(k) - f(k+dk)\right]}{dk}\frac{F}{\hbar} + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

BTE in 6-dimensional phase space

Classical vs. Quantum transport Equations

→ Conservation in a classical system via Hamilton's formalism $\dot{q}_i = \frac{\partial H}{\partial p_i}, \qquad \dot{p}_i = -\frac{\partial H}{\partial q_i}$

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f \quad \Leftrightarrow \quad \frac{\partial f}{\partial t} + \sum_{i=1}^{3N}\left(\frac{\partial H}{\partial p_i}\frac{\partial f}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial f}{\partial p_i}\right) = 0$$

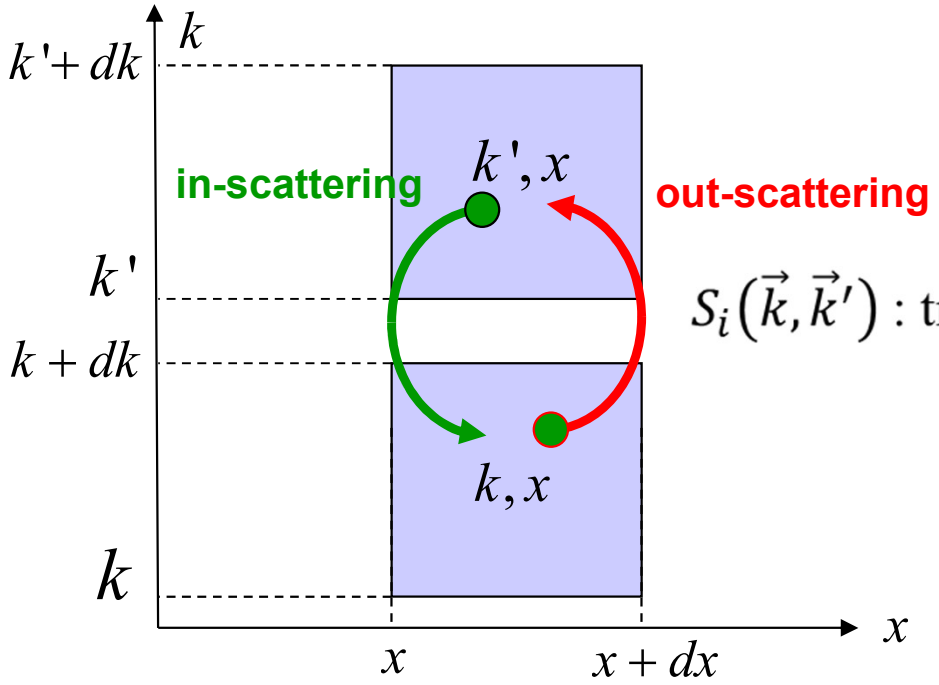
$$\frac{\partial f}{\partial t} + \{H, f\} = 0$$

→ Conservation in a quantum system (correspondence principle)

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho]$$

- But in transport the main issue is : $\left.\frac{\partial f}{\partial t}\right|_{coll}$

Collision term - scatterings



$S_i(\vec{k},\vec{k}')$: transition rate
from an occupied state k
to an available state k'

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \sum_i \left[\int f(\vec{k}')\, S_i(\vec{k}',\vec{k})\, d\vec{k}' - \int f(\vec{k})\, S_i(\vec{k},\vec{k}')\, d\vec{k}' \right] = \hat{C}\, f$$

in-scattering *out-scattering* *collision operator*

In non-degenerate fermion gas: $\max f(\vec{r},\vec{k},t) > 0.1$

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \sum_i \left[\int f(\vec{k}')\left[1 - f(\vec{k})\right] S_i(\vec{k}',\vec{k})\, d\vec{k}' - \int f(\vec{k})\left[1 - f(\vec{k}')\right] S_i(\vec{k},\vec{k}')\, d\vec{k}' \right]$$

It turns out to be a non linear tem…

BTE solutions: At thermal equilibrium

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

- **At thermal equilibrium:** Equilibrium distributions are solutions (Boltzmann, FD, BE)

Eg.: Electrons obey the Fermi-Dirac statistics:

$$f\left(\vec{r},\vec{k},t\right) = f_0\left(\vec{r},\vec{k}\right) = \left[1+\exp\left(\frac{E\left(\vec{r},\vec{k}\right)-E_f}{k_B T}\right)\right]^{-1}$$

$$\begin{cases} E_f \text{ is the Fermi level} \\ E\left(\vec{r},\vec{k}\right) = E_p\left(\vec{r}\right) + \varepsilon\left(\vec{k}\right) \end{cases}$$

Total energy

Potential energy (bottom of CB)

Kinetic energy

Ex:

$$\varepsilon\left(\vec{k}\right) = \frac{\left(\hbar k\right)^2}{2m^*}$$

- At thermal equilibrium: $\left.\frac{\partial f}{\partial t}\right|_{coll} = 0$

$$\left.\frac{\partial f}{\partial t}\right|_{coll} = \sum_i \left[\int f\left(\vec{k}'\right) S_i\left(\vec{k}',\vec{k}\right) d\vec{k}' - \int f\left(\vec{k}\right) S_i\left(\vec{k},\vec{k}'\right) d\vec{k}'\right] = \hat{C}\, f$$

Linear response (close to equilibrium regime)

☞ **At eq.:** $f_0(\vec{r},\vec{k}) \equiv \exp\left(\frac{\mu - \varepsilon_C - \varepsilon_k}{k_B T}\right)$ $\qquad \varepsilon_k = \frac{1}{2}m(v^2) = \frac{(\hbar k)^2}{2.m}$ ➔$f_0(r, v(k)) \approx \exp\left(-\frac{m(v)^2}{2.k_B T}\right)$

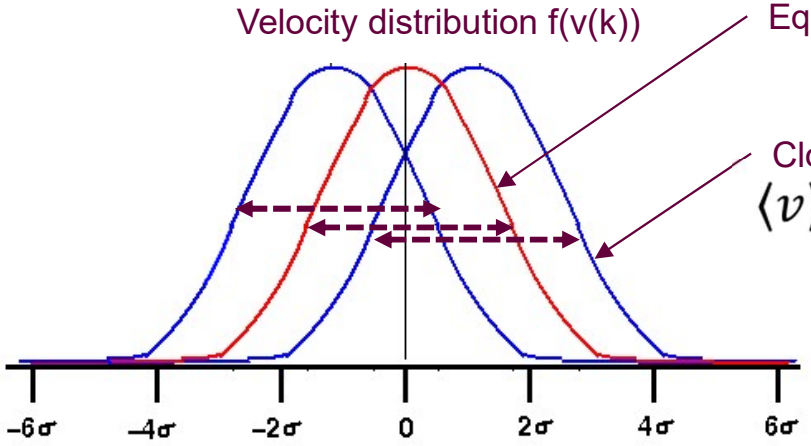
☞ **linear response:**

- **Steady state**
- **Small perturbations**

$$\begin{cases} f(x,v) = f_0(x,v) + f_1 \approx f_0 \gg f_1 \\ \frac{df}{dx} \approx \frac{df_0}{dx} \gg \frac{df_1}{dx} \\ \frac{df}{dv} \approx \frac{df_0}{dk} \gg \frac{df_1}{dv} \end{cases}$$

☞ **Shifted gaussian distributions?**

$$f(v) = f_0 + f_1 \equiv \exp\left(-\frac{m(v - \langle v\rangle)^2}{2k_B T}\right)$$



BTE at low field: Drift term derivation

Electric force: $\vec{F} = -q\vec{E}$

Current density: $\vec{J}(\vec{r}) = -q\iiint f_1(\vec{k},\vec{r})\vec{v}(\vec{k})n(\vec{k})d^3\vec{k}$ with $f_1 = f - f_{equi} = f - f_0$

Assumptions:

(i) Non degenerate N-type semiconductor
(ii) Parabolic and isotropic energy band (constant and isotropic mass)
(iii) Stationary regime (∂f/∂t = 0), without generation
(iv) Relaxation time depending on electron kinetic energy ε
(v) Uniform doping and temperature (no gradients in real space)
(vi) Uniform, constant and low electric field (< 1 kV/cm)

$$\left.\frac{\partial f}{\partial t}\right|_{coll} \approx \frac{f - f_0}{\tau(\varepsilon)} = \frac{f_1}{\tau}$$

(iii) + (v) $\Rightarrow$ $\frac{1}{\hbar}\vec{\nabla}_{\vec{k}} f \cdot \vec{F} + \frac{f_1}{\tau} = 0$

(i) $\Rightarrow$ $f_0(\vec{k}) \approx \exp\left(\frac{E_f - E_c - \varepsilon}{k_B T}\right)$

(vi) $\Rightarrow$ $f = f_0 + f_1 \approx f_0$

$\Rightarrow \vec{\nabla}_{\vec{k}} f = \frac{\partial f_0}{\partial \varepsilon}\vec{\nabla}_{\vec{k}}\varepsilon = -\frac{f_0}{k_B T}\hbar\vec{v}$

Thus, using (iv) $f_1 = -q\tau(\varepsilon)\frac{f_0}{k_B T}\vec{E}\cdot\vec{v}$ so $J_x = \frac{q^2 E_x}{k_B T}\iiint \tau(\varepsilon) f_0(\vec{k}) v_x^2 n(\vec{k}) d^3\vec{k}$

BTE: solutions

$$\frac{\partial f}{\partial t} = -\vec{v} \cdot \vec{\nabla}_r f - \frac{\vec{F}}{\hbar} \cdot \vec{\nabla}_k f + \left.\frac{\partial f}{\partial t}\right|_{coll}$$

- **At thermal equilibrium:** Equilibrium distributions are solutions (Boltzmann, FD, BE)

- **Close to equilibrium:** BTE ➔ Drift/Diffusion eq., Hydrodynamic model

- **Far from equilibrium** the shape of *f* is unknown !

  Complex (linear ?!) PDE with 7 degrees of freedom t,x,y,z,k_x,k_y,k_z
  Even with simplification in the real space the direct discretization leads to huge Matrices

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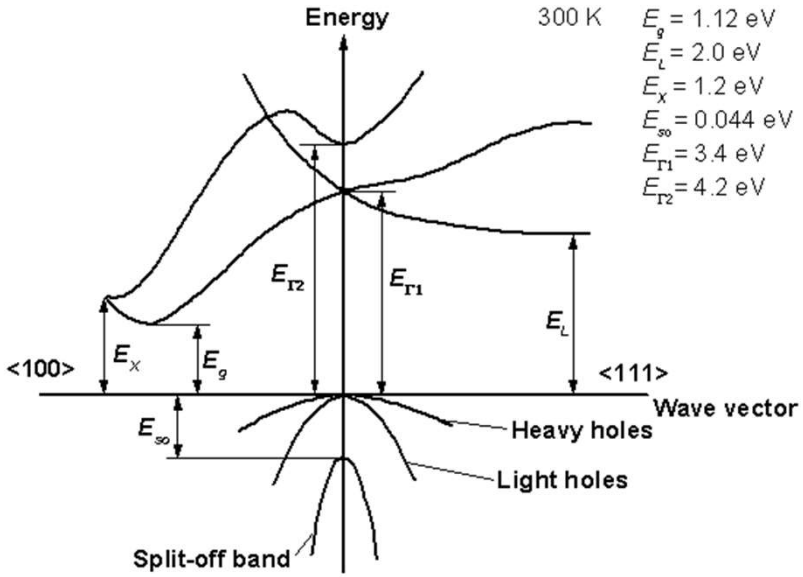
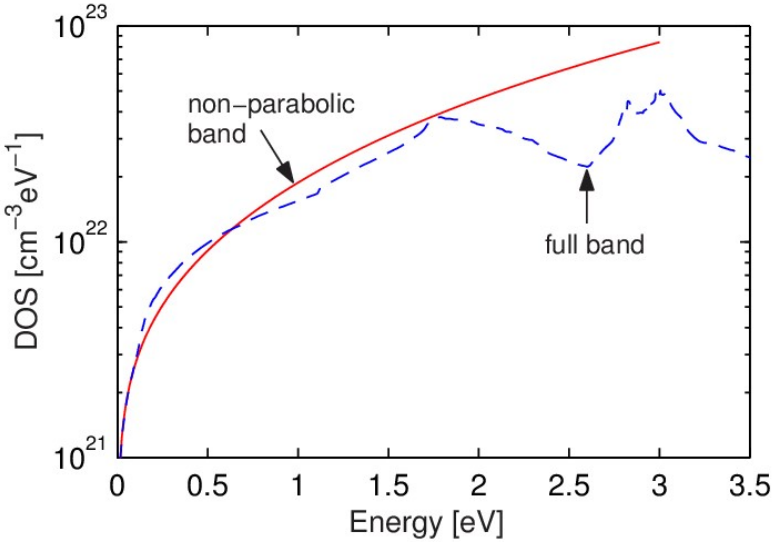
Dispersion: Electron in Silicon

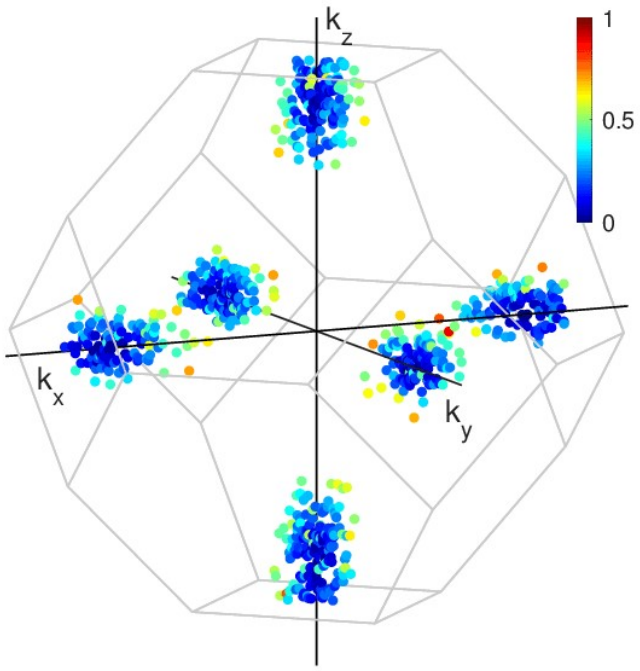


http://www.ioffe.ru/SVA/NSM/Semicond/Si/Figs/121.gif

Analitytical modeling:
Non parabolic and anisotropic modeling

$$E\left(1+\alpha E\right)=\frac{\hbar^2}{2m_0}\left(\frac{k_x^{\,2}}{m_l}+\frac{k_y^{\,2}}{m_t}+\frac{k_z^{\,2}}{m_t}\right)$$





Pop, Eric & Goodson, Kenneth. (2022). Self-heating and scaling of thin body transistors /.

Collision term – scatterings

Transition rate:
(for mechanism *i*)

$$S_i\left(\vec{k},\vec{k}'\right)=\frac{2\pi}{\hbar}\left|\left\langle\vec{k}'\right|H_i\left|\vec{k}\right\rangle\right|^2\rho_{k'}\,\delta\left(E'-E\right)$$

(Fermi golden rule)

matrix element of H_i ; DOS (spin…)

Fermi golden rule, main features:

- 1st order, time dependant, perturbation theory,
- Scattering between two Bloch (plane) waves with momentum k and k' (conservation OK but real space ?) $\psi_{\mathbf{k}}\left(\mathbf{r}\right)=u_{\mathbf{k}}\left(r\right)e^{i\mathbf{k}.\mathbf{r}}$

- Time between two scatterings in the limit: t →∞ (to ensure energy conservation),
- Independant scattering mechanisms.

For electrons: possible collision mechanisms (collision ≡ interaction ≡ scattering):

- electron-phonon scattering
- electron-impurity scattering
- **electron-electron scattering (difficult !!)**
- alloy scattering (in SiGe, AlGaAs,…)
- …

$$\longrightarrow S_i\left(\vec{k},\vec{k}'\right)\longrightarrow\left.\frac{\partial f}{\partial t}\right|_{coll}$$

➢ But matrix element H_i ????

