Kinetic and Macroscopic Models for Semiconductors

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Literature

Main reference

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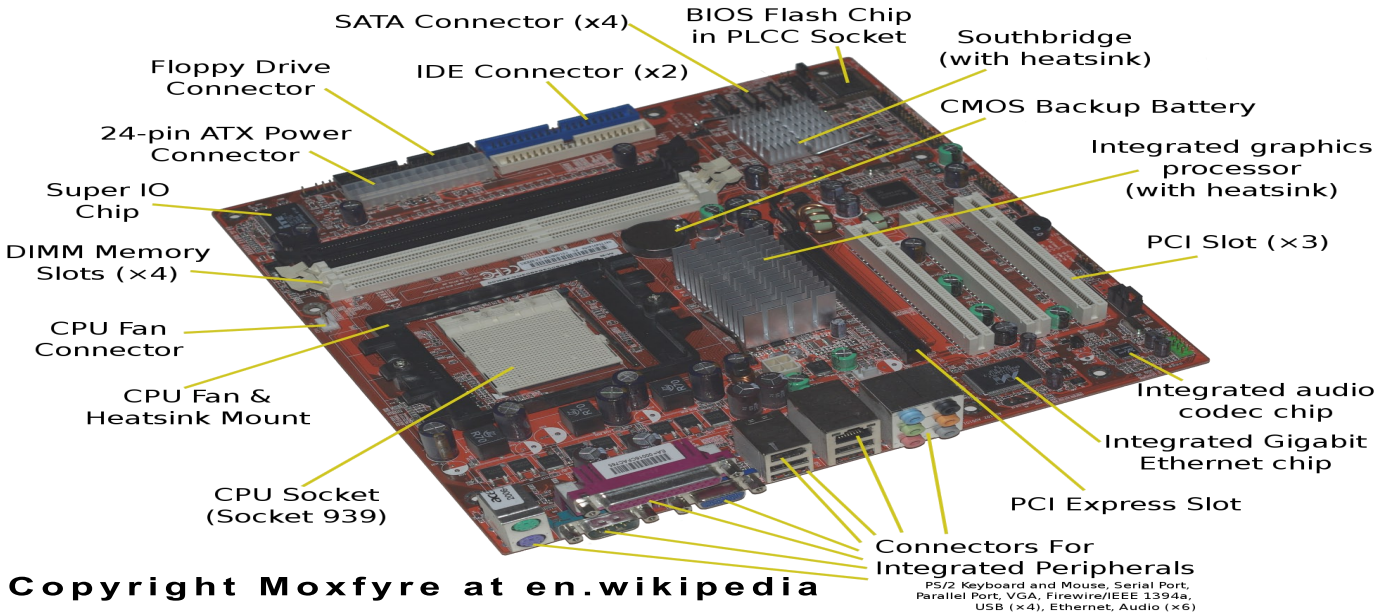
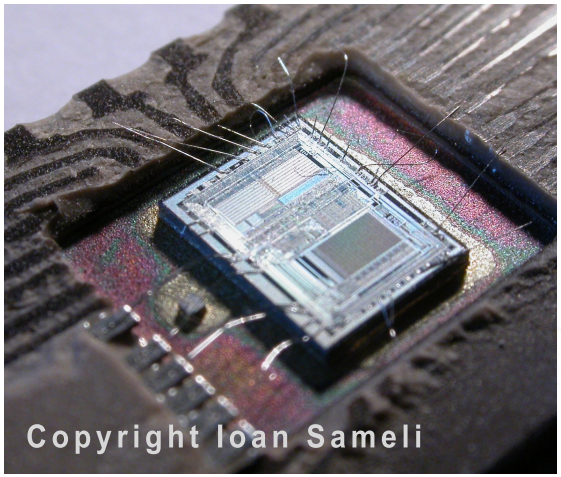
  - M. Lundstrom. *Fundamentals of Carrier Transport.* Cambridge, 2000.
- Kinetic semiconductor models:
  - P. Markowich, C. Ringhofer, and C. Schmeiser. *Semiconductor Equations.* Vienna, 1990.
- Macroscopic semiconductor models:
  - P. Degond. Mathematical modelling of microelectronics semiconductor devices. Providence, 2000.
  - F. Brezzi, L. Marini, S. Micheletti, P. Pietra, R. Sacco, and S. Wang. Discretization of semiconductor device problems. Amsterdam, 2005.

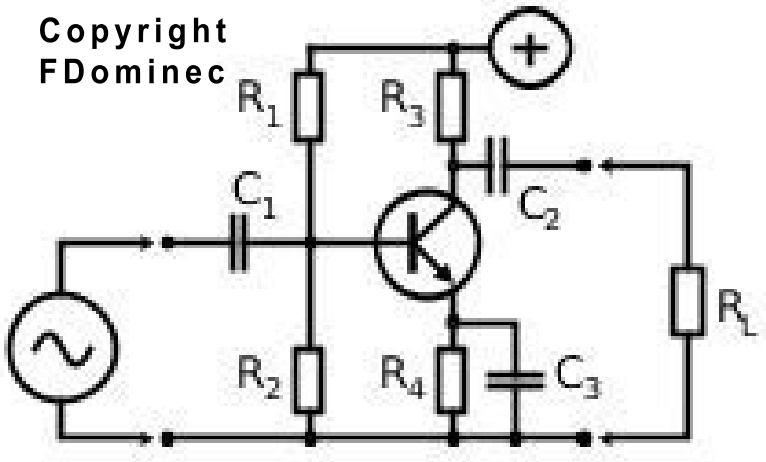
From motherboard to transistor



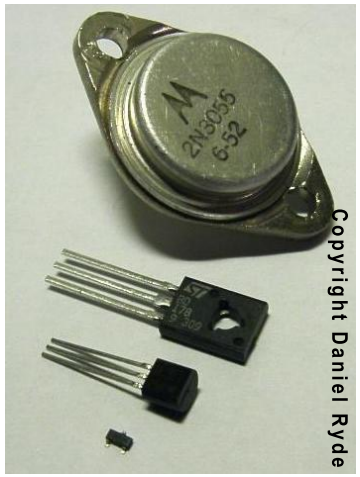
Processor



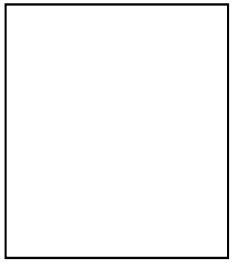
Electric circuit



Transistor



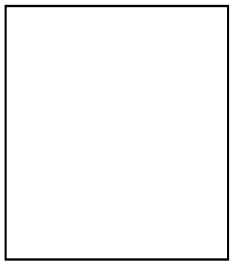
History of Intel processors

1971 

4004

108 KHz, 2250 transistors,

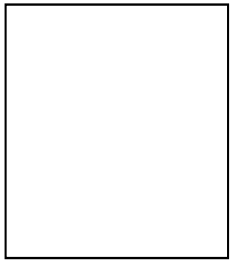
feature size: 10μm (1μm$= 10^{-6}$m)

1982 

80286

12 MHz, 134,000 transistors,

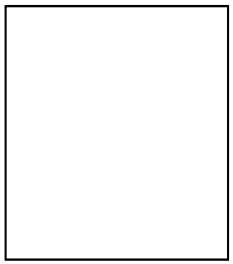
feature size: 1.5μm

1996 

Pentium 2

66 MHz, 7,500,000 transistors,

feature size: 0.35μm

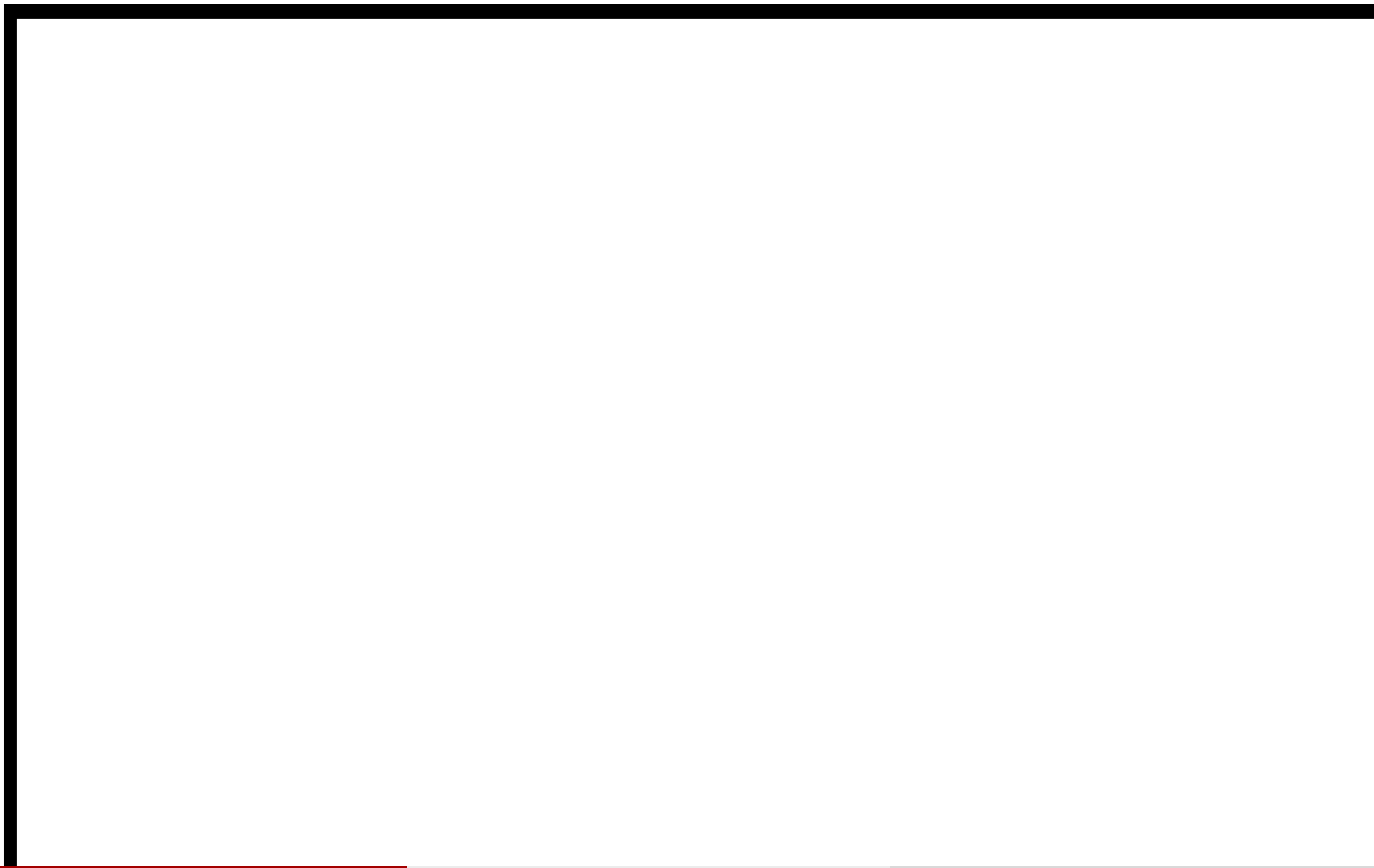
2011 

Core i7

3.5 GHz, 2,600,000,000 transistors,

feature size: 0.032μm$= 32$nm

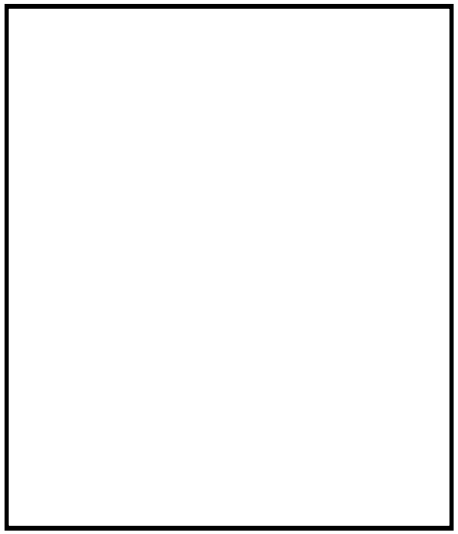
Channel lengths 2000–2016



Challenges in semiconductor device design

Future processors (2012):

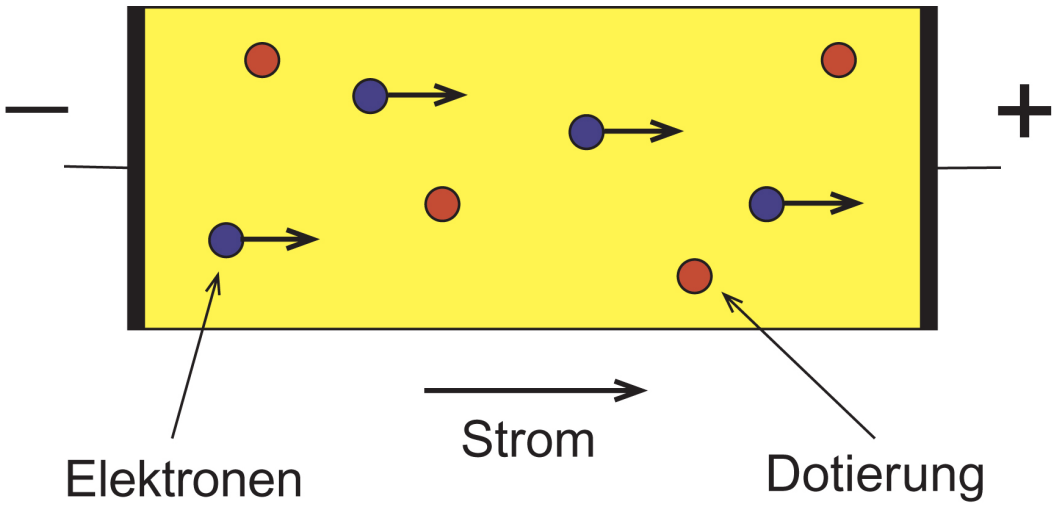
- Number of transistors $> 2{,}000{,}000{,}000$
- Transistor feature size 22 nm
- Highly-integrated circuits:
  power density $> 100\,\mathrm{W/cm^2}$



