Monte Carlo Simulation of Electron Transport in Semiconductor Nanodevices

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Research topics

Modelling and simulation of transport in semiconductor nanodevices

☞ Different kind of devices:

→ **in strong connection with industrial R&D:**

- "conventional" transistors (MOSFET, HEMT, …): towards nm scale

→ **more advanced devices for nanoelectronics:**

- quantum dots and single electron devices
- quantum wires, carbon nanotubes and related devices
- resonant tunelling diode

☞ Different approaches to transport modelling:

- Semi-classical Boltzmann transport equation (Monte Carlo)
- Single electron tunnelling (Master equation and Monte Carlo)
- Quantum transport equations
  - Non-Equilibrium Green function (tight-binding)
  - Wigner function (Monte Carlo)

☞ Device simulator associated with these modelling techniques:

Members of the group

Permanent researchers:

Valérie Aubry-Fortuna
Arnaud Bournel
Sylvie Galdin-Retailleau
Johann Sée
Philippe Dollfus

Engineer:

Christophe Chassat

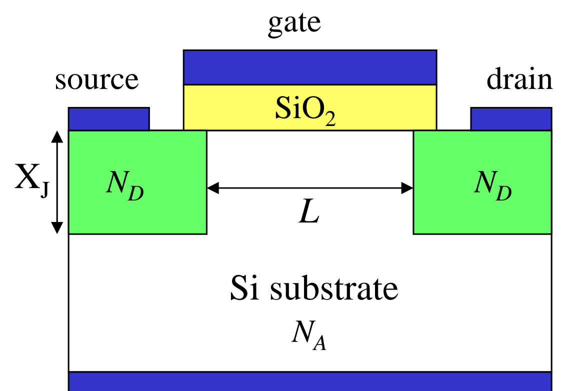
PhD students:

Emmanuel Fuchs (also with ST, Grenoble) **[compact modelling of nano-MOSFETs]**
Jérôme Saint Martin **[ballistic effects and quantization effects in nano-MOSFETs]**
Marie-Anne Jaud (also with CEA-LETI, Grenoble) **[quantum corrections in MC algorithms]**
Do Van Nam (also with IOP, Hanoi) **[quantum transport in nanodevices, NEGF]**
Hugues Cazin (also with CEA-SCM, Saclay) **[transport in carbon nanotubes and transistors]**
Damien Querlioz **[quantum transport, Wigner function]**
Audrey Valentin **[single-electron devices, QDs]**
Karim Huet (also with ST, Grenoble) **[device simulation using full-band description]**

Microelectronics and CMOS limits

The top-down approach in microelectronics:

Downscaling of CMOS devices

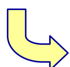


CMOS requires very good and reproducible device characteristics:

– high I_{on} (rapidity)
– low I_{off} (power consumption)
– well calibrated V_T

Downscaling in the nanometer range makes difficult to meet the CMOS requirements:

– gate tunneling leakage (ultra-thin oxide)
– short-channel effects (degradation of current control)
– access resistances
– quantum effects (charge control and transport)
– interface and doping fluctuations (fluctuations of device characteristics)
– …



the concept of CMOS is questionable at the nanometer scale

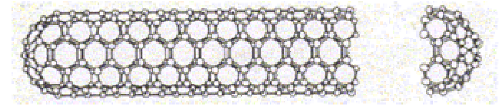
The future: nanoelectronics and bottom-up

The bottom-up approach:

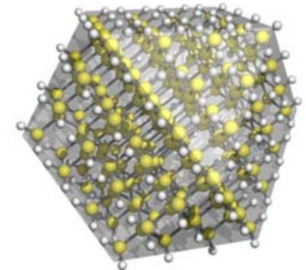
1) Introduction of nano-objects in conventional devices and circuits
   → new functionalities

2) New concepts of devices and circuits based on nano-objects, molecules,…
   → post-CMOS architectures

Possible candidates:



☞ Carbone nanotube (CNT)
- semiconducting CNT : excellent transport properties → channel of FET
- metallic CNT : interconnects

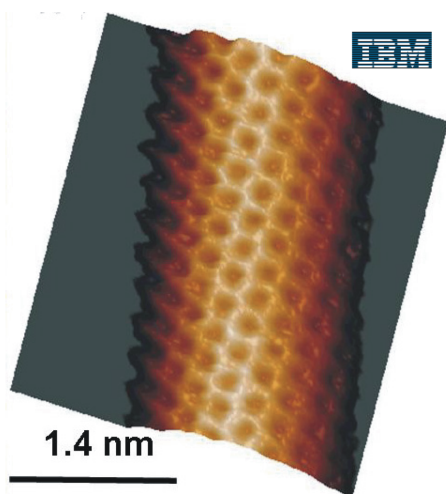


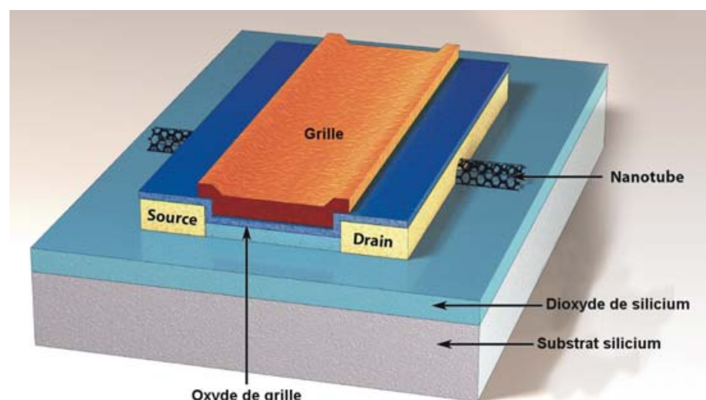
☞ silicon or germanium nanocrystal (NC)
- Coulomb blockade effect, improved current control
- "Single-electron" devices and circuits

⇒ Promising demonstrations of devices
⇒ compatible with silicon technology

The evolution of microelectronics: towards nanoelectronics

carbone nanotubes and applications





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2. Classical transport: the Boltzmann transport equation
- **distribution Function and transport equation**
- **Scattering**
- **Solution: the particle Monte Carlo method**
- **Examples of applications: MOSFET, CNT**

Second part: **3. Quantum transport: the Wigner transport equation**
- **Wigner function and transport equation**
- **Solution: the particle Monte Carlo method**
- **Examples of applications: RTD**

Third part: **4. Coulomb blocade in conducting island: principle**

[*5. Electronic structure of semiconductor quantum dot*]

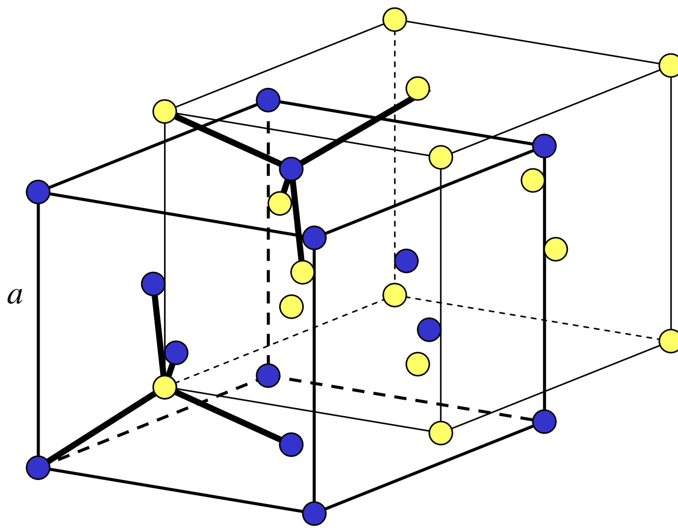
6. Single electron tunneling: I-V characteristics
- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Examples: MISiIM**

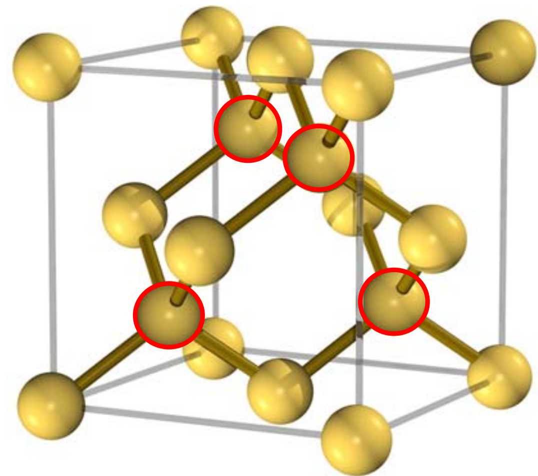
1. From the crystal to the transport equation

The semiconductor crystal

* Most usual semiconductors have a diamond-like (Si, Ge) or zinc-blende-like (GaAs) structure

* Diamond and zinc-blende crystal = 2 fcc lattices:
1 is displaced 1 quarter of the length along the diagonal





tetrahedral bonding with 4 nearest neighbors

Si: $\begin{cases} a = 0.543 \text{ nm} \\ 5\times10^{22} \text{ atoms / cm}^3 \end{cases}$

The semiconductor crystal

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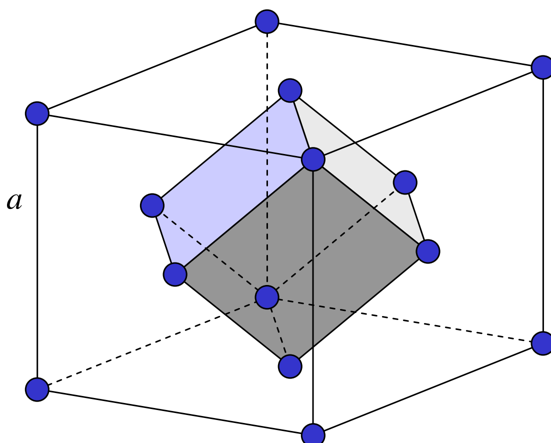
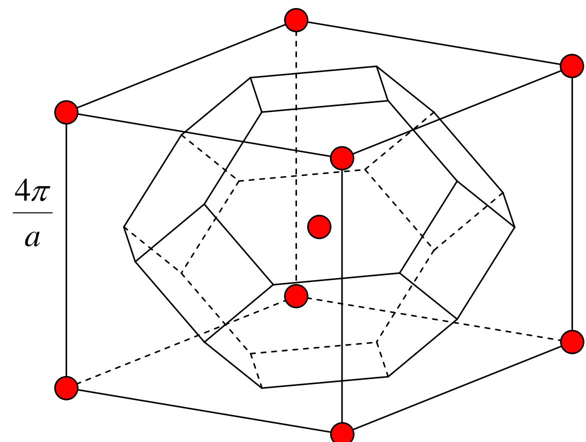
Lattice (fcc) → **Reciprocal Lattice (bcc)**





primitive unit cell (Bravais cell)
= rhomboedron

1st Brillouin zone
= ocatedron with truncated corners

cubic semiconductors (2 fcc latices):
N_u = 2 atoms per unit cell

The crystal Hamiltonian

For an assembly of atoms in a crystal:

$$H = \sum_{l} \frac{p_l^2}{2M} + \frac{1}{2}\sum_{l,m} U\left(\vec{R}_l - \vec{R}_m\right) + \sum_{i} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i,j} W\left(\vec{r}_i - \vec{r}_j\right) + \sum_{i,l} V\left(\vec{r}_i - \vec{R}_l\right)$$

Where l and m label the nuclei, i and j label the electrons, p is the momentum

M is the nucleus mass and m is the electron mass

$\vec{R}$ is the position of a nucleus and $\vec{r}$ is the position of an electron

$\frac{p_l^2}{2M}$ .... is the kinetic energy of the nucleus l

$\frac{p_i^2}{2m}$ .... is the kinetic energy of the electron i

$U\left(\vec{R}_l - \vec{R}_m\right)$ .... is the interaction potential between nuclei l and m

$W\left(\vec{r}_i - \vec{r}_j\right) = \frac{q^2 / 4\pi\varepsilon_0}{\left|\vec{r}_i - \vec{r}_j\right|}$ is the interaction potential between electrons i and j

$V\left(\vec{r}_i - \vec{R}_l\right)$ .... is the interaction potential between electron i and nucleus l

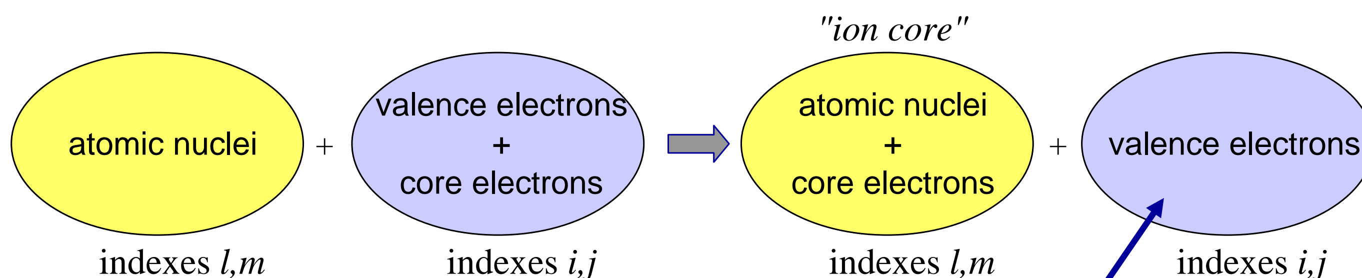
Schrödinger equation: $H\Psi = E\Psi$

The crystal Hamiltonian: approximations

☞ 1st approximation:

* Core electrons are strongly linked to the nucleus which forms an « ion core » labeled by indexes *l* and *m*.

* In the previous equations the indexes *i* and *j* only label valence electrons which is the main sub-system of interest in transport problems.



System of interest for transport problems

The crystal Hamiltonian: approximations

☞ 2nd approximation: ("adiabatic" or "Born-Oppenheimer")

↳ electrons much slower than ions

⇒ Electrons can instantaneously adjust their motion to that of the ions.

⇒ Thus the wave function is approximately of the form:

$$\Psi = \Psi_e\left(\vec{r},\vec{R}_0\right)\Psi_{ion}\left(\vec{R}\right)$$

where:
$\Psi_{ion}(\vec{R})$ is the wavefunction for all the ions (independent on electron position)
$\Psi_e(\vec{r},\vec{R}_0)$ is the wavefunction for electrons (instantaneously dependent on ion position)

$$H = H_{ion}\left(\vec{R}\right)+H_e\left(\vec{r},\vec{R}_0\right)+H_{e-ion}\left(\vec{r},\delta\vec{R}\right) \quad \text{with} \quad \delta\vec{R}=\vec{R}-\vec{R}_0=\vec{S}$$

$H_{ion}\left(\vec{R}\right)=\sum_l \frac{p_l^2}{2M}+\frac{1}{2}\sum_{l,m}U\left(\vec{R}_l-\vec{R}_m\right)$ acts only on the ions

$H_e\left(\vec{r},\vec{R}_0\right)=\sum_i \frac{p_i^2}{2m}+\frac{1}{2}\sum_{i,j}\frac{q^2/4\pi\varepsilon_0}{\left|\vec{r}_i-\vec{r}_j\right|}+\sum_{i,l}V\left(\vec{r}_i-\vec{R}_{0_l}\right)$ acts only on the electrons

$H_{e-ion}\left(\vec{r},\delta\vec{R}\right)$ is the effect of ion displacement on electrons (usually small perturbation)

The crystal Hamiltonian: approximations

$H_{ion}\left(\vec{R}\right)\Psi_{ion}\left(\vec{R}\right)=E_{ion}\,\Psi_{ion}\left(\vec{R}\right)$ is a purely ionic Schrödinger equation

$H_e\left(\vec{r},\vec{R}_0\right)\Psi_e\left(\vec{r},\vec{R}_0\right)=E_e\,\Psi_e\left(\vec{r},\vec{R}_0\right)$ is a purely electronic Schrödinger equation

☞ 3rd approximation: ("Mean-field" or "Hartree-Fock" or "one-electron")

↳ The electron-electron interaction is averaged and considered as a perturbation

$\Psi_e\left(\vec{r},\vec{R}_0\right)=\prod_i \Psi_i\left(\vec{r}_i,\vec{R}_0\right)$ where Ψ_i is the wave function of electron *i*

$H_{e_i}\left(\vec{r}_i,\vec{R}_0\right)\Psi_i\left(\vec{r},\vec{R}_0\right)=E_{e_i}\,\Psi_i\left(\vec{r},\vec{R}_0\right)$ is a one-electron equation

$H_{e_i}\left(\vec{r}_i,\vec{R}_0\right)=\frac{p_i^2}{2m}+\sum_l V\left(\vec{r}_i-\vec{R}_{0_l}\right) \longrightarrow V_c\left(\vec{r}\right)=\sum_l V\left(\vec{r}_i-\vec{R}_{0_l}\right)$

is the (periodic) crystal potential

➡ $\left[\frac{p^2}{2m}+V_c\left(\vec{r}\right)\right]\Psi\left(\vec{r}\right)=E\,\Psi\left(\vec{r}\right)$ ➡ **Band Structure of the crystal**

The crystal Hamiltonian: approximations

$$\left[\frac{p^2}{2m}+V_c(\vec{r})\right]\Psi(\vec{r})=E\,\Psi(\vec{r})$$

is the electron equation for an ideal non perturbated crystal
(T = 0, frozen atoms, no impurity, infinite crystal,…)

By including all sources of perturbation:

$$\left[\frac{p^2}{2m}+V_c(\vec{r})\;+\;V_{scatt}(\vec{r})\;+\;V_{ext}(\vec{r})\right]\Psi(\vec{r})=E\,\Psi(\vec{r})$$

is the full one-electron equation

scatterings (phonon, impurity,…) → V_{scatt}

"external" fields (heterojunction, bias voltage,…) → V_{ext}

Usual approximation:

Weak perturbations → transitions between allowed states of ideal crystal

(no effect on the band structure)

The crystal Hamiltonian: summary

	Treatment:
☞ ion equation: (all ions) ➡ $H_{ion}(\vec{R})\,\Psi_{ion}(\vec{R})=E_{ion}\,\Psi_{ion}(\vec{R})$ gives the **phonon spectra**	**quantum**
☞ electron equation: (one electron) $\left[\frac{p^2}{2\;m}+V_c(\vec{r})\;+\;V_{scatt}(\vec{r})\;+\;V_{ext}(\vec{r})\right]\Psi(\vec{r})=E\;\;\Psi(\vec{r})$ ➡ $\left[\frac{p^2}{2m}+V_c(\vec{r})\right]\Psi(\vec{r})=E\,\Psi(\vec{r})$ gives the **band structure** $V_{scatt}(\vec{r})$ and $V_{ext}(\vec{r})$ are considered as weak perturbations	**quantum**
➡ $V_{scatt}(\vec{r})$: **scatterings** (transitions between allowed states)	**quantum**
➡ $V_{ext}(\vec{r})$: **transport phenomena**	**classical or quantum**

Semiconductor band structure

$$\left[\frac{p^2}{2m}+V_c(\vec{r})\right]\Psi(\vec{r})=E\,\Psi(\vec{r})$$

periodic crystal potential

Bloch functions ⇒

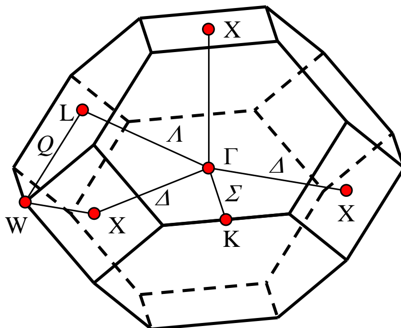
$$\Psi_{\vec{k}}(\vec{r})\equiv\exp\left(i\vec{k}\cdot\vec{r}\right)u_{\vec{k}}(\vec{r})$$

where $u_{\vec{k}}(\vec{r})$ has the periodicity of $V_c(\vec{r})$

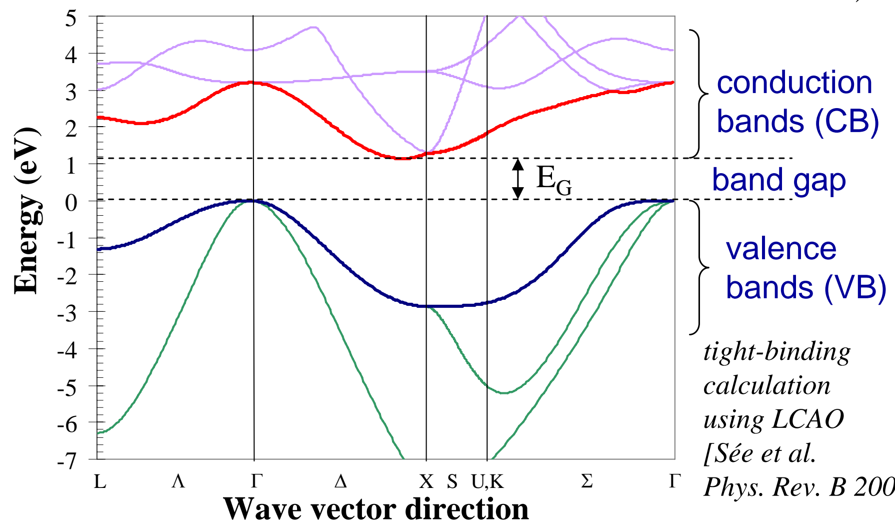
$$\left(\text{normalisation}\Rightarrow\Psi_{\vec{k}}(\vec{r})=\frac{1}{\sqrt{N_c}}\exp\left(i\vec{k}\cdot\vec{r}\right)u_{\vec{k}}(\vec{r})\right)$$

(u_k is normalized to 1 in the unit cell)

The first Brillouin zone



Bandstructure of silicon :



tight-binding calculation using LCAO [Sée et al. Phys. Rev. B 2002]

Effective mass end equi-energy surfaces in band extrema

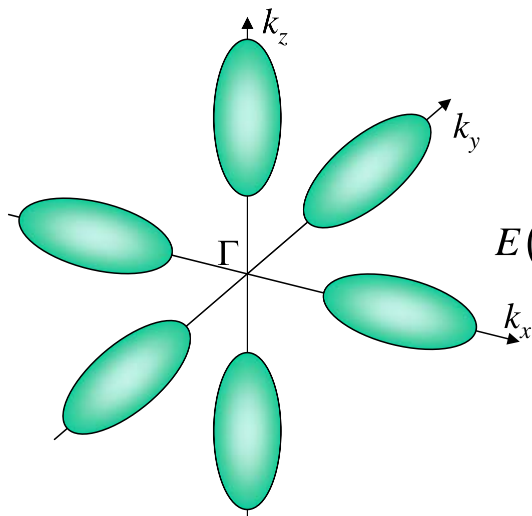
Conduction band of GaAs:

→ 1 spherical valley in Γ
(+ satellite L and X valleys)

$$E=\frac{\hbar^2}{2m^*}k^2 \quad \text{or} \quad E\,(1+\alpha E)=\frac{\hbar^2}{2m^*}k^2$$