Pertubation potential and matrix element

Evaluation of the coupling constant D_q:

* Electrostatic force (polar material): physical models exist

→ acoustic intravalley (piezoelectric): $D_{\mathbf{q}} = 2\sqrt{\pi}\,\frac{e P_z}{\varepsilon}\left(\frac{q^2}{q^2 + q_s^2}\right)$ $\quad q_s = \sqrt{\frac{e^2 n}{\varepsilon k_B T}}$

(P_z = piezoelectric Const, q_s = inverse screening length)

→ optical intravalley (polar optical): $\left|\left\langle \vec{k}' \right| H_{op} \left| \vec{k} \right\rangle\right|^2 = \frac{2\pi e^2 \hbar\omega}{q^2}\left(\frac{1}{\varepsilon_{hf}} - \frac{1}{\varepsilon_{lf}}\right)$

(ε_{hf} and ε_{lf} = high frequency and low frequency permittivity)

* Deformation potential D_q: empirical paramters

$\Delta E = D_{\mathbf{q}} \cdot u$ (Energy change associated with a displacement u of an atom)

$\mathbf{q} = \mathbf{k}' - \mathbf{k}$

→ optical/acoustic intervalley: (large q) $\quad \hbar\omega_q = \text{Const} \quad D_{\mathbf{q}} = D_0 + \cancel{D_1 q} + \ldots$ with D_0 in eV/cm

→ acoustic intravalley: (small q) $\quad \hbar\omega_q = \hbar v_s q \quad D_{\mathbf{q}} = \cancel{D_0} + D_{ac} q$ with D_{ac} in eV

sound velocity

We have all needed information to calculate the electron-phonon scattering rates

Electron-phonon scattering

$$S_i\left(\vec{k},\vec{k}'\right)=\frac{2\pi}{\hbar}\left|\left\langle\vec{k}'\right|H_i\left|\vec{k}\right\rangle\right|^2\rho_{k'}\,\delta\left(E'-E\right)$$

→ the energy of each mode ω_q is quantized according to:

$$E=\hbar\omega_{\mathbf{q}}\left[n_{\mathbf{q}}+\frac{1}{2}\right]$$

→ the quantum of energy is a boson particle called ***phonon***, whose number is given by:

$$n_{\mathbf{q}}=\frac{1}{\exp\left(\dfrac{\hbar\omega_{\mathbf{q}}}{k_B T}\right)-1}$$

General expression for transition probability per unit of time from **k** to **k'** (per unit of volume *d***k'**)

$$S_{el-ph}\left(\mathbf{k},\mathbf{k}'\right)=\frac{\hbar}{8\pi^2}\,\frac{1}{\rho\hbar\omega_{\mathbf{q}}}\,\underbrace{D_{\mathbf{q}}^2\,\mathcal{G}\left(\mathbf{k},\mathbf{k}'\right)}_{\text{dependent on phonon process}}\left[n_{\mathbf{q}}+\frac{1}{2}\pm\frac{1}{2}\right]\delta\left(E'-E\mp\hbar\omega\right)$$

$\left\{\begin{array}{l}\text{+ : emission}\\ \text{- : absorption}\end{array}\right.$

where ρ is the mass density $D_{\mathbf{q}}$ is the coupling constant

$$\mathcal{G}\left(\mathbf{k},\mathbf{k}'\right)=\left|\int_{cell}d\mathbf{r}\;u_{\mathbf{k}'}^{*}\left(\mathbf{r}\right)u_{\mathbf{k}}\left(\mathbf{r}\right)\exp\left[i\,\mathbf{G}\cdot\mathbf{r}\right]\right|^2$$ is the overlap factor

Electron-phonon scattering

Evaluation of the overlap factor $$\mathcal{G}(\mathbf{k},\mathbf{k}') = \left| \int_{cell} d\mathbf{r}\, u^{*}_{\mathbf{k}'}(\mathbf{r})\, u_{\mathbf{k}}(\mathbf{r}) \right|^2$$

* Electrons:

→ intravalley process in Γ valley (GaAs): $$\mathcal{G}(\mathbf{k},\mathbf{k}') = \frac{\left[(1+\alpha E)^{1/2}(1+\alpha E')^{1/2} + \alpha (EE')^{1/2}\cos\theta\right]^2}{(1+2\alpha E)(1+2\alpha E')}$$

→ intravalley process in X valleys (Si):

→ intervalley process:

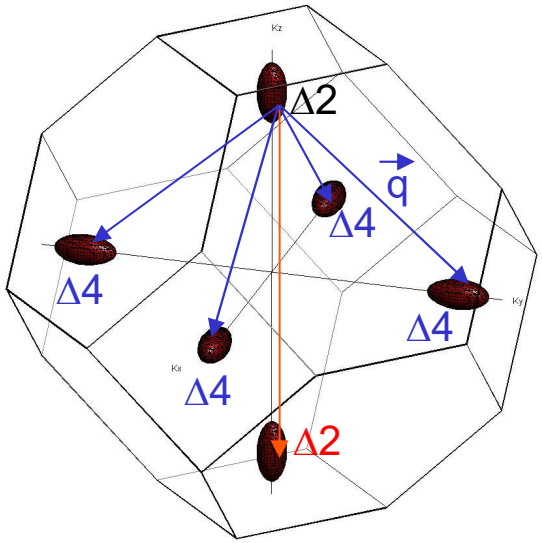
$$\mathcal{G}(\mathbf{k},\mathbf{k}') \approx \text{constant} \approx 1$$

* Holes:

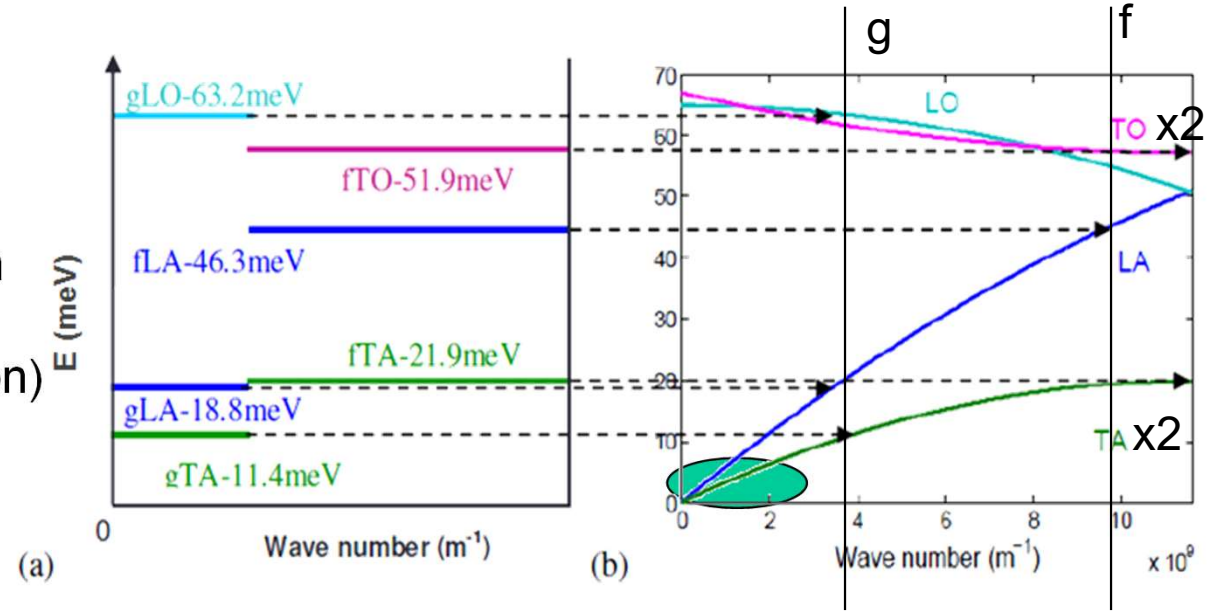
→ intravalley process: $$\mathcal{G}(\mathbf{k},\mathbf{k}') = \frac{1}{4}\left(1+3\cos^2\theta\right)$$

→ intervalley process (hh↔lh): $$\mathcal{G}(\mathbf{k},\mathbf{k}') = \frac{3}{4}\sin^2\theta$$

Electron-phonon scattering in Si



typical phonon spectrum (along 1 direction)



Classification of phonon processes:

* *2 physical mechanisms of interaction*:
  - Deformation potential (all SC)
  - Electrostatic force (polar SC, e.g. GaAs)
* *2 types of phonon mode (branche):*
  - Acoustic modes
  - Optical modes
* *2 types of transition:*
  - intra-valley (small q)
  - inter-valley (large q)

Monte Carlo method: example of scattering rates (1)

Electron-phonon interaction by deformation potential coupling

* Acoustic intravalley scattering

→ small energy and small wave vector phonon ⇒ $n_{\mathbf{q}} = \left[\exp\left(\frac{\hbar\omega_{\mathbf{q}}}{k_B T}\right) - 1\right]^{-1} \approx \frac{k_B T}{\hbar\omega_{\mathbf{q}}}$

$\hbar\omega_q = \hbar v_S q$

→ the exchange of energy is neglected (**elastic approximation**, $E' = E$)
and both emission and absorption are considered through the same process

$$S_{ac}(\mathbf{k},\mathbf{k}') = \frac{k_B T}{4\pi^2}\frac{D_{ac}^2}{\rho\hbar v_s^2}\delta(E'-E) \quad \text{with} \quad E(1+\alpha E) = \frac{\hbar^2}{2m_0}\left(\frac{k_x^{\,2}}{m_l} + \frac{k_y^{\,2}}{m_t} + \frac{k_z^{\,2}}{m_t}\right)$$

$$\lambda_{ac}(\vec{k}) = \int S_{ac}(\vec{k},\vec{k}')\,d\vec{k}' \longrightarrow \text{change of variables:}$$

$$\vec{k}' \to E,\theta,\varphi \qquad d\vec{k} = J(E,\theta,\varphi)\,dE\,d\theta\,d\varphi$$

$$J(E,\theta,\varphi) = \sqrt{2}\left(\frac{m_0}{\hbar^2}\right)^{3/2}(1+2\alpha E)\sqrt{E(1+\alpha E)}\sin\theta\left(\frac{\sin^2\theta}{m_t} + \frac{\cos^2\theta}{m_l}\right)^{-3/2}$$

$$\lambda_{ac}(E) = \int S_{ac}(\vec{k},\vec{k}')\,J(E,\theta,\varphi)\,dE\,d\theta\,d\varphi$$

$$\lambda_{ac}(E) = \frac{\sqrt{2}}{\pi}\frac{k_B T}{\rho\hbar^4 v_s^2}\,m_{DOS}^{3/2}\,D_{ac}^2\,(1+2\alpha E)\sqrt{E(1+\alpha E)}$$

Monte Carlo method: example of scattering rates (2)

Electron-phonon interaction by deformation potential coupling

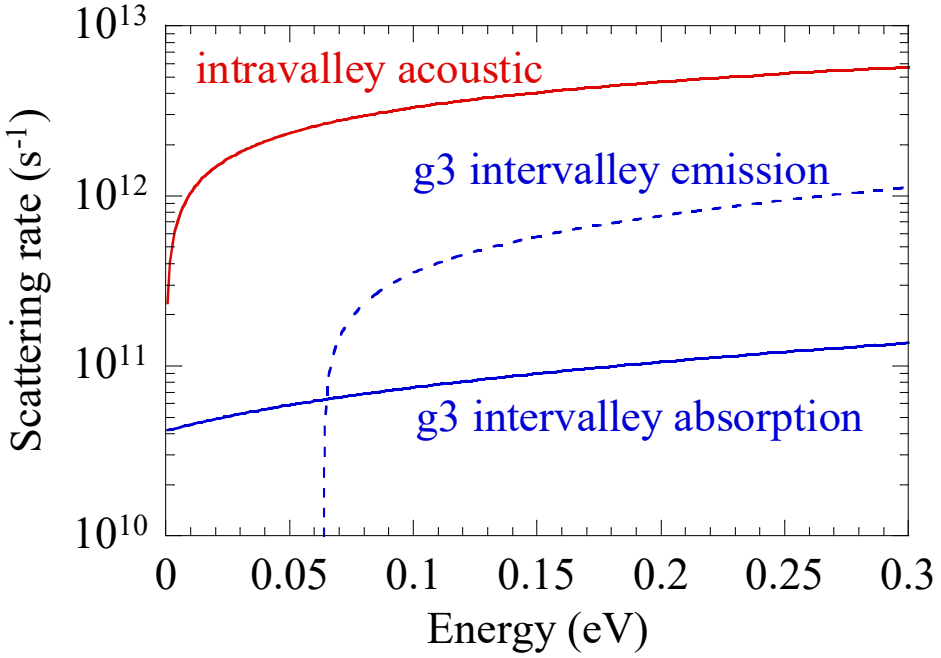
* Intervalley scattering (Z_{iv} possible final valleys)

zero order process: $D_{\mathbf{q}} = D_0$

$$S_{iv_0}(\mathbf{k},\mathbf{k}') = Z_{iv}\frac{\hbar}{8\pi^2}\frac{D_0^2}{\rho\hbar\omega_{iv}}\left[n_{\mathbf{q}}+\frac{1}{2}\pm\frac{1}{2}\right]\delta\left(E'-E\mp\hbar\omega\right)$$

$\begin{cases} + : \text{emission} \\ - : \text{absorption} \end{cases}$

$$\lambda_{iv_0}(E) = \frac{Z_{iv}}{\sqrt{2}\,\pi\,\rho\hbar^3\,\omega_{iv}}\,m_{DOS}^{3/2}\,D_0^2\left[n_{\mathbf{q}}+\frac{1}{2}\pm\frac{1}{2}\right]\left[1+2\alpha\left(E\mp\hbar\omega\right)\right]\sqrt{\left(E\mp\hbar\omega\right)\left(1+\alpha\left(E\mp\hbar\omega\right)\right)}$$



example: Si ($T = 300\text{K}$)

$D_{ac} = 9$ eV

$D_0 = 3.4\times10^8$ eV/cm

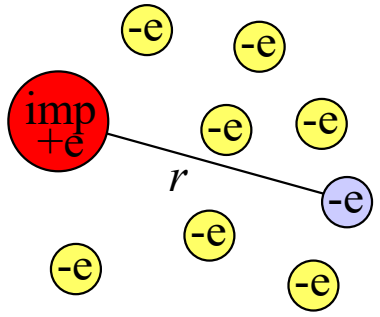
intervalley (Δ-Δ) phonons:

g1	$\hbar\omega_{iv} = 11.4$ meV
g2	$\hbar\omega_{iv} = 18.8$ meV
g3	$\hbar\omega_{iv} = 63.2$ meV
f1	$\hbar\omega_{iv} = 21.9$ meV
f2	$\hbar\omega_{iv} = 46.3$ meV
f3	$\hbar\omega_{iv} = 59.1$ meV

Electron-impurity scattering

* For 1 ionized impurity:

(Brooks-Herring model)



$$H_{el-imp} = U_{coul}(r) = \frac{e}{4\pi\varepsilon}\frac{\exp(-r/L_D)}{r}$$

L_D = Debye length
= screening length

$$L_D = \frac{1}{q_s} = \sqrt{\frac{\varepsilon k_B T}{e^2 n}}$$

n = electron density

$\exp(-r/L_D)$ accounts for screening effects due to other electrons

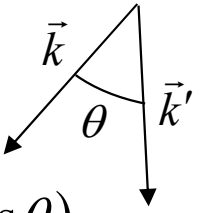
$$S_{el-imp}(\mathbf{k},\mathbf{k}') = \frac{1}{V}\frac{1}{4\pi^2\hbar}\frac{e^4}{\varepsilon^2}\frac{1}{\left(q^2+q_s^2\right)^2}\delta(E'-E)$$

elastic process

$$\vec{q} = \vec{k}' - \vec{k} \quad , |\vec{k}'| = |\vec{k}|$$

$$q^2 = |\vec{k}' - \vec{k}|^2 = 2k^2(1-\cos\theta)$$

$$E' = E$$



* For N_{imp} impurities: $N_{imp} = N_{dop}\,V$

$$S_{el-imp}(\mathbf{k},\mathbf{k}') = \frac{N_{dop}}{4\pi^2\hbar}\frac{e^4}{\varepsilon^2}\frac{1}{\left(q^2+q_s^2\right)^2}\delta(E'-E)$$

Electron transport in semiconductor nanodevices using the Monte Carlo method

1. Stochastic solution

2. Boltzmann Transport Equation

3. BTE Inputs: Dispersion and Scattering

4. BTE Solution: Particle Monte Carlo method

- **Frozen field**
- **Device simulation**

5. BTE Applications and Examples

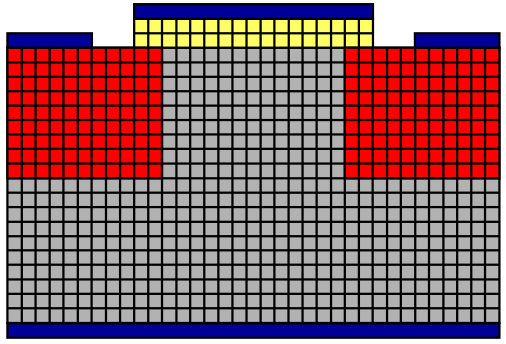
Solving the BTE for device simulation (in frozen field E)

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \sum_i \left[\int f\left(\vec{k}'\right) S_i\left(\vec{k}',\vec{k}\right) d^3\vec{k}' - \int f\left(\vec{k}\right) S_i\left(\vec{k},\vec{k}'\right) d^3\vec{k}'\right]$$

Starting from an

- initial solution
- boundary conditions

How to calculate the time evolution of the distribution function f inside the device with a constant electric field (frozen field?

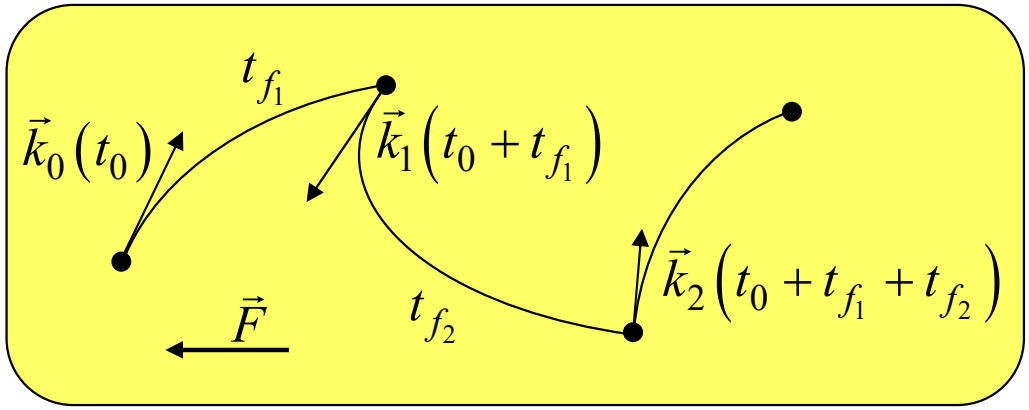


Indeed, the BTE is a rather complicated integro-differential equation ➔ direct (deterministic) solution is complex

- simplifying approximations of *f*: drift-diffusion (DD) and hydro-dynamic (HD) approaches
- statistical solution: **Monte Carlo methods (MC)**

The particle Monte Carlo method

☞ $f\left(\vec{r},\vec{k},t\right)$ → assembly of individual particles

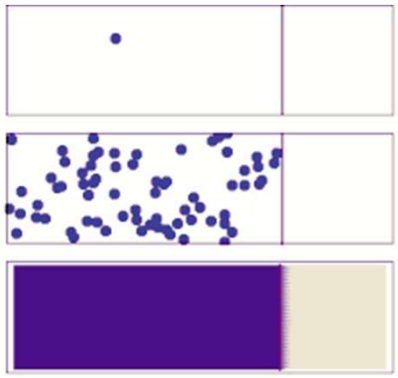


carrier trajectory:
succession of free flights
interrupted by
instantaneous scatterings

☞ **Statistical solution**

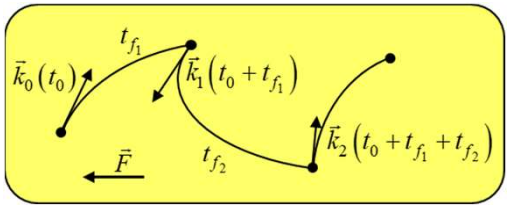
scattering rates $\lambda_i\left(\vec{k}\right)$ → random selection of → { - time of free flights t_f - type of scattering i - effect of scattering (ΔE, θ) }

(Monte Carlo algorithm)



Equivalence between BTE and particle MC trajectories

Is BTE equivalent to MC ?



