Physics-based Modelling of Quantum Transport in Nanostructured Devices

A. Heigl and G. Wachutka

Institute for Physics of Electrotechnology
Munich University of Technology

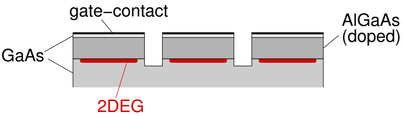
27 March 2007

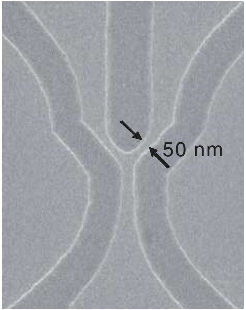
TECHNISCHE UNIVERSITÄT MÜNCHEN

TECHNISCHE UNIVERSITÄT MÜNCHEN

Motivation

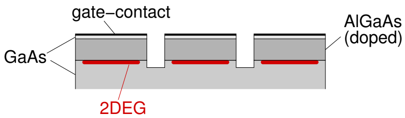
The realization and optimization of novel nanodevice concepts (e.g. y-branch switch) require the predictive simulation of quantum-ballistic transport processes.

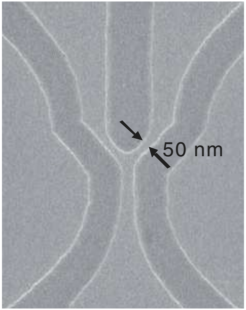




Motivation

The realization and optimization of novel nanodevice concepts (e.g. y-branch switch) require the predictive simulation of quantum-ballistic transport processes.





Other devices of interest

- Resonant structures for optical devices like lasers (QCLs).
- Further shrinking of nanoscale transistors needs full quantum mechanical treatment.

Nanoscale Device Simulation

Statistical properties in nanodimensions?

- Only a small number of free particles is existing in the active region of modern devices.
- Device lengths are smaller than the mean free path of electrons.
- The distance between impurities is in average 100 nm for a doping concentration of $10^{15}\,\mathrm{cm}^{-3}$.

TECHNISCHE UNIVERSITÄT MÜNCHEN

Nanoscale Device Simulation

Statistical properties in nanodimensions?

- Only a small number of free particles is existing in the active region of modern devices.
- Device lengths are smaller than the mean free path of electrons.
- The distance between impurities is in average 100 nm for a doping concentration of $10^{15}\,\text{cm}^{-3}$.

Quantum mechanical treatment?

In the case of strongly confined systems charge distribution and transport cannot be correctly described without the use of quantum mechanics.

TECHNISCHE UNIVERSITÄT MÜNCHEN

Nanoscale Device Simulation

Statistical properties in nanodimensions?

- Only a small number of free particles is existing in the active region of modern devices.
- Device lengths are smaller than the mean free path of electrons.
- The distance between impurities is in average 100 nm for a doping concentration of $10^{15}\,\text{cm}^{-3}$.

Quantum mechanical treatment?

In the case of strongly confined systems charge distribution and transport cannot be correctly described without the use of quantum mechanics.

Quantummechanical particles themselves have inherently statistical character!

TECHNISCHE UNIVERSITÄT MÜNCHEN

Basics of Quantum Transport

Classification by transport mechanisms

- Dissipative transport.
- Ballistic transport ($L_{device} \approx \lambda_{free}$).
- Quantumballistic transport ($L_{device} \ll \lambda_{free}$).

Basics of Quantum Transport

Classification by transport mechanisms

- Dissipative transport.
- Ballistic transport ($L_{device} \approx \lambda_{free}$).
- Quantumballistic transport ($L_{device} \ll \lambda_{free}$).

Classification by application

- Interference effects (e.g. resonant tunneling diodes).
- Coulomb blockade (e.g. single electron transistors or quantum dots).
- Mesoscopic devices (e.g. quantum waveguides).