Some key problems:

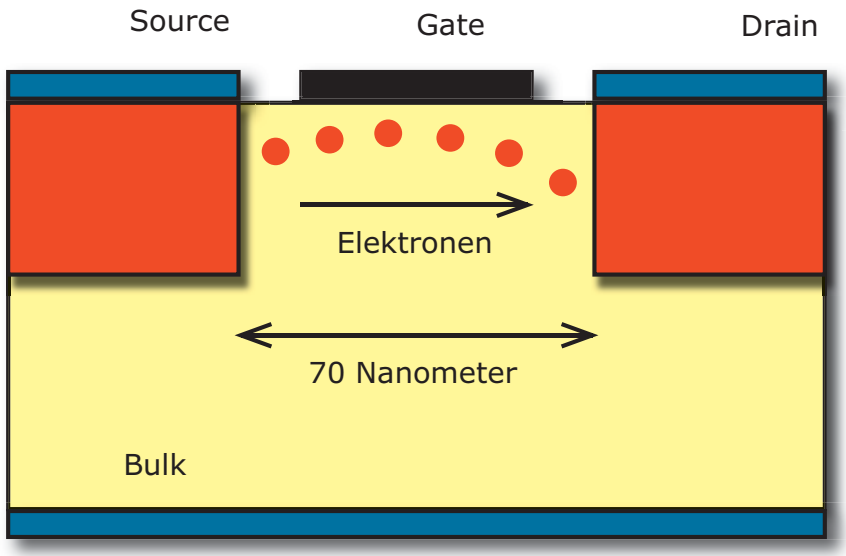
Decreasing power supply	$\longrightarrow$	noise effects
Increasing frequencies	$\longrightarrow$	multi-scale problems
Increasing design variety	$\longrightarrow$	need of fast and accurate simulations
Increasing power density	$\longrightarrow$	parasitic effects (heating, hot spots)

What are semiconductors?



- Non-conducting at temperature $T = 0\,\mathrm{K}$, conducting at $T > 0$ (heat, light etc.)
- Modern definition: energy gap of order of a few eV
- Basis material: Silicon, Germanium, GaAs etc.
- Doping of the basis material with other atoms, gives higher conductivity
- Modeled by doping concentration $C(x)$

How does a semiconductor transistor work?



- MOSFET = Metal-Oxide Semiconductor Field-Effect Transistor
- Source and drain contact: electrons flow from source to drain
- Gate contact: applied voltage controls electron flow
- Advantage: small gate voltage controls large electron current
- Used as an amplifier or switch

Objectives

- Introduce into the basics of semiconductor physics
- Modeling of electron transport through semiconductors by kinetic equations
- Modeling of macroscopic electron transport (numerically cheaper than kinetic models)
- Modeling of quantum transport and quantum diffusion effects
- Numerical approximation of macroscopic models (finite-element and finite-difference methods)

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What do we need from physics?

Newton's law:

$x(t)$: spatial variable, $v(t)$: velocity, m: mass, F: force

$$\dot{x} = v, \quad m\dot{v} = F, \quad t > 0$$

Schrödinger equation:

- Schrödinger equation for wave function ψ:

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi - qV(x,t)\psi \quad \text{in } \mathbb{R}^3$$

  where $\hbar = h/2\pi$, q: elementary charge, $V(x,t)$: potential
- Interpretation of wave function:

$$\text{particle density: } n = |\psi|^2, \quad \text{current density: } J = -\frac{\hbar}{m}\text{Im}(\overline{\psi}\nabla\psi)$$

- Stationary equation: $\psi(x,t) = e^{-iEt/\hbar}\phi(x)$ gives eigenvalue problem

$$-\frac{\hbar^2}{2m}\Delta\phi - qV(x)\phi = E\phi, \quad E: \text{ energy}$$

Classical particle transport

- Given ensemble of M particles of mass m moving in a vacuum
- Trajectory $(x(t), v(t)) \in \mathbb{R}^3 \times \mathbb{R}^3$ computed from Newton's equations

$$\dot{x} = v, \;\; m\dot{v} = F, \;\; t > 0, \quad x(0) = x_0, \;\; v(0) = v_0$$

- Force: $F = \nabla V(x,t)$, $V(x,t)$: electric potential
- $M \gg 1$: use statistical description with probability density $f(x,v,t)$

Theorem (Liouville)

Let $\dot{x} = X(x,v)$, $\dot{v} = V(x,v)$. If

$$\frac{\partial X}{\partial x} + \frac{\partial V}{\partial v} = 0 \quad \textit{then} \quad f(x(t), v(t), t) = f_I(x_0, v_0), \;\; t > 0$$

$\rightarrow$ Assumption satisfied if $F = F(x,t)$

Vlasov equation

- Differentiation of $f(x(t), v(t), t) = f_I(x_0, v_0)$ gives Vlasov equation:

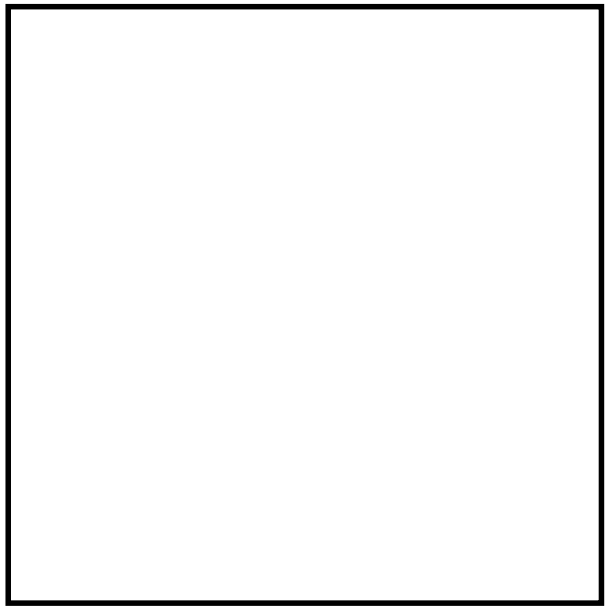
$$0 = \frac{d}{dt} f(x(t), v(t), t) = \partial_t f + \dot{x} \cdot \nabla_x f + \dot{v} \cdot \nabla_v f$$
$$= \partial_t f + v \cdot \nabla_x f + \frac{1}{m} \nabla_x V(x, t) \cdot \nabla_v f$$

- Moments of $f(x, v, t)$:

$$\text{Particle density:} \quad n(x, t) = \int_{\mathbb{R}^3} f(x, v, t) dv$$
$$\text{Current density:} \quad J(x, t) = \int_{\mathbb{R}^3} v f(x, v, t) dv$$
$$\text{Energy density:} \quad (ne)(x, t) = \int_{\mathbb{R}^3} \frac{m}{2} |v|^2 f(x, v, t) dv$$

- Electrons are quantum mechanical objects: quantum description needed!

Electrons in a semiconductor



- Semiconductor = ions (nuclei + core electrons) and valence electrons
- State of ion-electron system described by wave function ψ
- Schrödinger eigenvalue problem:

$$-\frac{\hbar^2}{2m}\Delta\psi - qV_L(x)\psi = E\psi, \quad x \in \mathbb{R}^3$$

- $V_L = V_{ei} + V_{eff}$: periodic lattice potential
  - V_{ei}: electron-ion Coulomb interactions
  - V_{eff}: effective electron-electron interactions (Hartree-Fock approx.)

Electrons in a semiconductor

Schrödinger eigenvalue problem:

$$-\frac{\hbar^2}{2m}\Delta\psi - qV_L(x)\psi = E\psi, \quad x \in \mathbb{R}^3$$

Theorem (Bloch)

Schrödinger eigenvalue problem in $\mathbb{R}^3$ can be reduced to Schrödinger problem on lattice cell, indexed by $k \in B$ (B: dual cell or Brillouin zone)

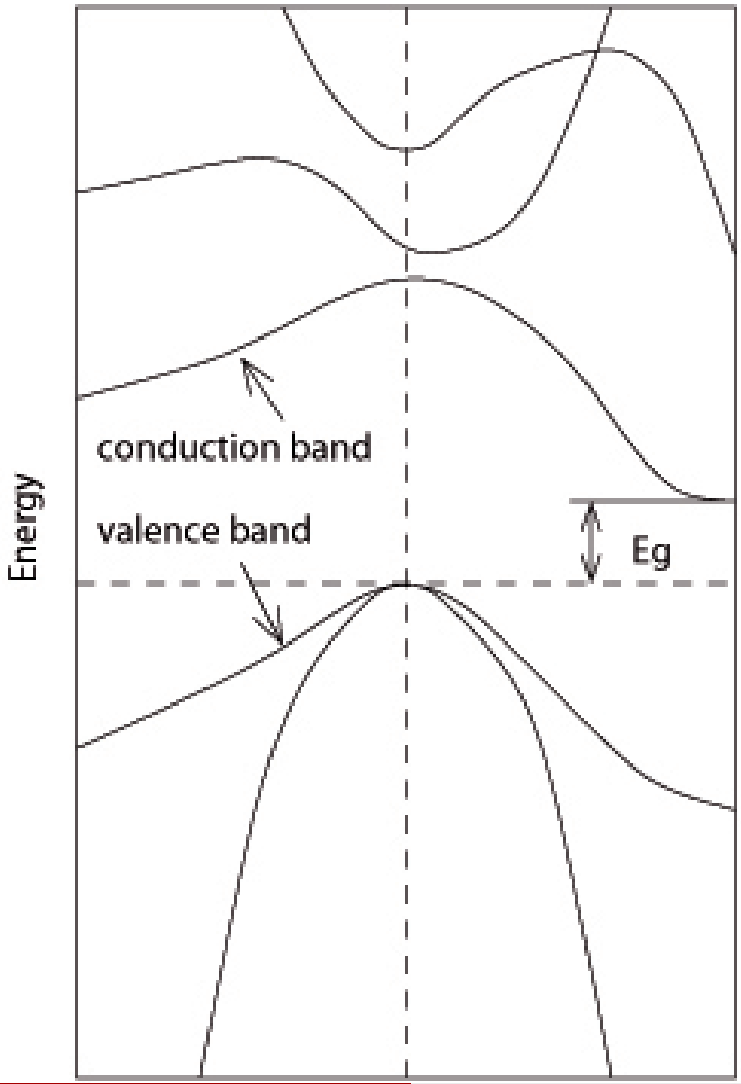
$$-\frac{\hbar^2}{2m}\Delta\psi - qV_L(x)\psi = E\psi, \quad x \in \text{cell}$$

- *For each k, there exists sequence $(E, \psi) = (E_n(k), \psi_{n,k})$, $n \in \mathbb{N}$*
- *$\psi_{n,k}(x) = e^{ik\cdot x}u_{n,k}(x)$, where $u_{n,k}$ periodic on lattice*
- *$E_n(k)$ is real, periodic, symmetric on Brillouin zone*

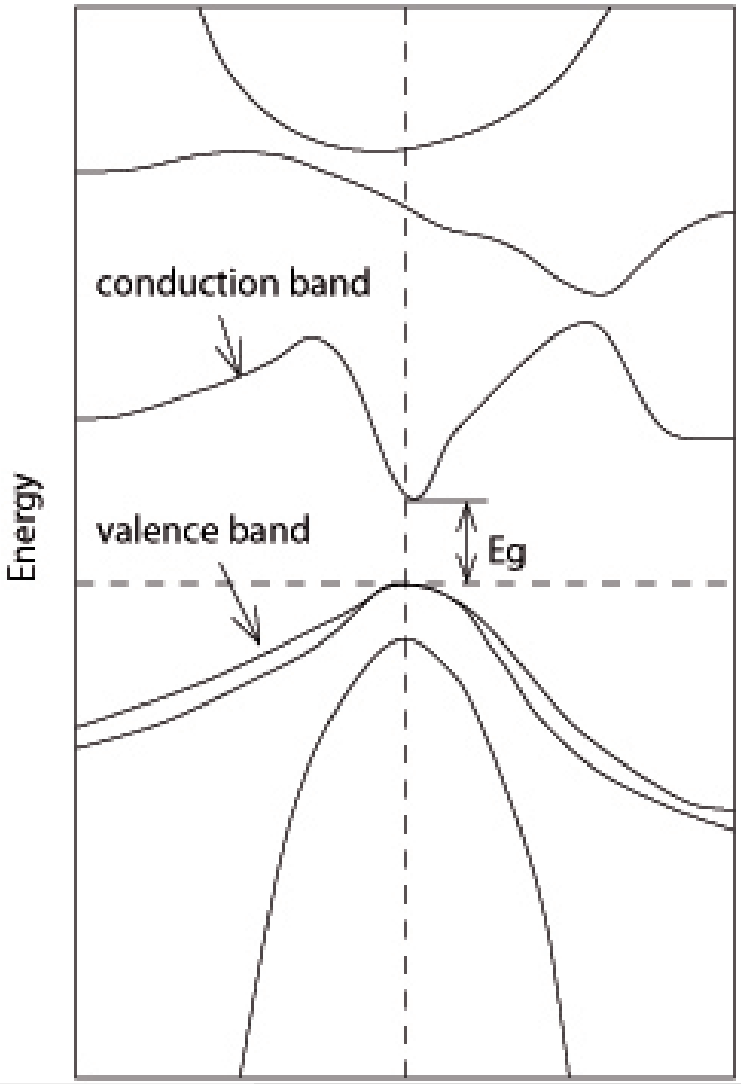
- $E_n(k) = n$-th energy band
- energy gap = all E^* for which there is no k with $E_n(k) = E^*$