(parabolic approximation) *(α = non parabolicity coefficient)*

with $m^*=m_\Gamma\ m_0=0.063m_0$ and $\alpha=0.58\ \text{eV}^{-1}$



Conduction band of Si:

→ 6 ellipsoidal Δ valleys (near X)

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

with $m_l=0.916\ ,\ m_t=0.019\ ,\ \alpha=0.5\ \ \text{eV}^{-1}$

Electron kinematics – acceleration effective mass

* velocity of an electron = group velocity of the wave packet:

$$v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial k} \quad \text{(1D)} \qquad \vec{v}_g = \frac{1}{\hbar}\vec{\nabla}_k E \quad \text{(3D)}$$

$$\left(\rightarrow \text{parabolic band}: \vec{v} = \frac{\hbar \vec{k}}{m^*} \right)$$

* velocity in k-space:

for an electron under the action of a force $\vec{F}$

$$dE = \vec{F}\, d\vec{r} = \vec{F}\, \vec{v}\, dt = \frac{\vec{F}}{\hbar} \cdot \frac{dE}{d\vec{k}} dt \quad \Rightarrow \quad \frac{d\vec{k}}{dt} = \frac{\vec{F}}{\hbar}$$

* acceleration in real-space:

$$\frac{dv}{dt} = \frac{1}{\hbar^2}\left(\frac{\partial^2 E}{\partial k^2}\right) F \quad \text{(1D)} \qquad \vec{\gamma} = \frac{d\vec{v}}{dt} = \left[\frac{1}{m^*}\right]\vec{F} \quad \text{(3D)}$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\left(\frac{\partial^2 E}{\partial k^2}\right) \qquad \left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2}\left(\frac{\partial^2 E}{\partial k_i\, \partial k_j}\right)$$

$$\gamma = \frac{dv}{dt} = \frac{1}{m^*} F$$

tensor of acceleration effective mass

Density of states in k-space

semiconductor of finite size $\Rightarrow$ **finite number of *k* values allowed**

* in a periodic linear (1D) chain of N atoms of length $L_x = N a$,
we impose periodic bounadry conditions:

$$\Psi(0) = \Psi(0 + N a) \Rightarrow u_k(0) = \exp(i k_x N a)\, u_k(N a) \Rightarrow \exp(i k_x N a) = 1$$

so only discrete values are possible: $k_x = n_x \dfrac{2\pi}{L_x}$, $n_x = 1, 2, 3, \ldots$

spin degeneracy $\Rightarrow$ 2 possible states in each space $\dfrac{2\pi}{L_x}$

$\rightarrow$ the density of states in *k*-space is $n(k_x) = 2 \times \dfrac{L_x}{2\pi}$

* in a 3D crystal of volume $\Omega = L_x L_y L_z$,

$\rightarrow$ the density of states in *k*-space is $n(\vec{k}) = 2 \times \dfrac{L_x}{2\pi} \times \dfrac{L_y}{2\pi} \times \dfrac{L_z}{2\pi} = \dfrac{V}{4\pi^3}$

$\rightarrow$ the density of states $n(E)$ in energy-space is deduced from:

$$\begin{cases} n(\vec{k})\, d\vec{k} = n(E)\, dE \\ E(\vec{k}) \end{cases}$$

$E(\vec{k})$ ← depends on the material

Density-of-states effective mass

→ Γ valley of GaAs (spherical): $E(\vec{k}) = \dfrac{\hbar^2}{2m^*}k^2$ (parabolic approximation)

the number of states in the range of energy $[E, E+dE]$ is: $n(E)dE = n(\vec{k})d\vec{k}$

1D gas (length L)

$$n(\vec{k})d\vec{k} = 2\frac{L}{2\pi}\times dk$$

$$n(E) = \frac{L}{\sqrt{2}\pi\hbar}(m^*)^{1/2}\frac{1}{E^{1/2}}$$

2D gas (surface A)

$$n(\vec{k})d\vec{k} = 2\frac{A}{4\pi^2}\times 2\pi k\, dk$$

$$n(E) = \frac{A}{\pi\hbar^2}m^*$$

3D gas (volume V)

$$n(\vec{k})d\vec{k} = 2\frac{V}{8\pi^3}\times 4\pi^2 k^2\, dk$$

$$n(E) = \frac{V\sqrt{2}}{\pi^2\hbar^3}(m^*)^{3/2}E^{1/2}$$

Density of states effective mass: $m_{DOS} = m^*$

Density-of-states effective mass

→ Δ valleys (6) of Si (ellipsoidal): $E(\vec{k}) = \dfrac{\hbar^2}{2m_0}\left(\dfrac{k_x^{\,2}}{m_l} + \dfrac{k_y^{\,2}}{m_t} + \dfrac{k_z^{\,2}}{m_t}\right)$

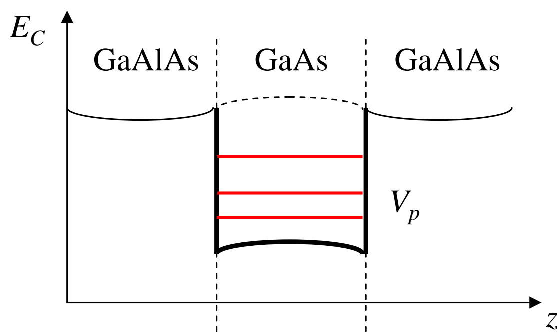
$$n(E) = 6\times\frac{V\sqrt{2}}{\pi^2\hbar^3}(m_0)^{3/2}\left(m_l^{1/2}m_t\right)^{3/2}E^{1/2}$$ ***(3D gas)***

$$n(E) = \frac{V\sqrt{2}}{\pi^2\hbar^3}(m_{DOS})^{3/2}E^{1/2}$$

$$m_{DOS} = m_0\left(6m_l^{1/2}m_t\right)^{2/3}$$

Quantum confinement: effective mass approximation

Example: GaAlAs/GaAs/GaAs heterostructure ⇒ Conduction band discontinuity



2-dimensional electron gas

Confinement potential V_p, which brokes the crystal periodicity

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_c(z)+V_p(z)\right]\Psi(z)=E\,\Psi(z)$$

Effective mass approximation (m^*)

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V_p(z)\right]F(z)=E\,F(z)$$

where ***F*(*z*) is the envelope function** of a bound state

→ The effect of the crystal is fully included in the effective mass m^*

$$\Psi_{\vec{k}}(\vec{r})=F(z)\exp(ik_x x)\exp(ik_y y)\;u_{\vec{k}_{xy}}(x,y)$$

Electron transport in semiconductor nanodevices

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- **Examples of applications: MOSFET, CNT**

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[5. *Electronic structure of semiconductor quantum dot*]

6. Single electron tunneling: I-V characteristics
- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Examples: MISiIM**

2. Classical transport: The Boltzmann Transport Equation

Distribution function

Classical approach:

The quantum properties of the electrons are neglected: one can specify at each time t the position $\vec{r}$ and the wave vector $\vec{k}$ (or the momentum $\vec{p}$).

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 related to the electron gas are deduced from the distribution function:

e.g.

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

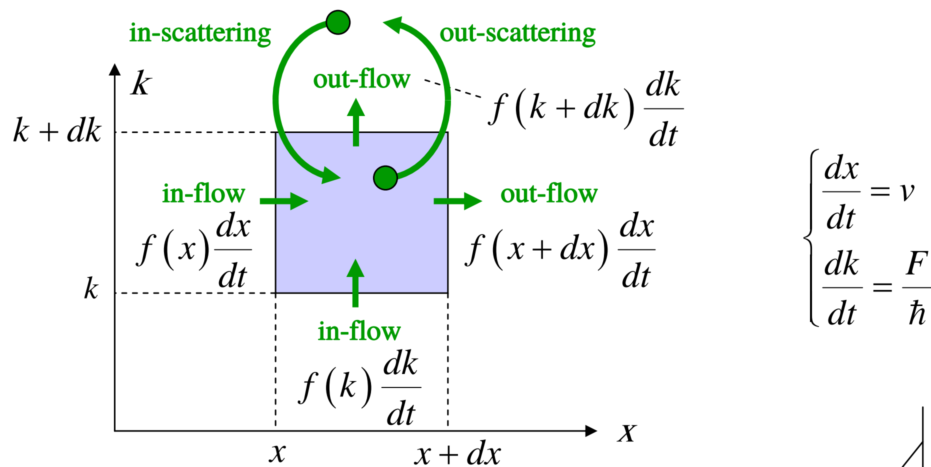
At thermal equilibrium electrons obey the Fermi-Dirac statistics:

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

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

total energy; potentiel energy (bottom of CB); kinetic energy

Boltzmann Transport Equation (BTE)



$$\begin{cases} \dfrac{dx}{dt} = v \\ \dfrac{dk}{dt} = \dfrac{F}{\hbar} \end{cases}$$

in and out scatterings

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

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

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

BTE in 6 dimensions phase space

Collision term - scatterings

Possible collision mechanisms (collision ≡ interaction ≡ scattering): $\longrightarrow S_i(\vec{k}, \vec{k}')$

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

Transition rate: (for mechanism *i*)

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

matrix element of H_i — DOS

(Fermi golden rule) (1st order perturbation theory)

Collision term in BTE (in $\vec{k}$):

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

collision operator

in non-degenerate electron gas: $f(\vec{r}, \vec{k}, t) << 1$

$$\left. \frac{\partial f}{\partial t} \right|_{coll} = \sum_i \left[\int f(\vec{k}')\, S_i(\vec{k}', \vec{k})\, d^3\vec{k}' - \int f(\vec{k})\, S_i(\vec{k}, \vec{k}')\, d^3\vec{k}' \right]$$

Electron-phonon scattering

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

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

$\varphi_{n_\mathbf{q}} = |n_\mathbf{q}\rangle =$ Hermitian polynomial of degree $n_\mathbf{q}$ in $\mathbf{q}$

→ 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'**)

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

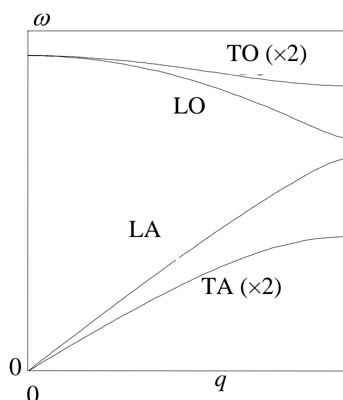
+ : emission
- : absorption

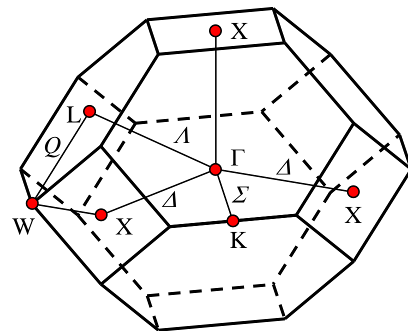
where ρ is the mass density $\quad D_\mathbf{q}$ is the coupling constant

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

Electron-phonon scattering

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)

Electron-phonon scattering

Evaluation of the overlap factor $\mathcal{G}(\mathbf{k},\mathbf{k}')$

* Electrons:

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

→ intravalley process in X valleys (Si):
→ intervalley process:
} $\mathcal{G}(\mathbf{k},\mathbf{k}') \simeq \text{constant} \simeq 1$

* 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

Evaluation of the coupling constant $D_{\mathbf{q}}$

* Deformation potential:

→ acoustic intravalley: (small q) $\hbar\omega_q = \hbar v_s q$ (sound velocity v_s) $D_{\mathbf{q}} = D_{ac}\, q$ with D_{ac} in eV

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

* Electrostatic force (polar material):

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

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

→ optical intravalley (polar optical): $D_{\mathbf{q}} = \dfrac{e\,\omega\sqrt{\rho}}{q}\left(\dfrac{1}{\varepsilon_{hf}} - \dfrac{1}{\varepsilon_{lf}}\right)$

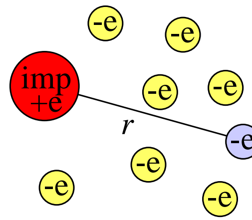
(ε_{hf} and ε_{lf} = high frequency and low frequency permittivity)

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

Electron-impurity scattering

* For 1 ionized impurity:

(Brooks-Herring model)



L_D = Debye length
= screening length

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

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

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

n = electron density

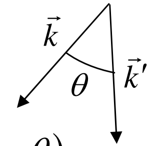
$$S_{el-imp}(\mathbf{k},\mathbf{k}') = \frac{1}{V}\frac{1}{4\pi^2\hbar}\frac{e^4}{\varepsilon^2}\frac{1}{\left(q^2+q_s^2\right)^2}\delta(E'-E)$$

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: $N_{imp} = N_{dop}\, V$

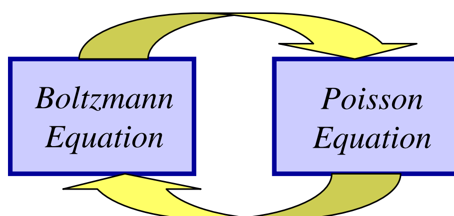
$$S_{el-imp}(\mathbf{k},\mathbf{k}') = \frac{N_{dop}}{4\pi^2\hbar}\frac{e^4}{\varepsilon^2}\frac{1}{\left(q^2+q_s^2\right)^2}\delta(E'-E)$$

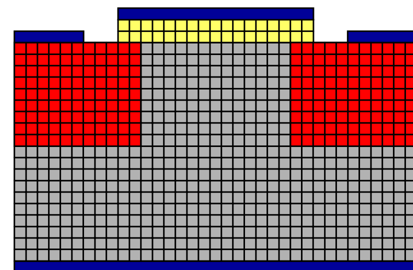
Solving the BTE for device simulation

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

Starting from an initial solution, we have all information needed to calculate the time evolution of the distribution function f inside a device:

- probabilities per time unit $S_i(\vec{k},\vec{k}')$ of scattering from state $\vec{k}$ to state $\vec{k}'$
- distribution of forces $\vec{F}$, e.g. by solving Poisson's equation





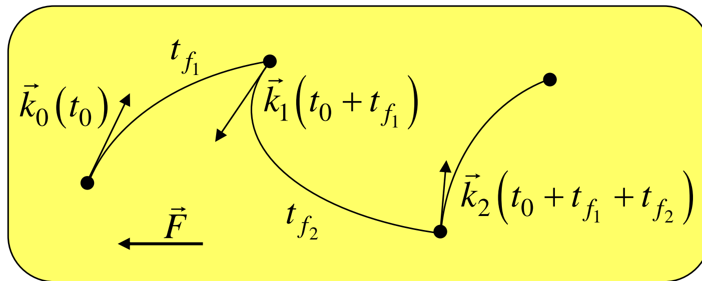
The BTE is a rather complicated integro-differential equation for *f* whose direct (deterministic) solution is impracticable in device simulation

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

The particle Monte Carlo method

Statistical solution: particle *Monte Carlo method*

- $f(\vec{r},\vec{k},t) \rightarrow$ assembly of individual particles
- 1 particle $\Leftrightarrow$ $\vec{r}(t),\ \vec{k}(t)$
- N particles allow us to reconstruct $f(\vec{r},\vec{k},t)$
  - $\rightarrow$ no complicated equation to solve
  - $\rightarrow$ same physical content as the deterministic solution
  - $\rightarrow$ suitable for device simulation



carrier trajectory: succession of free fights interrupted by instantaneous scatterings

scattering rates $\lambda_i(\vec{k})$ ⇒ 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 $(\vec{r},\vec{k})$

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

the calculation of:	*requires*	*the knowledge of:*
$\frac{d\vec{k}(t)}{dt}=\frac{1}{\hbar}\frac{d\vec{p}(t)}{dt}=\frac{q}{\hbar}\vec{F}$	→	nothing on the material
$\frac{d\vec{r}(t)}{dt}=\vec{v}(t)=\frac{1}{\hbar}\frac{\partial E}{\partial \vec{k}}$	→	band structure $E(\vec{k})$
scatterings $E \rightarrow E'$, $\vec{k} \rightarrow \vec{k}'$	→	scattering rates $\lambda_i(\vec{k})$

$\lambda_i(\vec{k})$ = 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*

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

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 ⇒ $n_{\mathbf{q}} = \left[\exp\left(\frac{\hbar\omega_{\mathbf{q}}}{k_B T}\right) - 1 \right]^{-1} \approx \frac{k_B T}{\hbar\omega_{\mathbf{q}}} - \frac{1}{2}$

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

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

$$\lambda_{ac}(\vec{k}) = \int S_{ac}(\vec{k},\vec{k}')\, d\vec{k}'$$

change of variables:

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

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

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

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

Monte Carlo method: example of scattering rates (2)

Electron-phonon interaction by deformation potential coupling

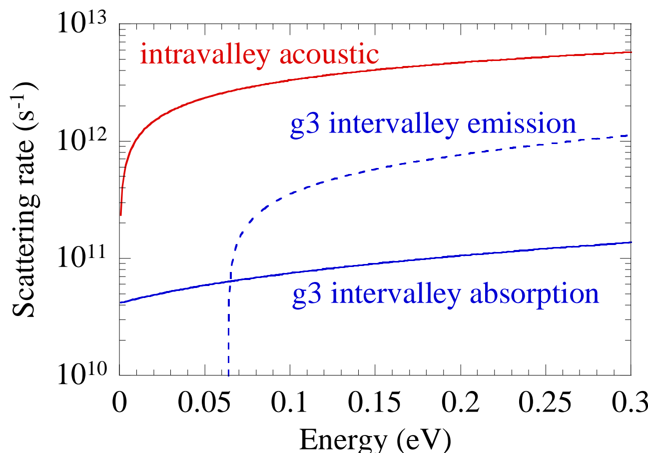
* Intervalley scattering (Z_{iv} possible final valleys)

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

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

{ + : emission; - : absorption

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



example: Si (T = 300K)

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

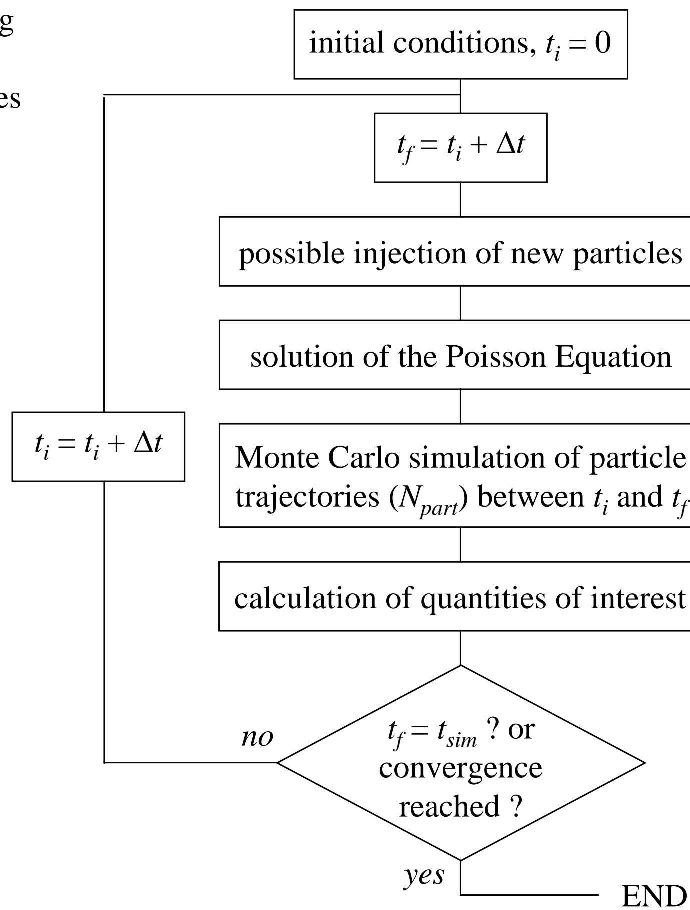
g3 $\hbar\omega_{iv} = 63.2$ meV

f1 $\hbar\omega_{iv} = 21.9$ meV

f2 $\hbar\omega_{iv} = 46.3$ meV

f3 $\hbar\omega_{iv} = 59.1$ meV

Monte Carlo method: flow chart



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

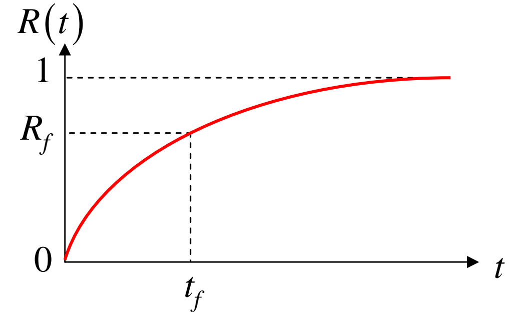
The probability that the free-fight time is less than t_f is: $R_f = R(t_f) = \int_0^{t_f} P(t)\,dt$

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 $P_r(R) = 1$



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

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

$$t_f = -\frac{\ln(R'_f)}{\lambda_0}$$

where $R'_f = 1 - R_f$

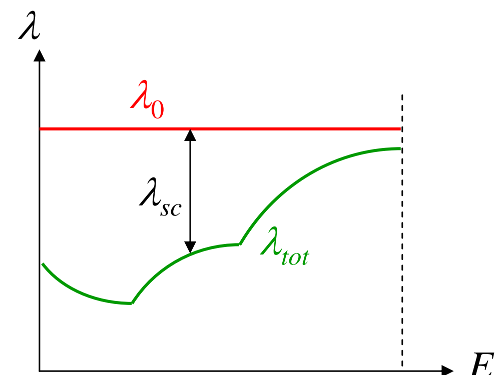
Monte Carlo method: selection of free-flight duration

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

solution: we introduce a new interaction

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

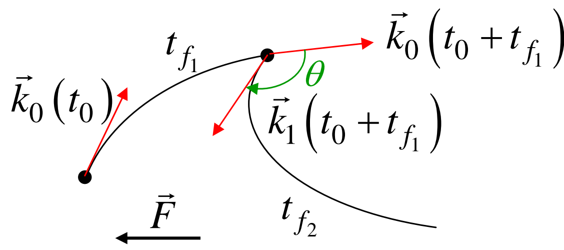
$$\lambda_{tot}(E) + \lambda_{sc}(E) = \text{Const} = \lambda_0$$



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

Monte Carlo method: selection of scattering event

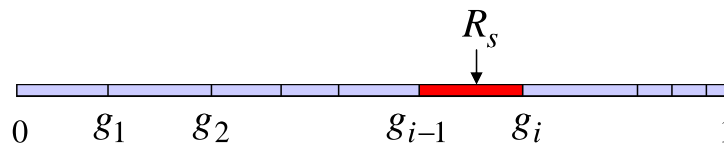
* **Type of scattering**: after each free flight, the electron undergoes a scattering event



of which type ?