TECHNISCHE UNIVERSITÄT MÜNCHEN

Basics of Quantum Transport

Classification by transport mechanisms

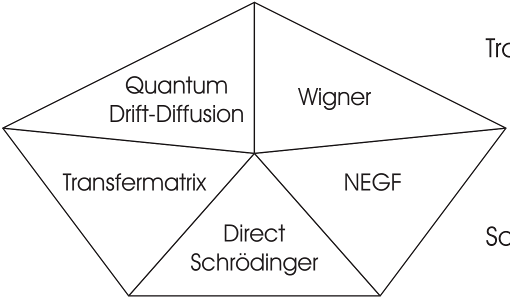
- Dissipative transport.
- Ballistic transport ($L_{device} \approx \lambda_{free}$).
- Quantumballistic transport ($L_{device} \ll \lambda_{free}$).

Classification by application

- Interference effects (e.g. resonant tunneling diodes).
- Coulomb blockade (e.g. single electron transistors or quantum dots).
- Mesoscopic devices (e.g. quantum waveguides).

The main goal are models to perform fast and yet accurate simulations.

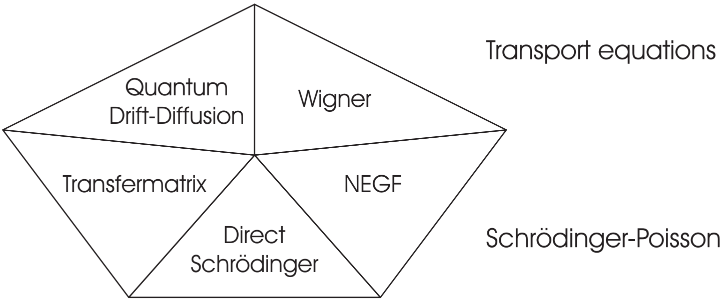
Approaches to Quantum Transport



Transport equations

Schrödinger-Poisson

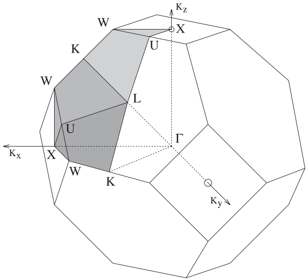
Approaches to Quantum Transport

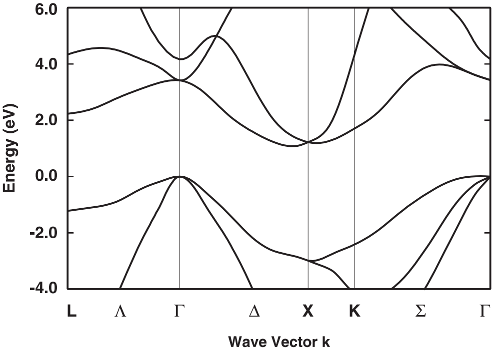


Only Schrödinger-Poisson-based methods are considered in the following.

TECHNISCHE UNIVERSITÄT MÜNCHEN

Electronic Bandstructure



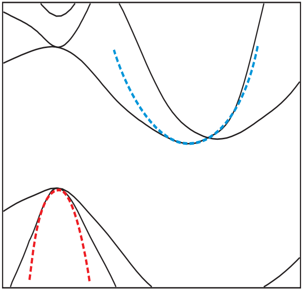


Due to the periodic lattice of semiconductor materials the single particle bulk states can be characterized by their (quasi-)momentum $\mathbf{p} = \hbar\,\mathbf{k}$.