$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \left.\frac{\partial f}{\partial t}\right|_{scatt} \quad \overset{?}{\Leftrightarrow} \quad \begin{cases} \dfrac{d\vec{k}_n(t)}{dt} = \dfrac{\vec{F}}{\hbar} + \left.\dfrac{\partial \vec{k}_n(t)}{\partial t}\right|_{scatt} \\ \dfrac{d\vec{r}_n(t)}{dt} = \vec{v}_n(t) \end{cases}$$

with $f(\vec{r},\vec{k},t) = \sum_n \delta(\vec{r}-\vec{r}_n(t))\,\delta(\vec{k}-\vec{k}_n(t))$ [1]

---

* Contribution of electron n: $\delta f_n(\vec{r},\vec{k},t) = \delta(\vec{r}-\vec{r}_n(t))\,\delta(\vec{k}-\vec{k}_n(t))$

$$\frac{\partial \delta f_n}{\partial t} = \vec{\nabla}_{r_n}\delta f_n \cdot \frac{d\vec{r}_n}{dt} + \vec{\nabla}_{k_n}\delta f_n \cdot \frac{d\vec{k}_n}{dt}$$

But [1] $\Rightarrow$ $\vec{\nabla}_{r_n} f = -\vec{\nabla}_r f$ and $\vec{\nabla}_{k_n} f = -\vec{\nabla}_k f$

* Hence, with MC trajectories: $\dfrac{\partial \delta f_n}{\partial t} = -\vec{\nabla}_r \delta f_n \cdot \vec{v}_n - \dfrac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k \delta f_n + \underbrace{\vec{\nabla}_{k_n}\delta f_n \cdot \left.\dfrac{\partial \vec{k}_n}{\partial t}\right|_{scatt}}_{\left.\dfrac{\partial \delta f_n}{\partial t}\right|_{scatt}}$

* Summing over $n \Rightarrow$ BTE is recovered

The particle Monte Carlo method

☞ **Statistical solution: particle *Monte Carlo method***

- $f\left(\vec{r},\vec{k},t\right) \rightarrow$ assembly of individual particles
- 1 particle $\Leftrightarrow \vec{r}\left(t\right),\ \vec{k}\left(t\right)$
- N particles allow us to reconstruct $f\left(\vec{r},\vec{k},t\right)=\sum_i \delta\left(r-r_i\left(t\right)\right)\delta\left(k-k_i\left(t\right)\right)$

  $\rightarrow$ no complicated equation to solve

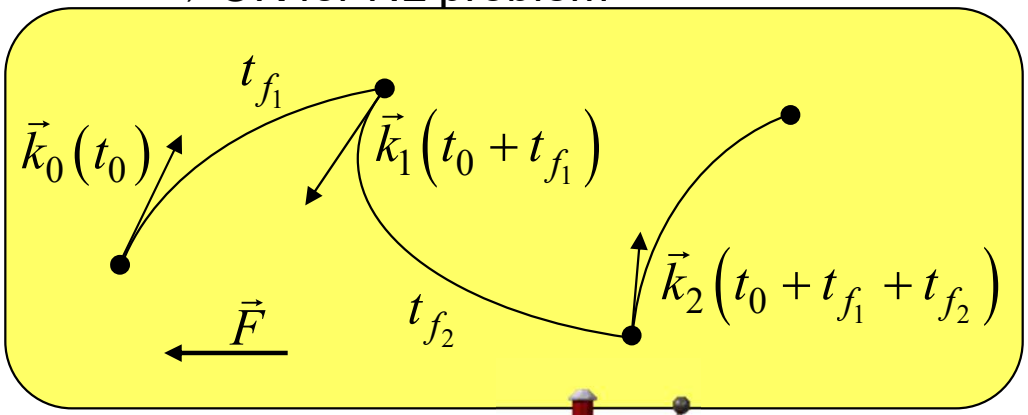
  $\rightarrow$ same physical (or even better) content as the deterministic solution

  $\rightarrow$ **complex scattering mechanism are easily implemented**

  $\rightarrow$ suitable for device simulation (even in 3D)

  $\rightarrow$ **no assumption about *f***

  $\rightarrow$ OK for NL problem



carrier trajectory: succession of free flights interrupted by instantaneous scatterings

scattering rates $\lambda_i\left(\vec{k}\right)$ ⇒ 

random selection of ⇒

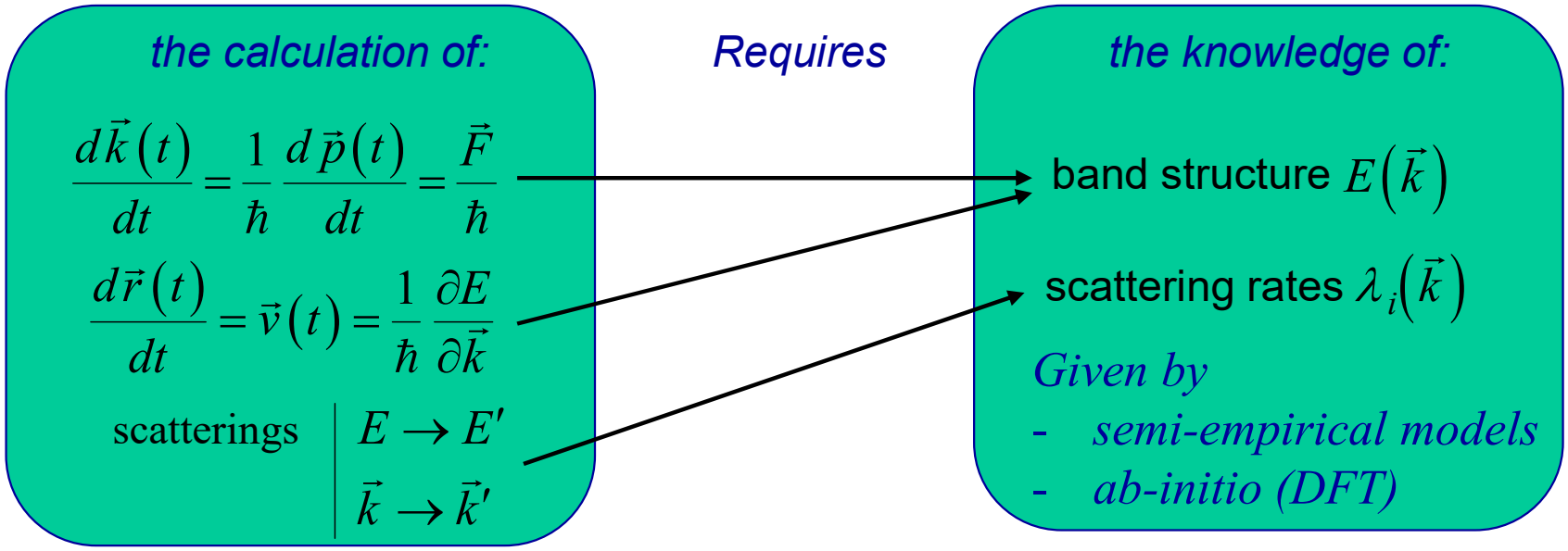
- time of free flights t_f
- type of scattering i
- effect of scattering (ΔE, θ)

(Monte Carlo algorithm)

The particle Monte Carlo method

1 particule is characterized at time *t* by $\left(\vec{r},\vec{k}\right)$

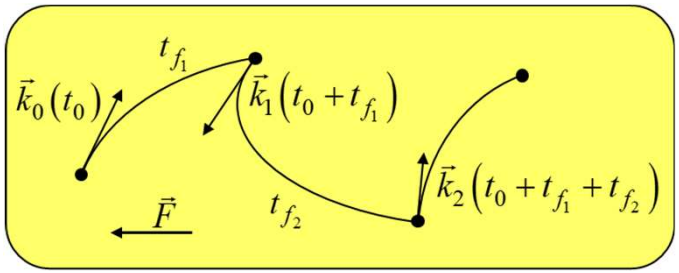
Problem : determination of $\vec{k}(t)$ and $\vec{r}(t)$ under the action of forces and scattering events



$\lambda_i\left(\vec{k}\right)$ = scattering rate of interaction process *i*
= probability per unit of time that an electron in state $\vec{k}$ scatters to any state $\vec{k}'$ by an interaction process of type *i*

$$\lambda_i\left(\vec{k}\right)=\int S_i\left(\vec{k},\vec{k}'\right)d\vec{k}'$$

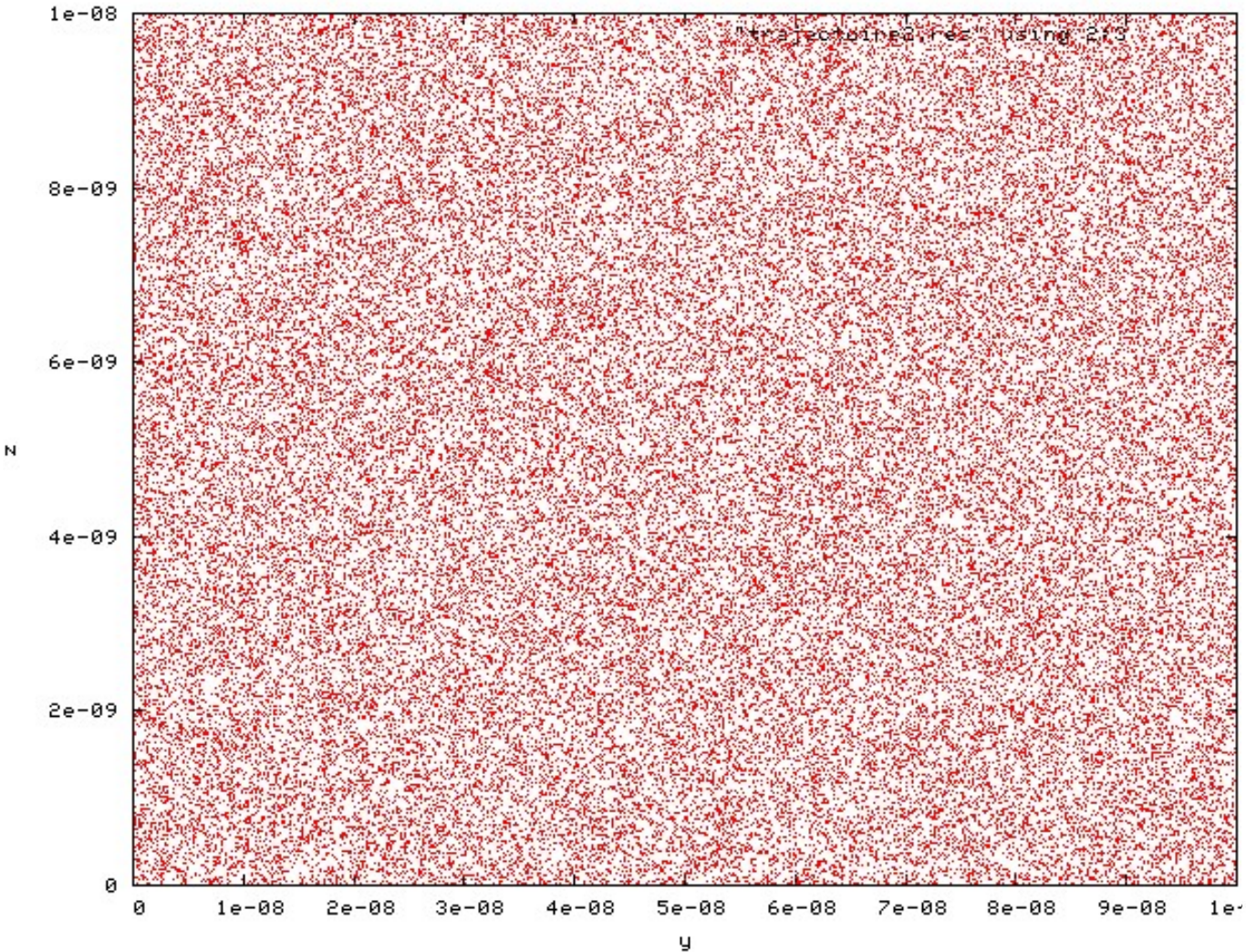
Diffusion: Illustration of trajectories

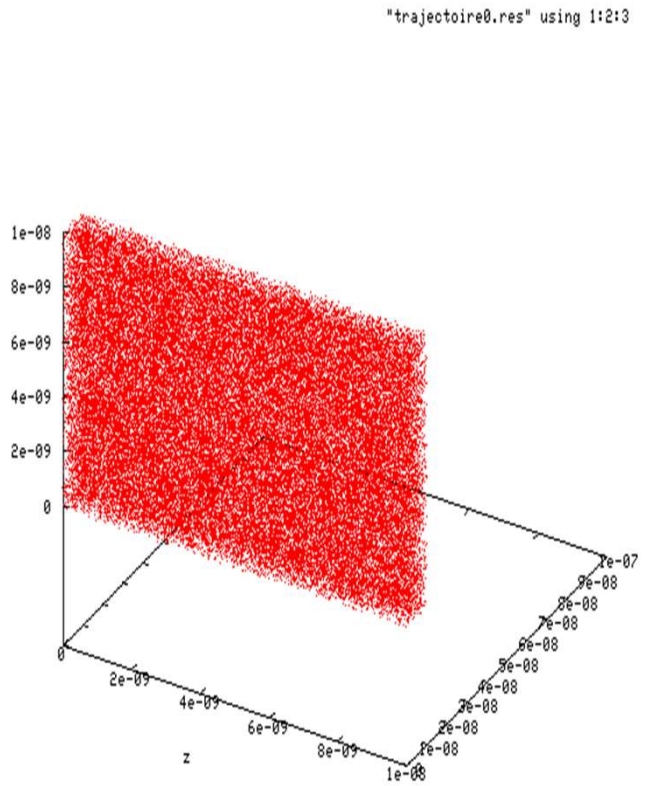


Intervalle du temps 1.e-13 s

Intervalle du temps 1.e-12 s

Intervalle du temps 1.e-11 s





Monte Carlo method: selection of free-flight duration

1. Suppose $\lambda_{tot}(E) = \sum_i \lambda_i(E) = \text{Const} = \lambda_0$

Consider n_{CF} = population of electrons that have not experienced any collision since t = 0
(CF = Collision-Free)

Each electron having the same scattering rate λ_0, the time rate of change of n_{CF} is:

$$\frac{dn_{CF}}{dt} = -\lambda_0 \, n_{CF} \quad \Rightarrow \quad n_{CF}(t) = n_{CF}(0)\exp(-\lambda_0 t)$$

→ The probability that an electron has a free flight (no collision) during the time t is therefore:

$$\frac{n_{CF}(t)}{n_{CF}(0)} = \exp(-\lambda_0 t)$$

→ The probability that an electron suffers a collision during the time interval dt is:

$$\lambda_0 \, dt$$

⇒ The probability that an electron suffers its first collision between t and $t + dt$ is:

$$P(t)dt = \exp(-\lambda_0 t) \times \lambda_0 \, dt$$

Monte Carlo method: selection of free-flight duration

The probability that the free-fight time is less than t_f is:

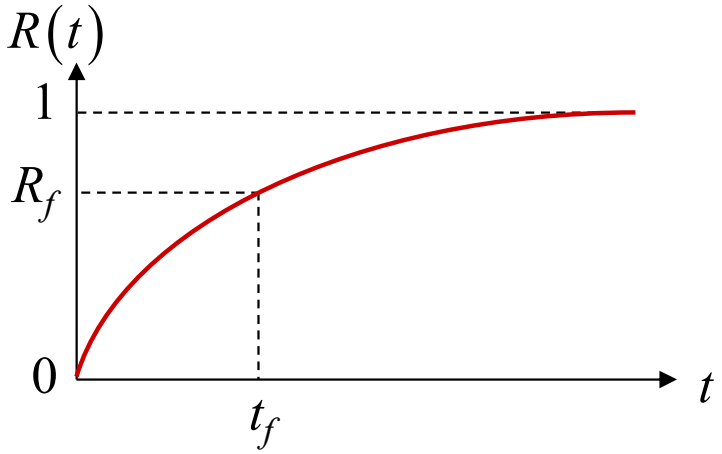
$$R_f = R(t_f) = \int_0^{t_f} P(t)\,dt$$

of course we have: $R(\infty) = \int_0^{\infty} P(t)\,dt = 1$

To select t_f according to $P(t)$

$\Leftrightarrow$

To select a random number R_f uniformly distributed between 0 and 1, i.e. according to $P_r(R) = 1$



$$P_r(R)\,dR = P(t)\,dt$$

$$\int_0^{R_f} dR = \int_0^{t_f} P(t)\,dt \quad \Rightarrow \quad R_f = 1 - \exp\left(-\lambda_0 t_f\right)$$

$$t_f = -\frac{\ln\left(R'_f\right)}{\lambda_0} \qquad \text{where} \quad R'_f = 1 - R_f$$

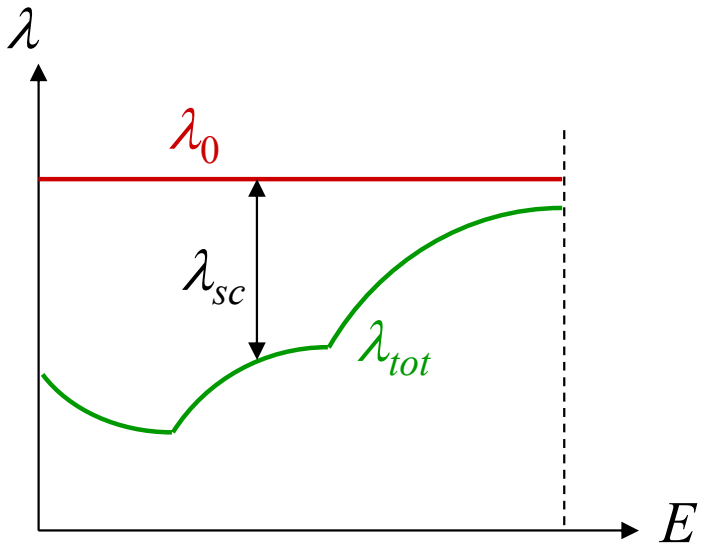
Monte Carlo method: selection of free-flight duration