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

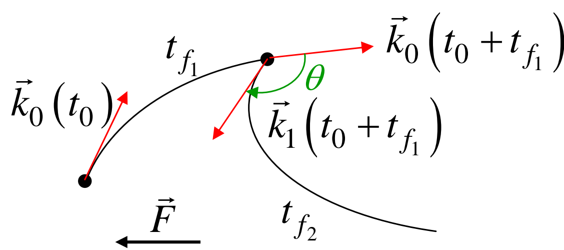
$$g_j(E)=\sum_{i=1}^{j}\lambda_i(E)/\lambda_0$$



→ 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



in case the case of phonon process: $E' = E \pm \hbar\omega_q$
in the case of other processes: $E' = E$

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

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

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

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

$$\begin{cases}P(\theta_s)=\dfrac{I(\theta_s,2\pi)}{I(\pi,2\pi)}=R_\theta & \to \theta_s\\[2ex] P_{\theta_s}(\varphi_s)=\dfrac{I(\theta_s,\varphi_s)}{I(\theta_s,2\pi)}=R_\varphi & \to \varphi_s\end{cases}$$

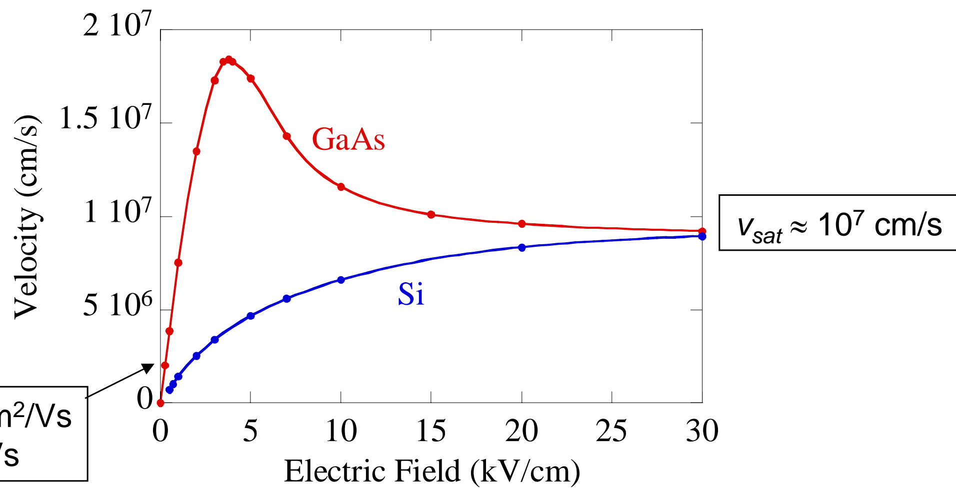
case of isotropic scattering:

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

Transport Monte Carlo simulation

Velocity-Field characteristics in uniform material – Stationary transport

(equilibrium between perturbation and relaxation effects)



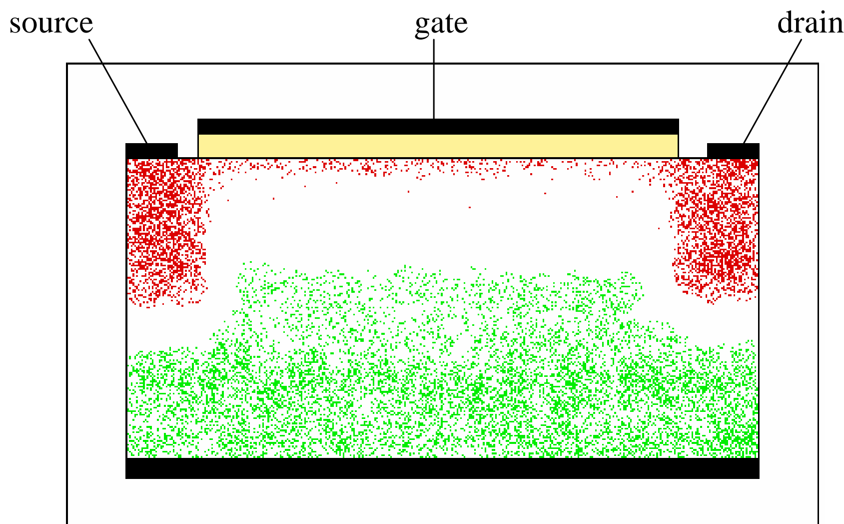
$v_{sat} \approx 10^7$ cm/s

μ (GaAs) ≈ 7000 cm²/Vs
μ (Si) ≈ 1500 cm²/Vs

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

Device Monte Carlo simulation: particle trajectories

N-channel MOSFET



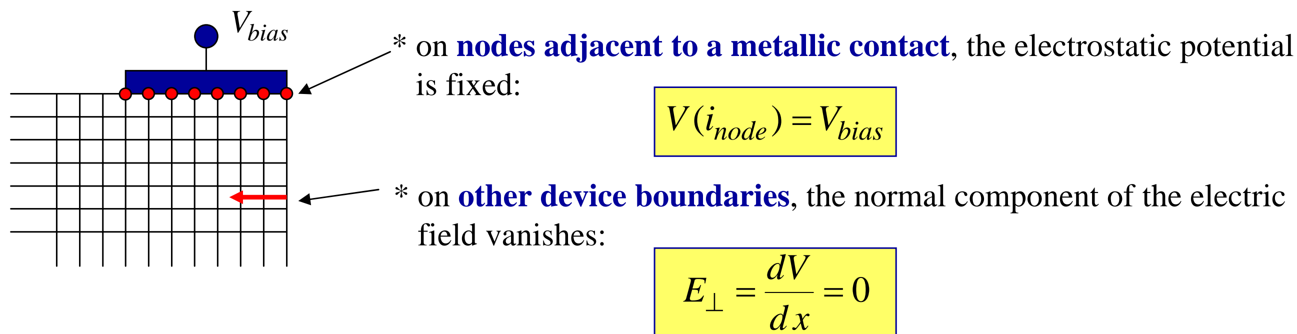
red dots: electrons
geen dots: holes

Possibility to make movies of particle motion in the working device

Monte Carlo method: boundary conditions

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

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



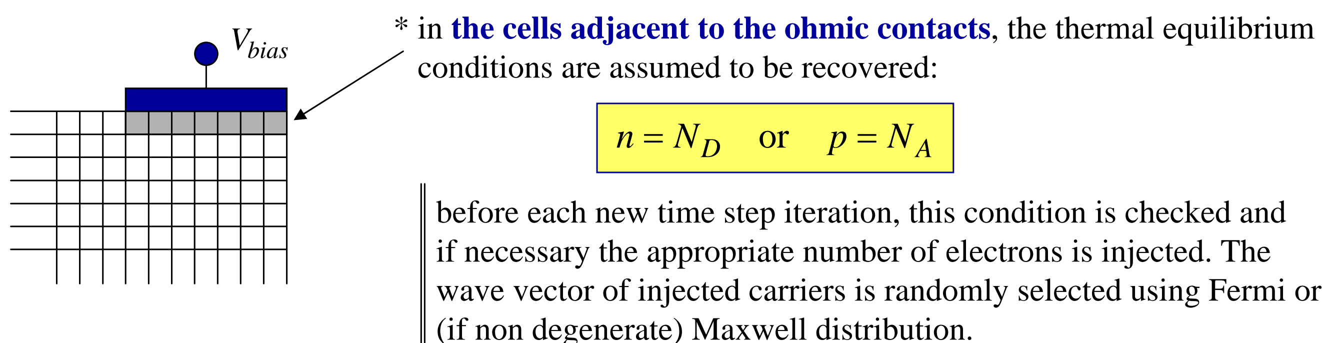
* on **nodes adjacent to a metallic contact**, the electrostatic potential is fixed:

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

* 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.

MOSFET architectures (N-channel)

Gate
Oxide
Source
Drain
N_D
N_D
N_A

Conventional Bulk MOSFET

Gate
Source
Drain
SiO_2

Single-Gate SOI MOSFET

Gate
Source
Drain
Gate

Double-Gate

Triple-Gate

Gate
Source
Drain

Study of nano-scaled DGMOS

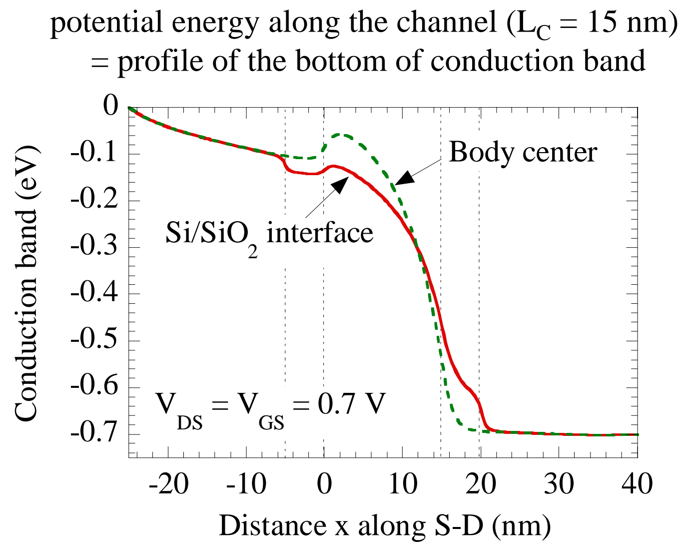
Study of DGMOS: I_D-V_{DS} characteristics

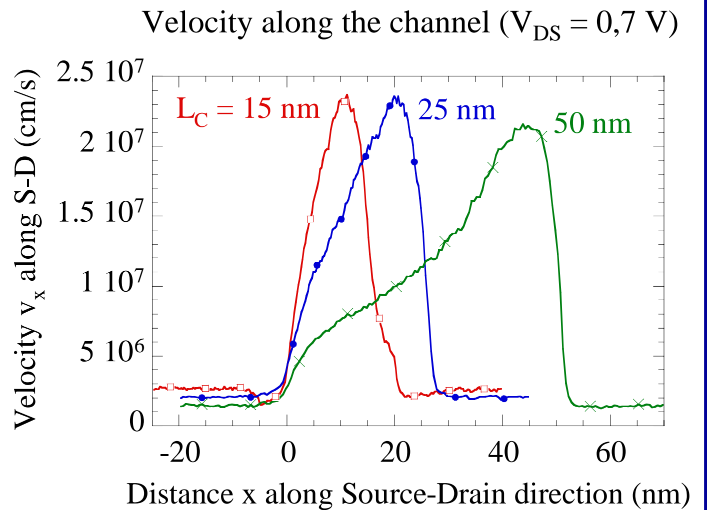
Drain characteristics for L_C = 15 nm

For L_C = 15 nm, 25 nm, 50 nm
Drain characteristics at V_{GS} = V_{DD}

Study of DGMOS: influence of gate length

Effective channel Length: L_C = 15 nm, 25 nm and 50 nm





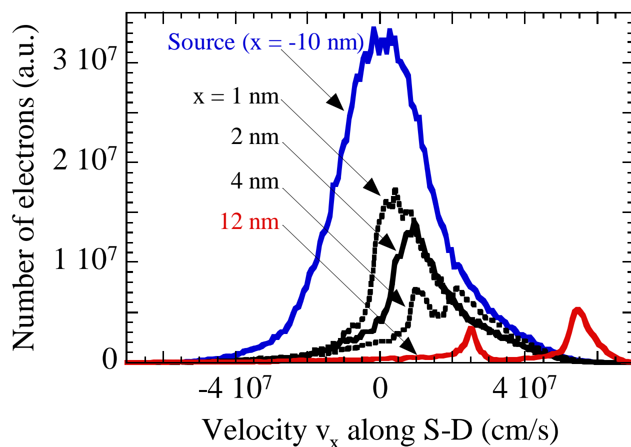
peak velocity > 2×10^7 cm/s
→ greater than saturation velocity = 10^7 cm/s

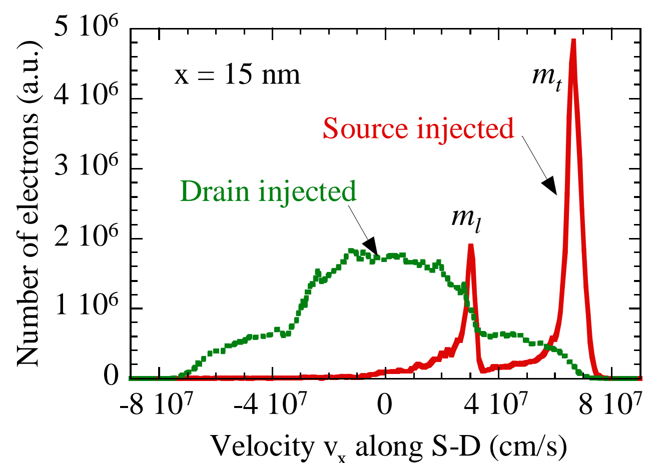
⇒ non stationary transport

Study of DGMOS: velocity distribution

L_C = 15 nm

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





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

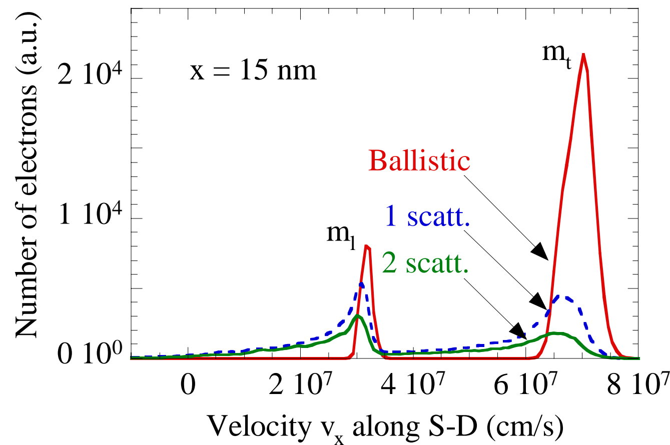
Study of DGMOS: velocity distribution

$L_C = 15$ nm

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

At the drain-end of the channel,

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

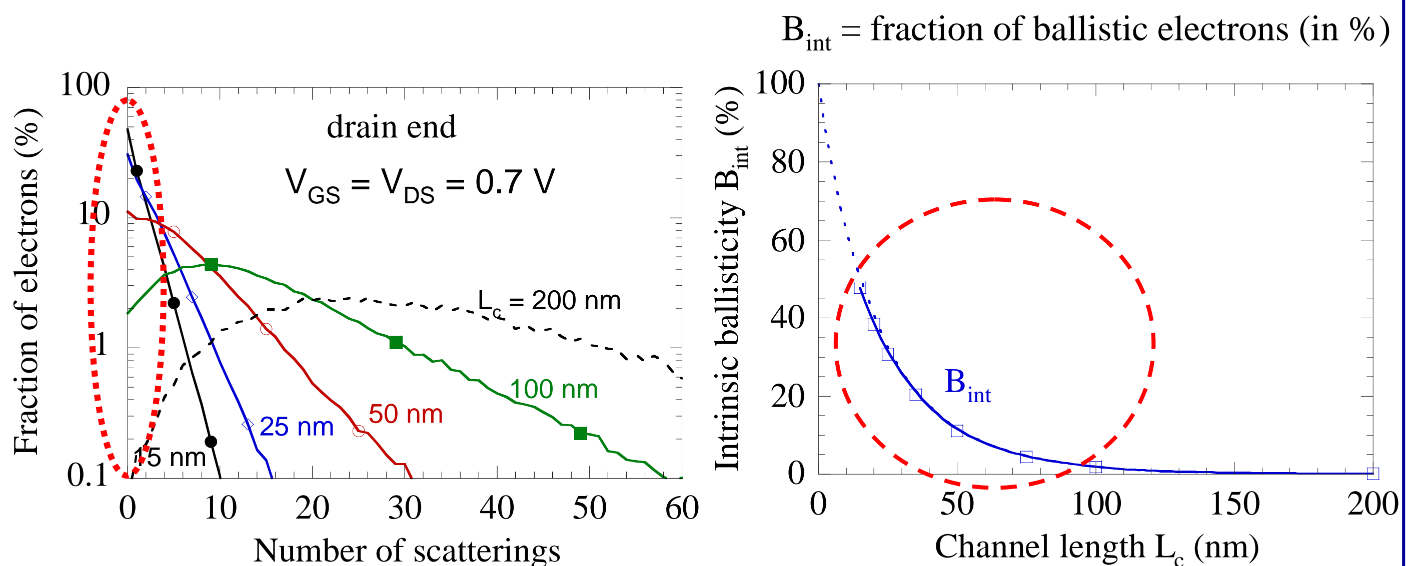


→ ballistic electrons form a large part of the velocity peaks in the distribution

Study of DGMOS: ballisticity

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

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



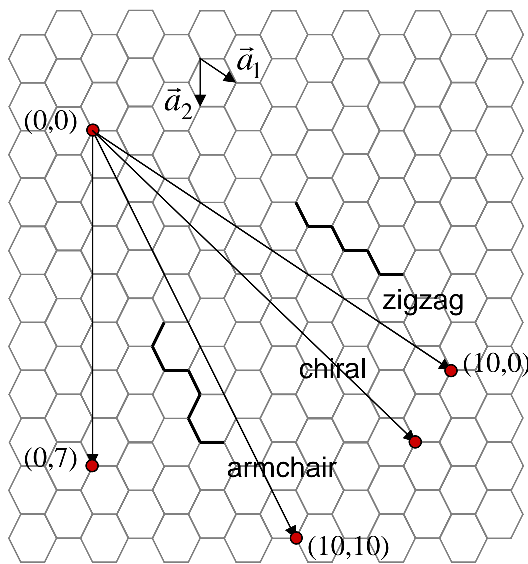
The ballisticity is becoming strong in nano-MOSFET

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

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

Structure of Carbon nanotubes

Rolling of a graphene sheet → Carbon nanotube (CNT)

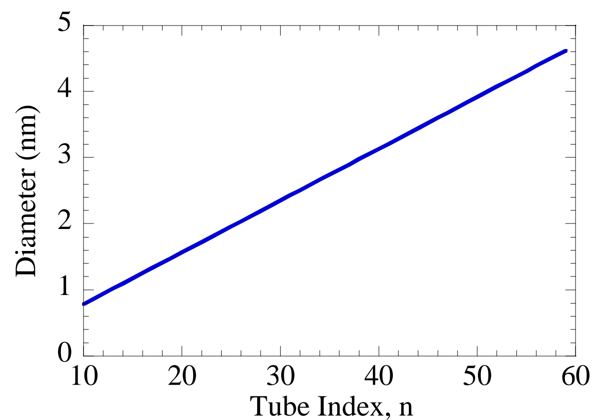


A CNT is characterized by *(n,m)*

- Here,

  we study **electron transport** in :

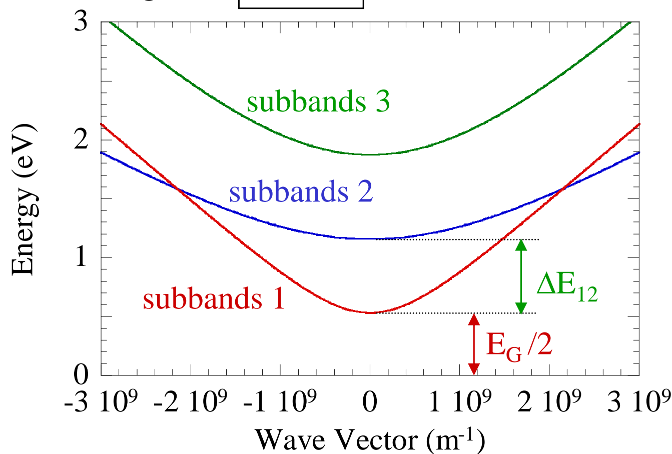
  - Single Wall
  - Zigzag ***(n,0)***
  - Semiconducting ***n ≠ 3p***
  - Index ***n*** ranging from 10 to 59



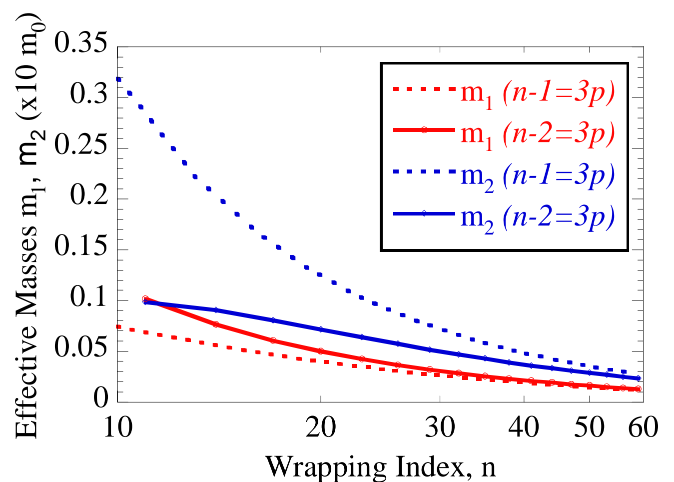
Conduction Band Structure of CNTs

- 2n subbands
- 2 equivalent valleys centered on 2 graphene K points

e. g. for $n = 10$

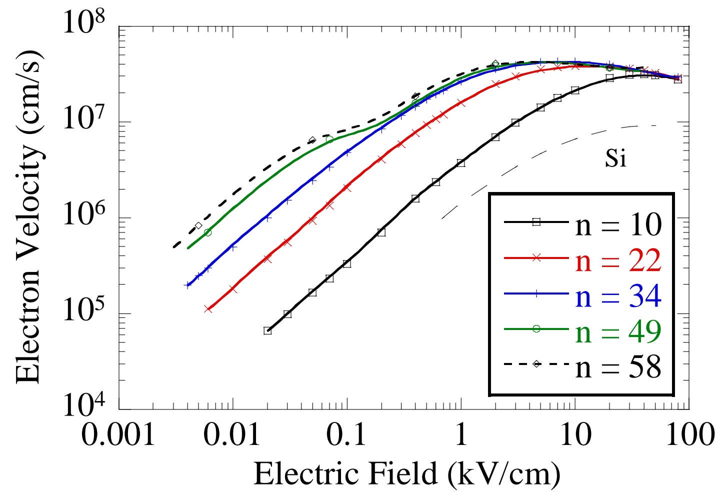


The three first subbands of each valley are considered in the calculation for all CNTs



Stationary transport

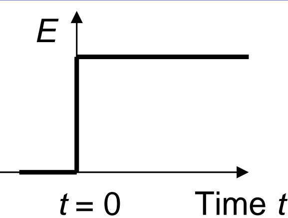
- **Velocity-Field characteristics (*T* = 300 K) *(n-1 = 3p)***