Effective Mass Approximation

In the vincinity of the band edges the true energy bands $\varepsilon_\nu(\mathbf{k})$ can be approximated by a parabolic function

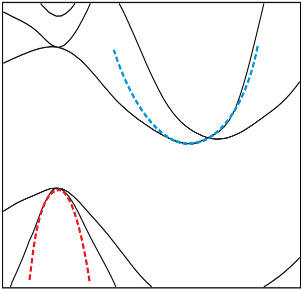
$$\tilde{\varepsilon}_\nu(\mathbf{k}) \approx \varepsilon_\nu(\mathbf{k}_v) + \frac{\hbar^2}{2} \cdot (\mathbf{k} - \mathbf{k}_v) \cdot \left[\frac{1}{m^*_{\nu,k_v}} \right] \cdot (\mathbf{k} - \mathbf{k}_v)$$



Effective Mass Approximation

In the vincinity of the band edges the true energy bands $\varepsilon_\nu(\mathbf{k})$ can be approximated by a parabolic function

$$\tilde{\varepsilon}_\nu(\mathbf{k}) \approx \varepsilon_\nu(\mathbf{k}_v) + \frac{\hbar^2}{2} \cdot (\mathbf{k} - \mathbf{k}_v) \cdot \left[\frac{1}{m^*_{\nu,k_v}}\right] \cdot (\mathbf{k} - \mathbf{k}_v)$$



where the effective particle mass tensor is defined as

$$\left[\frac{1}{m^*_{\nu,k_v}}\right]_{ij} = \frac{1}{\hbar^2} \cdot \left.\frac{\partial^2 \varepsilon_\nu(\mathbf{k})}{\partial k_i \partial k_j}\right|_{\mathbf{k}=\mathbf{k}_v}$$

⇒ free electron model as reference system

TECHNISCHE UNIVERSITÄT MÜNCHEN

The Schrödinger-Poisson System (1)

The effective mass approximation leads to a single particle Schrödinger equation for the electron wavefunctions $\psi_j(x)$ in a confined nanodevice with distributed space charge:

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*}\nabla + V_{eff}(x)\right]\cdot\psi_j(x) = \varepsilon_j\psi_j(x)$$

with the effective potential $V_{eff} = -qV + V_{xc}[n] + V_H + \dots$

TECHNISCHE UNIVERSITÄT MÜNCHEN

The Schrödinger-Poisson System (1)

The effective mass approximation leads to a single particle Schrödinger equation for the electron wavefunctions $\psi_j(x)$ in a confined nanodevice with distributed space charge:

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*}\nabla + V_{eff}(x)\right]\cdot\psi_j(x) = \varepsilon_j\psi_j(x)$$

with the effective potential $V_{eff} = -qV + V_{xc}[n] + V_H + \dots$

Density functional theory

- Electrostatic potential V induced by external fields and internal charge densities.
- Exchange-correlation potential $V_{xc}[n]$ describing electron-electron interactions (without classical Coulomb interaction).
- Confinement potential V_H of the heterostructure.

The Schrödinger-Poisson System (2)

The effect of mobile charges and fixed background charges on the effective potential V_{eff} has to be self-consistently calculated via the Poisson equation

$$\operatorname{div}\left(\varepsilon \nabla V\right) = q \cdot \left(n - p + N_A^+ - N_D^-\right)$$

The Schrödinger-Poisson System (2)

The effect of mobile charges and fixed background charges on the effective potential V_{eff} has to be self-consistently calculated via the Poisson equation

$$\operatorname{div}\left(\varepsilon \nabla V\right) = q \cdot \left(n - p + N_A^+ - N_D^-\right)$$

Note:

Since all the quantities on the right-hand side may exponentially depend on the potential, we have to cope with a highly nonlinear problem!

Calculation of Electron Density

The electron density is calculated via the wavefunctions and their corresponding occupation probabilities

$$n(x) = 2 \sum_j f_j \, |\psi_j(x)|^2$$

with the statistical weight f_j. That is, for example, the Fermi-Dirac distribution

$$f_j = f_{FD}(\varepsilon_j, \mu) = \frac{1}{1 + \exp\left[(\varepsilon_j - \mu)/kT\right]}$$

for local thermodynamic equilibrium.