2. BUT $\lambda_{tot}(E) = \sum_i \lambda_i(E)$ is not constant

solution: we introduce a new interaction

⇒ fictitious interaction: **self-scattering** $\lambda_{sc}(E)$

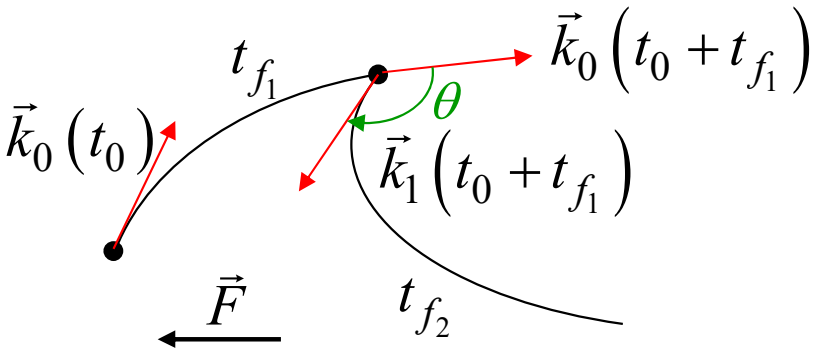
$$\lambda_{tot}(E) + \lambda_{sc}(E) = \text{Const} = \lambda_0$$



(if selected this interaction has no effect on the electron state)

Monte Carlo method: selection of scattering event

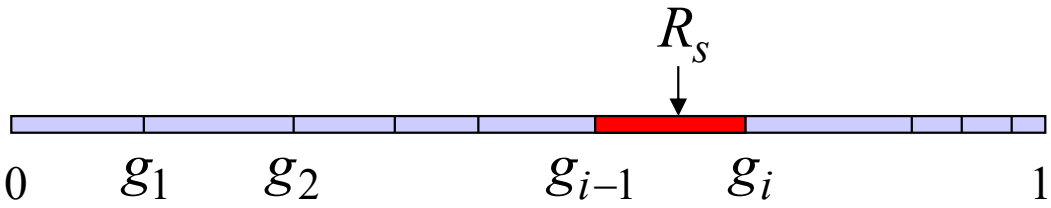
*** Type of scattering**: after each free flight, the electron undergoes a scattering event



of which type ?

selection using a random number R_s uniformly distributed between 0 and 1:

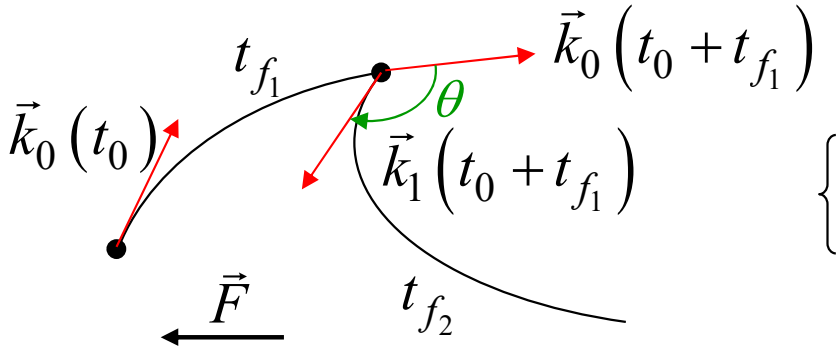
$$g_j(E) = \sum_{i=1}^{j} \lambda_i(E)/\lambda_0$$



$\rightarrow$ in this case the scattering process *i* is selected

Monte Carlo method: selection of scattering event

*** Effect of selected scattering**: deviation of the wave vector and possible energy exchange



$$\begin{cases} \text{in case the case of phonon process: } E' = E \pm \hbar\omega_q \\ \text{in the case of other processes: } \quad E' = E \end{cases}$$

$$\lambda_i(\vec{k}) = \int S_i(\vec{k},\vec{k}')\, d\vec{k}' = \iiint S_i(k,k',\theta,\varphi)\, dk' \sin\theta \; d\theta \, d\varphi$$

$$= \iiint S_i(E,E',\theta,\varphi) J(E,\theta,\varphi)\, dE' \sin\theta \; d\theta \, d\varphi = A(E) \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\varphi \, B(\theta,\varphi)$$

$$I(\theta_s,\varphi_s) = \int_0^{\theta_s} d\theta \sin\theta \int_0^{\varphi_s} d\varphi \, B(\theta,\varphi)$$

selection of θ_s and φ_s with random numbers R_θ and R_φ :

case of isotropic scattering:

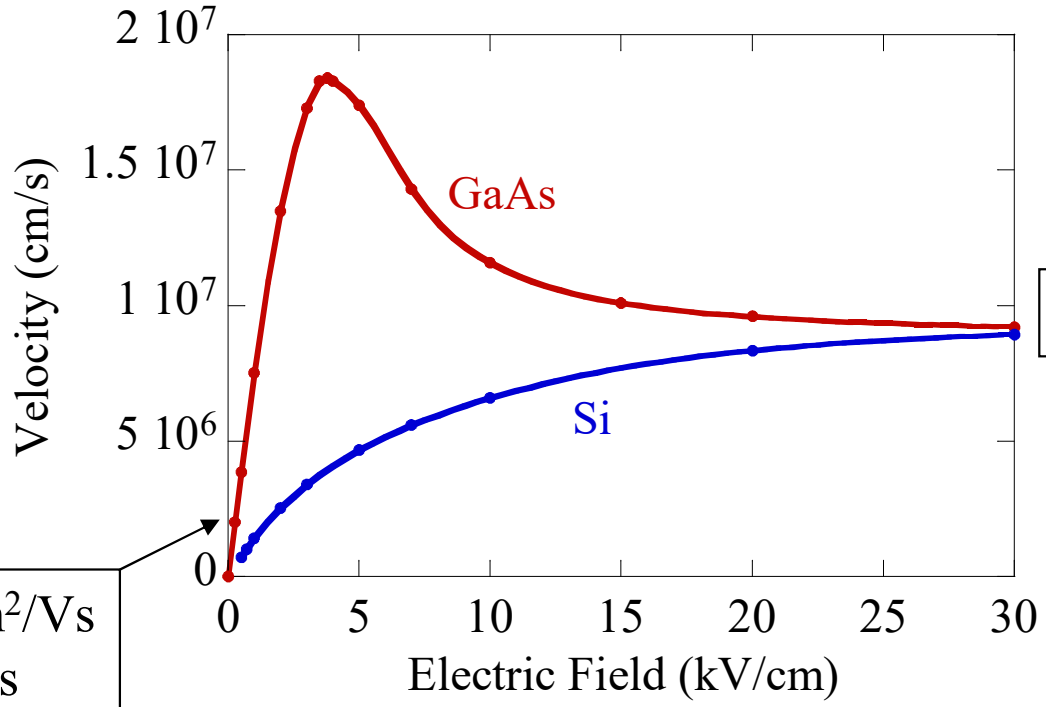
$$\begin{cases} P(\theta_s) = (1-\cos\theta_s)/2 \\ P(\varphi_s) = \varphi_s / 2\pi \end{cases} \Rightarrow \begin{cases} \cos\theta_s = 1 - 2R_\theta \\ \varphi_s = 2\pi R_\varphi \end{cases}$$

$$\begin{cases} P(\theta_s) = \dfrac{I(\theta_s,2\pi)}{I(\pi,2\pi)} = R_\theta \rightarrow \theta_s \\ P_{\theta_s}(\varphi_s) = \dfrac{I(\theta_s,\varphi_s)}{I(\theta_s,2\pi)} = R_\varphi \rightarrow \varphi_s \end{cases}$$

Transport Monte Carlo simulation

Velocity-Field characteristics in uniform material – Stationary transport

(equilibrium between perturbation and relaxation effects)

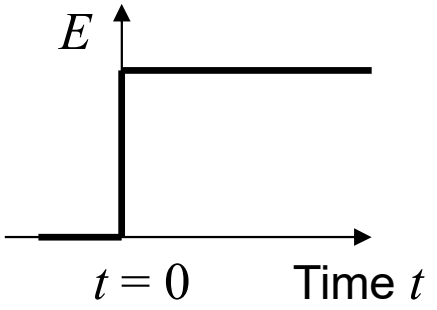


$v_{sat} \approx 10^7$ cm/s

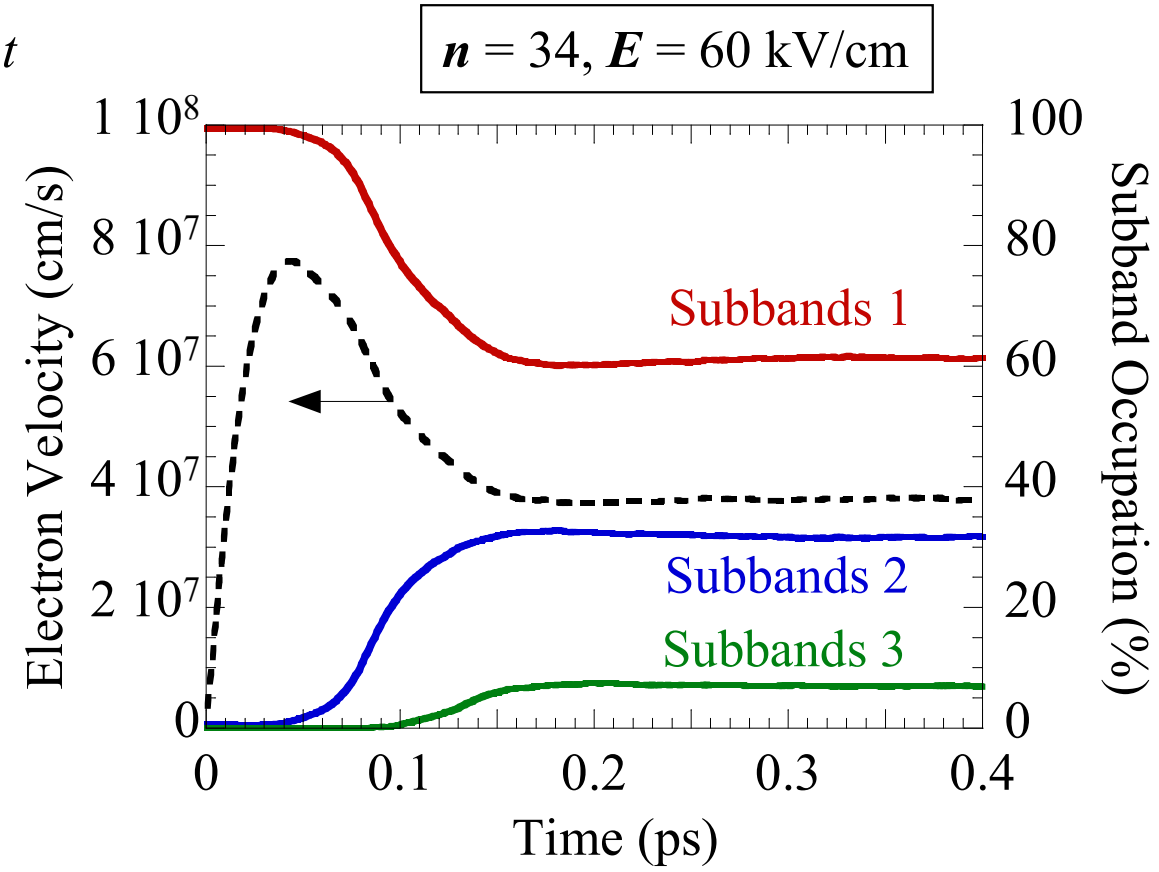
μ (GaAs) ≈ 7000 cm^2/Vs
μ (Si) ≈ 1500 cm^2/Vs

↳ Extraction of intrinsic transport parameters (mobility, relaxation times, saturation velocity,…)

CNT: Transient behaviour



- Response to a step field
- Time evolution of average electron velocity



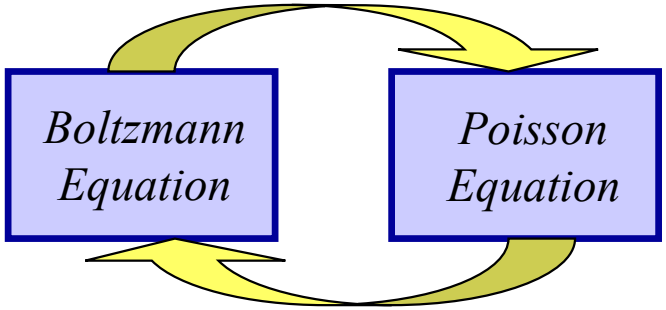
→ **Transient effect during 0.1 ps before reaching the stationary state**

→ **High Velocity Overshoot : $v_{peak} = 7.8\times10^7$ cm/s for $n = 34$**

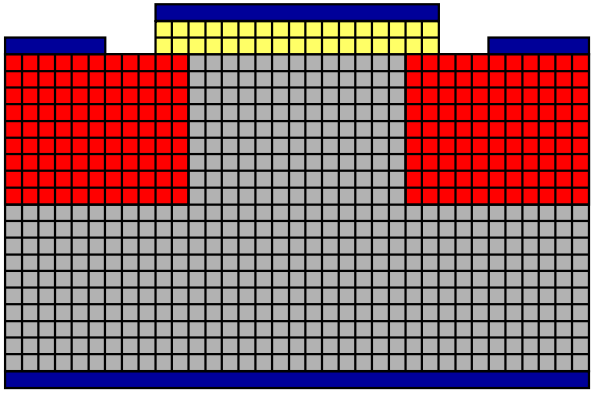
$v_{stat} = 3.8\times10^7$ cm/s

Solving the BTE for device simulation

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \sum_i \left[\int f\left(\vec{k}'\right) S_i\left(\vec{k}',\vec{k}\right) d^3\vec{k}' - \int f\left(\vec{k}\right) S_i\left(\vec{k},\vec{k}'\right) d^3\vec{k}'\right]$$



$$div(\epsilon.\vec{E}) = \rho(f)$$



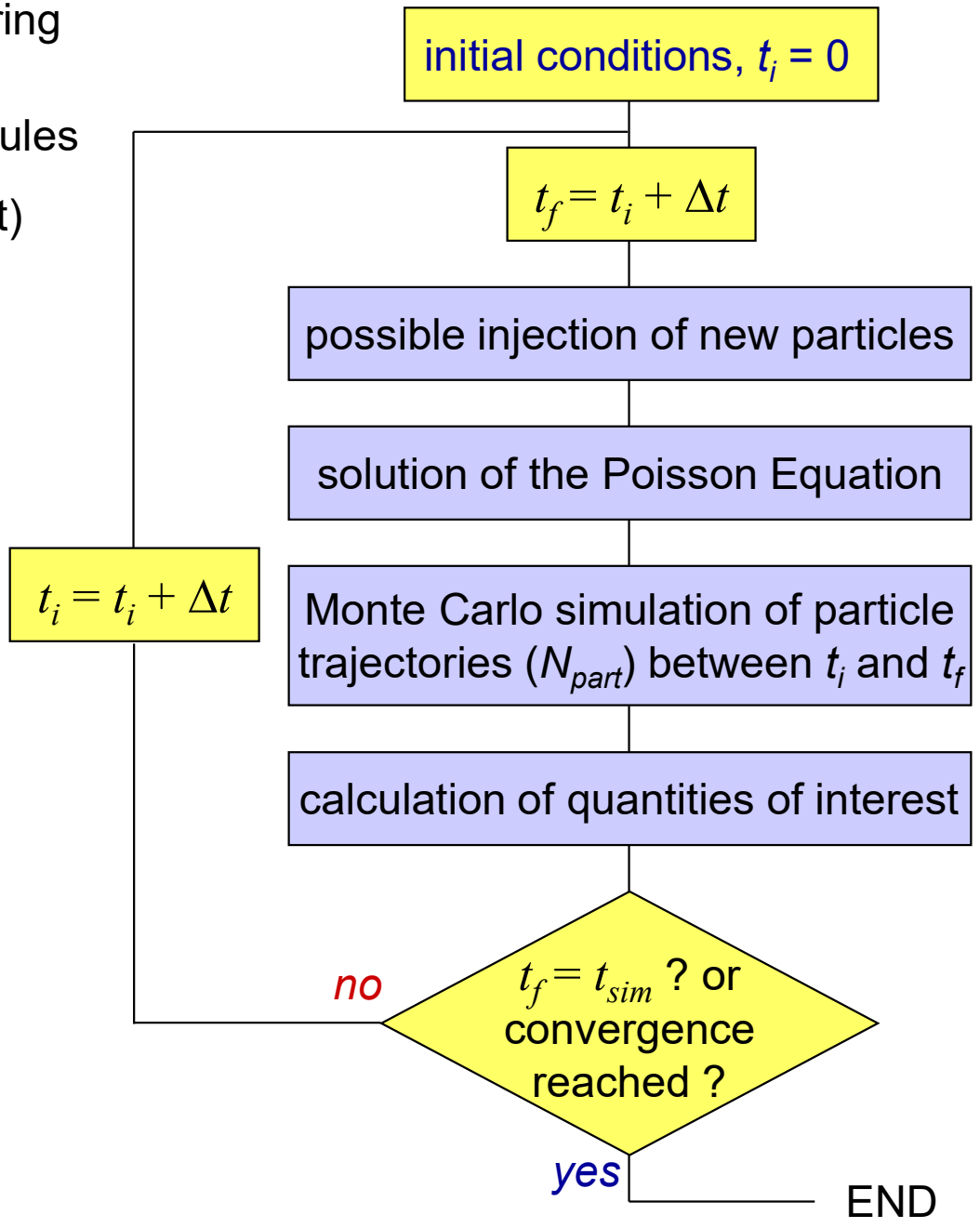
- distribution of forces $\vec{F} = -e\vec{E}$ by solving Poisson's equation

- statistical solution: **Monte Carlo methods (MC)**
- Direct solution of the Poisson equation

Monte Carlo method: flow chart

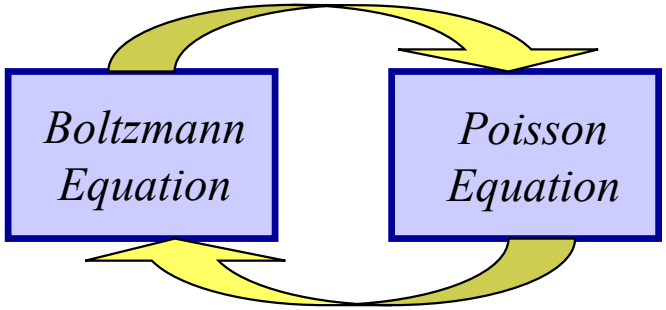
For the simulation during a time t_{sim} of a device containing N_{part} particules

(N_{part} is not constant)