Maximum Stationary Velocity : v_{max} = 3.43×10⁷cm/s for *n* = 10

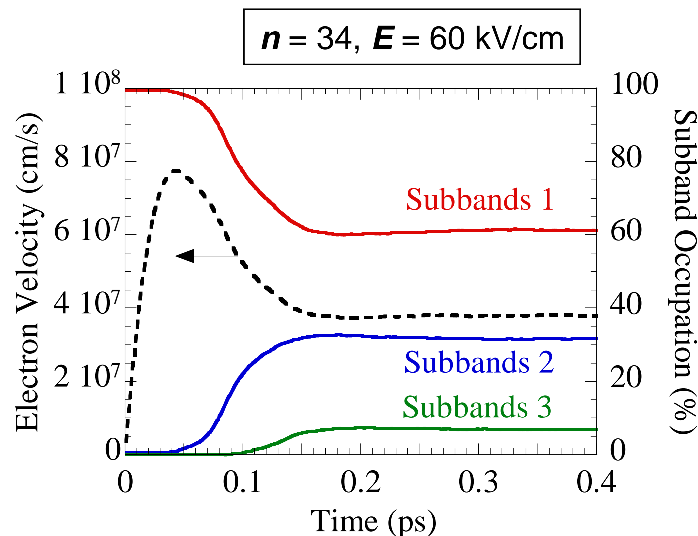
Maximum Low-Field Mobility : μ = 4×10³ cm²/Vs for *n* = 10
μ = 1.41×10⁵ cm²/Vs for *n* = 58
(μ = 1500 cm²/Vs for Si)

Transient behaviour



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

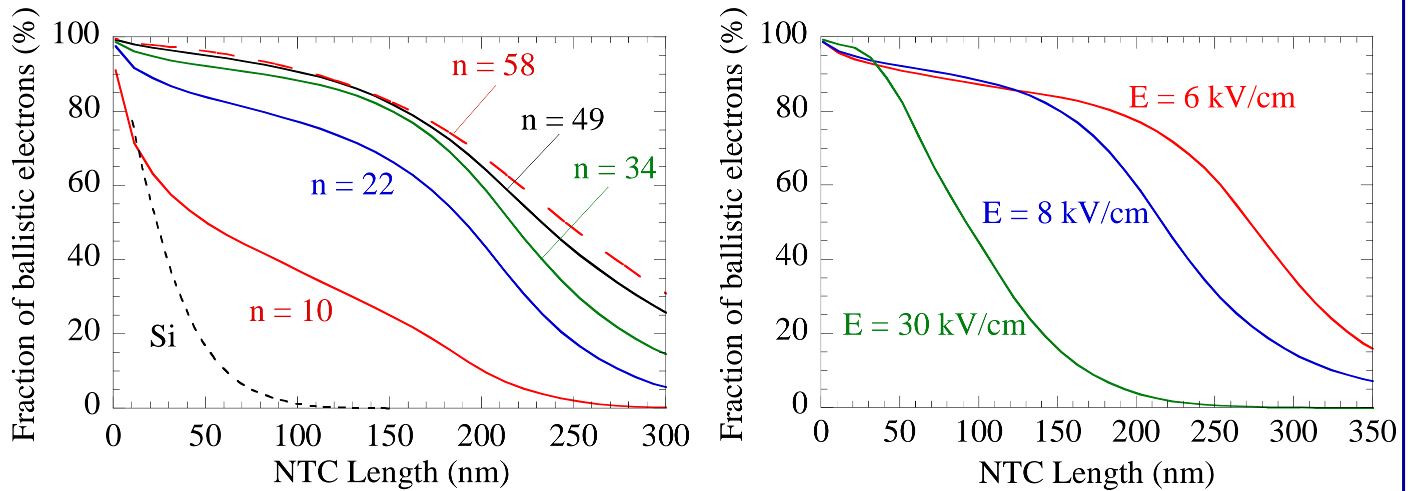
n = 34, ***E*** = 60 kV/cm



High Velocity Overshoot : ***vpeak* = 7.8×10⁷ cm/s for *n* = 34**
***vstat* = 3.8×10⁷ cm/s**

Transient behaviour

▪ **Fraction of ballistic electrons as a function of CNT length**



The ballistic transport is strongly dependent :

☞ **the *CNT diameter* (effective masses)**

☞ **the *Electric Field* (occurring of intervalley scattering)**

Electron transport in semiconductor nanodevices

Contents

First part: **1. From the crystal to the transport equation**

2. Classical transport: the Boltzmann transport equation
- **distribution Function and transport equation**
- **Scattering**
- **Solution: the particle Monte Carlo method**
- **Examples of applications: MOSFET, CNT**

Second part: **3. Quantum transport: the Wigner transport equation**
- **Wigner function and transport equation**
- **Solution: the particle Monte Carlo method**
- **Examples of applications: RTD**

Third part: **4. Coulomb blocade in conducting island: principle**

[*5. Electronic structure of semiconductor quantum dot*]

6. Single electron tunneling: I-V characteristics
- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Examples: MISiIM**

3. Quantum transport: The Wigner Transport Equation

The Wigner formalism of quantum transport is based on a function defined in a (**r**,**p**) phase space in strong analogy with the classical description of transport.

↳ It looks very appropriate to deal with space-dependent problems (device simulation)

The Wigner Function

- Semi-classical picture: electrons are described by specifying the distribution function
- Quantum mechanical picture: the phase relationship between the different states must be specified

for an electron with the wave function $\sum_{\mathbf{k}} a_{\mathbf{k}} |\mathbf{k}\rangle$

the density matrix is defined as $\rho(\mathbf{k},\mathbf{k}') = a_{\mathbf{k}}\, a^{*}_{\mathbf{k}'}$

(*in semi-classical approach, assuming the phase relaxation length to be very short,* $f(\mathbf{k})$ *is given by the diagonal elements of* $\rho(\mathbf{k},\mathbf{k})$)

For any operator $\mathcal{A}$: $\langle \mathcal{A} \rangle = Tr(\rho\mathcal{A})$

<u>Elementary definition</u> 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:

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

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

Some properties of the Wigner Function

* with this definition, we have: $\iint f_w(\mathbf{r},\mathbf{k})\,d\mathbf{k}\,d\mathbf{r} = 1$

* For an N particle system, we have: $\iint \left[N\, f_w(\mathbf{r},\mathbf{k})\right] d\mathbf{k}\,d\mathbf{r} = N$

$N \times f_w$ can be compared with the occupation number of quantum state **k**

*** Particle density in real and reciprocal space**

$$\int f_w(\mathbf{r},\mathbf{k})\,d\mathbf{k} = |\Psi(\mathbf{r})|^2 = n(\mathbf{r})$$

$$\int f_w(\mathbf{r},\mathbf{k})\,dr = \frac{1}{(2\pi)^3}\int dr_1 \int dr_2 \exp\left(-i\mathbf{k}\cdot(\mathbf{r}_2-\mathbf{r}_1)\right)\psi(\mathbf{r}_2)\,\Psi^*(\mathbf{r}_1)$$

$$= |\Phi(\mathbf{k})|^2 = n(\mathbf{k})$$

*** Mean value of an operator $\mathcal{A}$ over a statistical ensemble**

$$\langle \mathcal{A}\rangle = Tr(\rho\mathcal{A}) = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle \mathbf{r}_1|\mathcal{A}|\mathbf{r}_2\rangle\langle \mathbf{r}_2|\Psi\rangle\langle\Psi|\mathbf{r}_1\rangle$$

using the $|\mathbf{r}\rangle$ representation

change in average **r** and relative **r**' position:

Some properties of the Wigner Function

$$\langle \mathcal{A}\rangle = \int d\mathbf{r}\int d\mathbf{r}'\,\mathcal{A}(\mathbf{r}-\mathbf{r}'/2,\mathbf{r}+\mathbf{r}'/2)\,\Psi(\mathbf{r}+\mathbf{r}'/2)\,\Psi^*(\mathbf{r}-\mathbf{r}'/2)$$

introduction of $\delta(\mathbf{r}'-\mathbf{r}'')$ to recover the Wigner function:

$$\langle \mathcal{A}\rangle = \int d\mathbf{r}\int d\mathbf{r}'\,\mathcal{A}(\mathbf{r}-\mathbf{r}'/2,\mathbf{r}+\mathbf{r}'/2)\int d\mathbf{r}''\,\delta(\mathbf{r}'-\mathbf{r}'')\Psi(\mathbf{r}+\mathbf{r}''/2)\,\Psi^*(\mathbf{r}-\mathbf{r}''/2)$$

$$\langle \mathcal{A}\rangle = \int d\mathbf{r}\int d\mathbf{r}'\,\mathcal{A}(\mathbf{r}-\mathbf{r}'/2,\mathbf{r}+\mathbf{r}'/2)\int d\mathbf{r}'' \times \frac{1}{(2\pi)^3}\int d\mathbf{k}\exp\left(i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r}'')\right)\Psi(\mathbf{r}+\mathbf{r}''/2)\,\Psi^*(\mathbf{r}-\mathbf{r}''/2)$$

$\delta(\mathbf{r}'-\mathbf{r}'')$

$$\langle \mathcal{A}\rangle = \int d\mathbf{r}\int d\mathbf{k}\,\mathcal{A}_w(\mathbf{r},\mathbf{k})\,f_w(\mathbf{r},\mathbf{k})$$

with

$$\mathcal{A}_w(\mathbf{r},\mathbf{k}) = \int d\mathbf{r}'\exp(-i\mathbf{k}\cdot\mathbf{r}')\,\mathcal{A}(\mathbf{r}-\mathbf{r}'/2,\mathbf{r}+\mathbf{r}'/2)$$

(Weyl-Wigner transform of $\mathcal{A}$)

⇒ Strong analogy between the Wigner function and the classical distribution function

Some properties of the Wigner Function

If $\mathcal{A}$ is only **r** dependent : $\mathcal{A}(\mathbf{r}) = \langle \mathbf{r} | \mathcal{A} | \mathbf{r} \rangle$

$$\langle \mathcal{A} \rangle = \int d\mathbf{r} \int d\mathbf{k}\ \mathcal{A}(\mathbf{r})\, f_w(\mathbf{r},\mathbf{k})$$

If $\mathcal{A}$ is only **k** dependent : $\mathcal{A}(\mathbf{k}) = \langle \mathbf{k} | \mathcal{A} | \mathbf{k} \rangle$

$$\langle \mathcal{A} \rangle = \int d\mathbf{r} \int d\mathbf{k}\ \mathcal{A}(\mathbf{k})\, f_w(\mathbf{r},\mathbf{k})$$

⇒ Complete analogy between the Wigner function and the classical distribution function

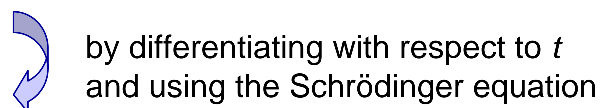
However, the Wigner function is not a distribution function (or a probability density) !

- it may assume negative values
- it would be in contradiction with the Heisenberg inequalities

(it is just mathematically used as a distribution function)

Dynamical equation of the Wigner Function

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



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

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

$$-\psi(\mathbf{r}+\mathbf{r}'/2,t)\left(H\psi^*(\mathbf{r}-\mathbf{r}'/2,t)\right)\Big]$$

where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) = H_0 + V(\mathbf{r})$

with $V(\mathbf{r})$ a general potential applied to the electron

We consider separately the effect of free electron term H_0 and of the potential $V(\mathbf{r})$

Dynamical equation of the Wigner Function

* free electron term ($H = H_0$)

$$i\hbar \frac{\partial f_w}{\partial t} = \frac{1}{(2\pi)^3} \int d\mathbf{r}' \exp(-i\mathbf{k}\cdot\mathbf{r}') \left[\left(-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}+\mathbf{r}'/2,t) \right) \psi^*(\mathbf{r}-\mathbf{r}'/2,t) - \psi(\mathbf{r}+\mathbf{r}'/2,t) \left(-\frac{\hbar^2}{2m} \nabla^2 \psi^*(\mathbf{r}-\mathbf{r}'/2,t) \right) \right]$$

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

(where $\nabla' \rightarrow$ derivation with respect to **r**')

integration by parts, assuming the wave function and its derivative to vanish at infinity, leads to:

$$\frac{\partial f_w}{\partial t} = -\frac{\hbar}{m} \mathbf{k} \cdot \frac{1}{(2\pi)^3} \int d\mathbf{r}' \exp(-i\mathbf{k}\cdot\mathbf{r}') \nabla \left[\psi(\mathbf{r}+\mathbf{r}'/2,t) \psi^*(\mathbf{r}-\mathbf{r}'/2,t) \right] = -\frac{\hbar}{m} \mathbf{k} \cdot \nabla f_w$$

Dynamical equation of the Wigner Function

* term including the effect of potential $V(\mathbf{r})$

$$i\hbar \left. \frac{\partial f_w}{\partial t} \right|_V = \frac{1}{(2\pi)^3} \int d\mathbf{r}' \exp(-i\mathbf{k}\cdot\mathbf{r}') \left[V(\mathbf{r}+\mathbf{r}'/2) \psi(\mathbf{r}+\mathbf{r}'/2,t) \psi^*(\mathbf{r}-\mathbf{r}'/2,t) - \psi(\mathbf{r}+\mathbf{r}'/2,t) V(\mathbf{r}-\mathbf{r}'/2) \psi^*(\mathbf{r}-\mathbf{r}'/2,t) \right]$$

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

inserting the plane wave representation of the *d* function leads to:

$$\left. \frac{\partial f_w}{\partial t} \right|_V = \int d\mathbf{k}' \; V_w(\mathbf{r},\mathbf{k}-\mathbf{k}') f_w(\mathbf{r},\mathbf{k}')$$

where $V_w(\mathbf{r},\mathbf{k}) = \frac{1}{i\hbar} \frac{1}{(2\pi)^3} \int d\mathbf{r}' \exp(-i\mathbf{k}\cdot\mathbf{r}') \left[V(\mathbf{r}+\mathbf{r}'/2) - V(\mathbf{r}-\mathbf{r}'/2) \right]$

is the **Wigner potential**

Dynamical equation of the Wigner Function

by including the free electron term, we have finally:

$$\frac{\partial f_w}{\partial t} + \frac{\hbar}{m}\,\mathbf{k}\cdot\nabla f_w = \int d\mathbf{k}'\; V_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}')$$

Wigner Transport Equation (WTE)

→ Dynamical equation for ballistic electrons moving in the potential $V(\mathbf{r})$

$$\hat{Q}[V]\, f_w(\mathbf{r},\mathbf{k}) = \int d\mathbf{k}'\; V_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}')$$

is the quantum evolution term of the Wigner function

Next steps:

* transforming the Wigner potential to see better the connection with BTE
* introduction of scatterings (collisions)
* solution of BTE for device simulation

Connection between Wigner TE and Boltzmann TE

The Wigner potential writes:

$$V_w(\mathbf{r},\mathbf{p}) = \frac{1}{i\hbar}\frac{1}{(2\pi)^3}\int d\mathbf{r}'\,\exp(-i\mathbf{k}\cdot\mathbf{r}')\, B_V(\mathbf{r},\mathbf{r}')$$

where $B_V(\mathbf{r},\mathbf{r}') = V(\mathbf{r}+\mathbf{r}'/2) - V(\mathbf{r}-\mathbf{r}'/2)$

Gradient expansion of the potential V: $\hat{V}_{\mp}(\mathbf{r},\mathbf{r}') = V(\mathbf{r}\pm\mathbf{r}'/2) - \nabla V(\mathbf{r})\cdot(\pm\mathbf{r}'/2)$

$$\hat{B}_V(\mathbf{r},\mathbf{r}') = \hat{V}_+(\mathbf{r},\mathbf{r}') - \hat{V}_-(\mathbf{r},\mathbf{r}')$$

$$\rightarrow B_V(\mathbf{r},\mathbf{r}') = \hat{B}_V(\mathbf{r},\mathbf{r}') + \underbrace{\nabla V(\mathbf{r})}_{-\mathbf{F}}\cdot\mathbf{r}'$$

by defining $\hat{V}_w(\mathbf{r},\mathbf{p}) = \frac{1}{i\hbar}\frac{1}{(2\pi)^3}\int d\mathbf{r}'\,\exp(-i\mathbf{k}\cdot\mathbf{r}')\,\hat{B}_V(\mathbf{r},\mathbf{r}')$

and given that $\frac{1}{i\hbar}\int d\mathbf{r}'\,\exp(-i\mathbf{k}\cdot\mathbf{r}')\,\nabla V(\mathbf{r})\cdot\mathbf{r}' = \frac{(2\pi)^3}{\hbar}\nabla V\,\delta'(\mathbf{k})$

→ we can separate the effect of the classical force **F** from quantum effects:

$$\int d\mathbf{k}'\; V_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}') = -\frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f_w + \int d\mathbf{k}'\; \hat{V}_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}')$$

Connection between Wigner TE and Boltzmann TE

Finally, the **WTE** writes:

$$\frac{\partial f_w}{\partial t} + \frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{r}} f_w + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f_w = \int d\mathbf{k}'\ \hat{V}_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}')$$

compared with the **BTE**:

$$\frac{\partial f}{\partial t} + \frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{r}} f + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f = 0$$

(without collision term)

If we can separate $V(\mathbf{r})$ into: $V(\mathbf{r}) = V_{slow}(\mathbf{r}) + V_{rapid}(\mathbf{r})$

V_{slow} → classical evolution; V_{rapid} → quantum evolution

$$\frac{\partial f_w}{\partial t} + \frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{r}} f_w - \frac{1}{\hbar}\nabla V_{slow}\cdot\nabla_{\mathbf{k}} f_w = \hat{Q}\left[V_{rapid}\right] f_w$$

Scattering in the Wigner Transport Equation

The simple method: instantaneous perturbation process

→ Boltzmann collision operator $\hat{C}$: it operates on the Wigner function f_w

$$\hat{C}\ f_w = \sum_i \Big[\int f_w(\mathbf{r},\mathbf{k}')\left[1-f_w(\mathbf{r},\mathbf{k})\right] S_i(\mathbf{k}',\mathbf{k})\, d\mathbf{k}' - \int f_w(\mathbf{r},\mathbf{k})\left[1-f_w(\mathbf{r},\mathbf{k}')\right] S_i(\mathbf{k},\mathbf{k}')\, d\mathbf{k}'\Big]$$

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

$$\frac{\partial f_w}{\partial t} + \frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{r}} f_w + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f_w = \hat{Q}\, f_w + \hat{C}\, f_w$$

Strong analogy between BTE and WTE

⇒ posibility of using the same numerical technique

Wigner Function and Green Functions

$$f_w = -i\hbar\, G^{<}$$

Monte Carlo solution of the WTE

$$\frac{\partial f_w}{\partial t} + \frac{\hbar}{m}\mathbf{k}\cdot\nabla_{\mathbf{r}} f_w + \frac{1}{\hbar}\mathbf{F}\cdot\nabla_{\mathbf{k}} f_w = \int d\mathbf{k}'\ \hat{V}_w(\mathbf{r},\mathbf{k}-\mathbf{k}')\, f_w(\mathbf{r},\mathbf{k}')$$

Idea : representing the Wigner fonction f_w as a sum of Dirac excitations in r et k, with an amplitude A (affinity) which changes

$$f_w(r,k) = \sum_i \delta(r-r_i)\,\delta(k-k_i)\,A_i$$

* pseudo-particule i characterized by :
- r_i → classical evolution
- k_i → classical evolution
- A_i → quantum evolution

The A_i may be negative

* classical limit : $A_i = 1$ ("real" particule)

⇒ We can use the standard Monte Carlo algorithm, by including the evolution of affinities

In a cell c(**r**,**k**) :

$$\sum_{i\in c(\mathbf{r},\mathbf{k})} \frac{dA_i}{dt} = \hat{Q}\left[V_{rapid}\right] f_w(\mathbf{r},\mathbf{k})$$

Interaction of a wave packet on a square barrier

Schrödinger 's equation:

Wigner's equation:

$p(x)$ (m^{-1}); axis values: 0, $5\ 10^7$, $1\ 10^8$; x (nm): 0, 40, 80, 120

t = 20 fs | t = 40 fs | t = 80 fs

⇒ Very good description of quantum effects using the Wigner's equation

GaAs/GaAlAs Resonant Tunneling Diode (RTD)

$N_D = 10^{18}\ at.cm^{-3}$ | $N_D = 10^{16}\ at.cm^{-3}$ | $N_D = 10^{18}\ at.cm^{-3}$

60nm | 9.5nm | 3nm | 5nm | 3nm | 9.5nm | 60nm

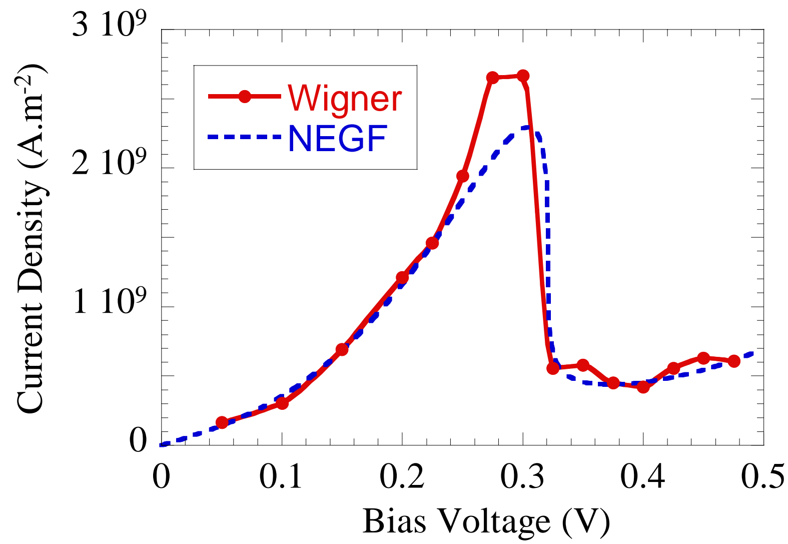
On-resonance (V = 0.3 V)