Calculation of Electron Density

The electron density is calculated via the wavefunctions and their corresponding occupation probabilities

$$n(x) = 2 \sum_j f_j \, |\psi_j(x)|^2$$

with the statistical weight f_j. That is, for example, the Fermi-Dirac distribution

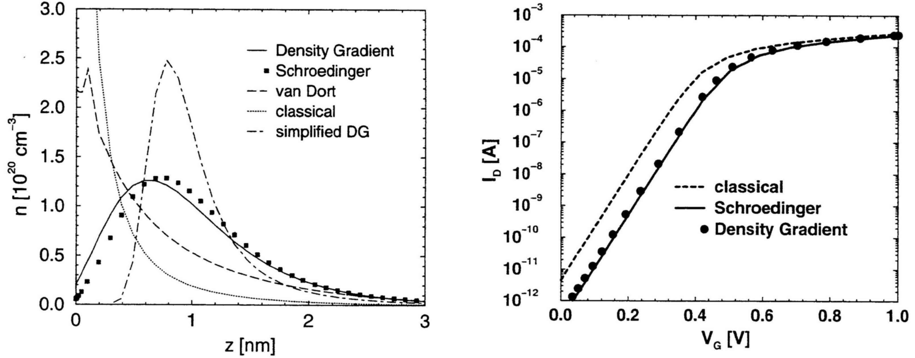
$$f_j = f_{FD}(\varepsilon_j, \mu) = \frac{1}{1 + \exp\left[\left(\varepsilon_j - \mu\right)/kT\right]}$$

for local thermodynamic equilibrium.

$|\psi_j(x)|^2$ expresses the wave character of electronic states visible in nanostructured devices.

Example: SOI-MOSFET

$$(L_{ch} = 80\text{nm},\ N_{ch} = 5 \cdot 10^{17}\text{cm}^{-3},\ t_{ox} = 1.5\text{nm},\ d_{body} = 5\text{nm})$$

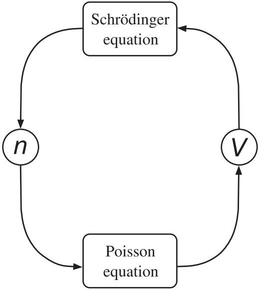


(A. Schenk, Proc. ESSDERC 2001, S. 9-16)

Self-Consistent Solution of Schrödinger-Poisson System

As it is impossible to solve the Poisson and Schrödinger equations simultaneously; no direct scheme can be applied.

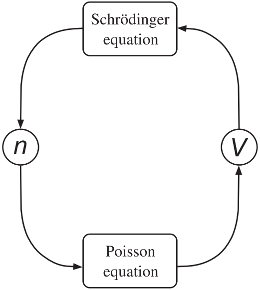
Since the calculation of the Jacobian matrix is prohibitive due to the effort of evaluating the charge densities, no standard Newton approach is applicable.



Self-Consistent Solution of Schrödinger-Poisson System

As it is impossible to solve the Poisson and Schrödinger equations simultaneously; no direct scheme can be applied.

Since the calculation of the Jacobian matrix is prohibitive due to the effort of evaluating the charge densities, no standard Newton approach is applicable.

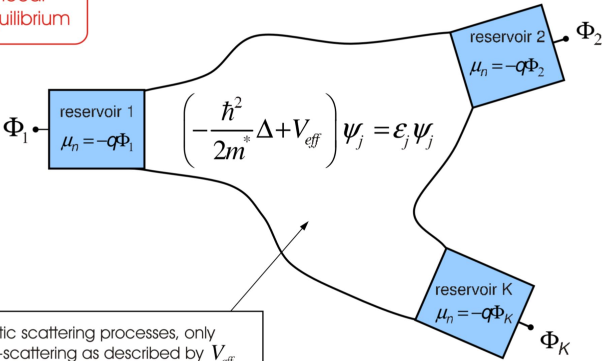


Methods

- Relaxation methods (e.g. modified Aitken Δ^2 method).
- Gummel iterations.
- Predictor-corrector approaches.