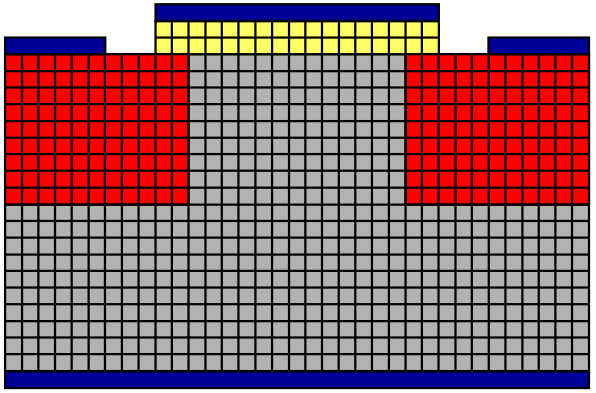


MC: sampling

$$\frac{\partial f}{\partial t} = -\vec{v}\cdot\vec{\nabla}_r f - \frac{\vec{F}}{\hbar}\cdot\vec{\nabla}_k f + \sum_i \left[\int f\left(\vec{k}'\right) S_i\left(\vec{k}',\vec{k}\right) d^3\vec{k}' - \int f\left(\vec{k}\right) S_i\left(\vec{k},\vec{k}'\right) d^3\vec{k}'\right]$$



$$div(\epsilon.\vec{E}) = \rho(f)$$



- Spatial discretization : $-\max \delta x$ = Debye length
  = screening length

$$L_D = \frac{1}{q_s} = \sqrt{\frac{\varepsilon k_B T}{e^2 n}}$$ n = electron density

- Time discretization : $-\max \delta t$ = dielectric relaxation time
  (or plasma oscillation)

$$\tau_D = \frac{\varepsilon_0 \varepsilon_{SC}}{\sigma_0} = \frac{\varepsilon_0 \varepsilon_{SC}}{qN_D \mu_n}$$

Space- and time-discretization issue: Debye length and Dielectric relaxation time

Consider an N-type homogeneous region

Under equilibrium:

- Equilibrium density: $n_0 = N_D$ Electric field: $E = 0$
- Conductivity: $\sigma_0 = q\, n_0\, \mu_n$

Small local desequilibrium: $n(x,t) = n_0 + \Delta n(x,t)$

$\Rightarrow$ An electric field builds up to restore the equilibrium according to the continuity equation:

$$\frac{\partial n(x,t)}{\partial t} = \frac{1}{q}\frac{\partial J(x,t)}{\partial x}$$

where the current density is: $J(x,t) = \sigma_0 E(x,t) + q\, D_n \frac{\partial n(x,t)}{\partial x}$

and the electric field obeys Poisson's Eq.: $\frac{\partial E(x,t)}{\partial x} = \frac{q}{\varepsilon_s\, \varepsilon_0}\left(n_0 - n(x,t)\right)$

Space- and time-discretization issue: Debye length and Dielectric relaxation time

By neglecting the second order terms, these 3 equations lead to:

$$\frac{\partial n(x,t)}{\partial t} = \frac{\sigma_0}{\varepsilon_s\,\varepsilon_0} n(x,\mathrm{t}) - D_n \frac{\partial^2 n(x,t)}{\partial x^2}$$

* Time desequilibrium → $$\frac{\partial n(x,t)}{\partial t} = \frac{\sigma_0}{\varepsilon_s\,\varepsilon_0} n(x,\mathrm{t}) \Rightarrow n(x,t) = n_0 \exp\left[-\frac{t}{\tau_D}\right]$$

$$\boxed{\tau_D = \frac{\varepsilon_s\,\varepsilon_0}{\sigma_0} = \frac{\varepsilon_s\,\varepsilon_0}{q\,\mu_n\,n_0}}$$ Dielectric Relaxation Time

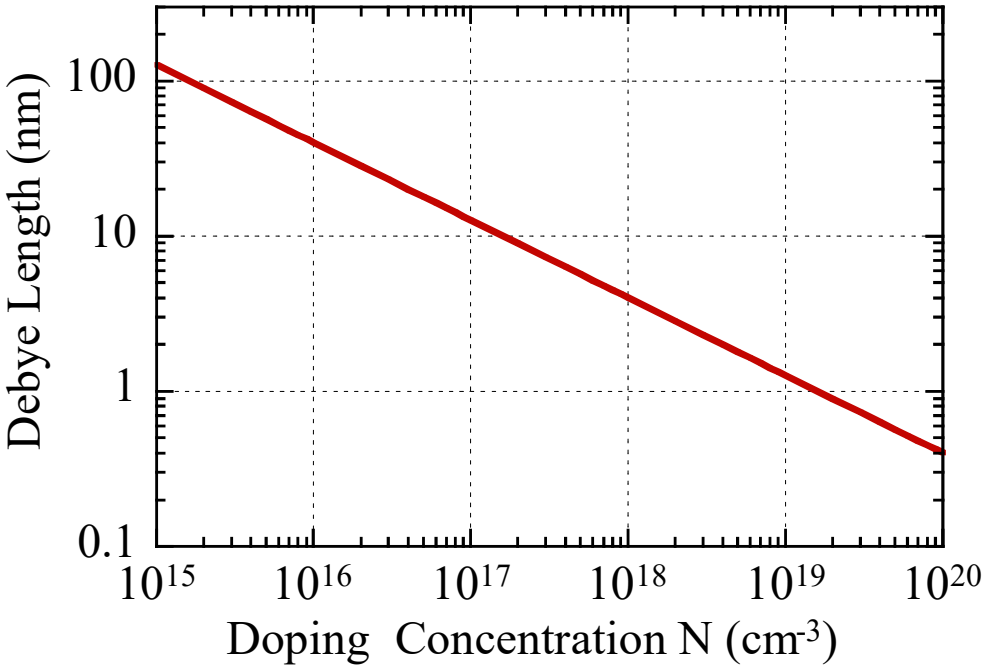
* Space desequilibrium → $$n(x,t) - \frac{\varepsilon_s\,\varepsilon_0}{\sigma_0}\frac{k_B T}{q^2}\frac{\partial^2 n(x,t)}{\partial x^2} \Rightarrow n(x,t) = n_0 \exp\left[-\frac{x}{L_D}\right]$$

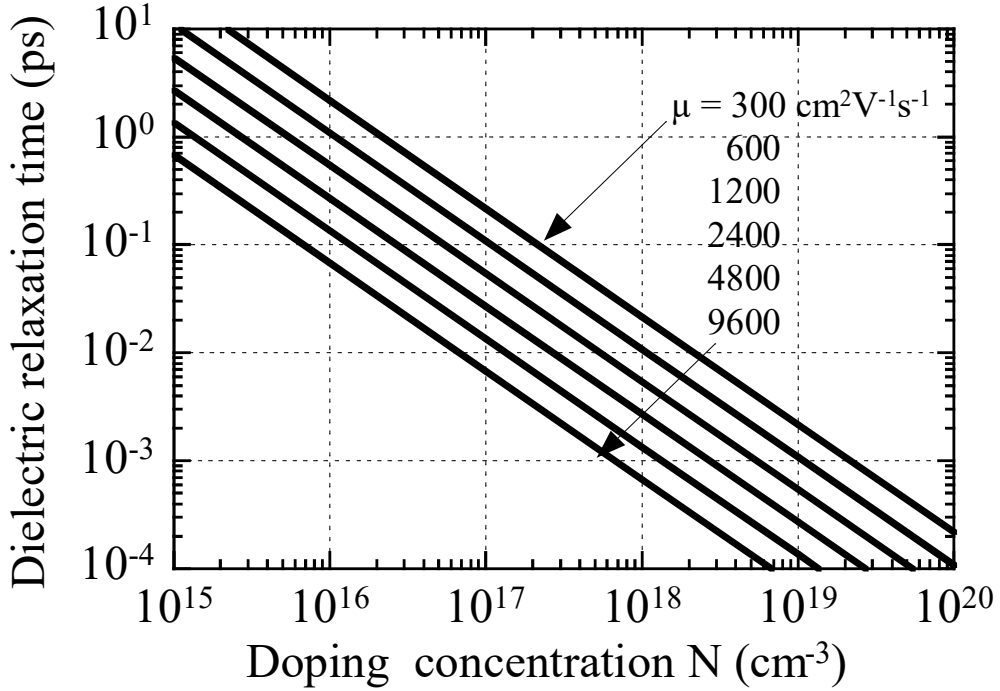
$$\boxed{L_D = \sqrt{\frac{\varepsilon_s\,\varepsilon_0\,k_B T}{q^2\,n_0}}}$$ Debye Length

Debye length and Dielectric relaxation time

$$L_D = \sqrt{\frac{\varepsilon_s \, \varepsilon_0 \, k_B T}{q^2 \, n_0}}$$

$$\tau_D = \frac{\varepsilon_s \, \varepsilon_0}{\sigma_0} = \frac{\varepsilon_s \, \varepsilon_0}{q \, \mu_n \, n_0}$$



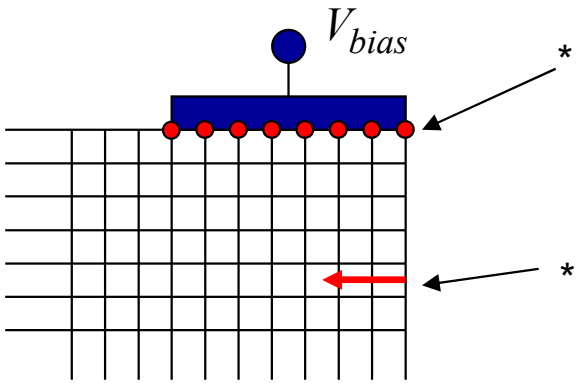


We have to satisfy: $\Delta x < L_D$ and $\Delta t < \tau_D$

boundary conditions

Device = open system for which appropriate boundary conditions must be applied

1. Boundary conditions for the solution of Poisson's equation:



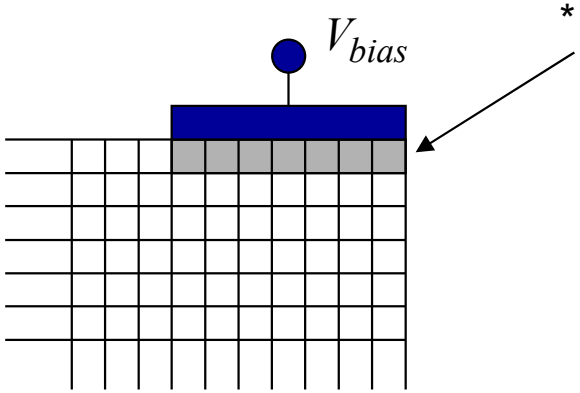
* on **nodes adjacent to a metallic contact**, the electrostatic potential is fixed:

$$V(i_{node}) = V_{bias}$$

* on **other device boundaries**, the normal component of the electric field vanishes:

$$E_{\perp} = \frac{dV}{dx} = 0$$

2. Conditions for carrier injection into the device:



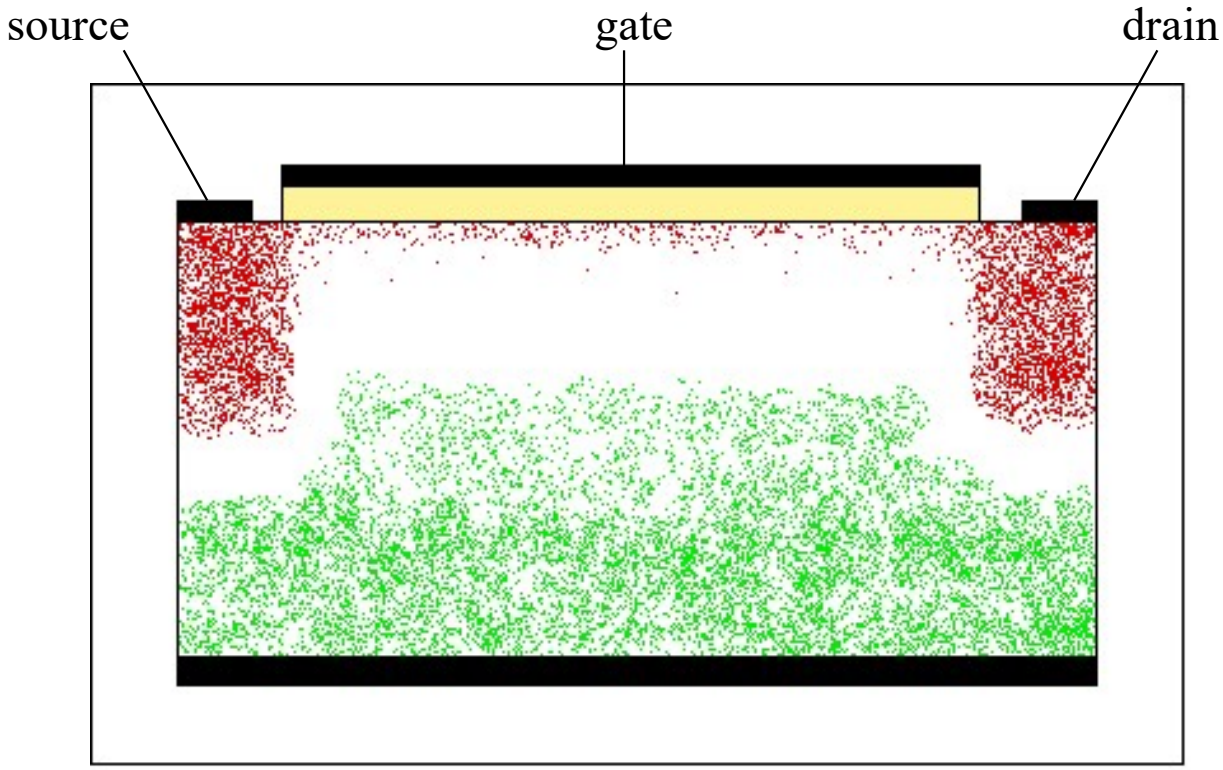
* in **the cells adjacent to the ohmic contacts**, the thermal equilibrium conditions are assumed to be recovered:

$$n = N_D \quad \text{or} \quad p = N_A$$

before each new time step iteration, this condition is checked and if necessary the appropriate number of electrons is injected. The wave vector of injected carriers is randomly selected using Fermi or (if non degenerate) Maxwell distribution.

Device Monte Carlo simulation: particle trajectories

N-channel MOSFET



red dots: electrons
green dots: holes

↳ Possibility to make movies of particle motion in the working device

Electron transport in semiconductor nanodevices using the Monte Carlo method

1. Stochastic solution

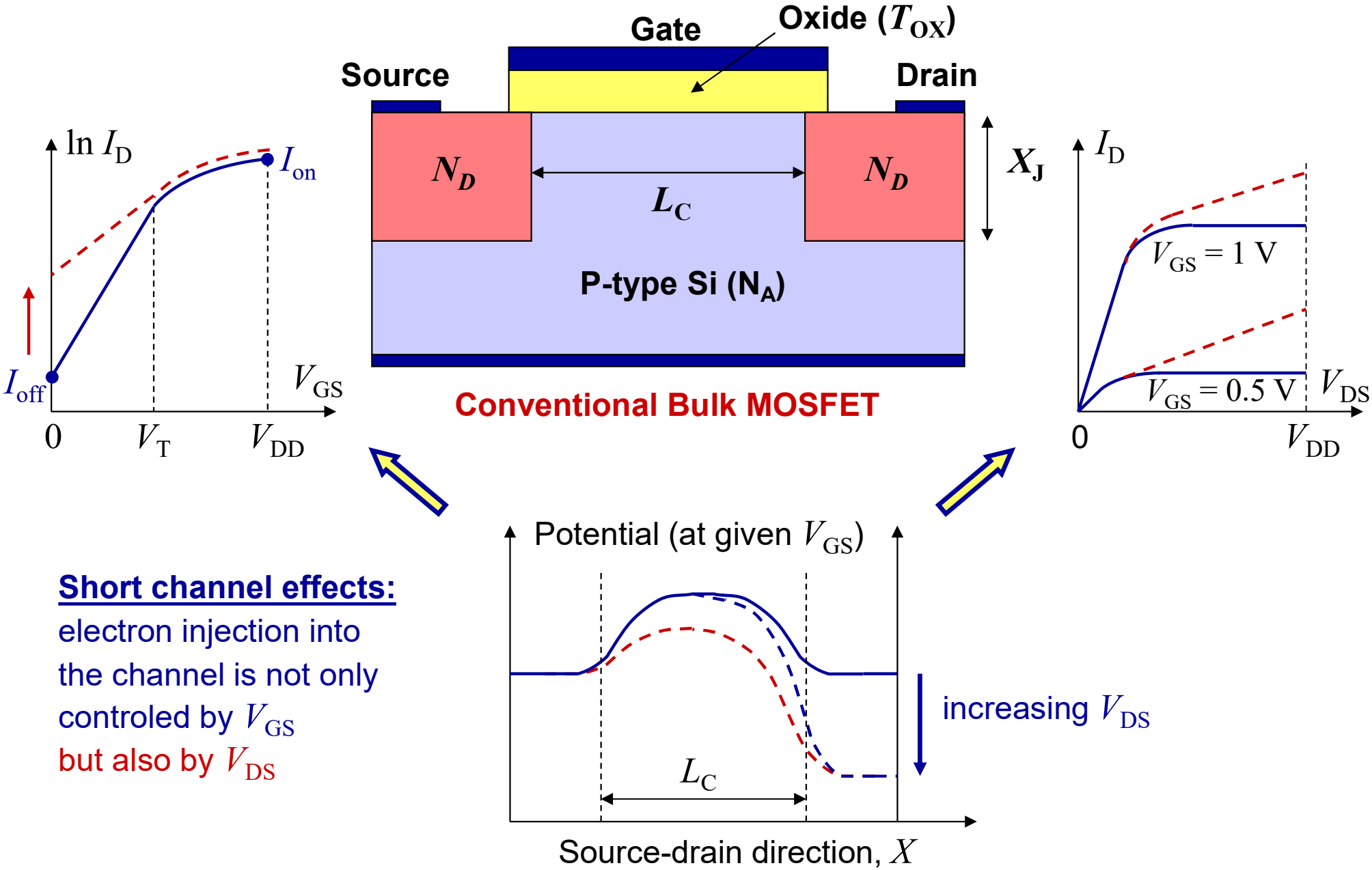
2. Boltzmann Transport Equation

3. BTE Inputs: Dispersion and Scattering

4. BTE Solution: Particle Monte Carlo method

5. BTE Applications and Examples

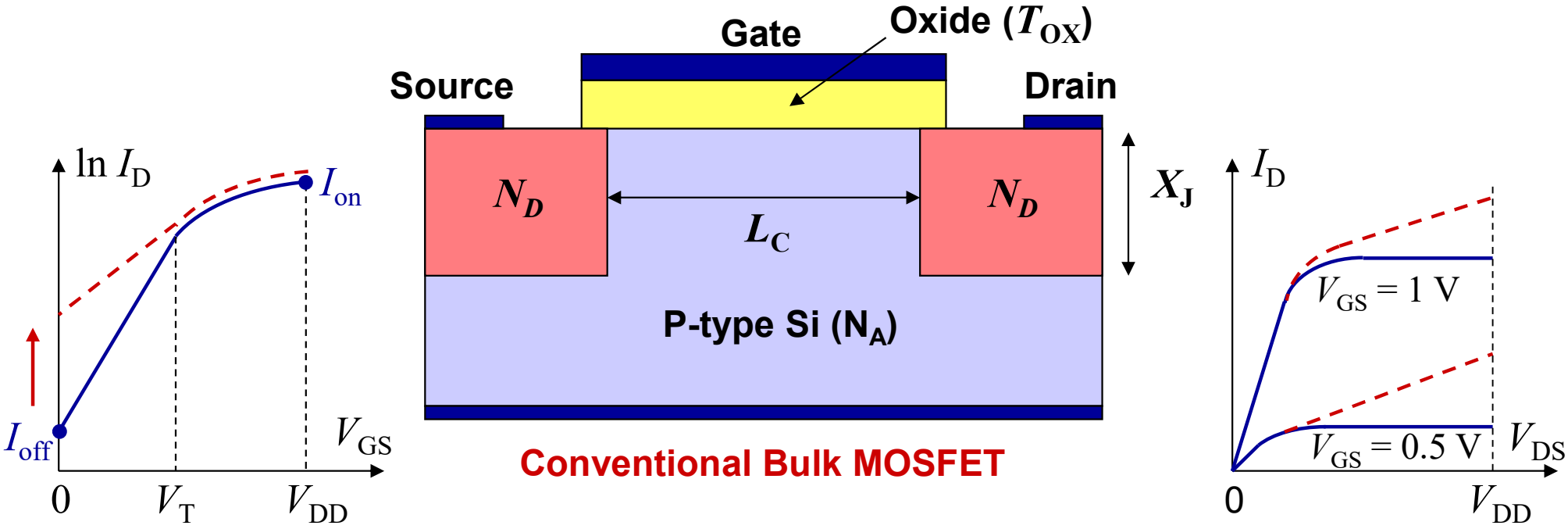
Conventional MOSFET architecture



Short channel effects:

electron injection into the channel is not only controled by V_{GS} but also by V_{DS}