E_C (eV): 0.3, 0.2, 0.1, 0, -0.1, -0.2, -0.3, -0.4, -0.5

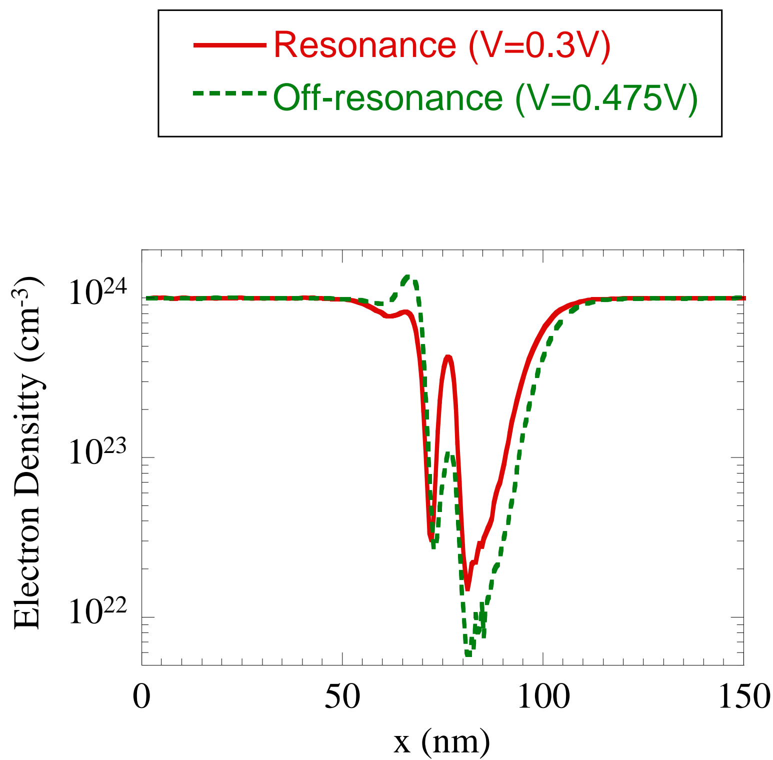
x (nm): 0, 50, 100, 150

I-V Characteristics

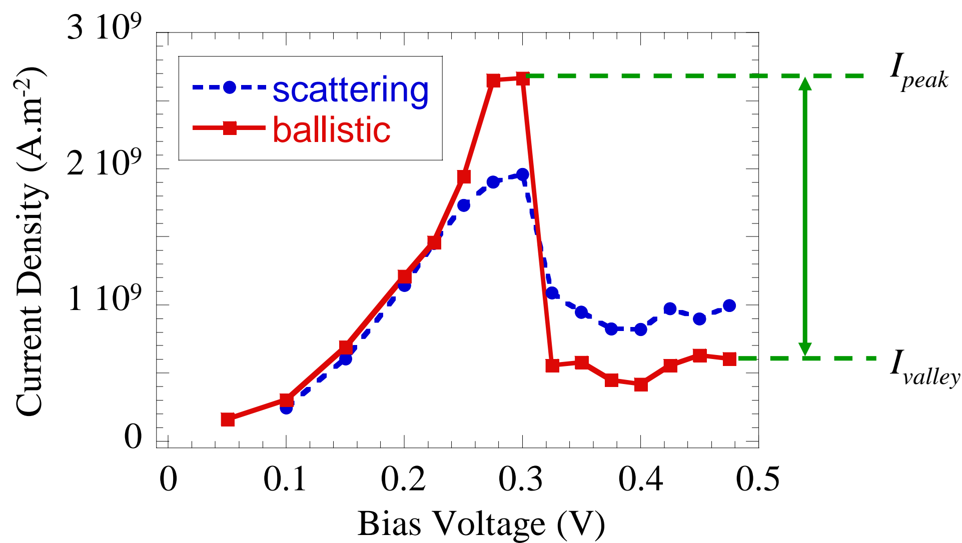
* Ballistic limit (no scattering)
* Comparison with Non-Equilibrium Green Function calculation



Electron Density



Effect of scattering



Scattering ⇒ reduction of Peak-to-Valley Ratio Ipeak/Ivalley

Transport in semiconductor nanodevices

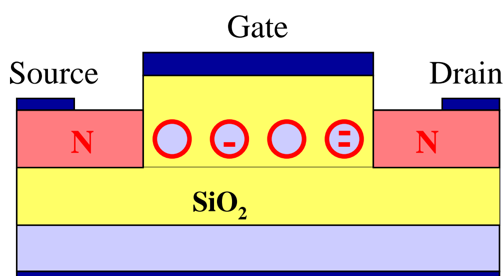
Third part: **Semiconductor quantum dots and Coulomb blockade for single-electron devices**

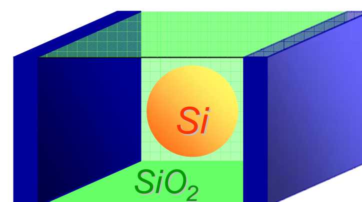
4. Coulomb blockade in conducting island: principle

5. Electronic structure of semiconductor quantum dot

6. Single electron tunneling: I-V characteristics

- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Example: MISiIM**

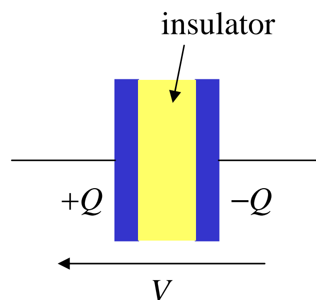




4. Coulomb blockade in conducting island: principle

The quantum capacitor

* Classical capacitor:



$$Q = C \cdot V$$

Displacement Current: $I(t) = \dfrac{dq}{dt}$

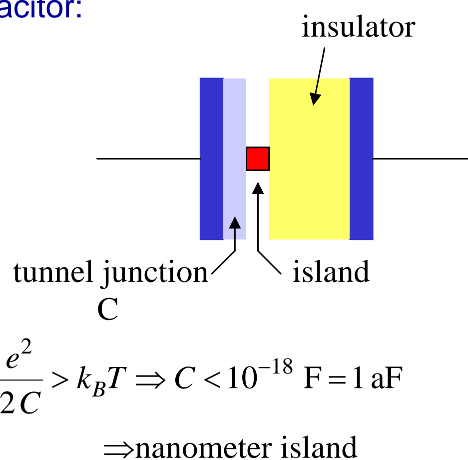
(no charge flow through the insulator)

Electrostatic energy in the capacitor:

$$E = \int_0^{\infty} V(t) I(t) dt = \frac{Q^2}{2C}$$

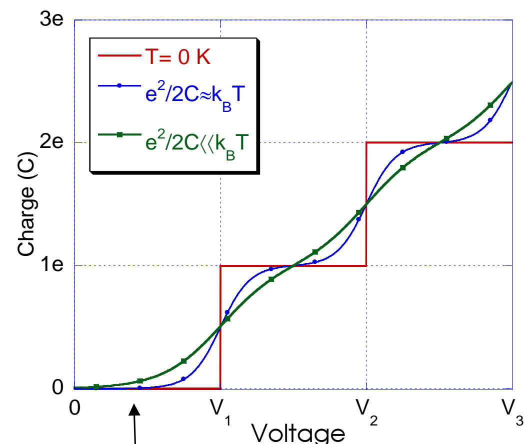
* Quantum capacitor:

$$\frac{e^2}{2C} \gg k_B T$$



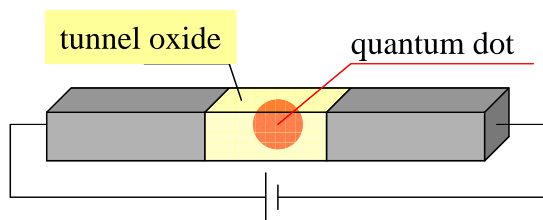
$$\frac{e^2}{2C} > k_B T \Rightarrow C < 10^{-18}\ \mathrm{F} = 1\,\mathrm{aF}$$

$\Rightarrow$nanometer island

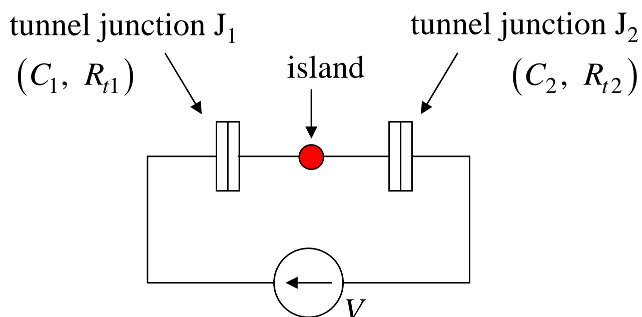


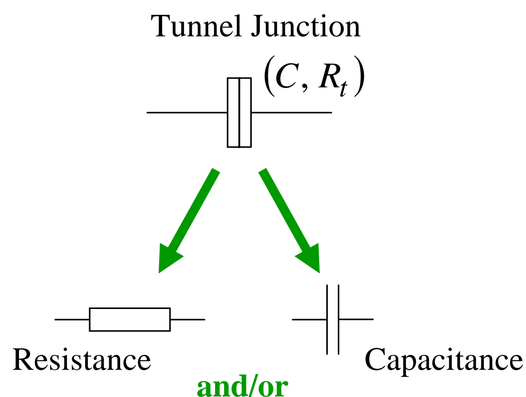
The double tunnel junction structure

island (or quantum dot) weakly coupled to to two leads to an external circuit via 2 tunnel junctions



$\Rightarrow$ control of the current electron by electron

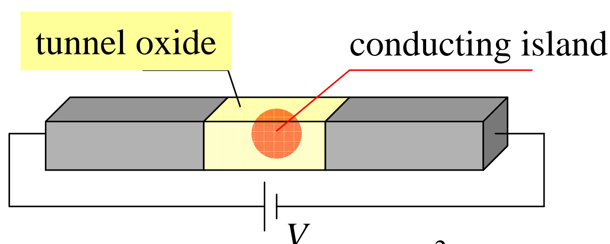


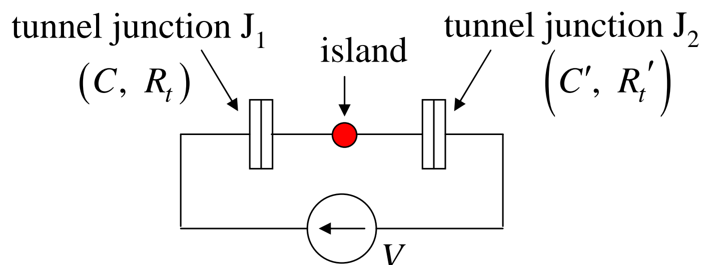


The principle of Coulomb blockade

Basic structure: The double tunnel junction

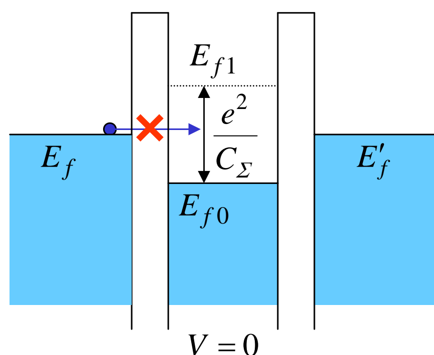
$\rightarrow$ conducting island weakly coupled to to 2 leads (external circuit) via 2 tunnel junctions





Charging energy : $E_{ch} = \dfrac{e^2}{C_\Sigma}$ (additional energy in the island for 1 additional electron)

where $C_\Sigma = C + C'$



Coulomb blockade effect may occur if :

$$\frac{e^2}{C_\Sigma} > k_B T$$

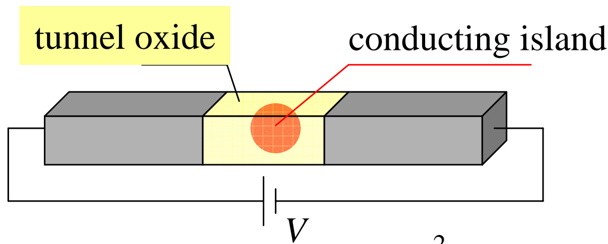
$$\Rightarrow C_\Sigma < 10^{-18}\ \mathrm{F} = 1\ \mathrm{aF} \quad (300\ \mathrm{K})$$

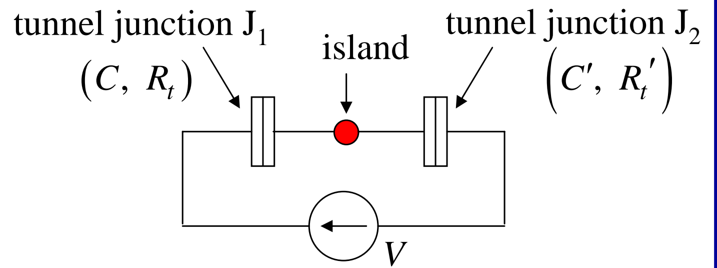
$\Rightarrow$ nanometer island

The principle of Coulomb blockade

Basic structure: The double tunnel junction

→ conducting island weakly coupled to to 2 leads (external circuit) via 2 tunnel junctions





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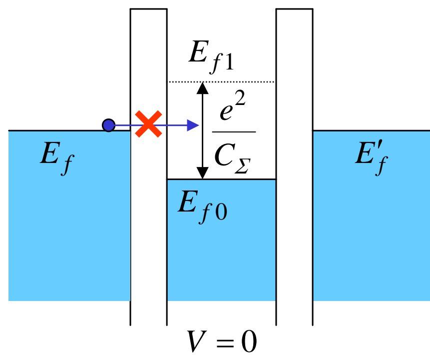
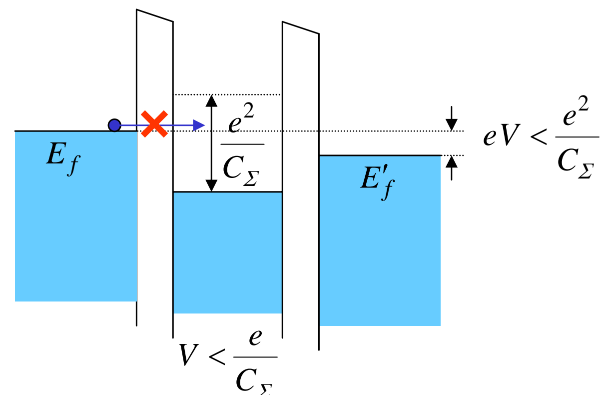
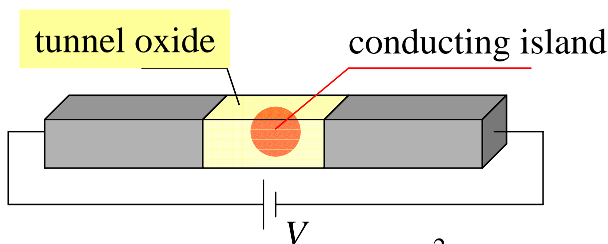


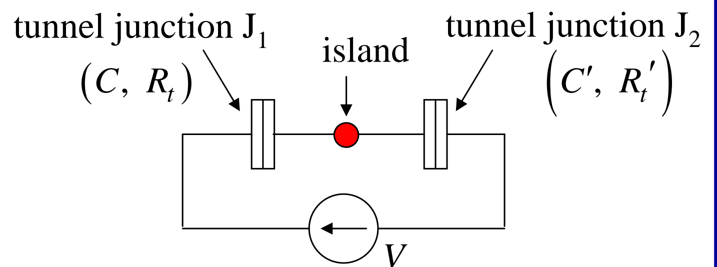


The principle of Coulomb blockade

Basic structure: The double tunnel junction

→ conducting island weakly coupled to to 2 leads (external circuit) via 2 tunnel junctions





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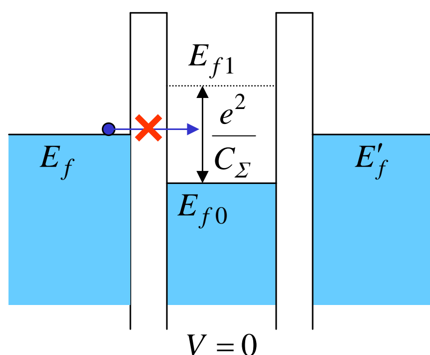
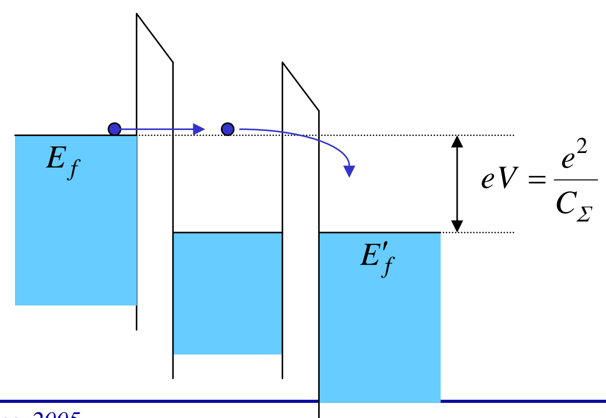
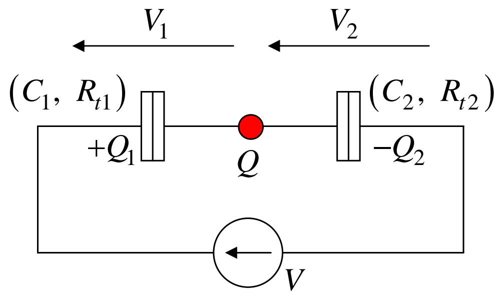




The MIMIM structure: electrical modelling



Basic equations:

$$\begin{cases} Q + Q_1 - Q_2 = 0 \\ Q = -n\,e \\ Q_1 = C_1 V_1 \\ Q_2 = C_2 V_2 \\ V = V_1 + V_2 \end{cases} \rightarrow \begin{cases} V_1 = (C_2 V + n\,e)/C_{eq} \\ V_2 = (C_1 V - n\,e)/C_{eq} \end{cases}$$

Basic idea:

@ a single electron tunneling through J_1 or J_2 is possible only if it leads to a **lower total energy**

Calculation of the total energy E of the system:

$$E = E_p + W$$

potential (electrostatic) energy — work done by the voltage source

* Potential energy:

$$E_p = \frac{Q_1^2}{2C_1} + \frac{Q_2^2}{2C_2} = \frac{C_1 V_1^2}{2} + \frac{C_2 V_2^2}{2}$$

i.e. with $C_{eq} = C_1 + C_2$:

$$E_p = \frac{1}{2C_{eq}}\left[C_1 C_2 V^2 + (n\,e)^2\right]$$

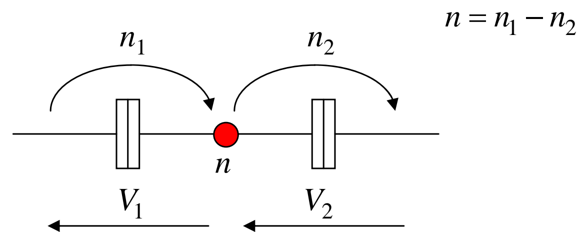
The MIMIM structure: electrical modelling

* Work done by the source:

$$W = \int V(t)\,I(t)\,dt = V\,\Delta Q \qquad \text{with} \quad V(t) = V = \text{Const}$$

$\rightarrow$ tunneling out the island via J_2: $(n_2 \rightarrow n_2 + 1 \Rightarrow n \rightarrow n - 1)$

$J_2 \equiv$ resistance
$J_1 \equiv$ capacitance



$$V_1 \rightarrow V_1 - \frac{e}{C_{eq}}$$

$$\Delta V_1 = -\frac{e}{C_{eq}} \Rightarrow \Delta Q_1 = -e\frac{C_1}{C_{eq}}$$

The voltage source compensate this charge variation by providing ΔQ_1
For n_2 electrons the source provide the work:

$$W_1 = -e\frac{C_1}{C_{eq}} n_2 V$$

$\rightarrow$ tunneling in the island via J_1:

$J_1 \equiv$ resistance
$J_2 \equiv$ capacitance

For n_1 electrons the source provide the work:

$$W_2 = -e\frac{C_2}{C_{eq}} n_1 V$$

The MIMIM structure: electrical modelling

* Total energy: Finally,

$$E = \frac{1}{2C_{eq}}\left[C_1 C_2 V^2 + (ne)^2\right] + e\frac{V}{C_{eq}}\left(n_1 C_2 + n_2 C_1\right)$$

* Possible transitions:

→ Junction 2:

$$n_2 \to n_2 + 1 \Rightarrow n \to n-1 \Rightarrow \Delta E_{n_2+1} = \frac{e}{2C_{eq}}\left[-(2n-1)e + 2VC_1\right]$$

$$n_2 \to n_2 - 1 \Rightarrow n \to n+1 \Rightarrow \Delta E_{n_2-1} = \frac{e}{2C_{eq}}\left[+(2n-1)e - 2VC_1\right]$$

→ Junction 1:

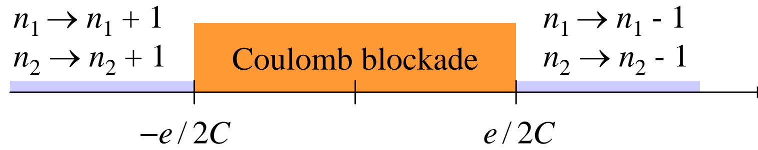
$$n_1 \to n_1 + 1 \Rightarrow n \to n+1 \Rightarrow \Delta E_{n_1+1} = \frac{e}{2C_{eq}}\left[+(2n+1)e + 2VC_2\right]$$

$$n_1 \to n_1 - 1 \Rightarrow n \to n-1 \Rightarrow \Delta E_{n_1-1} = \frac{e}{2C_{eq}}\left[-(2n-1)e - 2VC_2\right]$$

Threshold voltages: $(\Delta E \le 0)$

$$\begin{cases} \Delta E_{n_2+1} < 0 \Rightarrow V < (2n-1)e/2C_1 \\ \Delta E_{n_2-1} < 0 \Rightarrow V > (2n+1)e/2C_1 \\ \Delta E_{n_1+1} < 0 \Rightarrow V < -(2n+1)e/2C_2 \\ \Delta E_{n_1-1} < 0 \Rightarrow V < -(2n-1)e/2C_2 \end{cases}$$

* For $n = 0$:



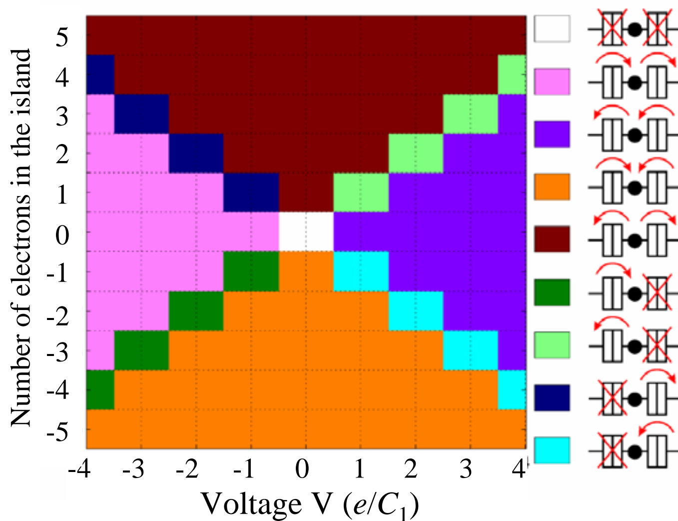
Coulomb blockade for:

$$|V| < V_{th} = \frac{e}{2C}$$

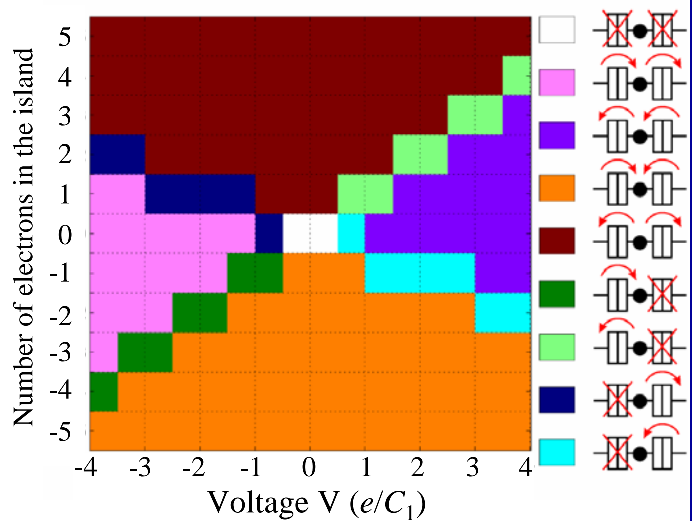
The MIMIM structure: electrical modelling