Quantum-Ballistic Model of Nanodevices

Coherent propagation of electron waves between charge reservoirs in local thermodynamic equilibrium



no inelastic scattering processes, only potential-scattering as described by V_{eff}

$\lambda_{coll} >> L_{device}$

Quantum-Ballistic Calculation of Currents

Basic hypothesis:

Between injecting and collecting contact, an electron stays in one fixed state ψ_k and adds to the current density the contribution

$$\vec{j}_k = -\frac{q}{2m^*}\left(\psi_k^* \frac{\hbar}{i}\nabla\psi_k - \psi_k \frac{\hbar}{i}\nabla\psi_k^*\right)$$

A statistical ensemble of electrons carries a total current density

$$\vec{j}(x) = \sum_k f_k \vec{j}_k(x)$$

where f_k is the occupation probability of state ψ_k.

TECHNISCHE UNIVERSITÄT MÜNCHEN

Quantum-Ballistic Calculation of Currents

Basic hypothesis:

Between injecting and collecting contact, an electron stays in one fixed state ψ_k and adds to the current density the contribution

$$\vec{j}_k = -\frac{q}{2m^*}\left(\psi_k^* \frac{\hbar}{i}\nabla\psi_k - \psi_k \frac{\hbar}{i}\nabla\psi_k^*\right)$$

A statistical ensemble of electrons carries a total current density

$$\vec{j}(x) = \sum_k f_k \vec{j}_k(x)$$

where f_k is the occupation probability of state ψ_k.

Problems:

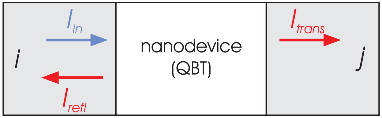
- How to find f_k?
- How to attach contacts to the Schrödinger-Poisson system?

The Landauer-Büttiker Approach (1)

Treat current calculation as scattering problem:

Transmission coefficient

$$T_{i \to j}(E) = \frac{I_{trans}}{I_{in}}$$

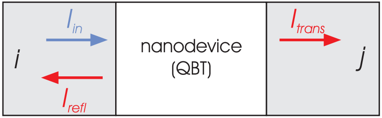


The Landauer-Büttiker Approach (1)

Treat current calculation as scattering problem:

Transmission coefficient

$$T_{i\to j}(E) = \frac{I_{trans}}{I_{in}}$$



Hypothesis

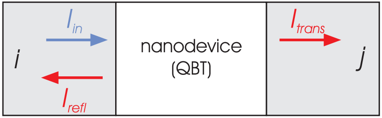
Injected electrons inherit statistical weight from their source i, which is assumed to follow a Fermi-Dirac distribution with electrochemical potential μ_i: $f_k = f_{FD}(\varepsilon_k, \mu_i)$

The Landauer-Büttiker Approach (1)

Treat current calculation as scattering problem:

Transmission coefficient

$$T_{i\to j}(E) = \frac{I_{trans}}{I_{in}}$$



Hypothesis

Injected electrons inherit statistical weight from their source i, which is assumed to follow a Fermi-Dirac distribution with electrochemical potential μ_i: $f_k = f_{FD}(\varepsilon_k, \mu_i)$

Current from terminal i to terminal j

$$I_{i\to j} = \frac{q}{\pi\hbar}\int_E T_{i\to j}(E)\cdot f_{FD}(E,\mu_i)dE$$

The Landauer-Büttiker Approach (2)

Total current collected by terminal j:

$$I_j = \sum_{i \neq j} (I_{i \to j} - I_{j \to i})$$

The Landauer-Büttiker Approach (2)

Total current collected by terminal j:

$$I_j = \sum_{i \neq j} (I_{i \to j} - I_{j \to i})$$

For elastic potential scattering $T_{i \to j}(E) = T_{j \to i}(E)$. Hence:

$$I_j = \frac{q}{\pi \hbar} \sum_i \int_E T_{i \to j}(E) \cdot \Big(f_{FD}(E, \mu_i) - f_{FD}(E, \mu_j) \Big) dE$$