Conventional MOSFET architecture



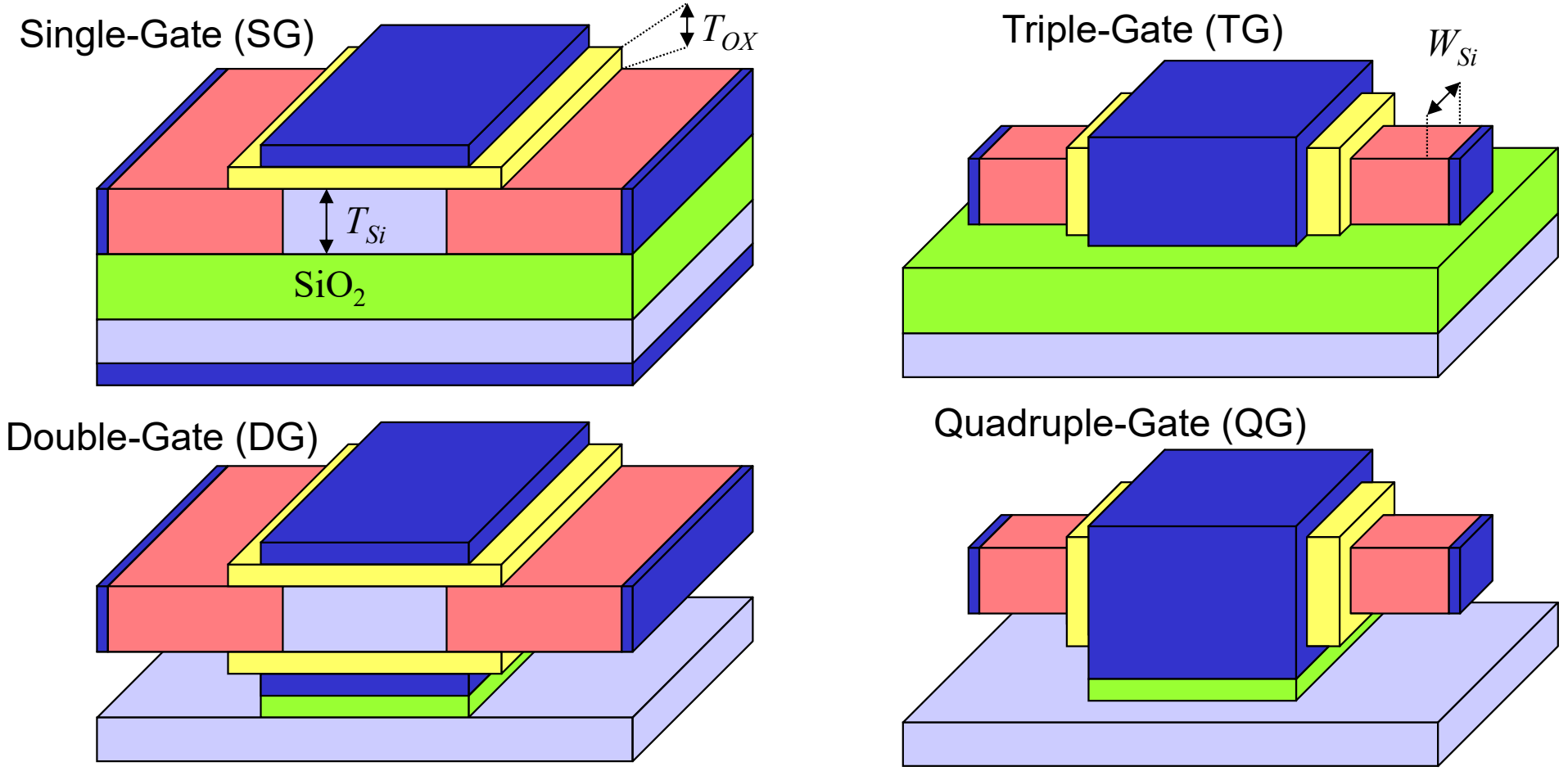
To control short-channel effects when reducing the gate and channel lengths in deca-nanometer transistors one needs:

- reduced T_{OX}, but then gate tunnelling leakage current occurs
- reduced X_J, but then access series resistance increases dramatically
- higher N_A, but then:
  - transport properties are degraded
  - sensitivity to doping fluctuations

↳ Needs for new materials and new device architectures

New MOSFET architectures on SOI substrate

Ultra-thin undoped channel & Multiple-Gate transistors

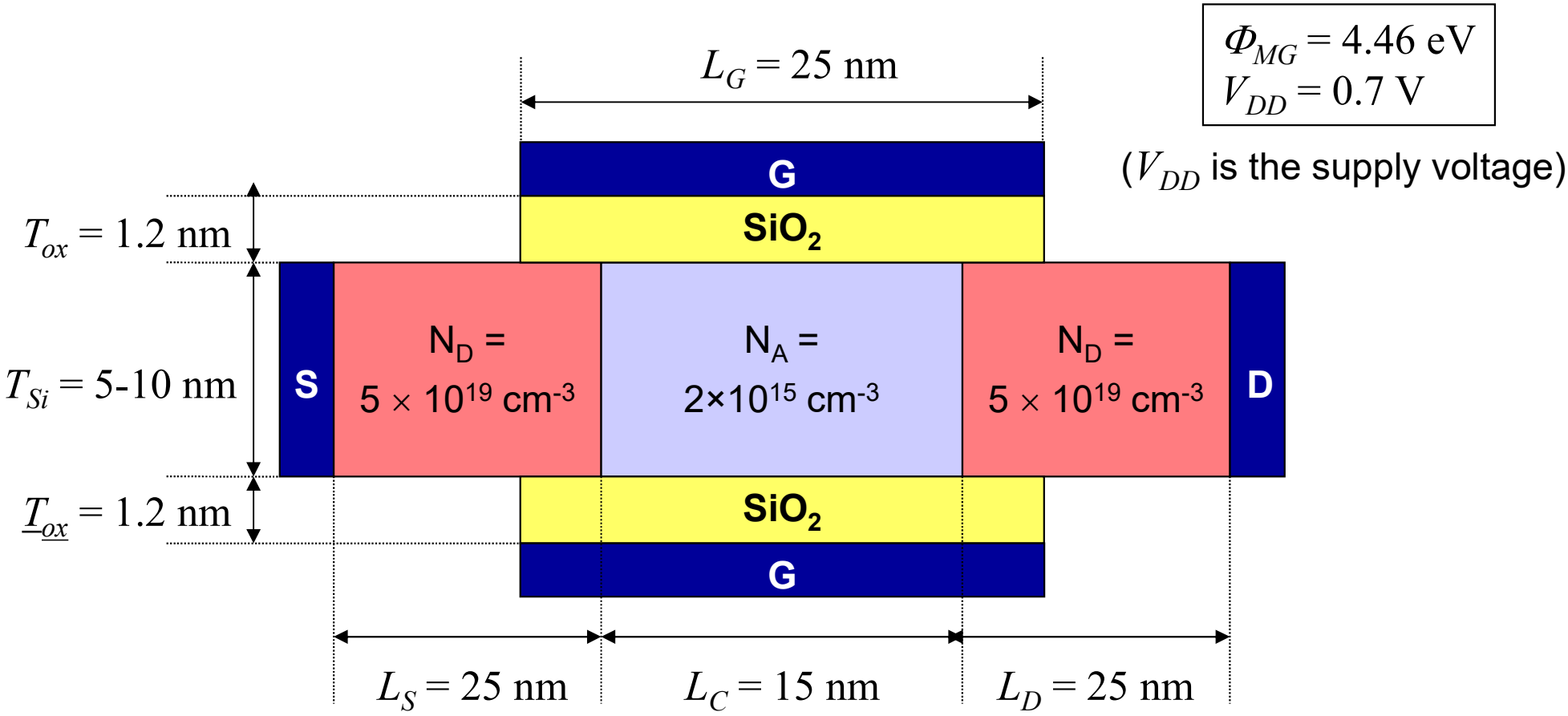


undoped channel ..... $\Rightarrow$ improved transport properties & lower fluctuations

thin channel ($T_{Si} < 10$ nm) ..... } $\Rightarrow$ improved control of short channel effects

multiple-gate ..... } $\Rightarrow$ less urgent reduction of T_{OX}

Nano-scaled DG-MOSFET

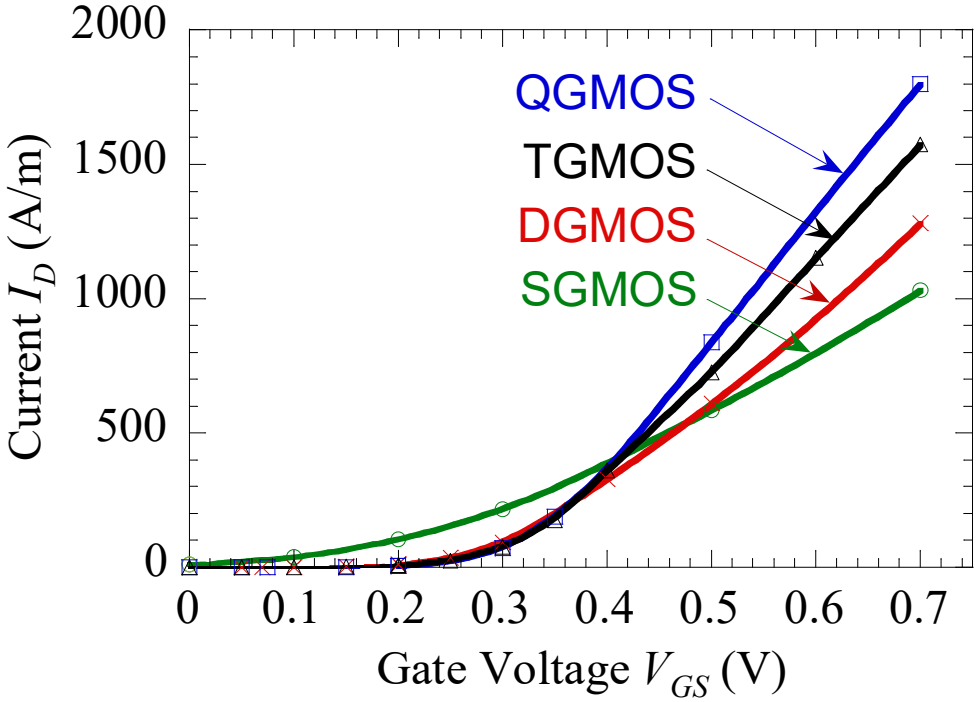


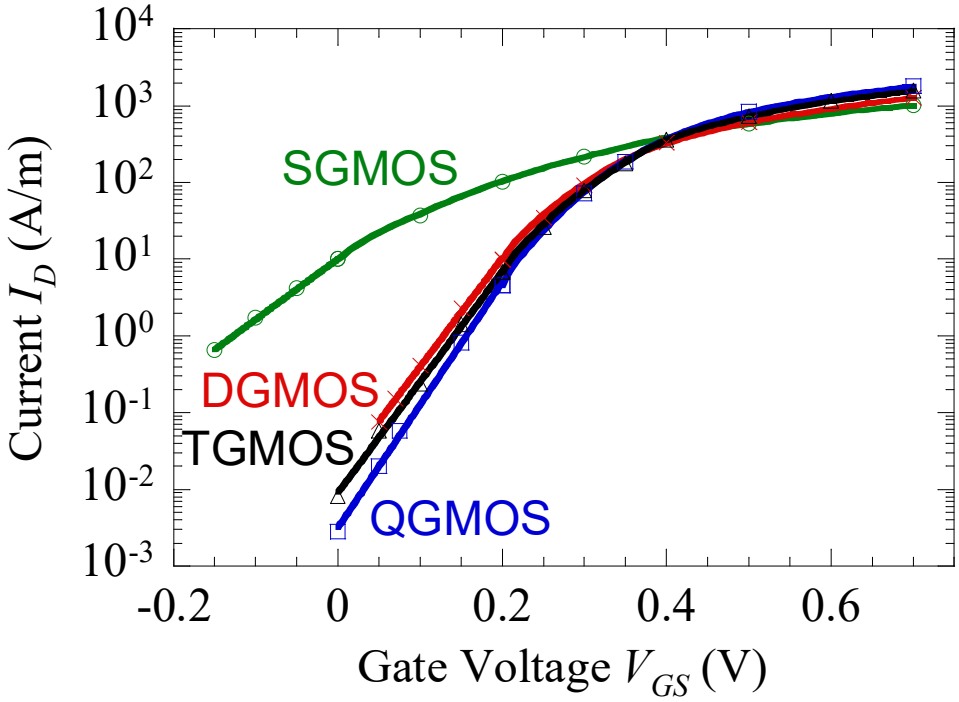
For comparison: similar design of SG, TG and QG transistors

Multiple-Gate MOSFETs: I_D-V_{GS} characteristics

$L_c = 15$ nm & $L_G = 25$ nm & $T_{Si} = 5$ nm

$V_{DS} = V_{DD} = 0.7$ V



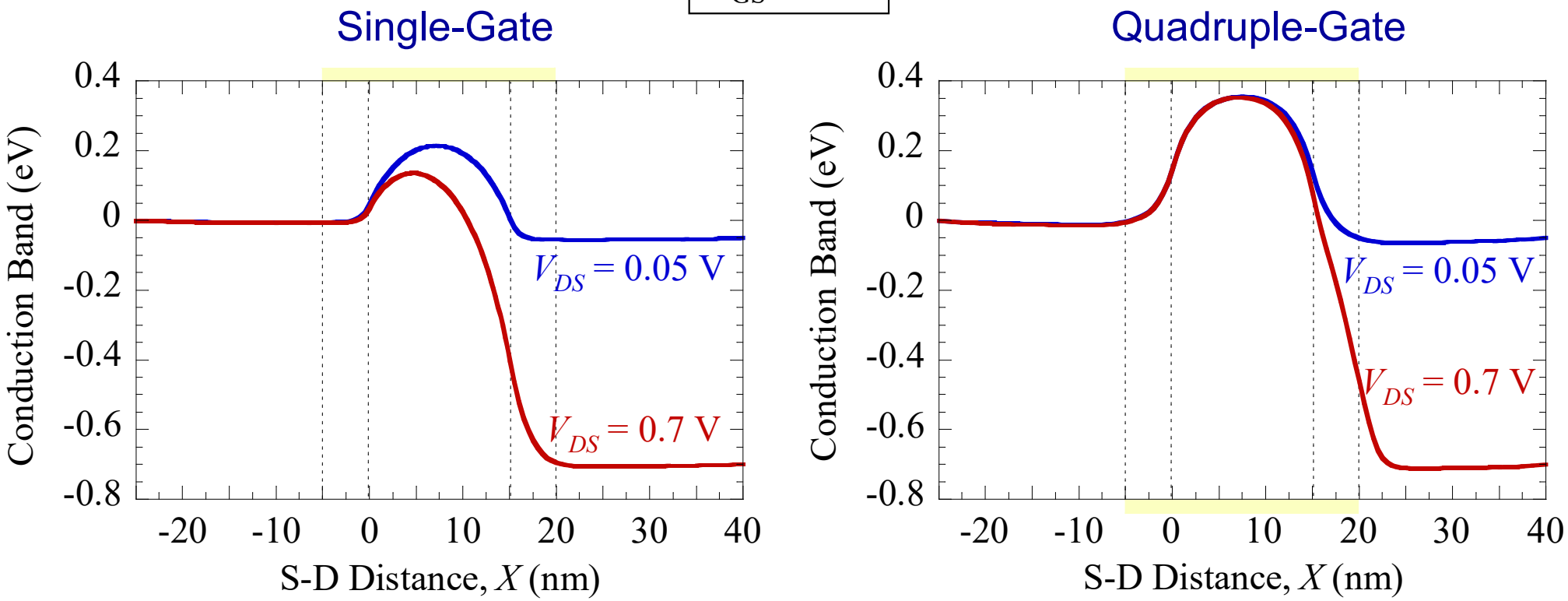


increasing the number of gates $\Rightarrow$ { * higher I_{on} ; * lower I_{off}

Multiple-Gate MOSFETs: Short-channel effects

$L_c = 15$ nm & $L_G = 25$ nm & $T_{Si} = 5$ nm

$V_{GS} = 0$ V

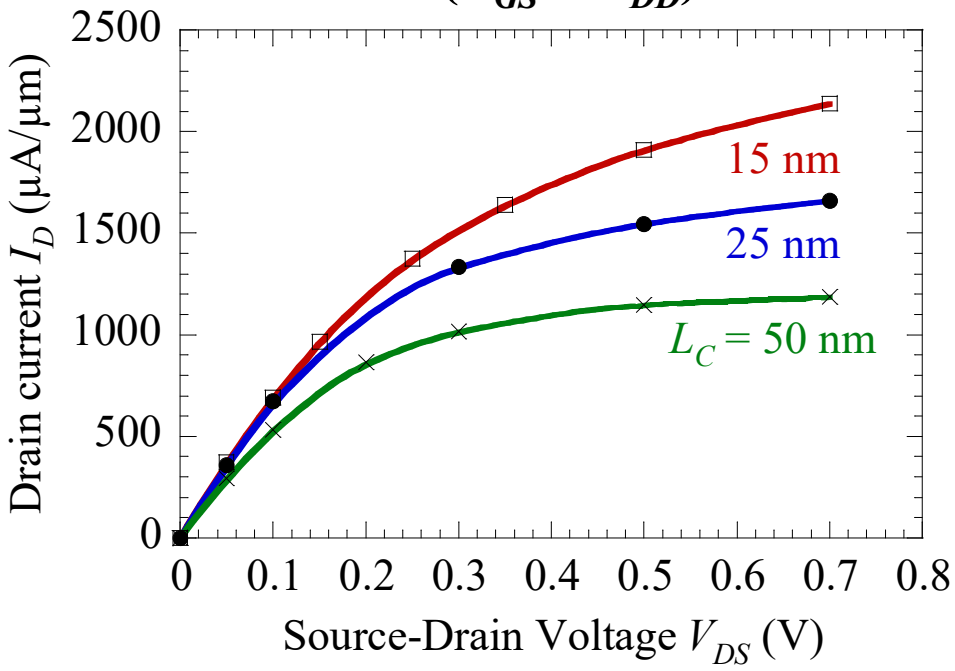


Drain-Induced Barrier Lowering (DIBL) is strongly reduced by using multiple gates