Energy bands

Silicon



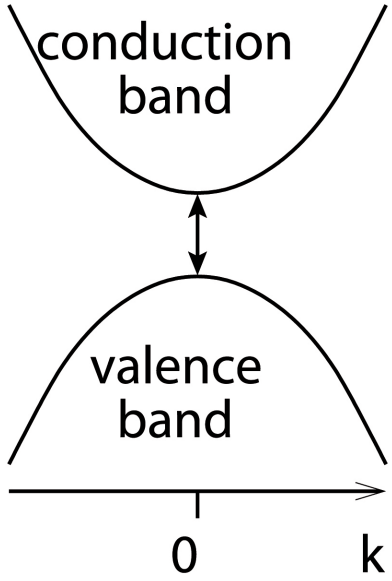
Gallium Arsenide



Parabolic band approximation

- Taylor expansion around $k = 0$ if $E(0) = 0$:

$$E(k) \approx E(0) + \nabla_k E(0) \cdot k + \frac{1}{2} k^\top \frac{d^2E}{dk^2}(0)k$$
$$= \frac{1}{2} k^\top \frac{d^2E}{dk^2}(0)k$$



- Diagonalization:

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2}(0) = \begin{pmatrix} 1/m_1^* & 0 & 0 \\ 0 & 1/m_2^* & 0 \\ 0 & 0 & 1/m_3^* \end{pmatrix} \overset{\text{isotropic}}{=} \begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix}$$

Parabolic band approximation

$$E(k) = \frac{\hbar^2}{2m^*}|k|^2$$

Semi-classical picture

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi - q(V_L(x) + V(x))\psi$$

where V_L: lattice potential, V: external potential

Theorem (Semi-classical equations of motion)

$$\hbar\dot{x} = \hbar v_n(k) = \nabla_k E_n(k), \quad \hbar\dot{k} = q\nabla_x V$$

- Momentum operator: $P\psi_{n,k} = (\hbar/i)\nabla\psi_{n,k}$
- Mean velocity: $v_n = \langle P\rangle/m = (\hbar/im)\int\overline{\psi}_{n,k}\nabla\psi_{n,k}dx$

Motivation of the formulas:

- Insert $\psi_{n,k}(x) = e^{ik\cdot x}u_{n,k}(x)$ in Schrödinger equation $\Rightarrow$ first eq.
- $\psi_{n,k}(x) = e^{ik\cdot x} \Rightarrow P\psi_{n,k} = \hbar k\psi_{n,k}$: $\hbar k$ = crystal momentum = p
- Newton's law: $\hbar\dot{k} = \dot{p} = F = q\nabla_x V$ gives second equation

Effective mass

- Semi-classical equations of motion:

$$\hbar\dot{x} = \hbar v_n(k) = \nabla_k E_n(k), \quad \hbar\dot{k} = q\nabla_x V$$

- Definition of effective mass m^*:

$$p = m^* v_n$$

- Consequence:

$$\dot{p} = m^* \frac{\partial}{\partial t} v_n = \frac{m^*}{\hbar} \frac{\partial}{\partial t} \nabla_k E_n = \frac{m^*}{\hbar} \frac{d^2 E_n}{dk^2} \dot{k} = \frac{m^*}{\hbar^2} \frac{d^2 E_n}{dk^2} \dot{p}$$

- Effective mass equation:

$$m^* = \hbar^2 \left(\frac{d^2 E_n}{dk^2} \right)^{-1}$$

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Semi-classical kinetic equations

- Semi-classical equations:

$$\hbar\dot{x} = \nabla_k E(k), \quad \hbar\dot{k} = q\nabla_x V(x), \quad p = m^* v$$

- Liouville's theorem: If (and this is true)

$$\frac{\partial}{\partial x}\nabla_k E(k) + \frac{\partial}{\partial k} q\nabla_x V(x) = 0 \quad \text{then} \quad f(x(t), k(t), t) = f_I(x_0, k_0)$$

- Semi-classical Vlasov equation:

$$0 = \frac{d}{dt} f(x,k,t) = \partial_t f + \dot{x}\cdot\nabla_x f + \dot{k}\cdot\nabla_k f = \partial_t f + v(k)\cdot\nabla_x f + \frac{q}{\hbar}\nabla_x V\cdot\nabla_k f$$

- Include collisions: assume that $df/dt = Q(f)$

Semi-classical Boltzmann equation

$$\partial_t f + v(k)\cdot\nabla_x f + \frac{q}{\hbar}\nabla_x V\cdot\nabla_k f = Q(f)$$

Poisson equation

- Electric force given by $E = E_{\text{ext}} + E_{\text{mean}}$
- Electric force between electrons given by Coulomb field:

$$E_c(x,y) = -\frac{q}{4\pi\varepsilon_s}\frac{x-y}{|x-y|^3}$$

- Mean-field approximation of electric field:

$$E_{\text{mean}}(x,t) = \int_{\mathbb{R}^3} n(y,t)E_c(x,y)dy \quad \Rightarrow \quad \operatorname{div} E_{\text{mean}} = -\frac{q}{\varepsilon_s}n$$

- External electric field generated by doping atoms:

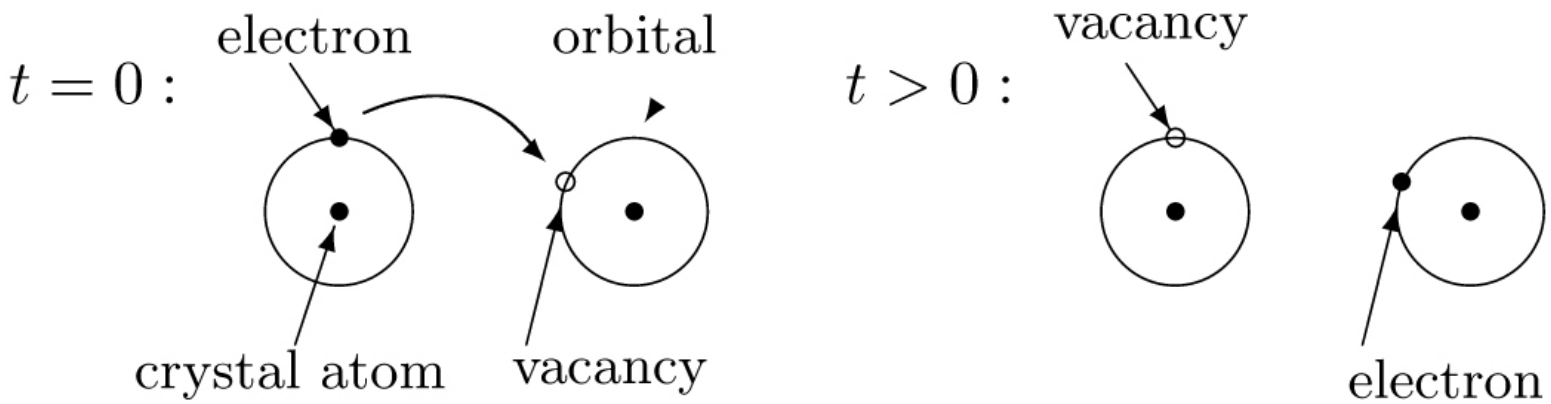
$$E_{\text{ext}}(x,t) = \frac{q}{4\pi\varepsilon_s}\int_{\mathbb{R}^3} C(y)\frac{x-y}{|x-y|^3}dy \quad \Rightarrow \quad \operatorname{div} E_{\text{ext}} = \frac{q}{\varepsilon_s}C(x)$$

- Since $\operatorname{curl} E = 0$, there exists potential V such that $E = -\nabla V$

Poisson equation

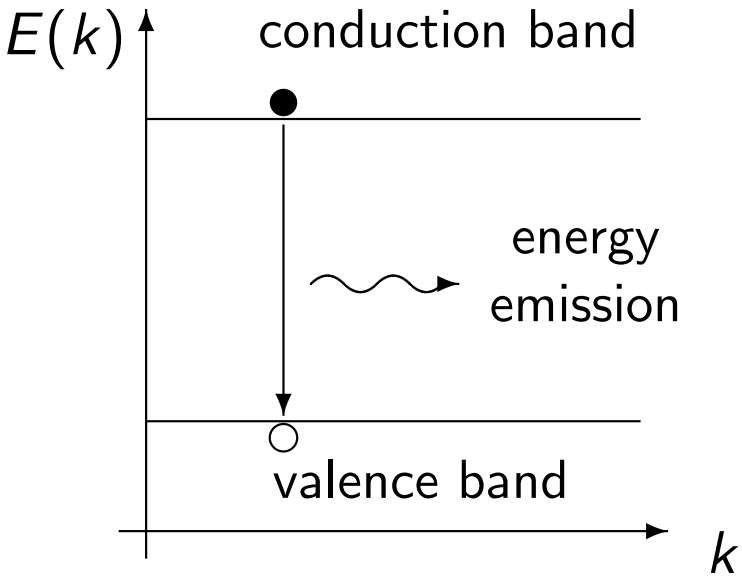
$$\varepsilon_s \Delta V = -\varepsilon_s \operatorname{div}(E_{\text{mean}} + E_{\text{ext}}) = q(n - C(x))$$

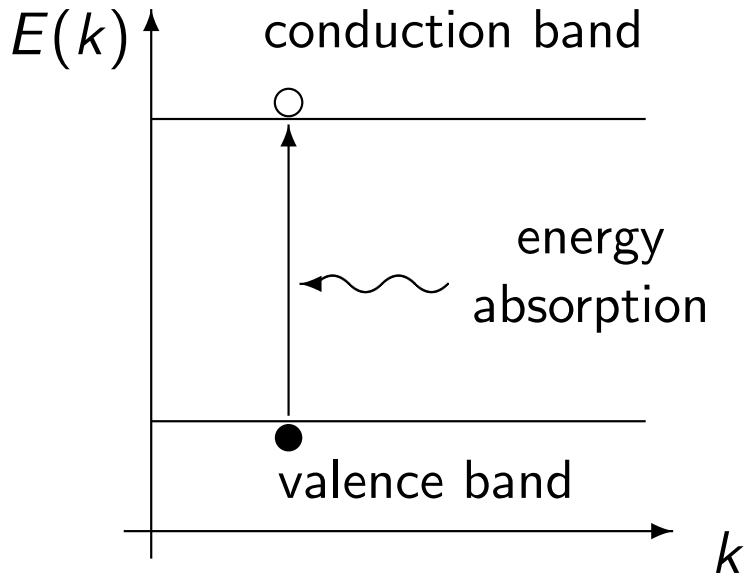
Holes



- Hole = vacant orbital in valence band
- Interpret hole as defect electron with positive charge
- Current flow = electron flow in conduction band and hole flow in valence band
- Electron density $n(x, t)$, hole density $p(x, t)$

Holes





- Recombination: conduction electron recombines with valence hole
- Generation: creation of conduction electron and valence hole
- Shockley-Read-Hall model:

$$R(n,p) = \frac{n_i^2 - np}{\tau_p(n + n_d) + \tau_n(p + p_d)}, \qquad n_i : \text{ intrinsic density}$$

Boltzmann distribution function

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f), \quad v(k) = \nabla_k E(k)/\hbar$$

- Definition of distribution function:

$$f(x,k,t) = \frac{\text{number of occupied states in } dx\,dk \text{ in conduction band}}{\text{total number of states in } dx\,dk \text{ in conduction band}}$$

- Quantum state has phase-space volume $(2\pi)^3$ (integrate $k \in B \sim (-\pi,\pi)^3$)
- Quantum state density (take into account electron spin):

$$N^*(x,k)dx\,dk = \frac{2}{(2\pi)^3} dx\,dk = \frac{1}{4\pi^3} dx\,dk$$

- Total number of electrons in volume $dx\,dk$:

$$dn = f(x,k,t)N^*(x,k)dx\,dk = f(x,k,t)\frac{dx\,dk}{4\pi^3}$$

- Electron density: $n(x,t) = \int_B dn = \int_B f(x,k,t)\frac{dk}{4\pi^3}$

Collision models

- Probability that electron changes state k' to k is proportional to

  occupation prob. $f(x,k',t) \times$ non-occupation prob.$(1-f(x,k,t))$

- Collisions between two electrons in states k and k':

$$\begin{aligned}(Q(f))(x,k,t) &= (\text{Probability } k' \to k) - (\text{Probability } k \to k') \\ &= \int_B \big(s(x,k',k)f'(1-f) - s(x,k,k')f(1-f')\big)\,dk'\end{aligned}$$

  where $f' = f(x,k',t)$, $s(x,k',k)$: scattering rate

- Important collision processes:
  - Electron-phonon scattering
  - Ionized impurity scattering
  - Electron-electron scattering

Scattering rates

Electron-phonon scattering:

- Collisions of electrons with vibrations of crystal lattice (phonons)
- Phonon emission: $E(k') - E(k) = \hbar\omega =$ phonon energy
- Phonon absorption: $E(k') - E(k) = -\hbar\omega$
- Phonon occupation number: $N = 1/(\exp(\hbar\omega/k_B T) - 1)$
- General scattering rate:

$$s(x,k,k') = \sigma\big((1+N)\delta(E'-E+\hbar\omega) + N\delta(E'-E-\hbar\omega)\big)$$

  where δ: delta distribution, $E' = E(k')$
- If phonon scattering elastic, $\hbar\omega \approx 0$: $s(x,k,k') = \sigma(x,k,k')\delta(E'-E)$

$$(Q_{\rm el}(f))(x,k,t) = \int_B \sigma(x,k,k')\delta(E'-E)(f'-f)dk'$$

- Elastic collisions conserve mass and energy:

$$\int_B Q_{\rm el}(f)dk = \int_B E(k)Q_{\rm el}(f)dk = 0$$

Scattering rates

Ionized impurity scattering:

- Collisions of electrons with ionized doping atoms: elastic scattering
- Collision operator

$$(Q(f))(x,k,t) = \int_B \sigma(x,k,k')\delta(E'-E)(f'-f)dk'$$

Electron-electron scattering:

- Electrons in states k' and k_1' collide and scatter to states k and k_1
- Elastic collisions: $s(x,k,k',k_1,k_1') = \sigma(x)\delta(E'+E_1'-E-E_1)$
- Collision operator:

$$(Q(f))(x,k,t) = \int_{B^3} s(x,k,k',k_1,k_1') \times \left(f'f_1'(1-f)(1-f_1) - ff_1(1-f')(1-f_1')\right)dk'\,dk_1\,dk_1'$$

- Mass and energy conservation: $\int_B Q(f)dk = \int_B E(k)Q(f)fdk = 0$

Summary

Electron motion in semi-classical approximation:

Semi-classical Boltzmann equation

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f), \quad x \in \mathbb{R}^3, \ k \in B$$

- B: Brillouin zone coming from crystal structure
- k: pseudo-wave vector, $p = \hbar k$: crystal momentum
- Mean velocity: $v(k) = \nabla_k E(k)/\hbar$
- Energy band $E(k)$; parabolic band approximation: $E(k) = \hbar^2 |k|^2 / 2m^*$
- Electric potential V computed from Poisson equation

$$\varepsilon_s \Delta V = q(n - C(x)), \quad C(x): \text{ doping profile}$$

- Electron density:

$$n(x,t) = \int_B f(x,k,t) \frac{dk}{4\pi^3}$$

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Why macroscopic models?

Semi-classical Boltzmann equation

$$\partial_t f + v(k)\cdot\nabla_x f + \frac{q}{\hbar}\nabla_x V\cdot\nabla_k f = Q(f), \quad x\in\mathbb{R}^3,\ k\in B\subset\mathbb{R}^3$$

- Semi-classical Boltzmann equation is (3+3)-dimensional: numerical simulations extremely time-consuming
- Often only macroscopic physical variables (particle density n, velocity u, energy ne) are of interest

$$(n, nu, ne) = \int_{\mathbb{R}^3} f(k)(1, k, \tfrac{1}{2}|k|^2)\frac{dk}{4\pi^3}$$

- Derive evolution equations by integrating Boltzmann equation over $k\in B$
- Depending on semiconductor application, derive various models $\longrightarrow$ leads to model hierarchy

Scaling of Boltzmann equation

$$\partial_t f + v(k)\cdot\nabla_x f + \frac{q}{\hbar}\nabla_x V\cdot\nabla_k f = Q(f), \quad \varepsilon_s \Delta V = q(n - C(x))$$

- Introduce reference values for

length	λ	time	τ
mean free path	$\lambda_c = u\tau = \lambda$	velocity	$u = \sqrt{k_B T_L/m^*}$,
wave vector	$k_0 = m^* u/\hbar$	potential	$U_T = k_B T_L/q$

- Scaled Boltzmann equation:

$$\partial_t f + v(k)\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f = Q(f)$$

- Scaled Poisson equation:

$$\lambda_D^2 \Delta V = n - C(x), \quad \lambda_D^2 = \frac{\varepsilon_s U_T}{q\lambda^2 k_0}$$

Objective: derive macroscopic equations by averaging over $k \in B$

Moment method

Boltzmann equation with parabolic band:

$$\partial_t f + k \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f = Q(f), \quad \lambda_D^2 \Delta V = n - C(x)$$

- Integrate over $k \in B$:

$$\partial_t \underbrace{\int_B f \frac{dk}{4\pi^3}}_{=n(x,t)} + \mathrm{div}_x \underbrace{\int_B kf \frac{dk}{4\pi^3}}_{=-J_n(x,t)} + \nabla_x V \cdot \underbrace{\int_B \nabla_k f \frac{dk}{4\pi^3}}_{=0} = \underbrace{\int_B Q(f) \frac{dk}{4\pi^3}}_{=0}$$

  $\longrightarrow$ Mass balance equation: $\partial_t n - \mathrm{div}\, J_n = 0$

- Multiply by k and integrate by parts:

$$\partial_t \underbrace{\int_B kf \frac{dk}{4\pi^3}}_{=-J_n(x,t)} + \mathrm{div}_x \underbrace{\int_B k \otimes kf \frac{dk}{4\pi^3}}_{=P} - \nabla_x V \cdot \underbrace{\int_B f \frac{dk}{4\pi^3}}_{=n} = \underbrace{\int_B kQ(f) \frac{dk}{4\pi^3}}_{=-W}$$

  $\longrightarrow$ Momentum balance equation: $\partial_t J_n - \mathrm{div}\, P + \nabla V \cdot J_n = W$

Moment method: closure problem

- Mass balance equation:

$$\partial_t n - \operatorname{div} J_n = 0$$

- Momentum balance equation:

$$\partial_t J_n - \operatorname{div} P + \nabla V \cdot J_n = W, \quad P = \int_B k \otimes k f \frac{dk}{4\pi^3}$$

- Energy balance equation (assuming energy conservation):

$$\partial_t \underbrace{\int_B \frac{|k|^2}{2} f \frac{dk}{4\pi^3}}_{=(ne)(x,t)} + \operatorname{div} \underbrace{\int_B \frac{k|k|^2}{2} \frac{dk}{4\pi^3}}_{=R} - \nabla V \cdot \underbrace{\int_B k f \frac{dk}{4\pi^3}}_{=-J_n} = \underbrace{\int_B \frac{|k|^2}{2} Q(f) \frac{dk}{4\pi^3}}_{=0}$$

$$\to \partial_t (ne) + \operatorname{div} R + \nabla V \cdot J_n = 0$$

Closure problem: P and R cannot be expressed in terms of n, J_n, ne

Solution of closure problem

Scaling of Boltzmann equation:

- Collision time $\tau_c = \tau/\alpha$: hydrodynamic scaling (long time scale)

$$\alpha\partial_t f + \alpha\big(v\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f\big) = Q(f), \quad \alpha = \frac{\lambda_c}{\lambda} = \text{Knudsen number}$$

- Collision time $\tau_c = \tau/\alpha^2$: diffusion scaling (very long time scale)

$$\alpha^2\partial_t f + \alpha\big(v\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f\big) = Q(f),$$

Equilibrium distribution (Maxwellian):

- Kinetic entropy: $S(f) = -\int_B f(\log f - 1 + E(k))dk$
- Given f, solve constrained maximization problem:

$$\max\left\{S(g) : \int_B \kappa(k) g\frac{dk}{4\pi^3} = \int_B \kappa(k) f\frac{dk}{4\pi^3},\ \kappa(k) = 1, k, \frac{1}{2}|k|^2\right\}$$

$\longrightarrow$ formal solution: Maxwellian $M[f] = \exp(\kappa(k)\cdot\lambda(x))$

Model hierarchy

Model hierarchy depends on ...

- diffusive or hydrodynamic scaling
- number of moments or weight functions

Hydrodynamic models:

- Weight functions 1, k: isothermal hydrodynamic equations for electron density n and current density J_n
- Weight functions 1, k, $\frac{1}{2}|k|^2$: full hydrodynamic equations for n, J_n, and energy density ne

Diffusive models:

- Weight function 1: drift-diffusion equations for n
- Weight functions 1, $\frac{1}{2}|k|^2$: energy-transport equations for n and ne

Model hierarchy

Diffusive models	*Hydrodynamic models*	*# Variables*
Drift-diffusion equations		1
Van Roosbroeck 1950	Isothermal hydrodynamic equations	4
Energy-transport equations		2
Stratton 1962	Full hydrodynamic equations	5
Fourth-order moment equations	*Blotekjaer 1970*	3
Grasser et al. 2001	Extended hydrodynamic equations	13
Higher-order moment equations	*Anile 1995*	
A.J./Krause/Pietra 2007	Higher-order hydrodynamic equations	
	Struchtrup 1999	

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   - Basics of semiconductor physics
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Derivation

$$\alpha^2 \partial_t f_\alpha + \alpha\big(v(k)\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_k f_\alpha\big) = Q(f_\alpha)$$

- Simplifications: parabolic band $E(k) = \frac{1}{2}|k|^2$ $(k\in\mathbb{R}^3)$, relaxation-time operator $Q(f) = (nM - f)/\tau$
- Maxwellian: $M(k) = (2\pi)^{-3/2}\exp(-\frac{1}{2}|k|^2)$, $\int_{\mathbb{R}^3} M(k)dk = 1$
- Electron density: $n_\alpha(x,t) = \int_{\mathbb{R}^3} f_\alpha(x,k,t)dk/4\pi^3$
- Moment equation: integrate Boltzmann equation over k

$$\alpha\partial_t \int_{\mathbb{R}^3} f_\alpha \frac{dk}{4\pi^3} + \mathrm{div}_x \int_{\mathbb{R}^3} k f_\alpha \frac{dk}{4\pi^3} = \frac{1}{\alpha\tau}\int_{\mathbb{R}^3}(nM - f_\alpha)\frac{dk}{4\pi^3}$$

- Derivation in three steps

Step 1: limit $\alpha\to 0$ in Boltzmann equation $\Rightarrow Q(f) = 0$
$\Rightarrow f = \lim_{\alpha\to 0} f_\alpha = nM$

Derivation

Step 2:

- Chapman-Enskog expansion $f_\alpha = n_\alpha M + \alpha g_\alpha$ in Boltzmann equation:

$$\alpha\partial_t f_\alpha + \big(k\cdot\nabla_x(n_\alpha M) + \nabla_x V\cdot\nabla_k(n_\alpha M)\big) + \alpha\big(k\cdot\nabla_x g_\alpha + \nabla_x V\cdot\nabla_k g_\alpha\big) = \alpha^{-1}Q(n_\alpha M) + Q(g_\alpha) = Q(g_\alpha)$$

- Limit $\alpha\to 0$ ($g = \lim_{\alpha\to 0} g_\alpha$): $Q(g) = (nM - g)/\tau$

$$Q(g) = k\cdot\nabla_x(nM) + \nabla_x V\cdot\nabla_k(nM) = k\cdot(\nabla_x n - n\nabla_x V)M$$

$$\Rightarrow\quad g = -\tau k\cdot(\nabla_x n - n\nabla_x V)M + nM,\quad M(k) = (2\pi)^{-3/2}e^{-|k|^2/2}$$

Step 3:

- Insert Chapman-Enskog expansion in Boltzmann equation:

$$\partial_t\int_{\mathbb{R}^3} f_\alpha\frac{dk}{4\pi^3} + \frac{1}{\alpha}\mathrm{div}_x\underbrace{\int_{\mathbb{R}^3} kn_\alpha M\frac{dk}{4\pi^3}}_{=0} + \mathrm{div}_x\int_{\mathbb{R}^3} kg_\alpha\frac{dk}{4\pi^3} = \frac{1}{\alpha^2\tau}\underbrace{\int_{\mathbb{R}^3} Q(f_\alpha)\frac{dk}{4\pi^3}}_{=0}$$

Derivation

$$\partial_t \int_{\mathbb{R}^3} (n_\alpha M + \alpha g_\alpha) \frac{dk}{4\pi^3} + \operatorname{div}_x \int_{\mathbb{R}^3} k g_\alpha \frac{dk}{4\pi^3} = 0$$

- Limit $\alpha \to 0$:

$$\partial_t \int_{\mathbb{R}^3} nM \frac{dk}{4\pi^3} + \operatorname{div}_x \int_{\mathbb{R}^3} kg \frac{dk}{4\pi^3} = 0$$

- Define current density $J_n = -\int_{\mathbb{R}^3} kg\,dk/4\pi^3$, insert expression for $g = -\tau k \cdot (\nabla_x n - n\nabla_x V)M + nM$:

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \tau \underbrace{\int_{\mathbb{R}^3} k \otimes kM \frac{dk}{4\pi^3}}_{=\mathrm{Id}} (\nabla_x n - n\nabla_x V)$$

Theorem (Drift-diffusion equations)

The formal limit $\alpha \to 0$ gives

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \tau(\nabla n - n\nabla V)$$

Bipolar drift-diffusion equations

$$\partial_t n - \operatorname{div} J_n = -R(n,p), \quad J_n = \tau(\nabla n - n\nabla V)$$
$$\partial_t p + \operatorname{div} J_p = -R(n,p), \quad J_n = -\tau(\nabla p + p\nabla V)$$
$$\lambda_D^2 \Delta V = n - p - C(x)$$

- Hole density modeled by drift-diffusion equations
- Shockley-Read-Hall recombination-generation term:

$$R(n,p) = \frac{np - n_i^2}{\tau_p(n + n_d) + \tau_n(p + p_d)}$$

with physical parameter n_i, τ_n, τ_p, n_d, p_d

- Auger recombination-generation term (high carrier densities):

$$R(n,p) = (C_n n + C_p p)(np - n_i^2)$$

with physical parameter C_n and C_p

- Equilibrium state: $np = n_i^2$ = intrinsic density

Drift-diffusion equations: summary

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V, \quad \lambda_D^2 \Delta V = n - C(x)$$