The Landauer-Büttiker Approach (2)

Total current collected by terminal j:

$$I_j = \sum_{i \neq j} (I_{i \to j} - I_{j \to i})$$

For elastic potential scattering $T_{i \to j}(E) = T_{j \to i}(E)$. Hence:

$$I_j = \frac{q}{\pi \hbar} \sum_i \int_E T_{i \to j}(E) \cdot \Big(f_{FD}(E, \mu_i) - f_{FD}(E, \mu_j) \Big) dE$$

Transferring this ideas to wavefunction representation gives

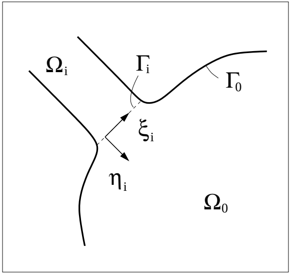
$$\vec{j}(x) = 2 \sum_{i,m} \int_E \vec{j}_{i,m,E}(x) \cdot f_{FD}(E, \mu_i) dE$$

with terminal i, injected mode m, energy E and the electrochemical potential μ_i of injecting terminal.

Building a Basis of Injected Electron States

Solve the Schrödinger-Poisson system subjected to scattering state boundary conditions along the contact interfaces:

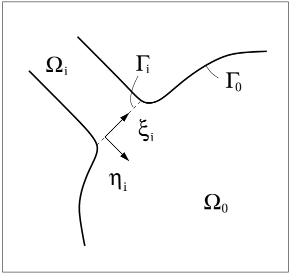
Contacts are connected to quantum-ballistic region by leads (i.e. electron waveguides), where the potential V_{eff} is not varying in transport direction.



Building a Basis of Injected Electron States

Solve the Schrödinger-Poisson system subjected to scattering state boundary conditions along the contact interfaces:

Contacts are connected to quantum-ballistic region by leads (i.e. electron waveguides), where the potential V_{eff} is not varying in transport direction.



The wavefunction of an electron state injected from terminal j reaches in the interior of lead i:

$$\varphi_j(\xi_i, \eta_i) = \delta_{ij} \cdot \chi_i(\xi_i) \cdot e^{+\imath k_i \eta_i} + s_{ij} \cdot \chi_i(\xi_i) \cdot e^{-\imath k_i \eta_i}$$

with longitudinal wavenumber k_i and transversal mode function $\chi_i(\xi_i)$.

Matching the Scattering Boundary Conditions

Using the wavefunctions $\varphi_j(\xi_i)$ in the leads as boundary values, a basis of wavefunctions in the active device area is calculated using

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*}\nabla + V_{eff} - E_i\right]\Phi_p = 0$$

with the total energy of the injected electron

$$E_i = \frac{\hbar^2 k_i^2}{2m^*} + \varepsilon_i$$

TECHNISCHE UNIVERSITÄT MÜNCHEN

Matching the Scattering Boundary Conditions

Using the wavefunctions $\varphi_j(\xi_i)$ in the leads as boundary values, a basis of wavefunctions in the active device area is calculated using

$$\left[-\frac{\hbar^2}{2}\nabla\frac{1}{m^*}\nabla + V_{eff} - E_i\right]\Phi_p = 0$$

with the total energy of the injected electron

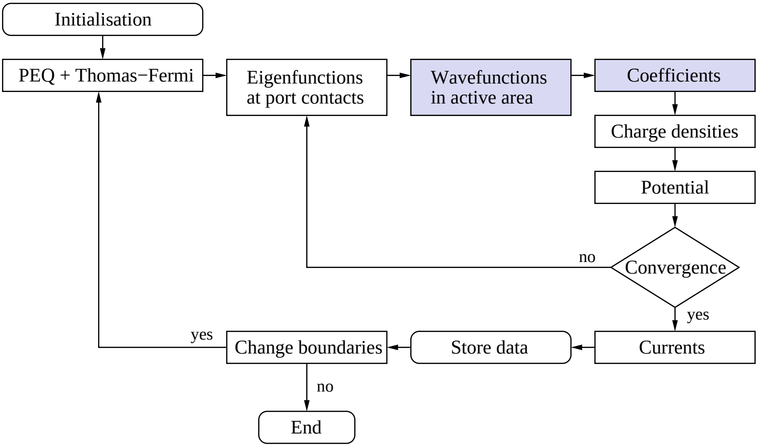
$$E_i = \frac{\hbar^2 k_i^2}{2m^*} + \varepsilon_i$$