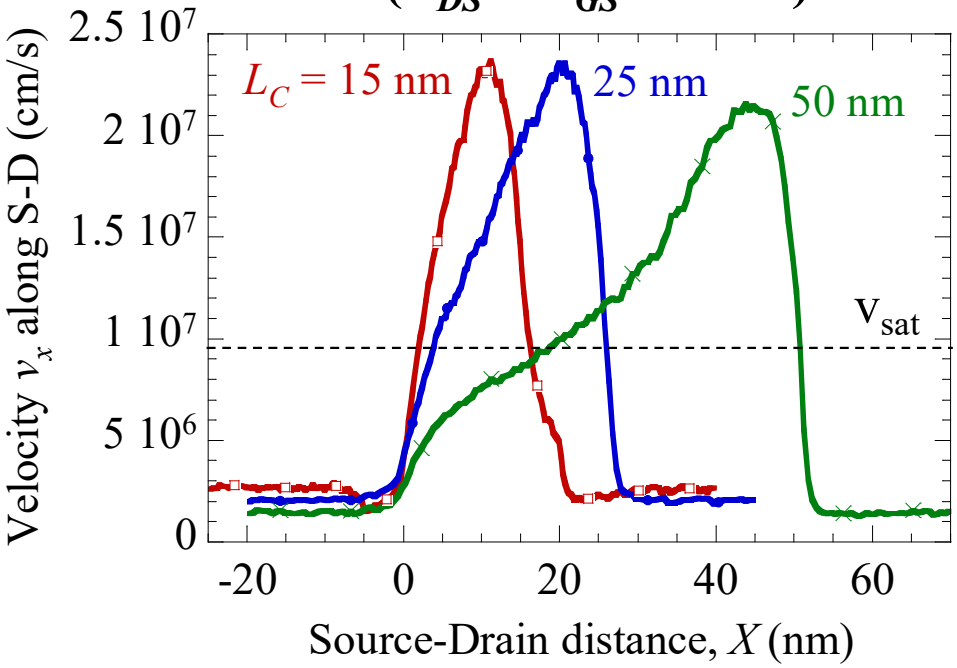
DGMOS: influence of gate length

Effective channel Length: L_C = 15 nm, 25 nm and 50 nm
T_{Si} = 10 nm

Drain characteristics
($V_{GS} = V_{DD}$)



Velocity along the channel
($V_{DS} = V_{GS} = 0.7$ V)



peak velocity > 2×10^7 cm/s
→ greater than saturation velocity = 10^7 cm/s

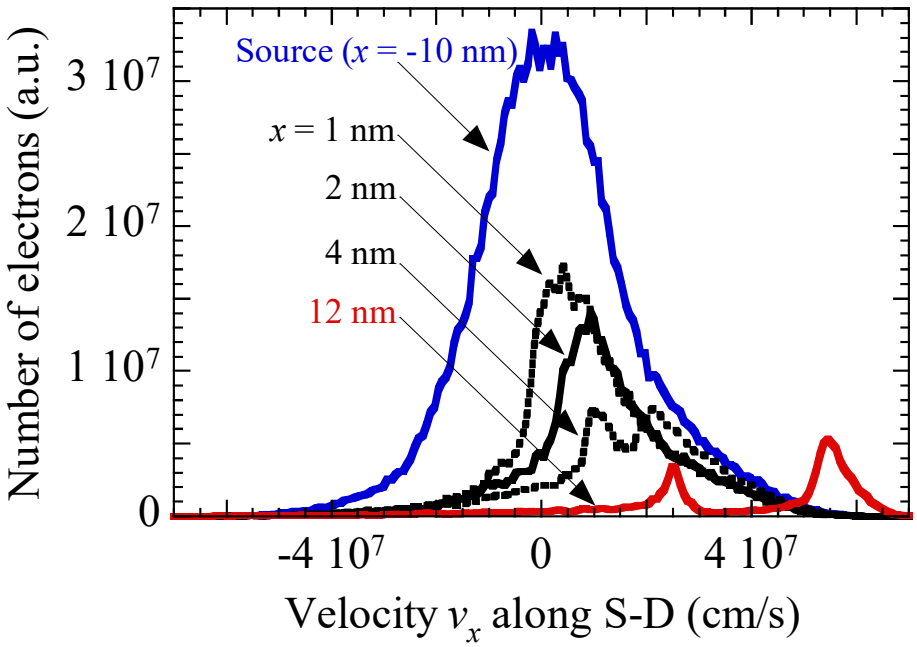
⇒ non stationary transport

DGMOS: velocity distribution

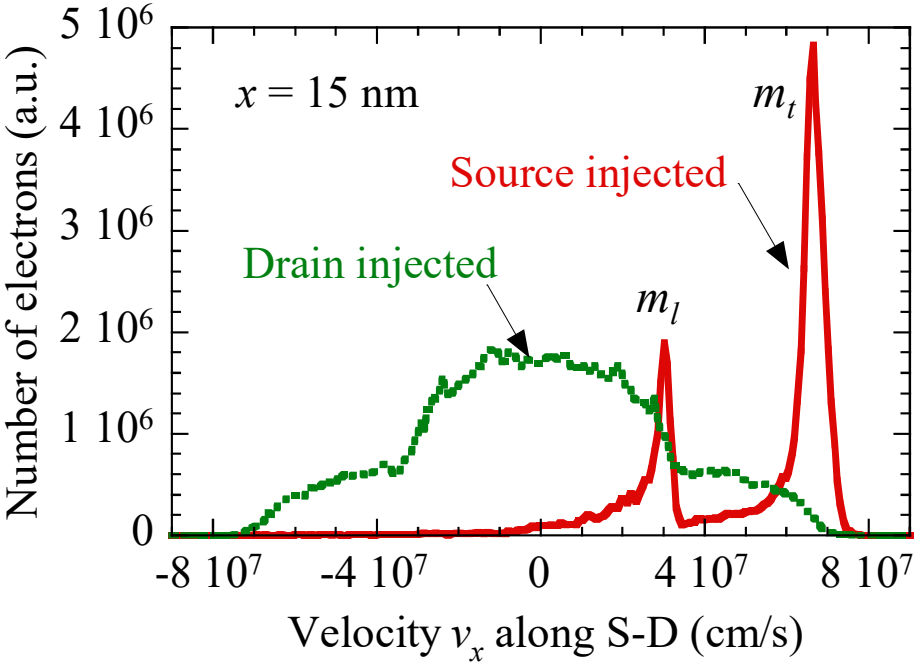
$L_C = 15$ nm

$V_{GS} = V_{DS} = V_{DD} = 0.7$ V

Evolution along the channel (electrons coming from the source)



At the drain-end of the channel



2 peaks corresponding to the velocity of ballistic electrons with either a transverse mass ($m_t = 0.19\ m_0$) or a longitudinal mass ($m_l = 0.916\ m_0$)

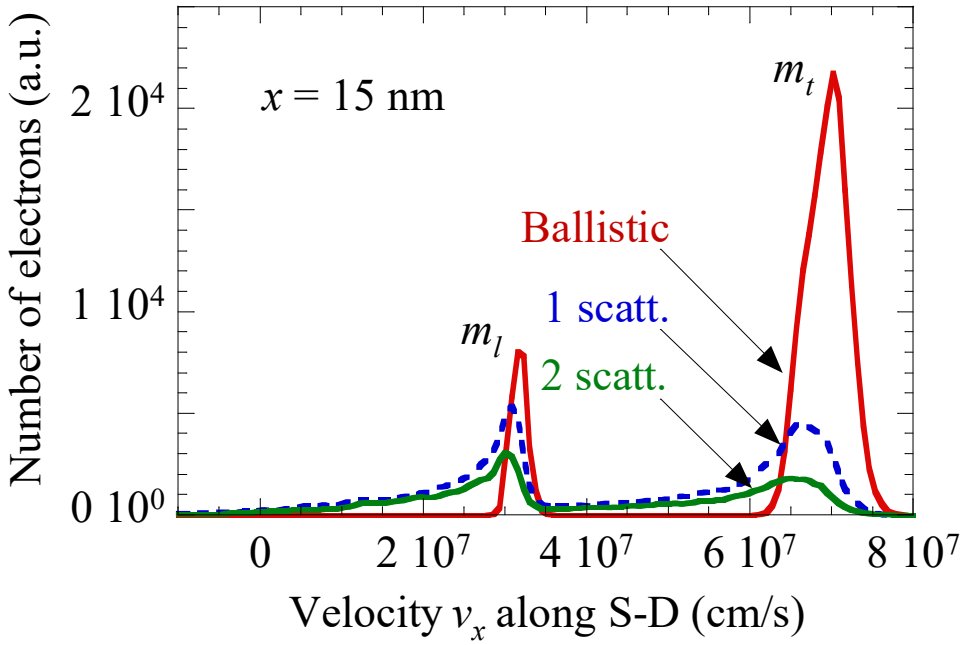
DGMOS: velocity distribution

$$L_C = 15 \text{ nm}$$

$$V_{GS} = V_{DS} = V_{DD} = 0.7 \text{ V}$$

At the drain-end of the channel,

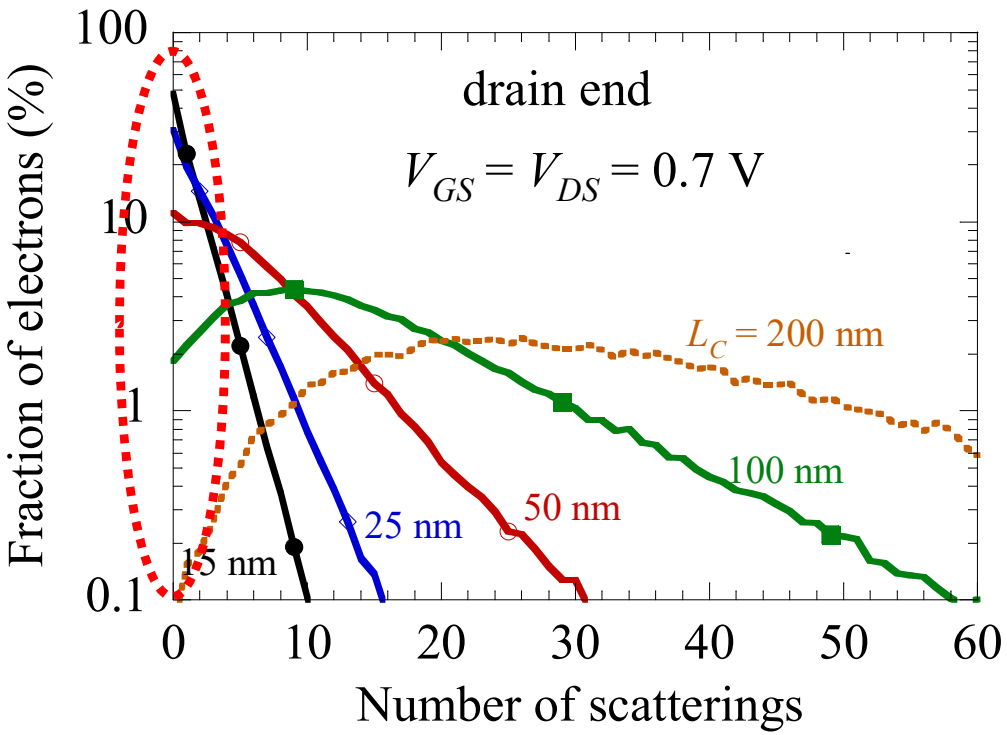
The part of purely ballistic, one-scattered and twice-scattered electrons:



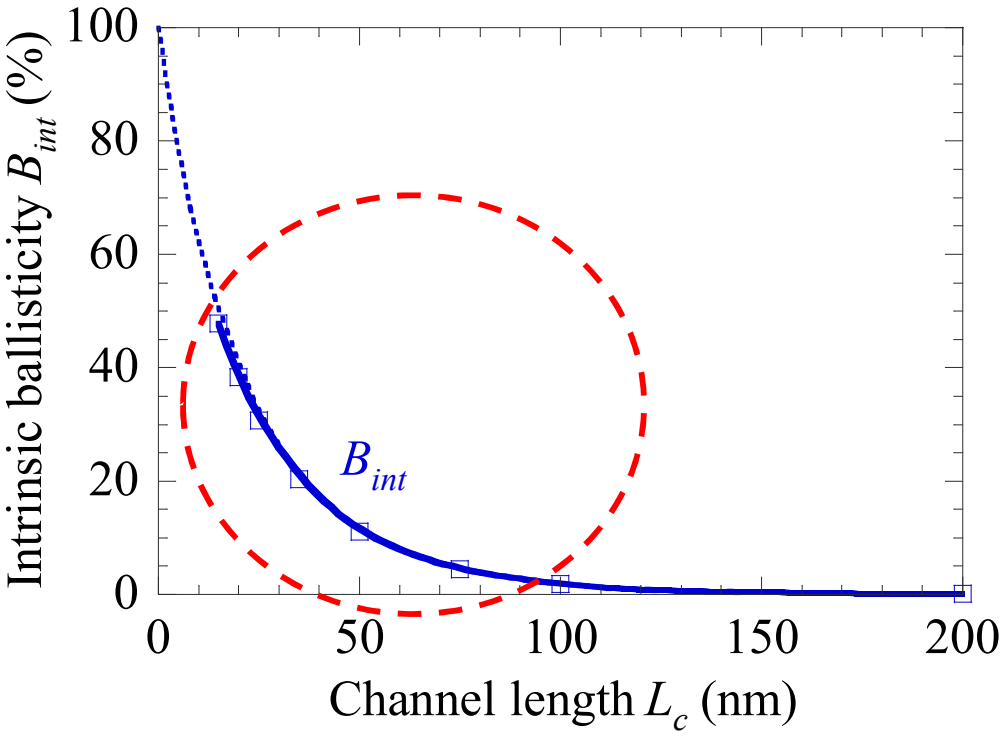
→ ballistic electrons form a large part of the velocity peaks in the distribution

DGMOS: ballisticity

$$V_{GS} = V_{DS} = V_{DD} = 0.7 \text{ V}$$



B_{int} = fraction of ballistic electrons (in %)



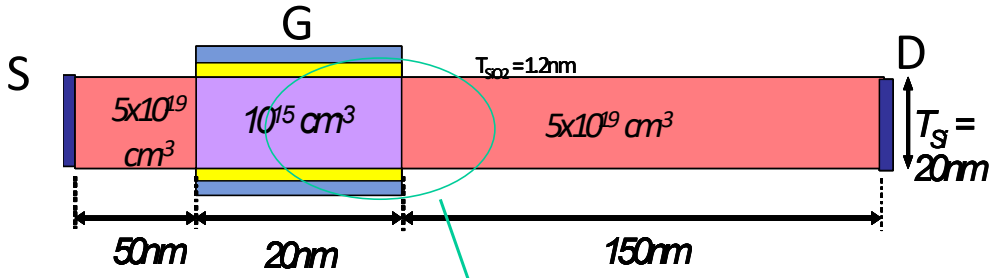
The ballisticity is becoming strong in nano-MOSFET

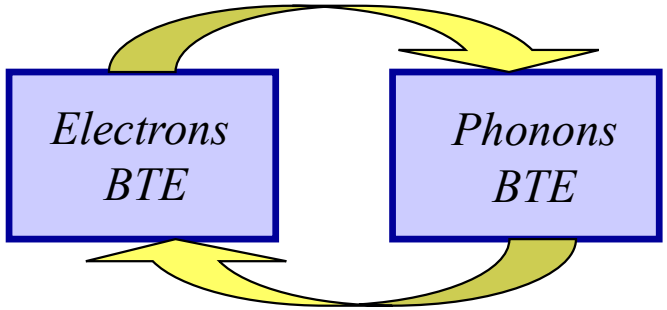
What about the validity of the approximation of semi-classical transport ?

(coherent transport, tunneling, quantum reflection,…?)