* For any n value:

Possible transitions in a MIMIM structure at $T = 0$ K

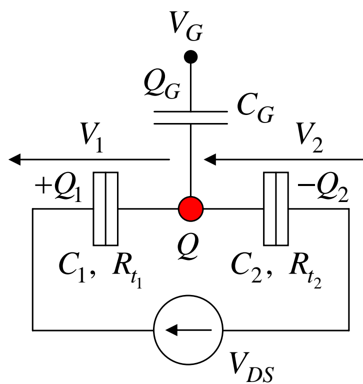


$C_2 = C_1$

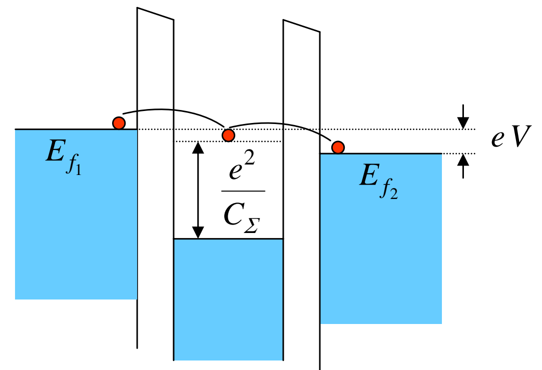


$C_2 = C_1 / 2$

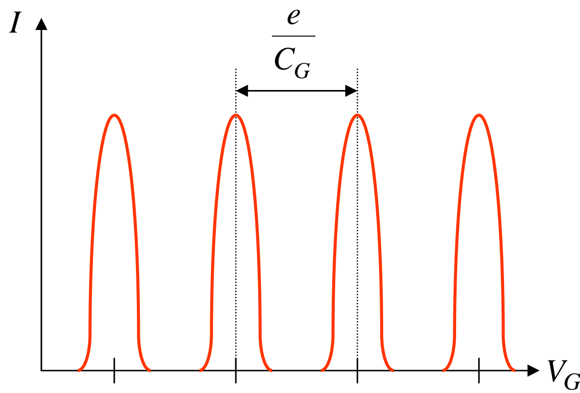
The Single Electron Transistor (SET)

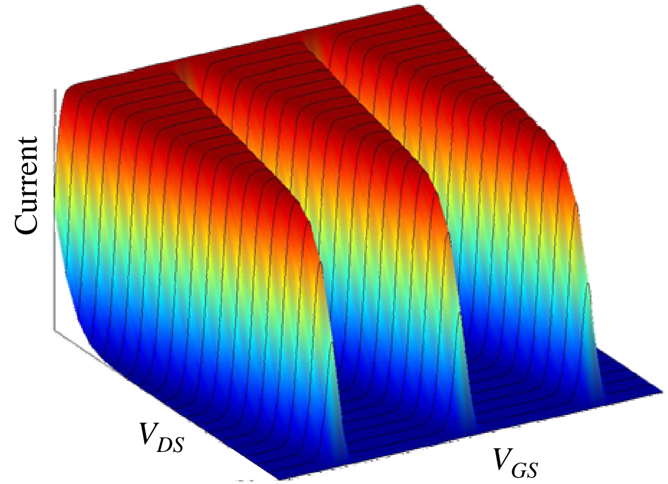


$$\begin{cases} Q = Q_2 - Q_1 - Q_G \\ Q = -n\,e + q_0 \\ Q_1 = C_1 V_1 \\ Q_2 = C_2 V_2 \\ Q_G = C_G \left(V_{GS} - V_2\right) \\ V_{DS} = V_1 + V_2 \end{cases}$$



The gate electrode allows controlling the Fermi level in the dot



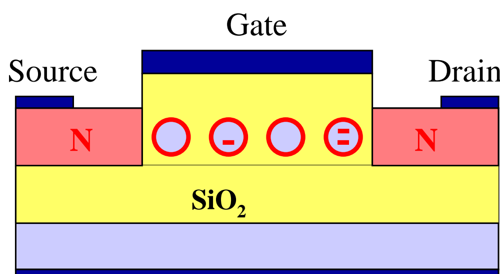


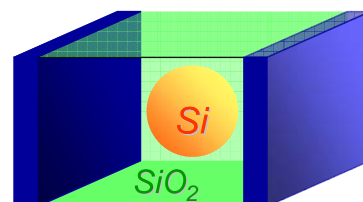
Third part: **Semiconductor quantum dots and Coulomb blockade for single-electron devices**

4. Coulomb blockade in conducting island: principle

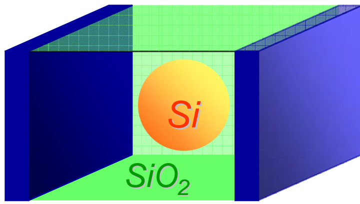
5. Electronic structure of semiconductor quantum dot

6. Single electron tunneling: I-V characteristics
- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Example: MISiIM**





Calculation of QD electronic structure



The problem : small number of electrons in a small SC QD

– nanometer size in semiconductor : quantization effect

→ **Shrödinger equation is to be solved**

– few electrons : Fermi statistics does not apply

→ **electostatic interaction is to be included properly**

Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} V_{conf}(\vec{r}_i) + \frac{1}{2}\frac{1}{4\pi\varepsilon\varepsilon_0}\sum_{i=1}^{N}\sum_{\substack{i=1 \\ j\neq i}}^{N} \frac{e^2}{\|\vec{r}_i - \vec{r}_j\|} + \sum_{i=1}^{N} V_{bias}(\vec{r}_i)$$

kinetic energy — confinement potential — interaction between electrons — bias potential

Schrödinger Equation:

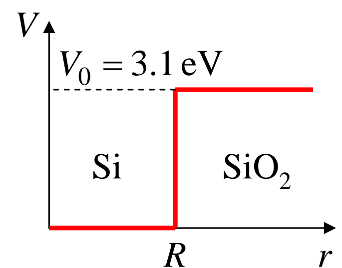
$$H\,\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = E\,\Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N)$$

Problem similar to the case of atoms

Electronic structure: Numerical techniques

The simplest case:

- spherical quantum dot
- 1 electron
- no bias



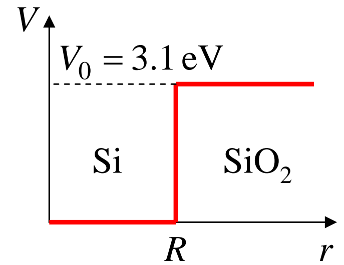
$$\left[-\frac{\hbar^2}{2}\nabla_{\vec{r}}\left(\frac{1}{m}\nabla_{\vec{r}}\right) + V_{conf}(\vec{r})\right]\Psi(\vec{r}) = E\,\Psi(\vec{r})$$

spherical symmetry → spherical harmonics

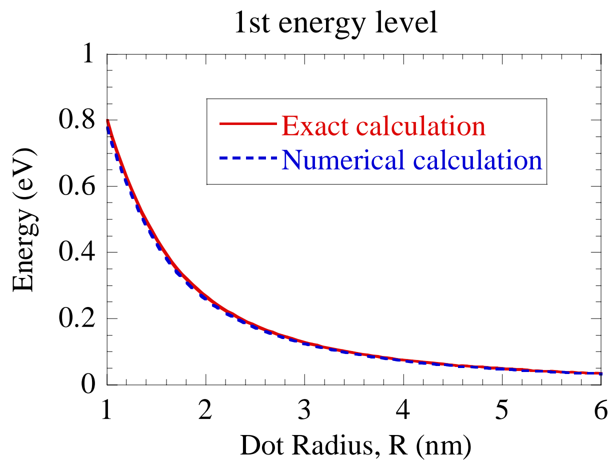
Electronic structure: Numerical techniques

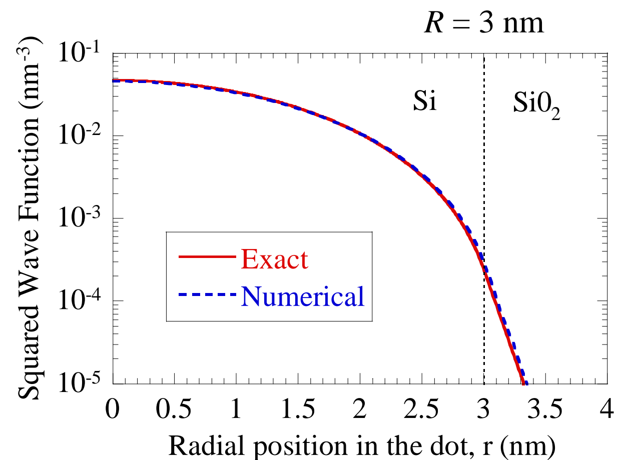
The simplest case:

- spherical quantum dot
- 1 electron
- no bias



$$\left[-\frac{\hbar^2}{2} \nabla_{\vec{r}} \left(\frac{1}{m} \nabla_{\vec{r}} \right) + V_{conf}\left(\vec{r}\right) \right] \Psi\left(\vec{r}\right) = E\,\Psi\left(\vec{r}\right)$$





possible application: basis functions for Hartree-Fock

Electronic structure: Numerical techniques

The general case: approximations are required to solve the Schrödinger Eq.

*** The Hatree method**

$$\psi\left(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\right) = \psi_1\left(\vec{r}_1\right)\psi_2\left(\vec{r}_2\right)\cdots\psi_N\left(\vec{r}_N\right)$$

- easy to implement
- w. function is not antisymetric (correlations not included)
- should be limited to $N = 2$

*** The Hatree-Fock method**

$$\psi\left(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N\right) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) & \cdots & \psi_1(\vec{r}_N) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) & \cdots & \psi_2(\vec{r}_N) \\ \cdots & \cdots & \cdots & \cdots \\ \psi_N(\vec{r}_1) & \psi_N(\vec{r}_2) & \cdots & \psi_N(\vec{r}_N) \end{vmatrix}$$

(Slater determinant)

- correct approach for any N
- w. function is antisymetric (correlations included)
- difficult to implement

*** The Density Functional Theory (DFT)**

It assumes the system can be fully described by the electron density

- rigorous for any N
- correlations included
- less information given: only total energy, no wave function

Electronic structure: Hartree method

Hartree : $\psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)\cdots\psi_N(\vec{r}_N)$

1 equation for each electron : $H_i\,\psi_i = E_i\,\psi_i$

with : $H_i = \dfrac{p_i^2}{2m} + V_{conf}(\vec{r}_i) + V_{inter_i}(\vec{r}_i)$ (no bias)

V_{inter_i} represents the interaction of electron *i* with the rest of the electronic cloud of density ρ_i

$$\rho_i(\vec{r}) = -e \sum_{\substack{j=0 \\ j\neq i}}^{N} \left|\psi_j(\vec{r})\right|^2 \quad \text{and} \quad \vec{\nabla}\left(\varepsilon\,\varepsilon_0\,\vec{\nabla}V_{inter_i}\right) = e\,\rho_i$$

system of coupled Poisson / Schrödinger equations

$$\begin{cases} \vec{\nabla}\left(\varepsilon\vec{\nabla}V_{inter_i}\right) = -\dfrac{e}{\varepsilon\,\varepsilon_0}\displaystyle\sum_{j\neq i}^{N}\left|\psi_j(\vec{r})\right|^2 \\ \dfrac{p_i^2}{2m}\psi_i + \left(V_{conf} + V_{inter_i}\right)\psi_i = E_i\,\psi_i \end{cases}$$

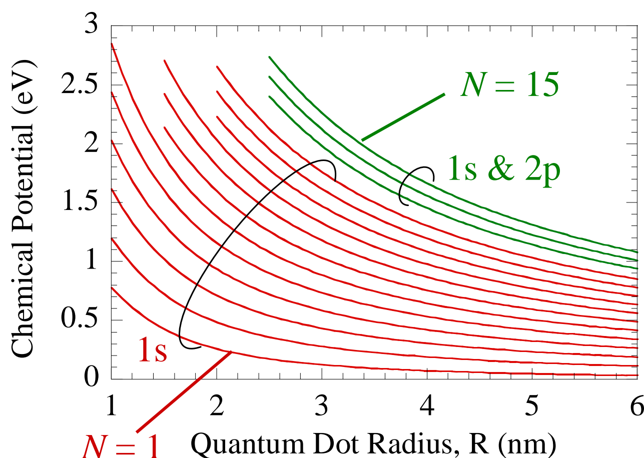
Electronic structure: results of Hartree

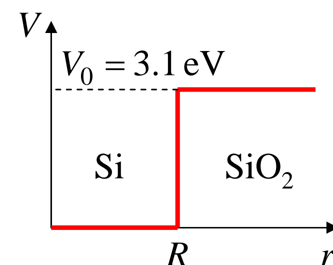
For a discrete number of electrons *N*, **the chemical potential** $\mu(N)$ is defined as the variation of total energy resulting from one additional electron:

$$\mu(N) = \frac{\partial E_{TOT}}{\partial N} \simeq \frac{E(N) - E(N-1)}{N-(N-1)} = E(N) - E(N-1)$$

spherical quantum dot

Chemical Potential as a function of QD radius for *N* = 1 to *N* = 15





(including the difference in effective mass and dielectric constant between Si and SiO_2)

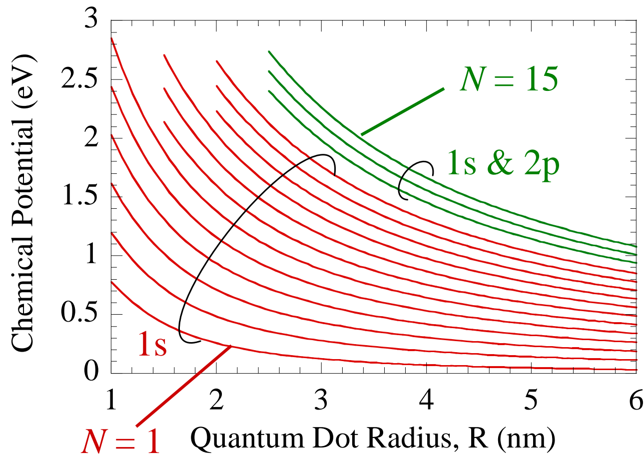
Electronic structure: results of Hartree

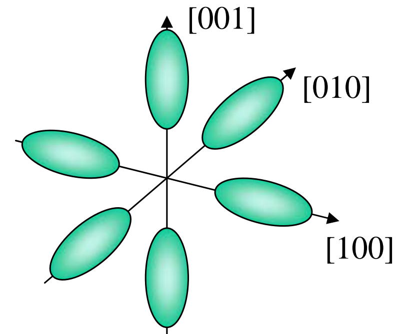
For a discrete number of electrons N, **the chemical potential** $\mu(N)$ is defined as the variation of total energy resulting from one additional electron:

$$\mu(N) = \frac{\partial E_{TOT}}{\partial N} \simeq \frac{E(N) - E(N-1)}{N-(N-1)} = E(N) - E(N-1)$$

spherical quantum dot

Chemical Potential as a function of QD radius for $N = 1$ to $N = 15$





* The 12 first electrons occupy the 1s orbital (6-fold degeneracy of Si conduction band and 2-fold spin degeneracy)

* The other electrons start to fill the 2p orbital

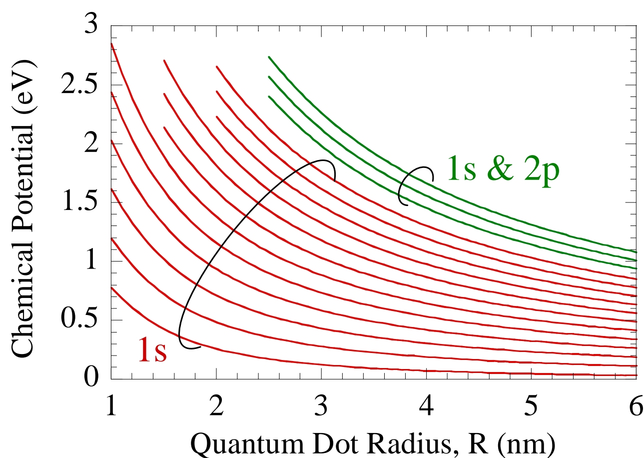
Electronic structure: results of Hartree

For a discrete number of electrons N, **the chemical potential** $\mu(N)$ is defined as the variation of total energy resulting from one additional electron:

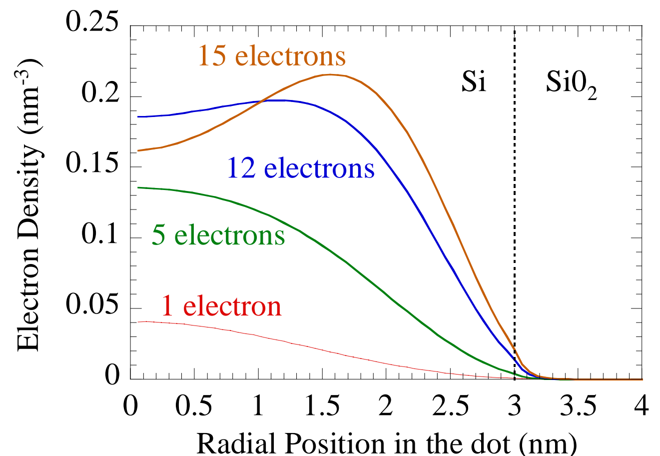
$$\mu(N) = \frac{\partial E_{TOT}}{\partial N} \simeq \frac{E(N) - E(N-1)}{N-(N-1)} = E(N) - E(N-1)$$

spherical quantum dot

Chemical Potential as a function of QD radius for $N = 1$ to $N = 15$



Electron Density for $R = 3$ nm



Electronic structure: Comparison Hartree / DFT

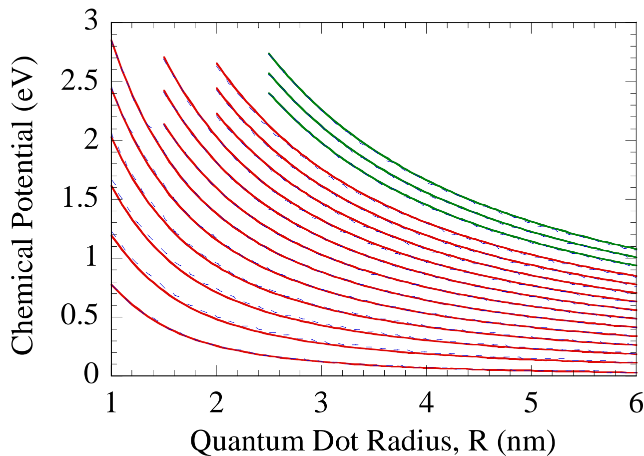
Validation of the Hartree method by comparison with Density Functional theory

DFT calculation : Kohn & Sham equations within Local Density Approximation (LDA)

→
- * Total electron energy and density in the dot for the fundamental state
- * Correct for any number of electrons
- * No information on the wave function (strictly speaking)

Chemical Potential as a function of QD radius for $N = 1$ to $N = 15$

[Sée et al., J. Appl. Phys. 92 (2002) 3141-3146]



☞ Excellent agreement

☞ The Hartree approximation is acceptable

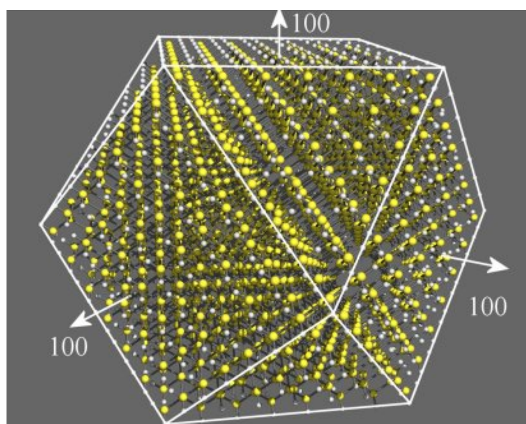
Validity of effective mass approximation

☞ Calculation of the first levels in Si-NC using 2 approaches :

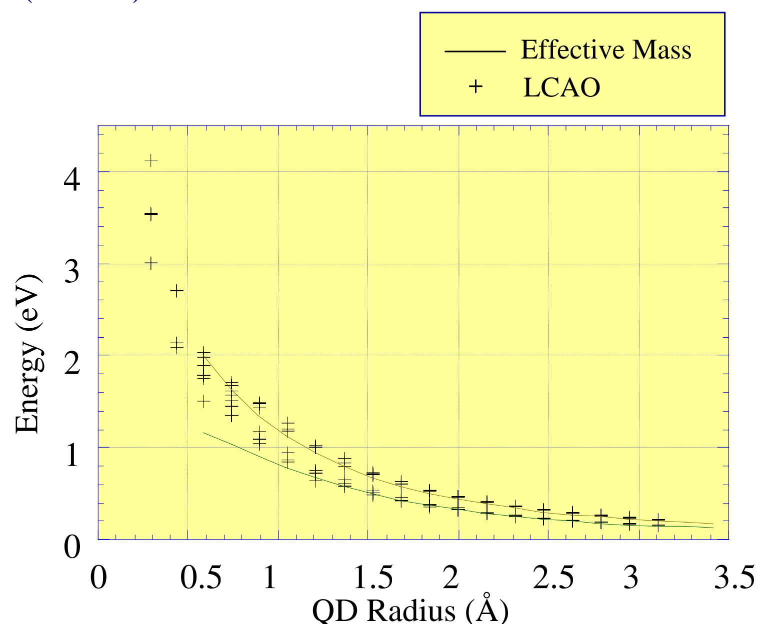
→ effective mass approximation (DFT)

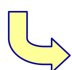
→ tight binding calculation (LCAO)

[Sée et al., Phys. Rev. B 66 (2002) 193307]