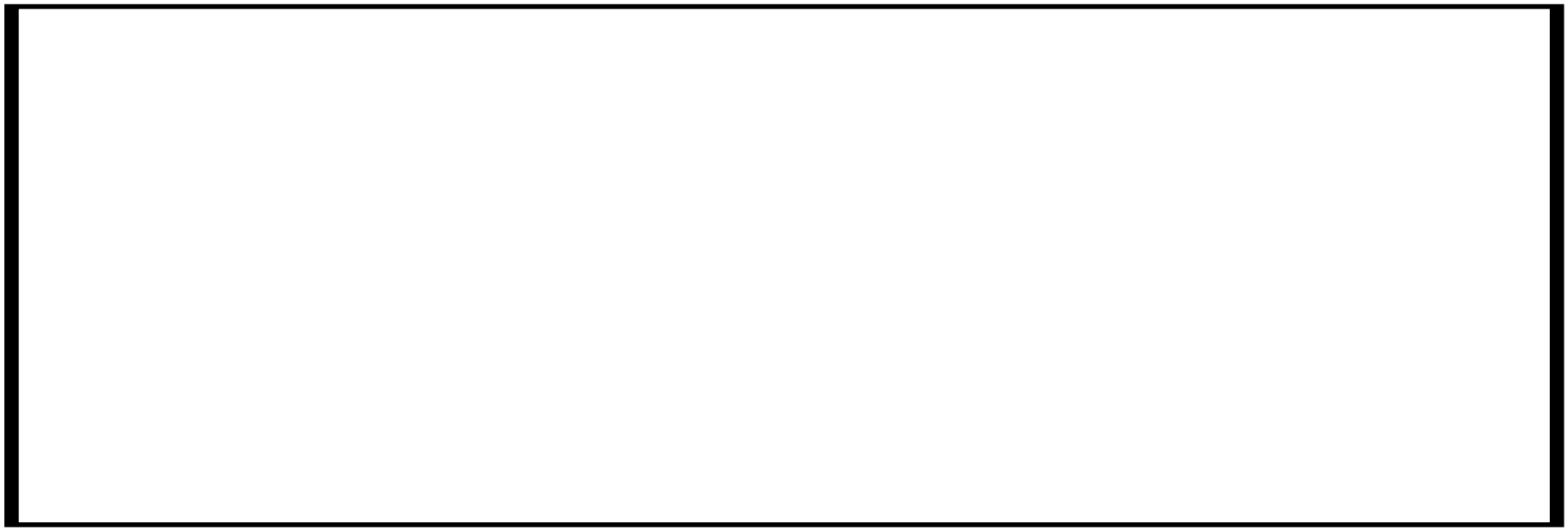
- Variables: electron density n, electric potential V
- $n\nabla V$: drift current, ∇n: diffusion current
- First proposed by van Roosbroeck 1950
- Rigorous derivation from Boltzmann equation: Poupaud 1992 (linear), Ben Abdallah/Tayeb 2004 (1D Poisson coupling), Masmoudi/Tayeb 2007 (multi-dimensional)
- Existence analysis: Mock 1972, Gajewski/Gröger 1986
- Numerical solution: Scharfetter/Gummel 1964, Brezzi et al. 1987

\+ well established, used in industrial semiconductor codes
\+ well understood analytically and numerically
\+ stable mixed finite-element schemes available
– satisfactory results only for lengths $> 1\,\mu$m
– no carrier heating (thermal effects)

Drift-diffusion models: extensions

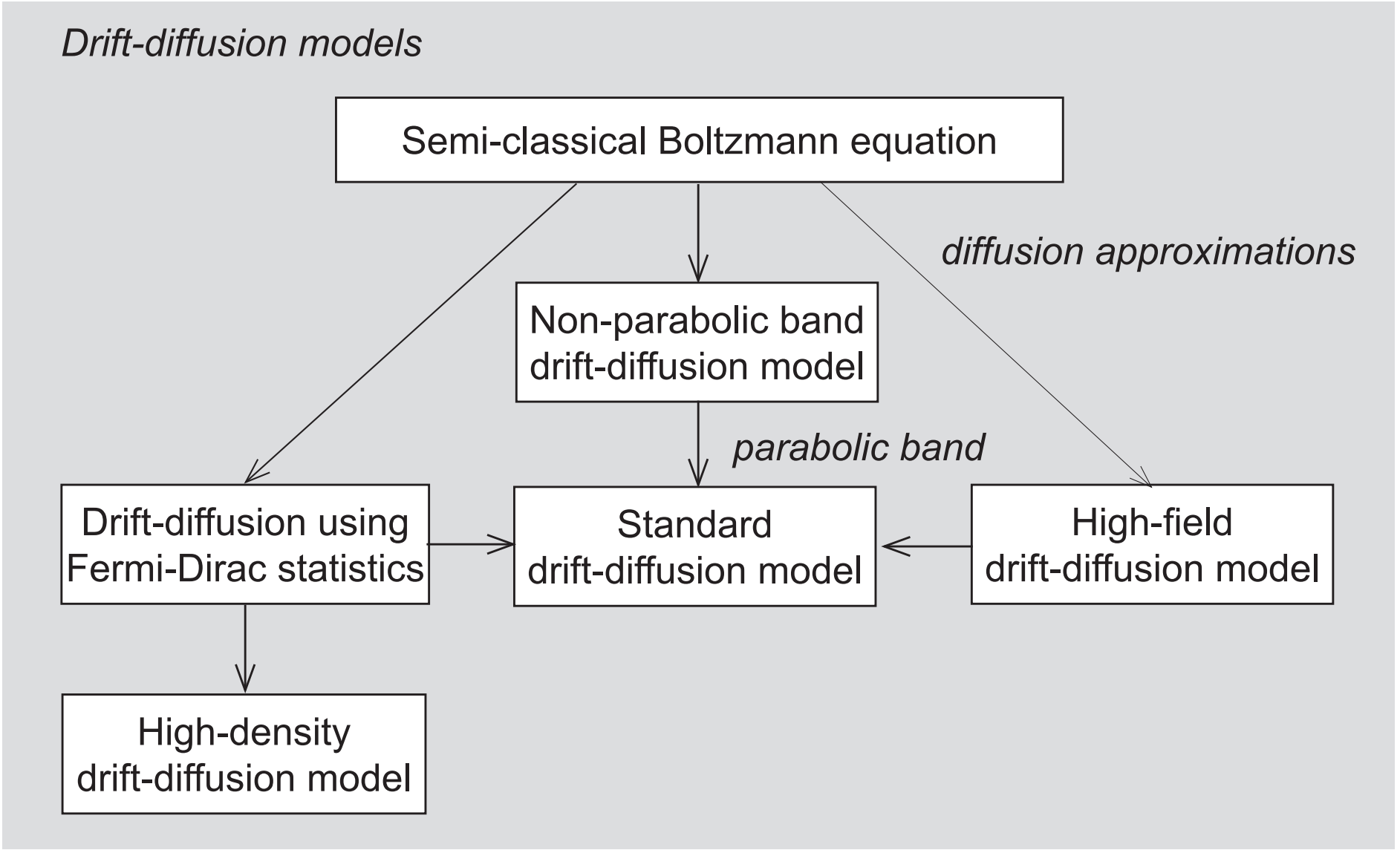
	Assumption:	Generalization:
①	Equilibrium given by Maxwellian M	Use Fermi-Dirac distribution
②	Parabolic-band approximation	Use non-parabolic bands
③	Scaling valid for low fields only	Devise high-field models
④	One moment (particle density) used	Use more moments

Comparison drift-diffusion and Monte-Carlo:



From: Grasser et al. 2005

Summary


Drift-diffusion models
Semi-classical Boltzmann equation
diffusion approximations
Non-parabolic band drift-diffusion model
parabolic band
Drift-diffusion using Fermi-Dirac statistics
Standard drift-diffusion model
High-field drift-diffusion model
High-density drift-diffusion model

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Semi-classical Boltzmann equation

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f)$$

- Collision operator: $Q(f) = Q_{\rm el}(f) + Q_{\rm ee}(f) + Q_{\rm in}(f)$

$$Q_{\rm el}(f) = \int_B \sigma_{\rm el}(k,k')\delta(E'-E)(f'-f)dk'$$

$$Q_{\rm ee}(f) = \int_{B^3} \sigma_{\rm ee}(,k,k',k_1,k_1')\delta(E'+E_1'-E-E_1) \times \big(f'f_1'(1-f)(1-f_1) - ff_1(1-f')(1-f_1')\big)dk'\,dk_1\,dk_1'$$

$$Q_{\rm in}(f) = \text{inelastic collisions (unspecified)}$$

- Scaling: $\alpha = \sqrt{\lambda_{\rm el}/\lambda_{\rm in}}$

$$\alpha^2\partial_t f + \alpha\big(v(k)\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f\big) = Q_{\rm el}(f) + \alpha Q_{\rm ee}(f) + \alpha^2 Q_{\rm in}(f)$$

Properties of elastic collision operator

$$Q_{\rm el}(f) = \int_B \sigma_{\rm el}(k,k')\delta(E'-E)(f'-f)dk', \quad \sigma(k,k') \text{ symmetric}$$

Proposition

- *Conservation properties:* $\int_B Q_{\rm el}(f)dk = \int_B Q_{\rm el}(f)E(k)dk = 0$ *for all* f
- *Symmetry:* $-Q_{\rm el}$ *is symmetric and nonnegative*
- *Kernel* $N(Q_{\rm el}) =$ *all functions* $F(x, E(k), t)$

Proof:

- Conservation and symmetry: use symmetry of $\sigma(k,k')$ and $\delta(E'-E)$
- Nonnegativity: show that

$$\int_B Q_{\rm el}(f)f dk = \frac{1}{2}\int_{B^2} \sigma_{\rm el}(k,k')\delta(E'-E)(f'-f)^2 dk'\,dk \geq 0$$

- Kernel: $Q_{\rm el}(f) = 0 \Rightarrow \delta(E'-E)(f'-f)^2 = 0 \Rightarrow f(k') = f(k)$ if $E(k') = E(k) \Rightarrow f$ constant on energy surface $\{k : E(k) = \varepsilon\}$

Properties of elastic collision operator

$$Q_{\rm el}(f) = \int_B \sigma_{\rm el}(k,k')\delta(E'-E)(f'-f)dk', \quad \sigma(k,k') \text{ symmetric}$$

Proposition

Equation $Q_{\rm el}(f) = h$ solvable iff $\int_B h(k)\delta(E(k)-\varepsilon)dk = 0$ for all ε

Proof:

- Fredholm alternative: $Q_{\rm el}$ symmetric $\Rightarrow$ $Q_{\rm el}(f) = h$ solvable iff $h \in N(Q_{\rm el})^\perp$
- Let $Q_{\rm el}(f) = h$ be solvable and let $h \in N(Q_{\rm el})^\perp$, $f = F(E) \in N(Q_{\rm el})$:

$$0 = \int_B hf dk = \int_B h(k) \int_{\mathbb{R}} F(\varepsilon)\delta(E(k)-\varepsilon)d\varepsilon\, dk$$
$$= \int_{\mathbb{R}} \int_B h(k)\delta(E(k)-\varepsilon)dk\, F(\varepsilon)d\varepsilon \;\Rightarrow\; \int_B h(k)\delta(E(k)-\varepsilon)dk = 0$$

- Conversely, show similarly that $h \in N(Q_{\rm el})^\perp$

Properties of electron-electron collision operator

$$Q_{\rm ee}(f) = \int_{B^3} \sigma_{\rm ee}(k,k',k_1,k_1')\delta(E'+E_1'-E-E_1)$$
$$\times\left(f'f_1'(1-f)(1-f_1) - ff_1(1-f')(1-f_1')\right)dk'\,dk_1\,dk_1'$$

Proposition

Let $\sigma_{\rm ee}$ be symmetric:

- *Conservation properties:* $\int_B Q_{\rm ee}(f)dk = \int_B Q_{\rm ee}(f)E(k)dk = 0\ \forall f$
- *Kernel $N(Q_{\rm ee})$ = Fermi-Dirac distributions $F(k)$,*

$$F(k) = 1/(1+\exp((E(k)-\mu)/T)) \quad \text{for arbitrary } \mu,\ T$$

Proof: Show that

$$\int_B Q_{\rm ee}(f)g dk = -\int_{B^4} \sigma_{\rm ee}\delta(E+E_1-E'-E_1')(g'+g_1'-g-g_1)$$
$$\times\left(f'f_1'(1-f)(1-f_1) - ff_1(1-f')(1-f_1')\right)dk^4$$

Conservation: take $g=1$ and $g=E$. Kernel: more difficult

Properties of electron-electron collision operator

$$Q_{\rm ee}(f) = \int_{B^3} \sigma_{\rm ee}(k,k',k_1,k_1')\delta(E'+E_1'-E-E_1)$$
$$\times\left(f'f_1'(1-f)(1-f_1) - ff_1(1-f')(1-f_1')\right)dk'\,dk_1\,dk_1'$$

Averaged collision operator:

$$S(\varepsilon) = \int_B Q_{\rm ee}(F)\delta(E-\varepsilon)dk$$

Proposition

Let $\sigma_{\rm ee}$ be symmetric:

- *Conservation properties:* $\int_{\mathbb{R}} S(\varepsilon)d\varepsilon = \int_{\mathbb{R}} S(\varepsilon)\varepsilon d\varepsilon = 0$
- *If $S(\varepsilon)=0$ for all ε then $F = 1/(1+\exp((E-\mu)/T))$ Fermi-Dirac*

Proof: similar as above

Derivation: general strategy

$$\alpha^2\partial_t f_\alpha + \alpha\big(v(k)\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_k f_\alpha\big) = Q_{\rm el}(f_\alpha) + \alpha Q_{\rm ee}(f_\alpha) + \alpha^2 Q_{\rm in}(f_\alpha)$$