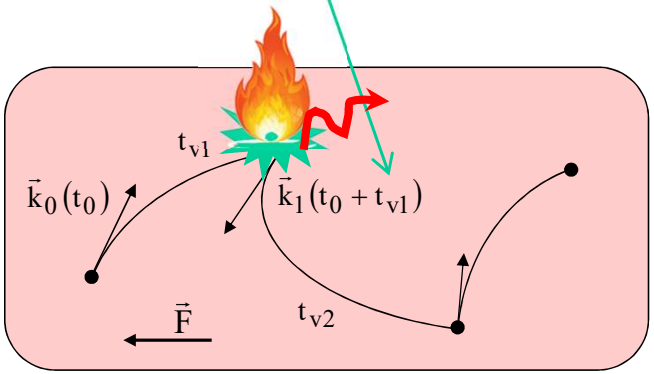
Self-heating in nano MOSFET

- DG MOSFET:





- Thermal generation



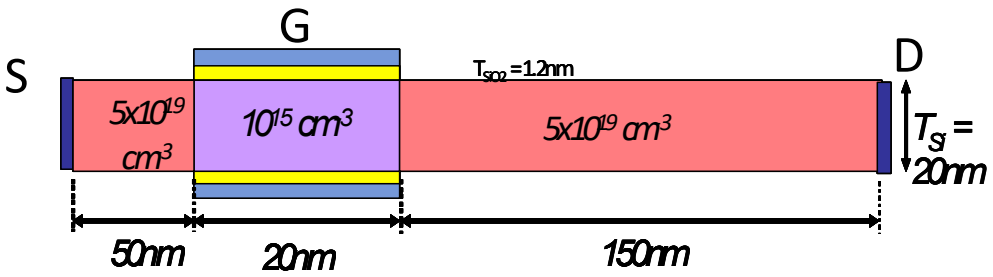
In Monte Carlo Simulation, phonon emissions are localized in (r and k)

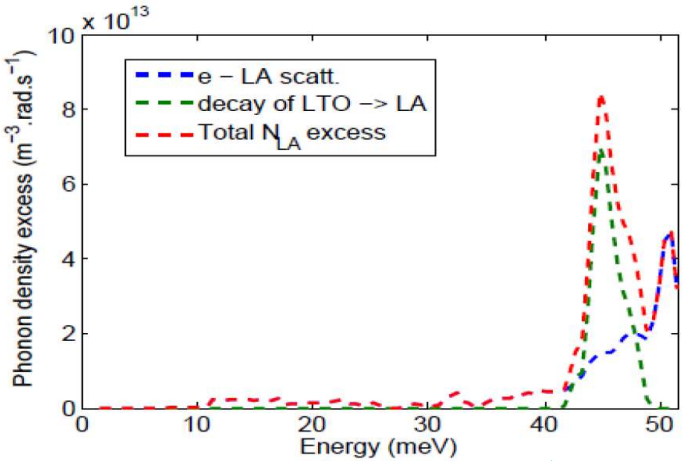
- Electro-thermal Simulation

Coupled solutions : MC for electron/Poisson + (direct) BTE for phonons

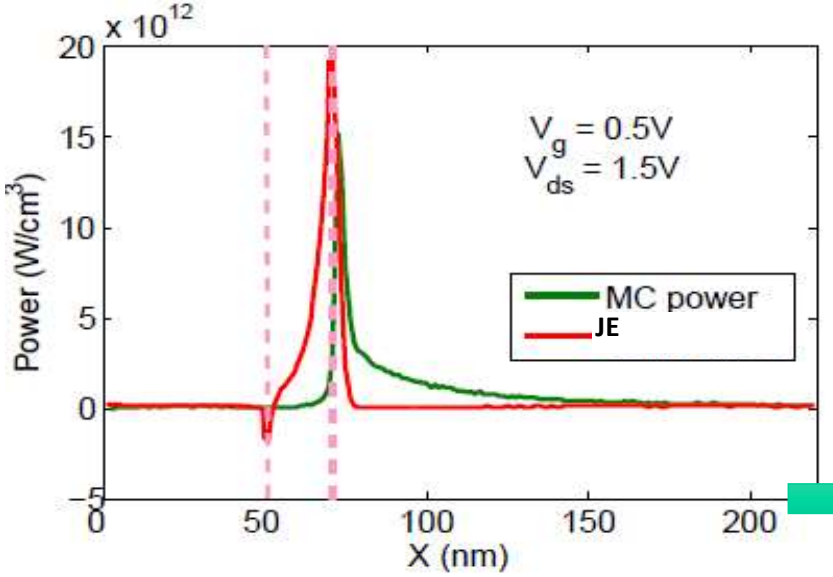
Self-heating in nano MOSFET

- DG MOSFET:

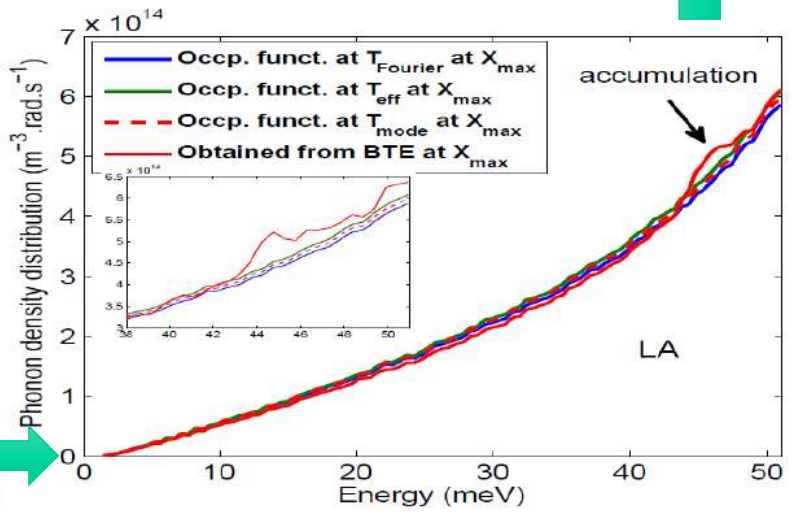




- Thermal generation



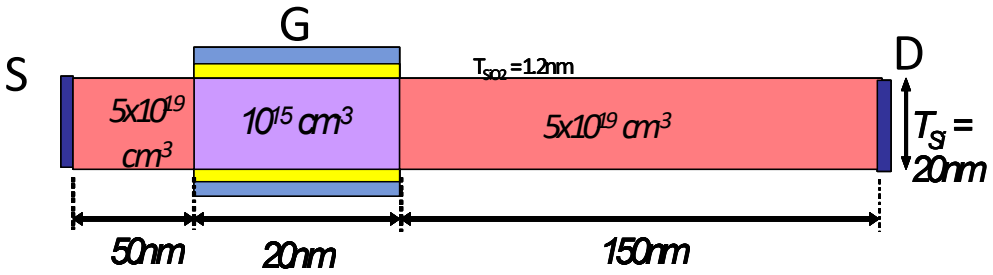
- Phonon spectrum

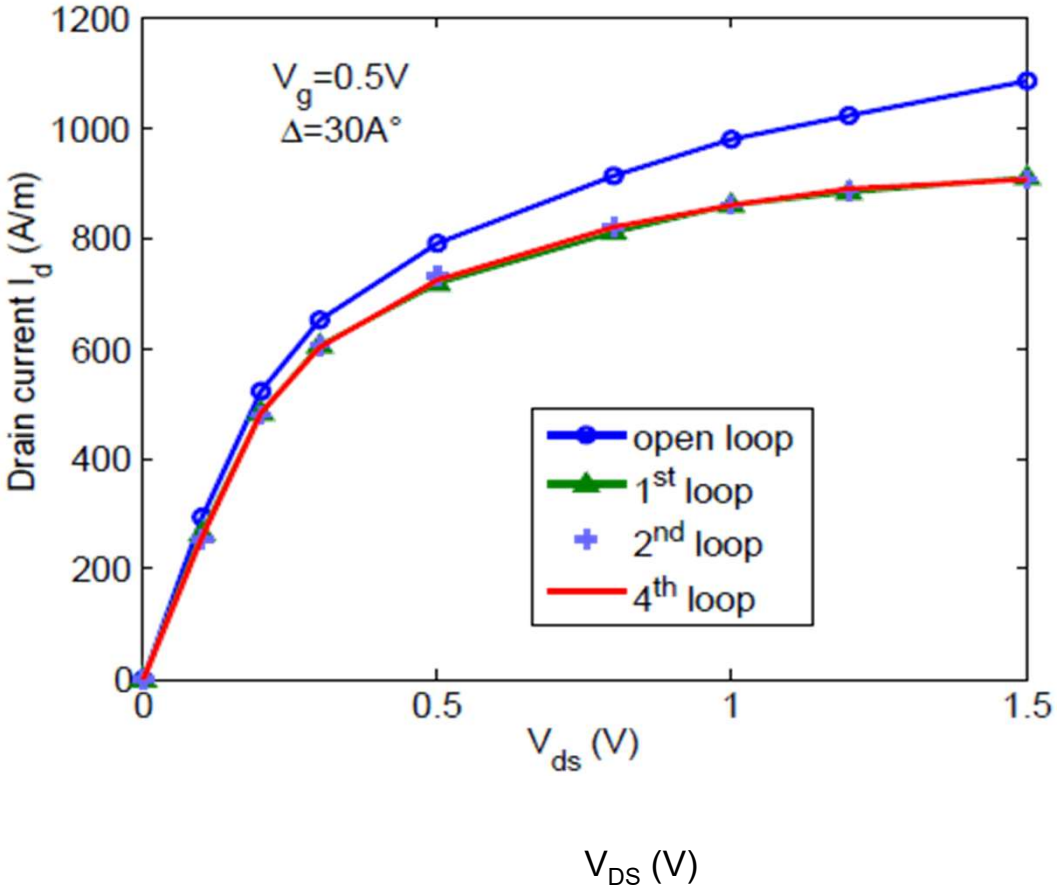


At the nanoscale, out of equilibrium (Rspace and E) effects occur

I-V Self-heating in nano MOSFET

- DG MOSFET:





V_{DS} (V)

CONCLUSION

Electron transport in semiconductor nanodevices using the Monte Carlo method

- **Particle Monte Carlo method is a stochastic solution of the BTE**
- **Random selection: free flight duration, scattering event, and the effect of scattering**
- **Only 2 BTE inputs: Dispersion and Scattering rates (empirical or ab-initio)**

- **Interest:**
  - **Easy to implement (few numerical issues)**
  - **No assumptions on *f* (all regime of transport)**
  - **Transient response available**
  - **Numerous and complex scattering events S(k,k') could be implemented**

➔ **For charged carriers: The feedback between $\vec{F}$ and *f* is an issue!**

Further readings:

- BTE/MC: *Fundamentals of Carrier Transport, Mark Lundstrom, Cambridge Univ. Press*
- MC: *Jacoboni, C., & Lugli, P. The Monte Carlo method for semiconductor device simulation. Springer Science & Business Media.*
- Wigner: *The Wigner Monte–Carlo Method for Nanoelectronic Devices: A Particle Description of Quantum Transport and Decoherence, Damien Querlioz&Philippe Dollfus, ISTE Ltd.*

The Wigner Function

Elementary definition of the **Wigner function** for an electron described by the wave function $\psi(\mathbf{r},t)$ normalized to 1 in the volume *V* of interest:

$$f_w(\mathbf{r},\mathbf{k},t) = \frac{1}{(2\pi)^3}\int d\mathbf{r}'\exp(-i\,\mathbf{k}\cdot\mathbf{r}')\left\langle \mathbf{r}+\mathbf{r}'/2\right|\rho(t)\left|\mathbf{r}-\mathbf{r}'/2\right\rangle$$

$$= \frac{1}{(2\pi)^3}\int d\mathbf{r}'\exp(-i\,\mathbf{k}\cdot\mathbf{r}')\,\psi(\mathbf{r}+\mathbf{r}'/2,t)\,\psi^*(\mathbf{r}-\mathbf{r}'/2,t)$$

1D system :

$$f_w(x,k,t) = \frac{1}{2\pi}\int dx'\exp(-i\,kx')\,\psi\left(x+\frac{x'}{2},t\right)\psi^*\left(x-\frac{x'}{2},t\right)$$

A piece of formalism…

CLASSICAL TRANSPORT

- **Boltzmann (1D): slowly varying potential** V

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\hbar} \nabla V \cdot \nabla_k f + \hat{C} f$$

local effect

collisions

QUANTUM TRANSPORT

- **Wigner's function de**fined from density matrix (and thus wave functions)
- **Wigner (1D):**

$$\frac{\partial f_w}{\partial t} + v \cdot \nabla_x f_w = \hat{Q}_V \ f_w + \hat{C} \ f_w$$

non local effect of potential V

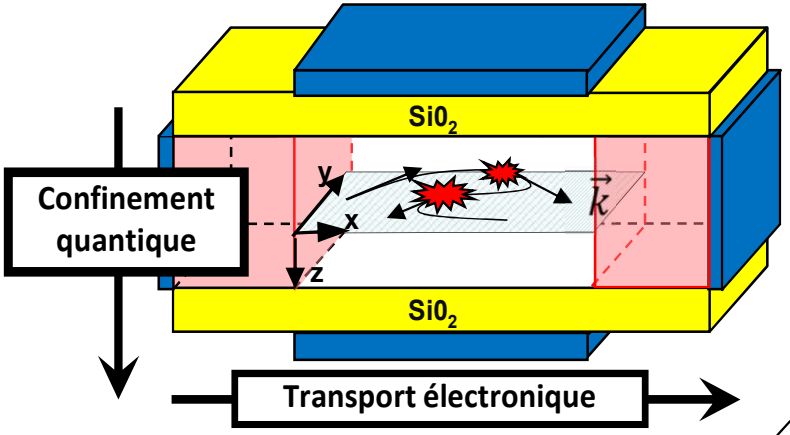
$$\hat{Q}_V \ f_w = \frac{1}{2\pi} \int dk' \ V_w(x, k - k') f_w(x, k')$$

Wigner's potential:

$$V_w(x,k) = \int dx' \sin(kx') \left[V\left(x + \frac{x'}{2}\right) - V\left(x - \frac{x'}{2}\right) \right]$$

- **$f_w \rightarrow f$ si V « classical »** *D. Querlioz et al. Physical Review B (2008)*
- **Strong analogy → simular resolution**

Quantum Monte Carlo simulation



D. Querlioz et al., IEEE Trans. on Electron Dev. (2007).

MONTE CARLO METHOD

Electron Transport 2Dk
BOLTZMAN / WIGNER

Electron density

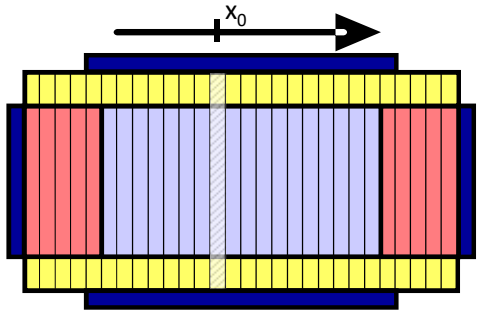
$n(x_0,z) \propto \sum_{N_{xo}} |\xi_n(x_0,z)|^2$

Poisson's equation

V(x,z)

$E_n(x)$, $\xi_n(x_0,z)$

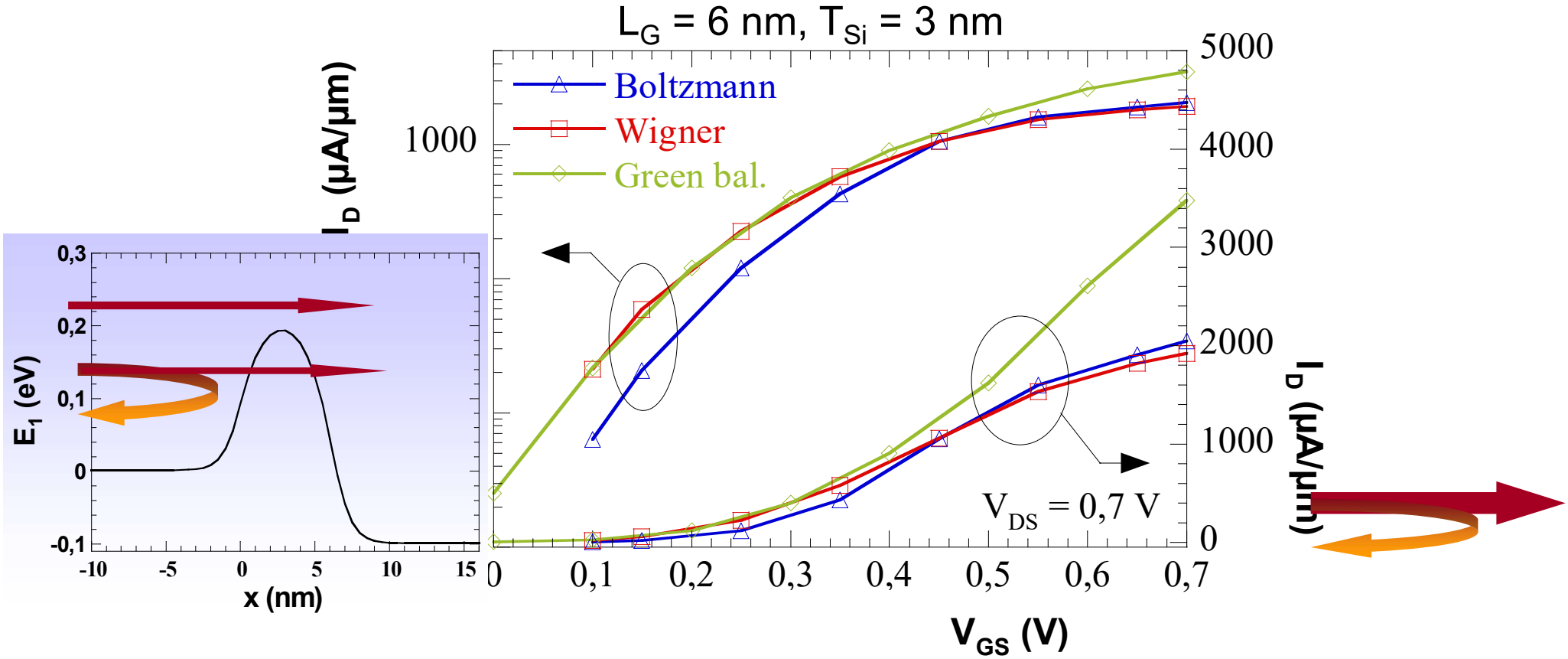
Schrödinger's Equation



Scattering: e^-_{2Dk} ↔ phonons 3Dk, impurities, rough interfaces

Full quantum code (confinement + transport) with scattering

Quantum Effects and I-V



- **OFF : Strong quantum effects (tunneling)**
- **ON : Scattering dominate**