The total wavefunction of an injected electron $\psi_j(x)$ is obtained by matching the linear combination

$$\psi_j(x) = \sum_{p=1}^{N} a_{jp}\Phi_p(x)$$

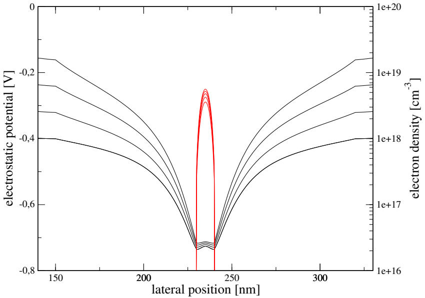
smoothly to the lead wavefunctions $\varphi_j(\xi_i, \eta_i)$.

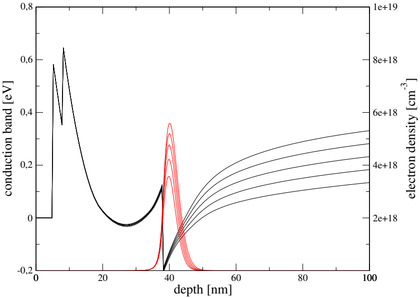
Iteration scheme for direct SPS



Simulation of 10nm quantumwire

AlGaAs layer is Si-doped ($N_D = 5 \cdot 10^{18} \text{cm}^{-3}$)

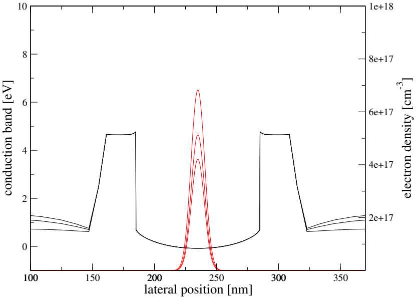


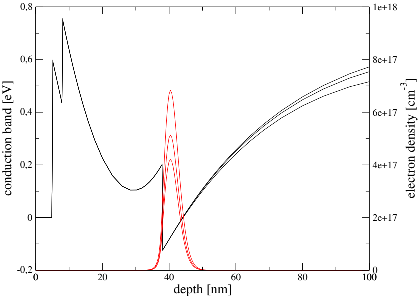


- Electron gas appears at a depth of 40nm.
- Surface states along etched trenches cause apparently reduced effective diameter of quantumwire.

Simulation of 100nm quantum-wire

AlGaAs layer is Si-doped ($N_D = 2 \cdot 10^{18}\text{cm}^{-3}$)

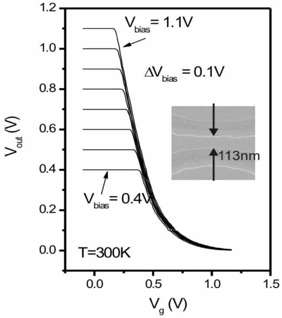


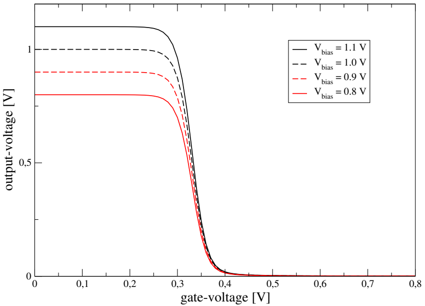


- Electron gas appears at a depth of 40nm.
- Surface energy pinning at -0.7eV due to etched trenches.