Set $\langle g\rangle = \int_B g(k)dk/4\pi^3$

Moment equations for moments $\langle f_\alpha\rangle$ and $\langle Ef_\alpha\rangle$:

$$\begin{aligned}
&\alpha^2\partial_t\langle E^j f_\alpha\rangle + \alpha{\rm div}_x\langle E^j v f_\alpha\rangle - \alpha\nabla_x V\cdot\langle\nabla_k E^j f_\alpha\rangle \\
&\quad = \langle E^j Q_{\rm el}(f_\alpha)\rangle + \alpha\langle E^j Q_{\rm ee}(f_\alpha)\rangle + \alpha^2\langle E^j Q_{\rm in}(f_\alpha)\rangle \\
&\quad = \alpha^2\langle E^j Q_{\rm in}(f_\alpha)\rangle, \quad j=0,1
\end{aligned}$$

Strategy of derivation:

- Step 1: formal limit $\alpha\to 0$ in Boltzmann equation
- Step 2: Chapman-Enskog expansion $f_\alpha = F + \alpha g_\alpha$
- Step 3: formal limit $\alpha\to 0$ in moment equations

References: Ben Abdallah/Degond 1996, Degond/Levermore/Schmeiser 2004

Step 1

$$\alpha^2\partial_t f_\alpha + \alpha\big(v(k)\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_k f_\alpha\big) = Q_{\rm el}(f_\alpha) + \alpha Q_{\rm ee}(f_\alpha) + \alpha^2 Q_{\rm in}(f_\alpha)$$

Step 1: $\alpha\to 0$ in Boltzmann equation $\Rightarrow Q_{\rm el}(f)=0$, where $f=\lim_{\alpha\to 0} f_\alpha$ $\Rightarrow f(x,k,t)=F(x,E(k),t)$

Step 2:

- Chapman-Enskog expansion $f_\alpha = F+\alpha g_\alpha$ in Boltzmann equation:

$$\alpha\partial_t f_\alpha + \big(v(k)\cdot\nabla_x F + \nabla_x V\cdot\nabla_k F\big) + \alpha\big(v(k)\cdot\nabla_x g_\alpha + \nabla_x V\cdot\nabla_k g_\alpha\big) = Q_{\rm el}(g_\alpha) + Q_{\rm ee}(f_\alpha) + \alpha Q_{\rm in}(f_\alpha)$$

- Formal limit $\alpha\to 0$ gives

$$Q_{\rm el}(g) = v(k)\cdot\nabla_x F + \nabla_x V\cdot\nabla_k F - Q_{\rm ee}(F)$$

- Operator equation solvable iff

$$\int_B \big(v(k)\cdot\nabla_x F + \nabla_x V\cdot\nabla_k F - Q_{\rm ee}(F)\big)\delta(E-\varepsilon)dk = 0 \quad \forall\varepsilon$$

Step 2

- Solvability condition for operator equation:

$$\int_B \big(v(k)\cdot\nabla_x F + \nabla_x V\cdot\nabla_k F - Q_{\rm ee}(F)\big)\delta(E-\varepsilon)dk = 0 \quad \forall\varepsilon$$

- Since $\nabla_k F = \partial_E F\nabla_k E$, $v = \nabla_k E$ and $H' = \delta$ (H: Heaviside fct.)

$$\begin{aligned}
&\int_B \big(v(k)\cdot\nabla_x F + \nabla_x V\cdot\nabla_k F\big)\delta(E-\varepsilon)dk \\
&\quad = \big(\nabla_x F + \partial_E F\nabla_x V\big)(\varepsilon)\cdot\int_B \nabla_k E\delta(E-\varepsilon)dk \\
&\quad = \big(\nabla_x F + \partial_E F\nabla_x V\big)(\varepsilon)\cdot\int_B \nabla_k H(E-\varepsilon)dk = 0
\end{aligned}$$

- Solvability condition becomes

$$\int_B Q_{\rm ee}(F)\big)\delta(E-\varepsilon)dk = 0$$

$\Rightarrow F_{\mu,T}$ = Fermi Dirac

Step 3

- Operator equation becomes (with $F_{\mu,T} = 1/(1+\exp((E(k)-\mu)/T))$)

$$Q_{\rm el}(g) = v(k)\cdot\nabla_x F_{\mu,T} + \nabla_x V\cdot\nabla_k F_{\mu,T} - \underbrace{Q_{\rm ee}(F_{\mu,T})}_{=0}$$

$$= F_{\mu,T}(1-F_{\mu,T})v(k)\cdot\left(\nabla_x\frac{\mu}{T} - \frac{\nabla_x V}{T} - E\nabla_x\frac{1}{T}\right)$$

Step 3: limit $\alpha\to 0$ in the moment equations

- Set $\langle g\rangle = \int_B g(k)dk/4\pi^3$. Moment equations for $j=0,1$:

$$\partial_t\langle E^j f_\alpha\rangle + \alpha^{-1}\underbrace{\langle E^j(v\cdot\nabla_x F_{\mu,T} + \nabla_x V\cdot\nabla_k F_{\mu,T})\rangle}_{=\langle E^j Q_{\rm el}(g)\rangle = 0}$$

$$+\langle E^j(v\cdot\nabla_x g_\alpha + \nabla_x V\cdot\nabla_k g_\alpha)\rangle = \langle E^j Q_{\rm in}(f_\alpha)\rangle$$

- Limit $\alpha\to 0$:

$$\partial_t\langle E^j F\rangle + \underbrace{\langle E^j(v\cdot\nabla_x g + \nabla_x V\cdot\nabla_k g)\rangle}_{=\mathrm{div}_x\langle E^j vg\rangle - \nabla_x V\cdot\langle\nabla_k E^j g\rangle} = \langle E^j Q_{\rm in}(F)\rangle$$

Step 3: balance equations

- Moment equation for $j = 0$:
  (assume mass conservation for inelastic scattering)

$$\partial_t \underbrace{\langle F \rangle}_{=n} + \mathrm{div}_x \underbrace{\langle vg \rangle}_{=-J_0} - \nabla_x V \cdot \underbrace{\langle \nabla_k g \rangle}_{=0} = \underbrace{\langle Q_{\mathrm{in}}(F) \rangle}_{=0}$$

- Moment equation for $j = 1$:

$$\partial_t \underbrace{\langle EF \rangle}_{=ne} + \mathrm{div}_x \underbrace{\langle Evg \rangle}_{=-J_1} - \nabla_x V \cdot \underbrace{\langle \nabla_k Eg \rangle}_{=-J_0} = \underbrace{\langle E^j Q_{\mathrm{in}}(F) \rangle}_{=W}$$

- Particle current density $J_0 = -\langle vg \rangle$
- Energy current density $J_1 = -\langle Evg \rangle$
- Energy relaxation term $W = \langle EQ_{\mathrm{in}}(F) \rangle$

Balance equations

$$\partial_t n - \mathrm{div}\, J_0 = 0, \quad \partial_t(ne) - \mathrm{div}\, J_1 + \nabla V \cdot J_0 = W$$

Step 3: current densities

$$J_0 = -\langle vg \rangle, \quad J_1 = -\langle Evg \rangle$$

where g is solution of

$$Q_{\rm el}(g) = F_{\mu,T}(1-F_{\mu,T})v(k)\cdot\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T} - E\nabla\frac{1}{T}\right)$$

- Let d_0 be solution of $Q_{\rm el}(d_0) = -F_{\mu,T}(1-F_{\mu,T})v(k)$. Then

$$g = -d_0\cdot\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T} - E\nabla\frac{1}{T}\right) + F_1, \quad F_1 \in N(Q_{\rm el})$$

- Insert into expressions for current densities:

$$J_0 = D_{00}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{01}\nabla\frac{1}{T}$$

$$J_1 = D_{10}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{11}\nabla\frac{1}{T}$$

- Diffusion coefficients:

$$D_{ij} = \langle E^{i+j}v\otimes d_0\rangle = \int_B E^{i+j}v\otimes d_0\frac{dk}{4\pi^3}$$

Summary

Energy-transport equations

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(ne) - \operatorname{div} J_1 + \nabla V \cdot J_0 = W, \quad x \in \mathbb{R}^3, \ t > 0$$

$$J_0 = D_{00}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{01}\nabla\frac{1}{T}, \quad J_1 = D_{10}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{11}\nabla\frac{1}{T}$$

- Electron and energy densities:

$$n(\mu, T) = \int_B F_{\mu,T}\frac{dk}{4\pi^3}, \quad ne(\mu, T) = \int_B E(k)F_{\mu,T}\frac{dk}{4\pi^3}$$

- Diffusion coefficients:

$$D_{ij} = \int_B E^{i+j} v \otimes d_0 \frac{dk}{4\pi^3}, \quad d_0 \text{ solves } Q_{\mathrm{el}}(d_0) = -F_{\mu,T}(1 - F_{\mu,T})v$$

- Energy-relaxation term:

$$W(\mu, T) = \int_B E(k)Q_{\mathrm{in}}(F_{\mu,T})\frac{dk}{4\pi^3}$$

References

Energy-transport equations

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(ne) - \operatorname{div} J_1 + \nabla V \cdot J_0 = W, \quad x \in \mathbb{R}^3, \ t > 0$$

$$J_0 = D_{00}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{01}\nabla\frac{1}{T}, \quad J_1 = D_{10}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{11}\nabla\frac{1}{T}$$

- First energy-transport model: Stratton 1962 (Rudan/Gnudi/Quade 1993)
- Derivation from Boltzmann equation: Ben Abdallah/Degond 1996
- Existence results:
  - Heuristic temperature model: Allegretto/Xie 1994
  - Uniformly positive definite diffusion matrix: Degond/Génieys/A.J. 1997
  - Close-to-equilibrium solutions: Chen/Hsiao/Li 2005
- Numerical approximations:
  - Mixed finite volumes: Bosisio/Sacco/Saleri/Gatti 1998
  - Mixed finite elements: Marrocco/Montarnal 1996, Degond/A.J./Pietra 2000, Holst/A.J./Pietra 2003-2004, Gadau/A.J. 2008

Relation to nonequilibrium thermodynamics

Energy-transport equations

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(ne) - \operatorname{div} J_1 + \nabla V \cdot J_0 = W, \quad x \in \mathbb{R}^3, \ t > 0$$

$$J_0 = D_{00}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{01}\nabla\frac{1}{T}, \quad J_1 = D_{10}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{11}\nabla\frac{1}{T}$$

- Balance equations = conservation laws of mass and energy (if no forces)
- Thermodynamic forces:

$$X_0 = \nabla(\mu/T) - \nabla V/T, \quad X_1 = -\nabla(1/T)$$

- Thermodynamic fluxes:

$$J_0 = D_{00}X_0 + D_{01}X_1, \quad J_1 = D_{10}X_0 + D_{11}X_1$$

- Density variables n, ne
- Entropy variables μ/T, $-1/T$

Properties of diffusion matrix

$$\mathcal{D} = (D_{ij}), \quad D_{ij} = \int_B E^{i+j} v \otimes d_0 \frac{dk}{4\pi^3} \in \mathbb{R}^{3\times 3}$$

and d_0 solves $Q_{\rm el}(d_0) = -F_{\mu,T}(1-F_{\mu,T})v(k)$

Proposition

- *$\mathcal{D}$ symmetric: $D_{01} = D_{10}$ and $D_{ij}^\top = D_{ji}$*
- *If $(d_0, E(k)d_0)$ linearly independent then $\mathcal{D}$ positive definite*

Proof:

- Symmetry: follows from symmetry of $Q_{\rm el}$
- Show that for $z \in \mathbb{R}^6$, $z \neq 0$,

$$z^\top \mathcal{D} z = \frac{1}{2}\int_{B^2} \sigma_{\rm el}(k,k')\delta(E'-E)\left|z\cdot\begin{pmatrix} d_0 \\ Ed_0\end{pmatrix}\right|^2 \frac{dk'\,dk}{4\pi^3 F(1-F)} > 0$$

since $z\cdot(d_0, Ed_0)^\top = 0$ would imply linear dependence of (d_0, Ed_0).