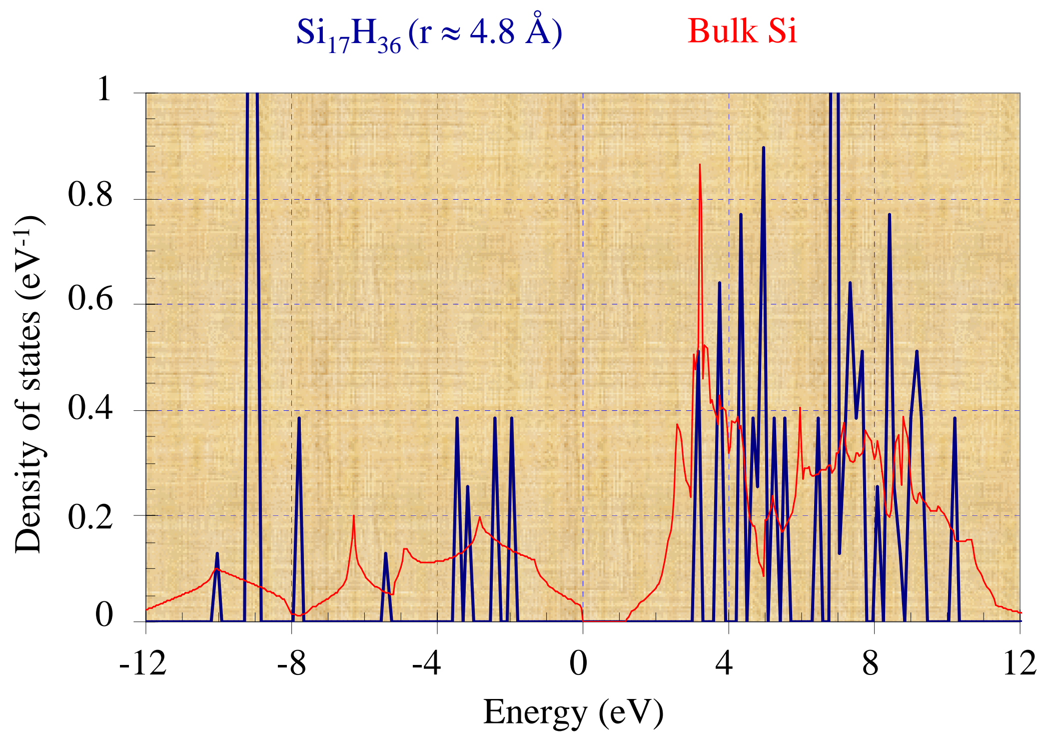
dangling bonds saturated with H atoms



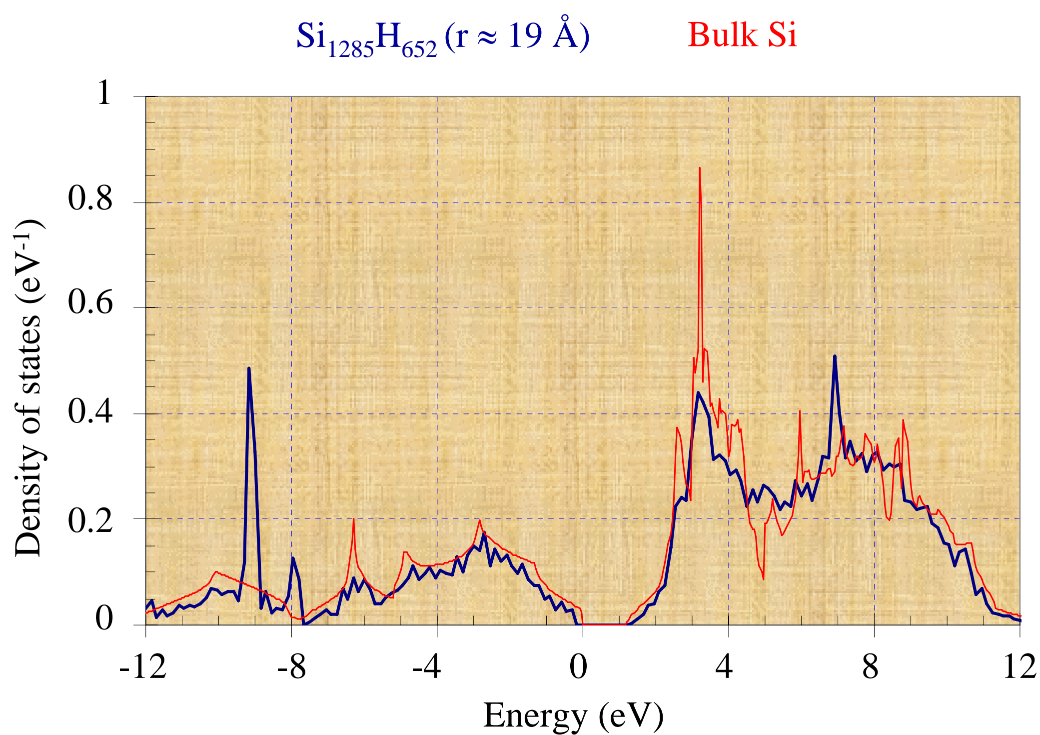


The effective mass approximation is correct for R > 1.5 nm

Electronic Structure: Density of States



Electronic Structure: Density of States

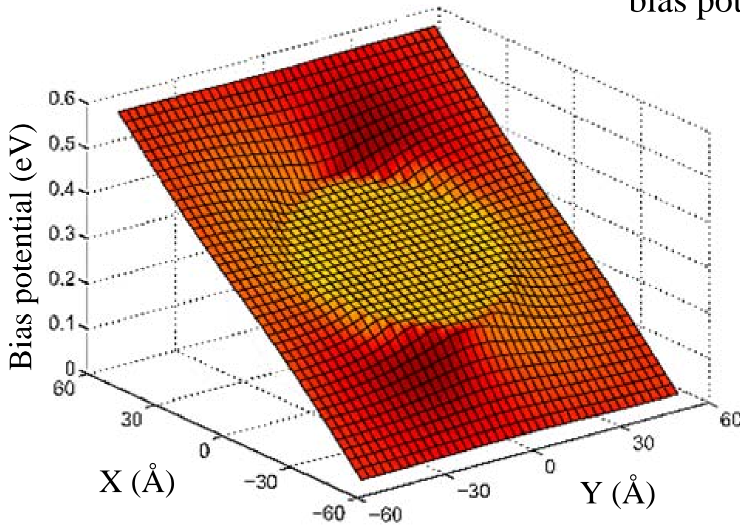


Electronic structure: Effect of bias (method)

For a biased quantum dot :

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} V_{conf}\left(\vec{r}_i\right) + \sum_{i=1}^{N} V_{bias}\left(\vec{r}_i\right) + \frac{1}{2}\frac{1}{4\pi\varepsilon\varepsilon_0}\sum_{i=1}^{N}\sum_{\substack{i=1\\ j\neq i}}^{N}\frac{e^2}{\left\|\vec{r}_i-\vec{r}_j\right\|}$$

bias potential



V_{bias} can be obtained from the following Poisson's equation:

$$\vec{\nabla}\left(\varepsilon\varepsilon_0\vec{\nabla}V_{bias}\right)=0$$

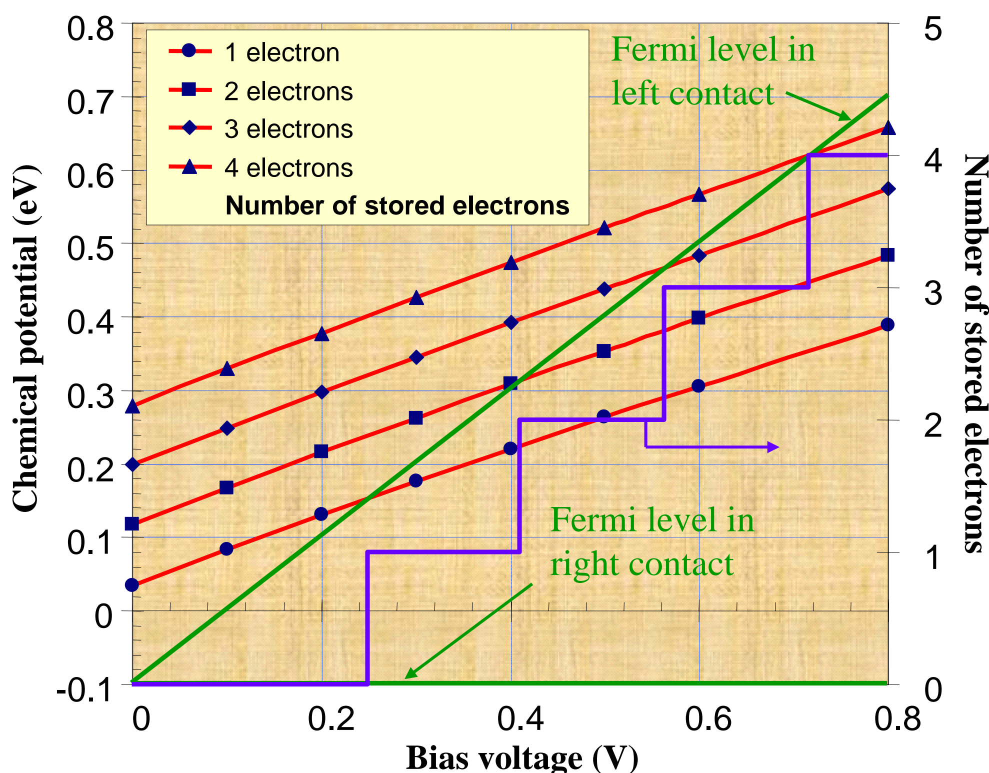
$$\text{with}\quad\begin{cases}V_{bias}\left(x=0,y,z\right)=0\\ V_{bias}\left(x=L,y,z\right)=V\end{cases}$$

→ all goes as if electrons evolve in a new effective potential $V_{conf} + V_{bias}$

Electronic structure: Effect of bias (result)

Energy level and maximum number of electrons stored in the dot

R = 6 nm

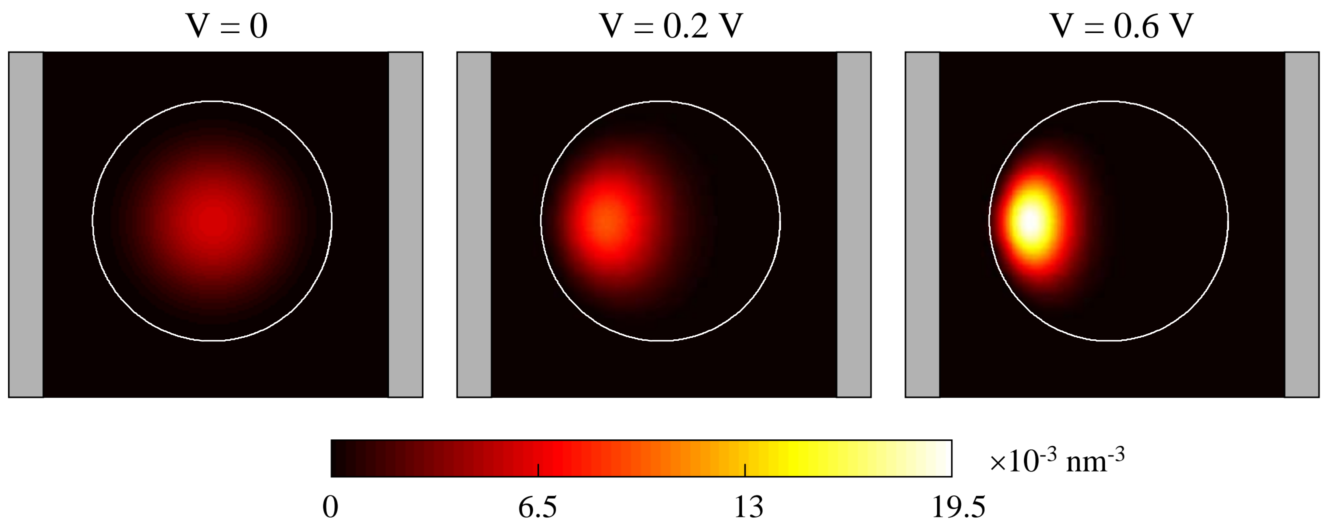


Electronic structure: Effect of bias (results)

Influence of bias on the density (wave function) in the dot

R = 6 nm

Example: electron density for 1 electron in the dot



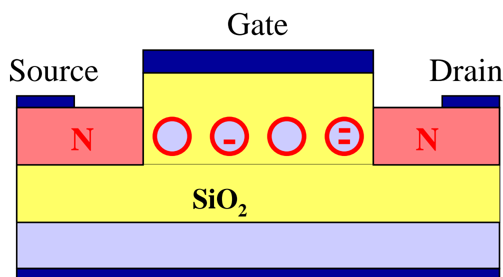
Electronic structure: Effect of bias (results)

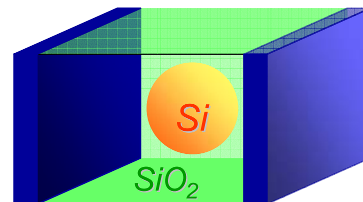
Third part: **Semiconductor quantum dots and Coulomb blockade for single-electron devices**

4. Coulomb blockade in conducting island: principle

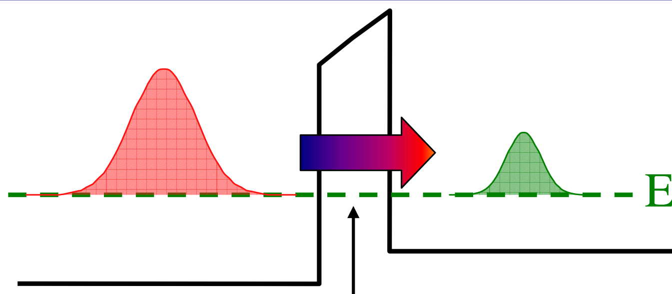
5. Electronic structure of semiconductor quantum dot

6. Single electron tunneling: I-V characteristics
- **Tunnel transfer hamiltonian**
- **Metallic vs Semiconductor quantum dot**
- **Monte Carlo simulation – Example: MISiIM**





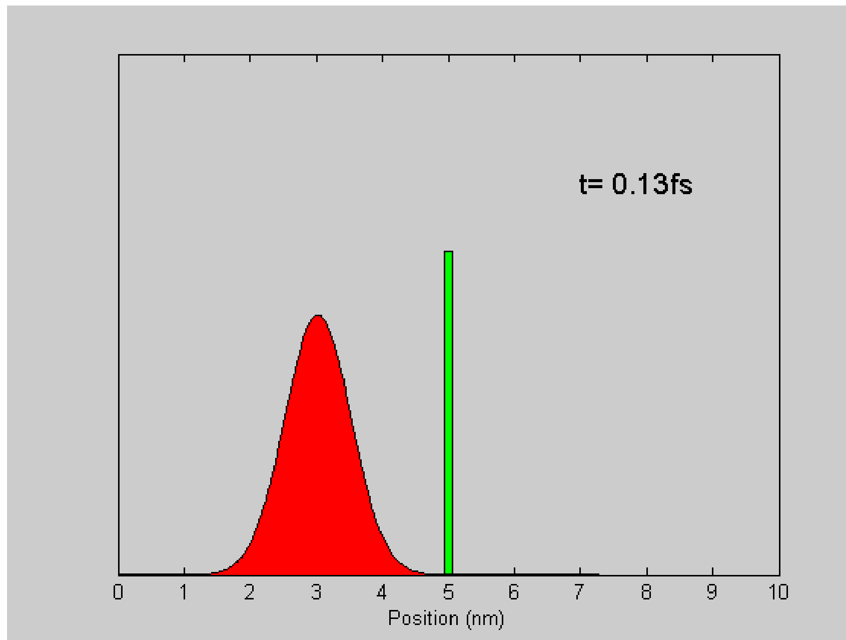
Single electron tunneling through a single barrier



* 1st method: (Schrödinger equation)
  - calculation of the eigen states of the system
  - transmission coefficient and probability current

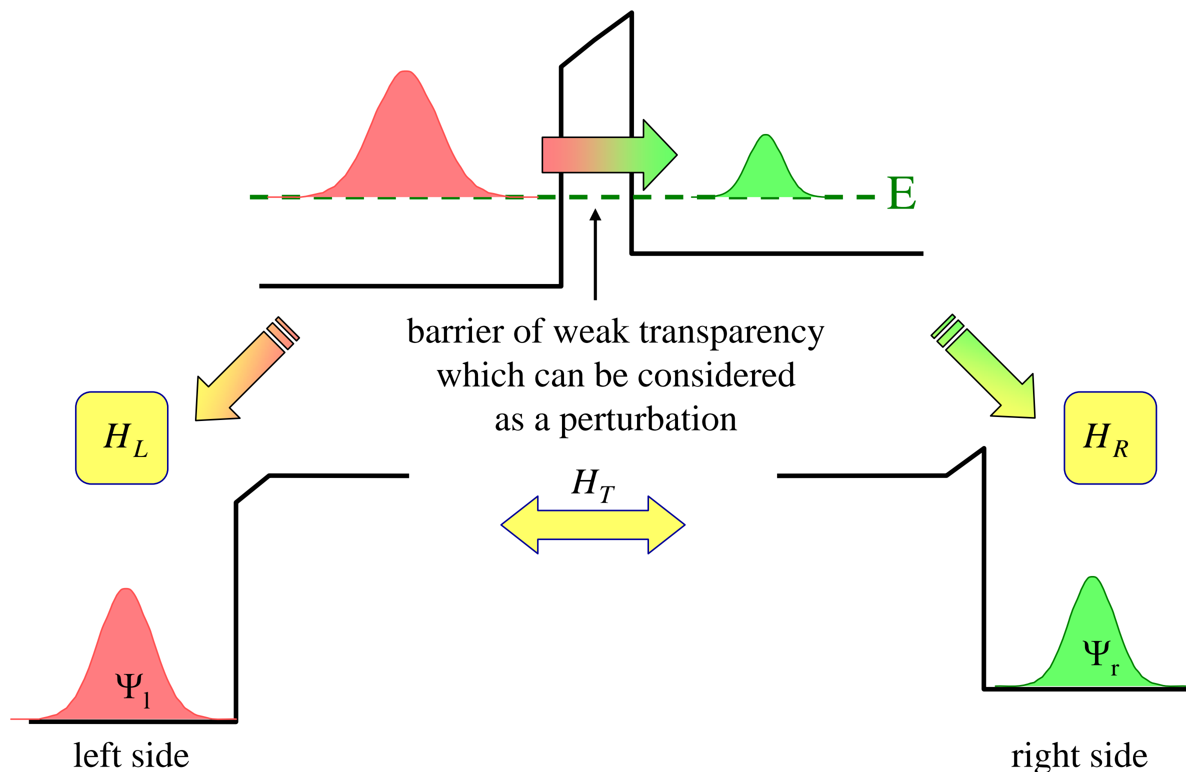
Single electron tunneling through a single barrier

Solution of Schrödinger equation for a 1D barrier



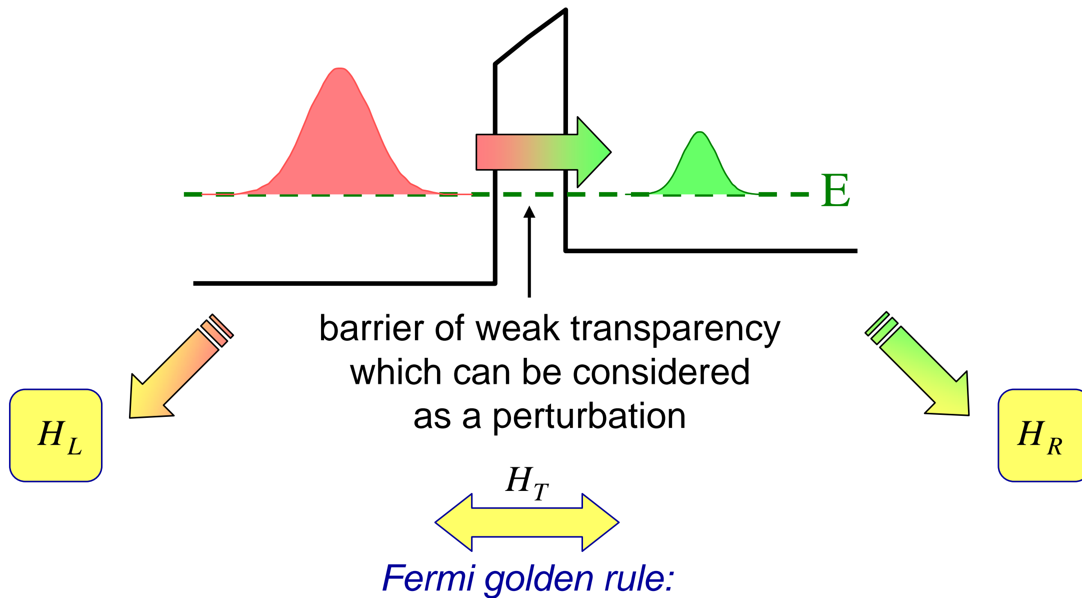
Single-electron tunneling

Tunnel Hamiltonian – Perturbative technique



Single-electron tunneling

Tunnel Hamiltonian – Perturbative technique



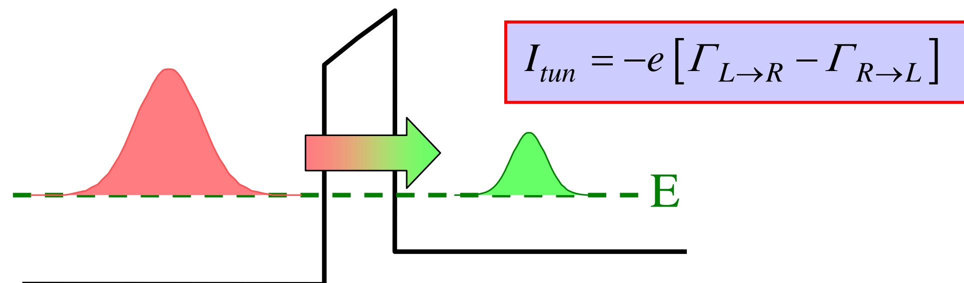
Fermi golden rule:

Probability per unit of time for an electron to have a tunnel event from a state k_L of the left side to a state k_R of the right side:

$$\delta^2 \Gamma_{k_L \to k_R} = \frac{2\pi}{\hbar} \left| \langle k_R | H_T | k_L \rangle \right|^2 \rho_L(E_L) \rho_R(E_R) f_L(E_L) \left[1 - f_R(E_R) \right] \delta(E_R - E_L)\, dE_L\, dE_R$$

Single-electron tunneling

Tunnel Hamiltonian – Perturbative technique



$$\delta^2 \Gamma_{k_L \to k_R} = \frac{2\pi}{\hbar} | M |^2 \rho_L(E_L) \rho_R(E_R) f_L(E_L) \left[1 - f_R(E_R) \right] \delta(E_R - E_L)\, dE_L\, dE_R$$

Total probability per unit of time: $\Gamma_{L \to R} = \int \delta^2 \Gamma_{k_L \to k_D}$

$$\Gamma_{L \to R} = \int \frac{2\pi}{\hbar} \left| \langle k_R | H_T | k_L \rangle \right|^2 \rho_L(E) \rho_R(E) f_L(E) \left[1 - f_R(E) \right] dE$$