Output characteristics

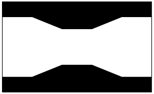
- Simulation performed with simulator SIMNAD (ETHZ).
- Measurements from Institute of Technische Physik, University of Würzburg.



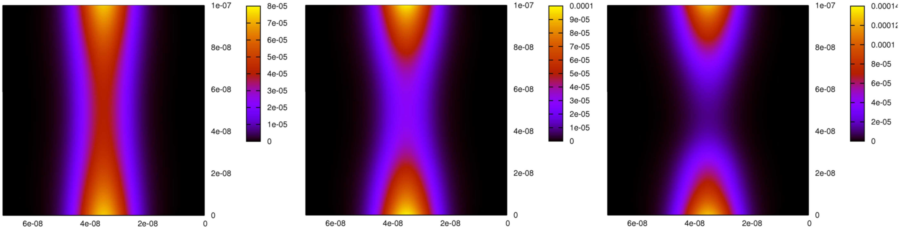


Fairly good agreement between measurement and simulation.

Quantumwire with constriction



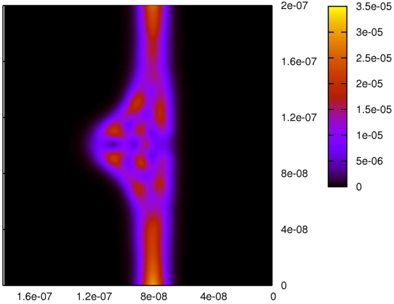
Confinement of quantumwires defined by etched trenches and voltages applied at gate contacts.

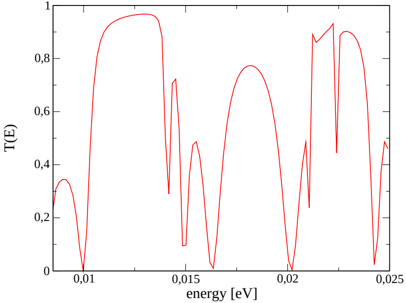


Non-linear effects are neglegible in the case of 'soft' constrictions.

T-stub structure

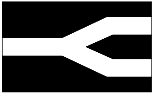
Electron distribution and transmission behaviour in the case of small source-drain voltages.



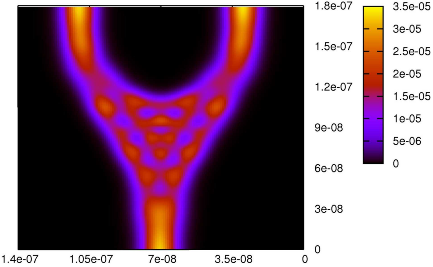


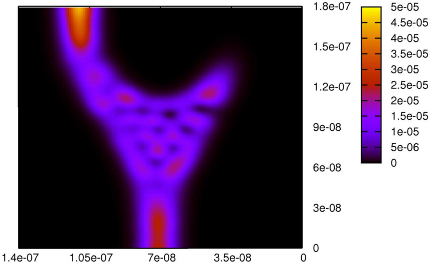
Electron density shows strong interference effects in active region.

Y-branch switch



Influence of non-symmetric gate voltages on a Y-branch structure have been analyzed.





Currents in branches can be completely turned off!

TECHNISCHE UNIVERSITÄT MÜNCHEN

Conclusion

Electronic devices in the decananometer regime and below require quantum-mechanical treatment of carrier distributions and current flow.

Conclusion

Electronic devices in the decananometer regime and below require quantum-mechanical treatment of carrier distributions and current flow.

Direct Schrödinger-Poisson scheme proves as an efficient and practical approach to real quantum-ballistic nanodevices with multiple contacts and gates.

Acknowledgement

This project is funded by the Bavarian Science Foundation within the research consortium for nanoelectronics (FORNEL).

Thank you for your interest!

Alexander Heigl
Institute for Physics of Electrotechnology
Munich University of Technology

heigl@tep.ei.tum.de