Properties of relaxation-time term

Inelastic (electron-phonon) collision operator:

$$Q_{\rm in}(f) = \int_B \big(s(k',k)f'(1-f) - s(k,k')f(1-f')\big)\,dk'$$
$$s(k,k') = \sigma\big((1+N)\delta(E'-E+E_{\rm ph}) + N\delta(E'-E-E_{\rm ph})\big)$$

where N: phonon occupation number, $E_{\rm ph}$: phonon energy

Proposition

W is monotone, $W(\mu,T)(T-1)\le 0$ for all $\mu\in\mathbb{R}$, $T>0$

Proof: After some manipulations,

$$W(\mu,T)(T-1) = \int_{B^2}(1-F)(1-F')\delta(E-E'+E_{\rm ph})E_{\rm ph}Ne^{-(E-\mu)/T}$$
$$\times\big(e^{E_{\rm ph}/T}-e^{E_{\rm ph}}\big)(T-1)\frac{dk'\,dk}{4\pi^3} \le 0$$

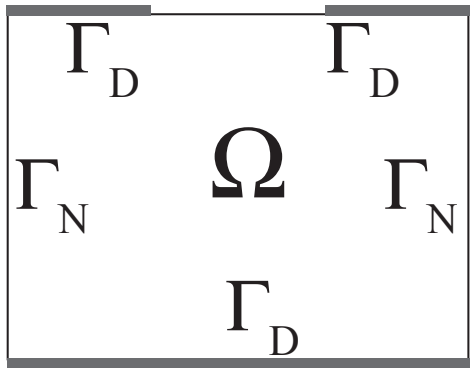
Boundary conditions

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(ne) - \operatorname{div} J_1 + \nabla V \cdot J_0 = W, \quad x \in \Omega, \ t > 0$$

$$J_0 = D_{00}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{01}\nabla\frac{1}{T}, \quad J_1 = D_{10}\left(\nabla\frac{\mu}{T} - \frac{\nabla V}{T}\right) - D_{11}\nabla\frac{1}{T}$$

- Dirichlet conditions at contacts Γ_D:

$$n = n_D, \quad T = T_D, \quad V = V_D \quad \text{on } \Gamma_D$$



- Neumann cond. at insulating boundary Γ_N:

$$J_0 \cdot \nu = J_1 \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N$$

- Improved boundary conditions for drift-diffusion (Yamnahakki 1995):

$$n + \alpha J_0 \cdot \nu = n_D \quad \text{on } \Gamma_D$$

(second-order correction from Boltzmann equation)

Open problem: improved boundary conditions for energy-transport

Explicit models: spherical symmetric energy band

Assumptions:

- $F_{\mu,T}$ approximated by Maxwellian $M = \exp(-(E-\mu)/T)$
- Scattering rate: $\sigma_{\rm el}(x,k,k') = s(x,E(k))$ for $E(k) = E(k')$
- Energy band spherically symm. monotone, $|k|^2 = \gamma(E(|k|))$, $k \in \mathbb{R}^3$

Proposition

$$\begin{pmatrix} n \\ ne \end{pmatrix} = \frac{e^{\mu/T}}{2\pi^2}\int_0^\infty e^{-\varepsilon/T}\sqrt{\gamma(\varepsilon)}\gamma'(\varepsilon)\begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} d\varepsilon$$

$$D_{ij} = \frac{e^{\mu/T}}{3\pi^3}\int_0^\infty e^{-\varepsilon/T}\frac{\gamma(\varepsilon)\varepsilon^{i+j}}{s(x,\varepsilon)\gamma'(\varepsilon)^2}d\varepsilon, \quad i,j=0,1$$

Proof: Use coarea formula for, for instance,

$$n = \int_{\mathbb{R}^3} e^{-(E(|k|)-\mu)/T}\frac{dk}{4\pi^3} = \frac{1}{4\pi^3}\int_0^\infty\int_{\{E(\rho)=\varepsilon\}}(\ldots)dS_\varepsilon\, d\varepsilon$$

Parabolic band approximation

Assumptions:

- Energy band: $E(k) = \frac{1}{2}|k|^2$, $k \in \mathbb{R}^3$
- Scattering rate: $s(x,\varepsilon) = s_1(x)\varepsilon^\beta$, $\beta \geq 0$

Proposition

$$n = NT^{3/2}e^{\mu/T}, \quad N = \frac{2}{(2\pi)^{3/2}} \text{ density of states}, \quad ne = \frac{3}{2}nT$$

$$\mathcal{D} = C(s_1)\Gamma(2-\beta)nT^{1/2-\beta}\begin{pmatrix} 1 & (2-\beta)T \\ (2-\beta)T & (3-\beta)(2-\beta)T^2 \end{pmatrix}$$

Proof: Since $\gamma(\varepsilon) = 2\varepsilon$,

$$n = \frac{\sqrt{2}}{\pi^2}e^{\mu/T}\int_0^\infty e^{-\varepsilon/T}\sqrt{\varepsilon}d\varepsilon = \frac{\sqrt{2}}{\pi^2}e^{\mu/T}T^{3/2}\Gamma(\tfrac{3}{2}) = \frac{2}{(2\pi)^{3/2}}T^{3/2}e^{\mu/T}$$

Parabolic band approximation

Scattering rate: $s(x,\varepsilon) = s_1(x)\varepsilon^\beta$, $\beta \geq 0$

Diffusion matrix: typical choices for β

$$\beta = \tfrac{1}{2}: \text{ Chen model } \mathcal{D} = \frac{\sqrt{\pi}}{2} C(s_1) n \begin{pmatrix} 1 & \frac{3}{2}T \\ \frac{3}{2}T & \frac{15}{4}T^2 \end{pmatrix}$$

$$\beta = 0: \text{ Lyumkis model } \mathcal{D} = C(s_1) n T^{1/2} \begin{pmatrix} 1 & 2T \\ 2T & 6T^2 \end{pmatrix}$$

Relaxation-time term:

$$W = -\frac{3}{2}\frac{n(T-1)}{\tau_\beta(T)}, \quad \tau_\beta(T) = C(\beta, s_1) T^{1/2-\beta}$$

Chen model: τ_β constant in T

Symmetrization and entropy

- Equations:

$$\partial_t \rho_j(u) - \operatorname{div} J_j + j\nabla V \cdot J_0 = W(u), \quad J_j = \sum_{i=0}^{1} D_{ji}\nabla u_i + D_{j0}\nabla V u_2$$

- Entropy variables $u_0 = \mu/T$, $u_1 = -1/T$
- $\rho(u)$ is monotone and there exists χ such that $\nabla_u \chi = \rho$

Symmetrization: dual entropy variables $w_0 = (\mu - V)/T$, $w_1 = -1/T$

- Symmetrized equations:

$$\partial_t b_j(w, V) - \operatorname{div} I_j = Q_j(w), \quad I_j = \sum_{i=0}^{1} L_{ij}(w, V)\nabla w_i$$

- New diffusion matrix (L_{ij}) symmetric, positive definite:

$$(L_{ij}) = \begin{pmatrix} D_{00} & D_{01} - D_{00}V \\ D_{01} - D_{00}V & D_{11} - 2D_{01}V + D_{00}V^2 \end{pmatrix}$$

- Advantage: convective terms $\nabla V/T$ and $\nabla V \cdot J_0$ eliminated

Symmetrization and entropy

- Dual entropy variables $w_0 = (\mu - V)/T$, $w_1 = -1/T$ well-known in nonequilibrium thermodynamics

Entropy (free energy):

$$E(t) = \int_{\mathbb{R}^3} \big(\rho(u)\cdot u - \chi(u)\big)dx + \frac{\lambda_D^2}{2}\int_{\mathbb{R}^3} |\nabla V|^2 dx$$

- Entropy inequality:

$$\frac{dE}{dt} + C\underbrace{\int_{\mathbb{R}^3} \big(|\nabla w_0|^2 + |\nabla w_1|^2\big)dx}_{\text{entropy production}} \le 0$$

- Advantage: estimates for w, allows to study long-time behavior
- existence of symmetrizating variables $\Leftrightarrow$ existence of entropy (hyperbolic systems: Kawashima/Shizuta 1988, parabolic systems: Degond/Génieys/A.J. 1997)

Drift-diffusion formulation

Drift-diffusion equations:

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - \frac{n}{T_L}\nabla V, \quad T_L = 1$$

Theorem

Let $F_{\mu,T}$ be approximated by a Maxwellian. Then

$$J_0 = \nabla D_{00} - \frac{D_{00}}{T}\nabla V, \quad J_1 = \nabla D_{10} - \frac{D_{10}}{T}\nabla V$$

Proof: Show that $\nabla_x d_0 = (\nabla(\mu/T) - E\nabla(1/T))d_0 + F_1$, $F_1 \in N(Q_{\rm el})^3$

- Variables $g_0 = D_{00}$, $g_1 = D_{10}$ "diagonalize" diffusion matrix
- Temperature $T = T(g_0, g_1)$ depends on new variables: invert

$$f(T) = \frac{g_1}{g_0} = \frac{\langle v \otimes d_0\rangle}{\langle Ev \otimes d_0\rangle}, \quad d_0 \text{ solves } Q_{\rm el}(d_0) = -vF$$

- f invertible if $\mathcal{D}$ pos. def. since $f'(T) = \det\mathcal{D}/T^2 D_{00}^2 > 0$

Drift-diffusion formulation

Assumptions: parabolic band and scattering rate with parameter β:

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(\tfrac{3}{2}nT) - \operatorname{div} J_1 + J_0 \cdot \nabla V = W(n,T)$$
$$J_j = \mu_0 \Gamma(2+j-\beta)\big(\nabla(nT^{1/2+j-\beta}) - nT^{-1/2+j-\beta}\nabla V\big), \quad j = 0,1$$

Chen model: $\beta = \frac{1}{2}$

$$J_0 = \mu^*\Big(\nabla n - \frac{n}{T}\nabla V\Big), \quad J_1 = \frac{3}{2}\mu^*\big(\nabla(nT) - n\nabla V\big), \quad \mu^* = \frac{\sqrt{\pi}}{2}\mu_0$$

Lyumkis model: $\beta = 0$

$$J_0 = \mu_0\Big(\nabla(nT^{1/2}) - \frac{n}{T^{1/2}}\nabla V\Big), \quad J_1 = 2\mu_0\big(\nabla(nT^{3/2}) - nT^{1/2}\nabla V\big)$$

Open problem: existence of solutions in general case

Numerical approximation: stationary equations

$$-\operatorname{div} J_0 = 0, \quad -\operatorname{div} J_1 + J_0 \cdot \nabla V = W(n,T)$$

$$J_0 = \mu^*\left(\nabla n - \frac{n}{T}\nabla V\right), \quad J_1 = \frac{3}{2}\mu^*\left(\nabla(nT) - n\nabla V\right)$$

Objective:

- Compute current densities J_i as function of applied voltage
- Precise and efficient numerical algorithm

Difficulties:

- Positivity of n and T? Lack of maximum principle
- Convection dominance due to high electric fields
- Standard finite elements give $n \in H^1 \Rightarrow J_0 \in L^2$ only

Solution:

- Construct positivity-preserving numerical scheme
- "Symmetrization" by exponential fitting: removes convection
- Mixed finite elements: higher regularity for J_j

Discretization of stationary equations

$$-\mathrm{div}\, J + cu = f, \quad J = \nabla u - \frac{u}{T}\nabla V$$

considered on triangulation of domain $\Omega = \cup_i K_i$

1. Exponential fitting:
   - Introduce local Slotboom variable $z = e^{-V/T}u$, $T = $ const. on each element K_i
   - Then $J = e^{V/T}\nabla z$ on K_i
2. Finite-element space:
   - $z_h \in H^1 \Rightarrow J_h \in L^2$ low current accuracy
   - Raviart-Thomas mixed finite elements (P_1 elements): $z_h \in L^2$ piecewise constant, $J_h \in H_{\mathrm{loc}}(\mathrm{div}) \rightarrow$ no M-matrix if $c > 0$
   - Marini-Pietra mixed finite elements (P_2 with 3 DOF): $z_h \in L^2$ piecewise constant, $J_h \in H_{\mathrm{loc}}(\mathrm{div}) \rightarrow$ yields M-matrix even if $c > 0$

Discretization of stationary equations

$$-\operatorname{div} J + cu = f, \quad J = \nabla u - \frac{u}{T}\nabla V$$

3. Hybridization and condensation:

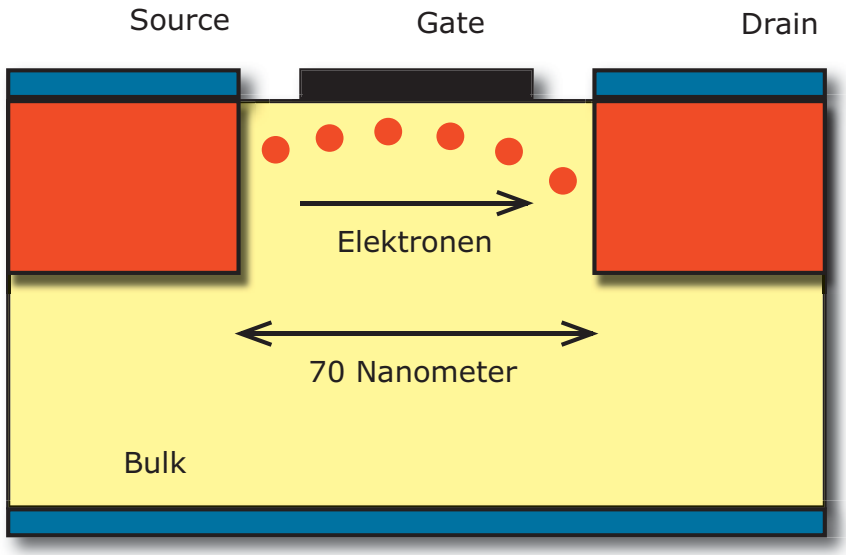
- Mixed finite-element scheme yields indefinite algebraic system $\longrightarrow$ hybridization
- Variables $J_h \in H_{\mathrm{loc}}(\mathrm{div})$, $u_h \in L^2$ und λ_h on surfaces
- Static condensation: reduce system for (J_h, z_h, λ_h)

$$\begin{pmatrix} A & \widetilde{B}^\top & -\widetilde{C}^\top \\ -B & D & 0 \\ C & 0 & 0 \end{pmatrix} \begin{pmatrix} J_h \\ z_h \\ \lambda_h \end{pmatrix} = \begin{pmatrix} 0 \\ f_h \\ 0 \end{pmatrix}$$

$\longrightarrow$ eliminate J_h, $z_h \Rightarrow M\lambda_h = g_h$, M is M-matrix
$\longrightarrow$ guarantees nonnegativity of λ_h (particle densities)

Simulation of field-effect transistors

MOSFET = Metal Oxide Semiconductor Field Effect Transistor
MESFET = Metal Semiconductor Field Effect Transistor



- Electron current from Source to Drain ($-$ to $+$)
- Current controlled by electric potential at Gate