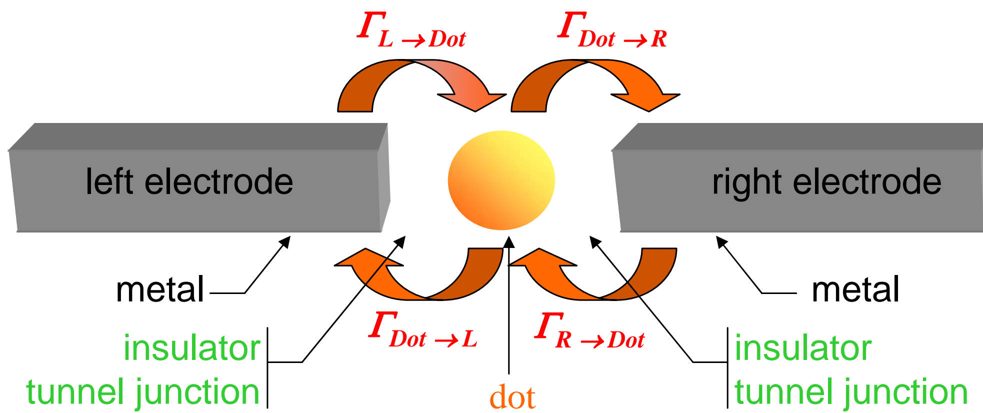
Matrix element (Bardeen):

$$M = \langle k_R | H_T | k_L \rangle = \frac{\hbar^2}{2} \iint_{S_B} \left[\psi_L [M_B]^{-1} \vec{\nabla} \overline{\psi_R} - \overline{\psi_R} [M_B]^{-1} \vec{\nabla} \psi_L \right] d\vec{S}$$

surface of the barrier

[J. Sée, PhD thesis, University Paris 11 (2003) ; Sée et al., to be published in IEEE-ED]

Single-electron tunneling



$$\Gamma_{elec \to dot} = \sum \frac{2\pi}{\hbar} |M|^2 \rho_{elec}(E) f_{elec}(E) l_{dot}(E)$$

number of free places on the level (l_{dot})

$$\Gamma_{dot \to elec} = \sum \frac{2\pi}{\hbar} |M|^2 \rho_{elec}(E) [1 - f_{elec}(E)] g_{dot}(E)$$

number of electrons on the level (g_{dot})

$$M = \langle k_{dot} | H_T | k_{elec} \rangle = \frac{\hbar^2}{2\, m_B} \iint_{S_B} \left[\psi_{elec} \vec{\nabla} \overline{\psi_{dot}} - \overline{\psi_{dot}} \vec{\nabla} \psi_{elec} \right] d\vec{S}$$

Hartree wave functions (ψ_{dot}); analytical expression (ψ_{elec})

Current: approximation of the tunnel resistance

Equations of the previous slide yield:

$$I = -e \frac{2\pi}{\hbar} \int |M|^2 \rho_L(E) \rho_R(E) [f_L(E) - f_R(E)] dE$$

where $f_{L/R}(E) = f\left(E - E_{F_{L/R}}\right) = \dfrac{1}{1 + \exp\left(\dfrac{E - E_{F_{L/R}}}{k_B T}\right)}$

* Approximation of low temperature:

$\Rightarrow$ Fermi functions are step functions

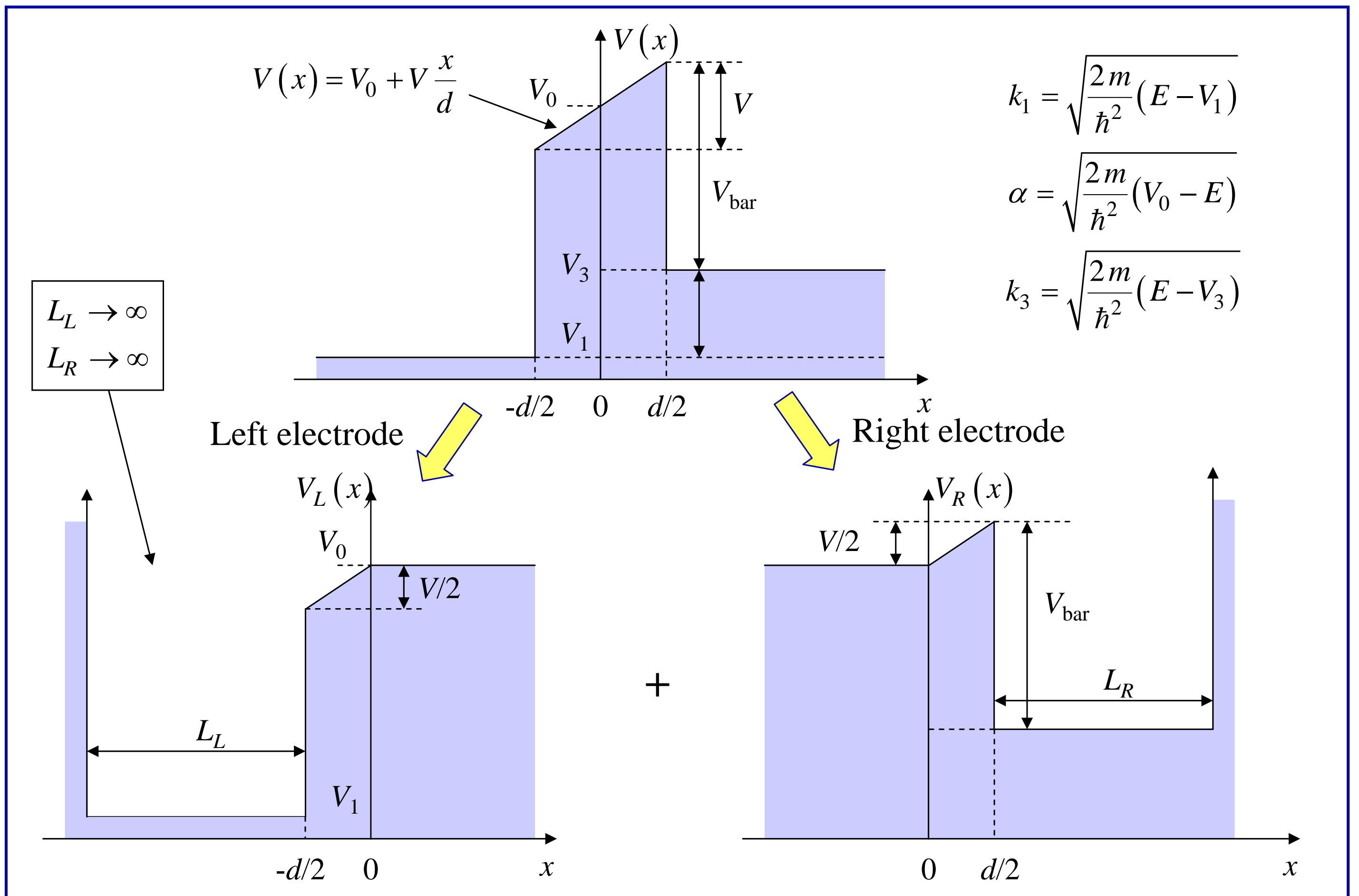
$$I \approx e \frac{2\pi}{\hbar} \int_{E_{F_L}}^{E_{F_R}} |M|^2 \rho_L(E) \rho_R(E)\, dE$$

* Approximation of low bias voltage: $-eV = E_{F_R} - E_{F_L}$ weak $\Rightarrow \begin{cases} \rho_R(E) \approx \text{const} = \rho_{R_0} \\ \rho_L(E) \approx \text{const} = \rho_{L_0} \\ |M|^2 \approx \text{const} \end{cases}$

$$I = \frac{V}{R_t}$$ where $$R_t = \frac{\hbar}{2\pi e^2 \rho_{R_0} \rho_{L_0} |M|^2}$$

is the tunnel resistance (hard approximation)

MIM structure: decomposition in 2 hamiltonians



MIM structure: wave functions

WKB approximation in the barrier: $\psi(x) \approx \psi(0)\exp\left(-\int_0^X \sqrt{\left(2m/\hbar^2\right)\left(V(x')-E\right)}\,dx'\right)$

$$\psi_L(x) = \begin{cases} A_L \sin\left[k_1\left(x + L_L + d/2\right)\right] & \text{if } -\left(L_L + d/2\right) \le x < -d/2 \\ A_L \sin\left[k_1 L_L\right] \exp\left[-\alpha \dfrac{2d}{3V}\dfrac{1}{\sqrt{V_0 - E}}\left(\left[\dfrac{x}{d}V + V_0 - E\right]^{3/2} - \left[-\dfrac{1}{2}V + V_0 - E\right]^{3/2}\right)\right] & \text{if } -d/2 \le x < 0 \\ A_L \sin\left[k_1 L_L\right] \exp\left[-\alpha \dfrac{2d}{3V}\dfrac{1}{\sqrt{V_0 - E}}\left(\left[V_0 - E\right]^{3/2} - \left[-\dfrac{1}{2}V + V_0 - E\right]^{3/2}\right)\right] & \text{if } 0 \le x \\ 0 & \text{otherwise} \end{cases}$$

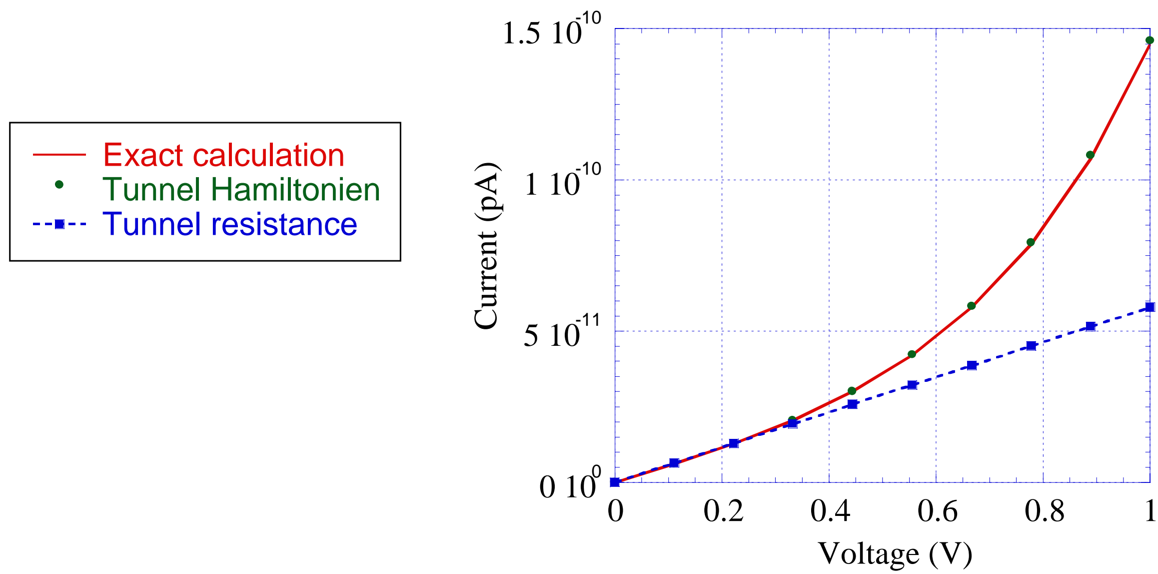
normalisation: $\left|A_L\right|^2_{L_L \to \infty} = \dfrac{2}{L_L}$

… and similar results for the right electrode

→ straightforward calculation of transition rates and current

Current: comparison of the methods (MIM structure)

Barrier Thickness : 2 nm
T = 300 K



Calculation of current: Monte Carlo

Exactly the same idea as for the Monte Carlo method for solving the BTE

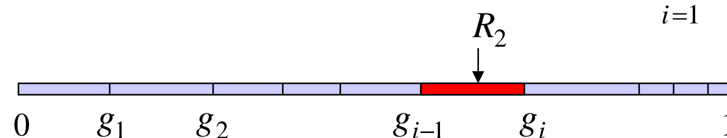
collision → tunneling event
time of free flight → time without tunneling event

⇒ series of "free flights" interrupted by tunneling events

using 2 random numbers R_1, R_2 :

$$t_f = -\frac{\ln(R_1)}{\sum_i \Gamma_i}$$

for a set of T possible tunneling events: $$g_j(E) = \frac{\sum_{i=1}^{j} \Gamma_i}{\sum_{i=1}^{T} \Gamma_i}$$



→ in this case the tunneling event i is selected

M-I-Si-I-M structure: I-V characteristics

Si quantum dot

V

Coulomb Blockade – Effect of temperature

dot radius: $R = 3$ nm
barrier thicknesses: $T_L = 1.5$ nm
$T_R = 1.2$ nm

T = 30 K
T = 100 K
T = 300 K

Current (pA)

Voltage (V)

Current-Voltage characteristics

Effect of the size of the quantum dot

barrier thicknesses: $T_L = 1.5$ nm
$T_R = 1.2$ nm

T = 30 K

R = 3 nm
R = 4 nm
R = 5 nm

Coulomb blockade

Current (pA)

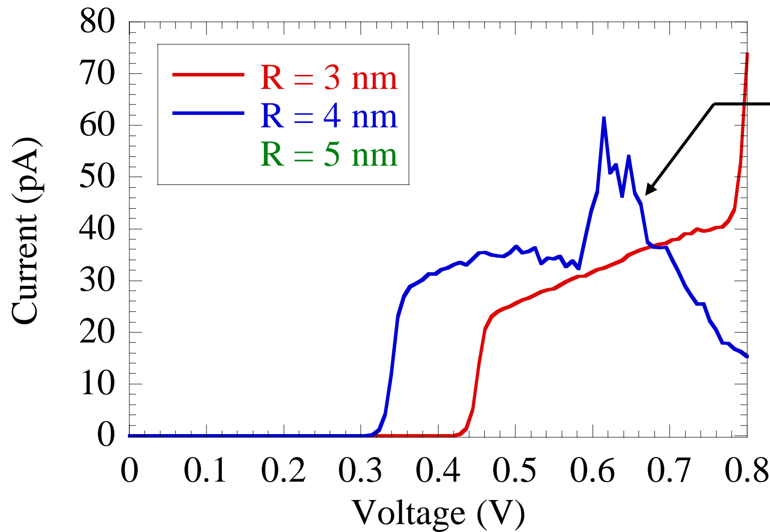
Voltage (V)

Current-Voltage characteristics

Effect of the size of the quantum dot

barrier thicknesses: $T_L = 1.5$ nm
$T_R = 1.2$ nm

T = 30 K



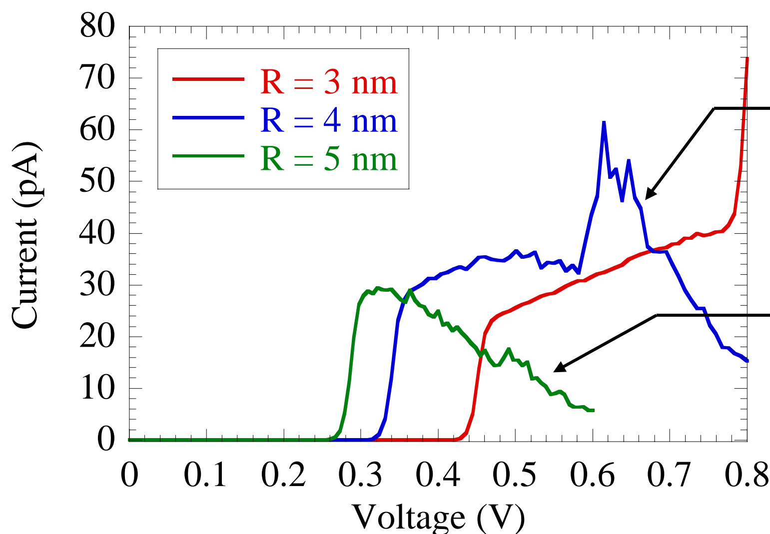
Effect of negative differential conductance

Current-Voltage characteristics

Effect of the size of the quantum dot

barrier thicknesses: $T_L = 1.5$ nm
$T_R = 1.2$ nm

T = 30 K

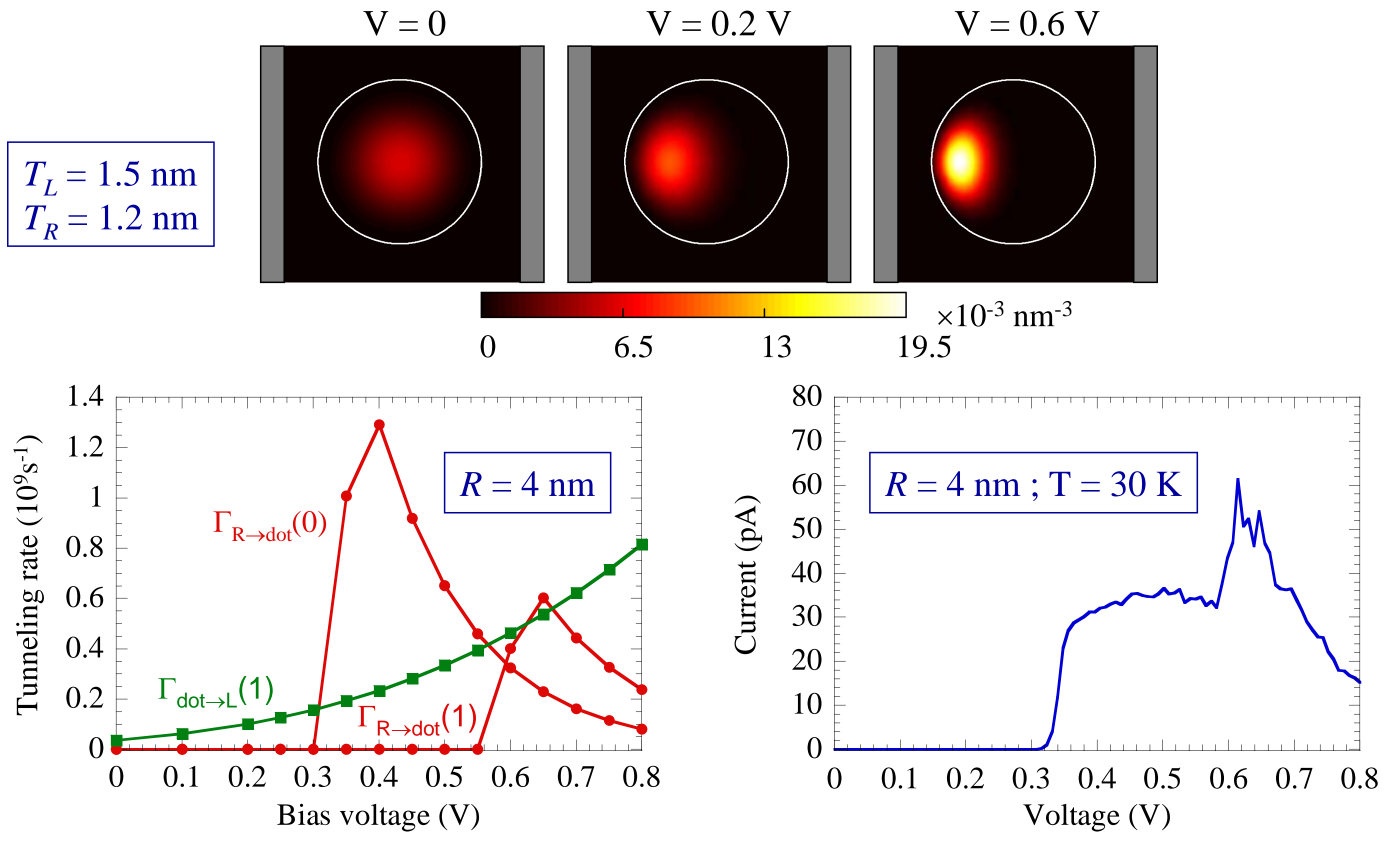


Effect of negative differential conductance

Stronger effect by increasing the dot size

Current-Voltage characteristics

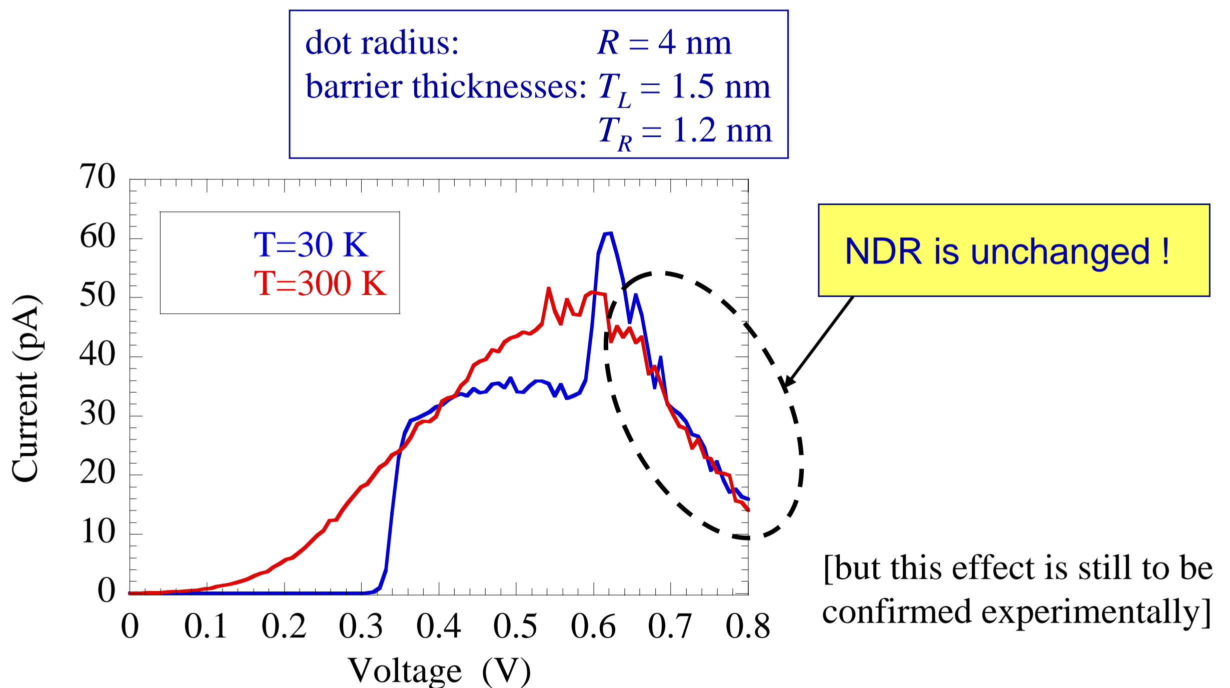
NDR effect is a consequence of bias influence on wave functions:



Current-Voltage characteristics

Influence of temperature on NDR effect

dot radius: R = 4 nm
barrier thicknesses: T_L = 1.5 nm
T_R = 1.2 nm



NDR is unchanged !

[but this effect is still to be confirmed experimentally]

Is the future of single-electron devices in the use of NDR instead of Coulomb staircase ?

Influence of the shape of the dot