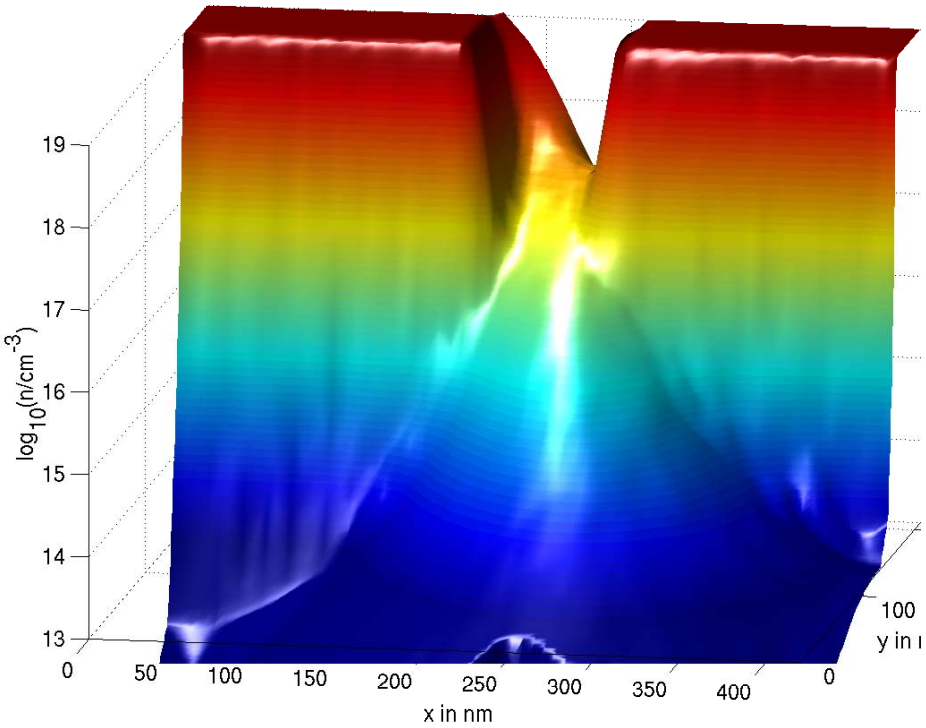
Iteration scheme:

- 2D: decoupling scheme (Gummel) and voltage continuation
- 3D: Newton scheme and adaptive voltage continuation

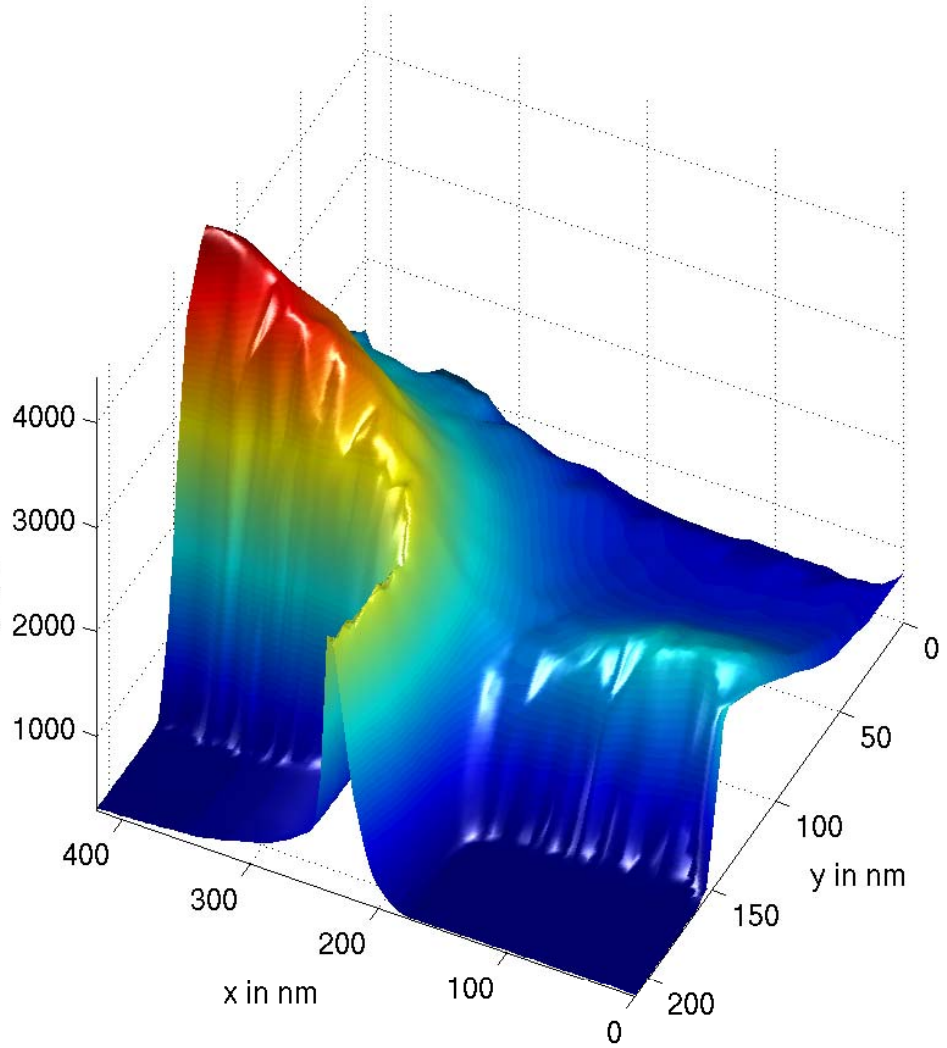
Simulation of 2D MOSFET

(Holst/A.J./Pietra 2003)

Electron density



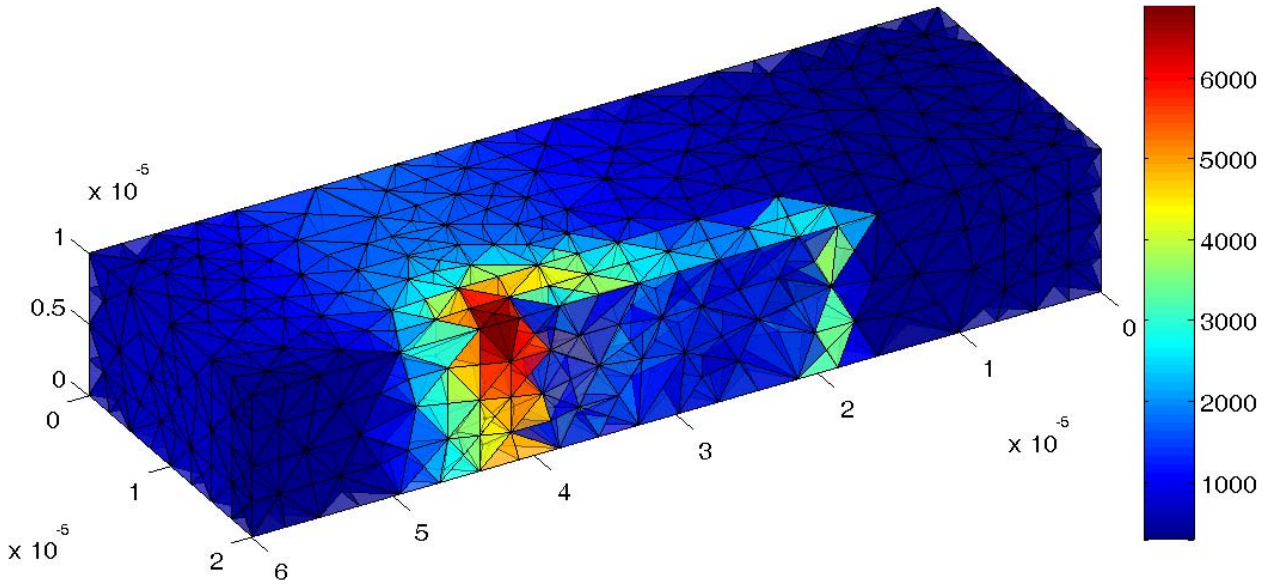
Temperature



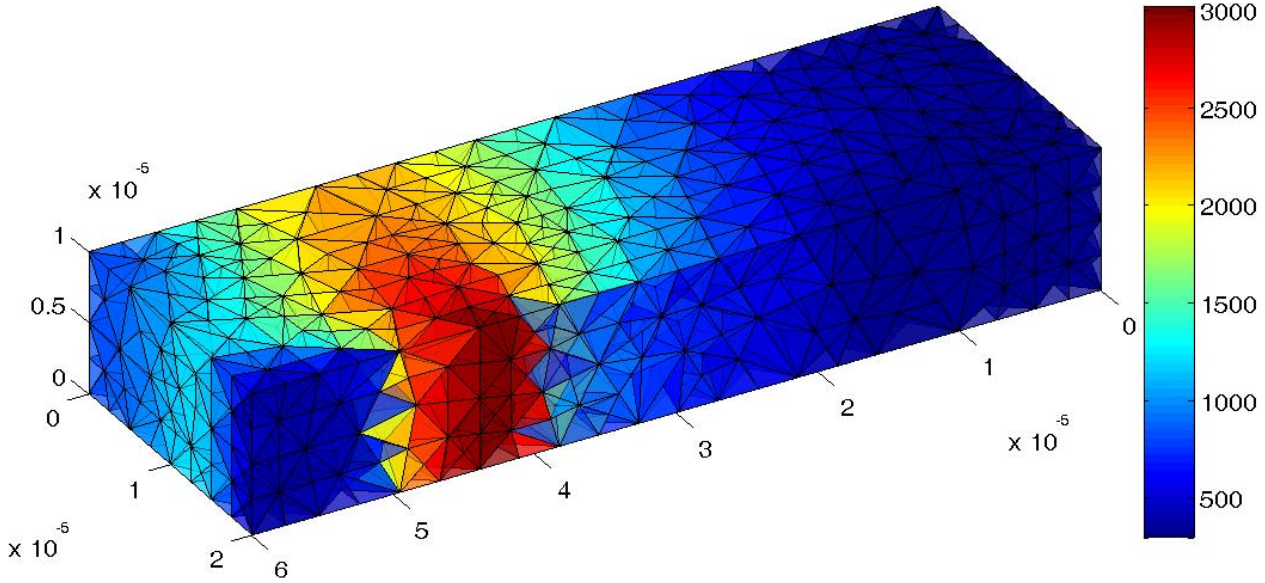
Simulation of 3D single-gate MESFET

(Gadau/A.J. 2008)

Off state

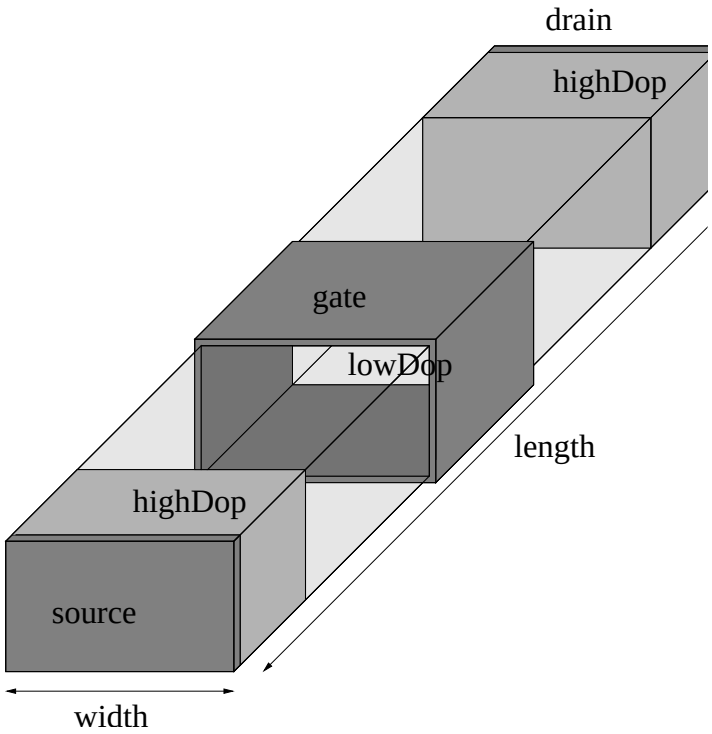


On state

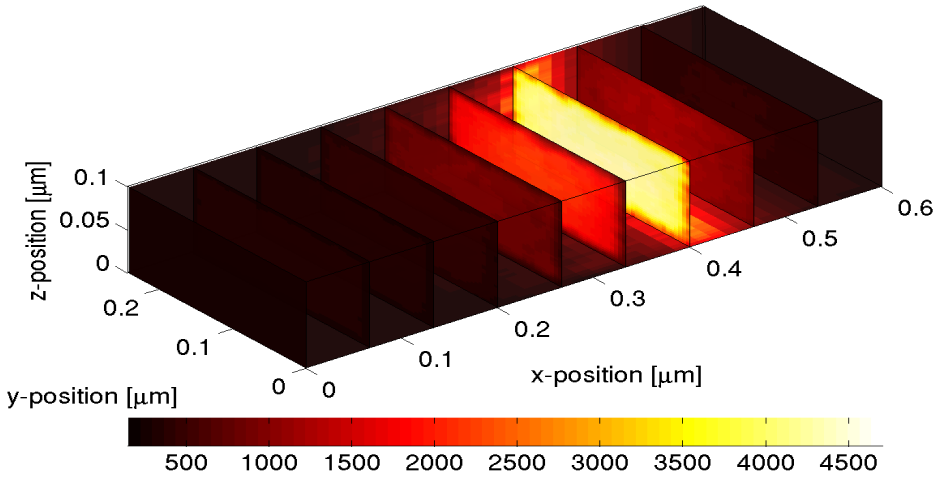


3D Gate-All-Around MESFET

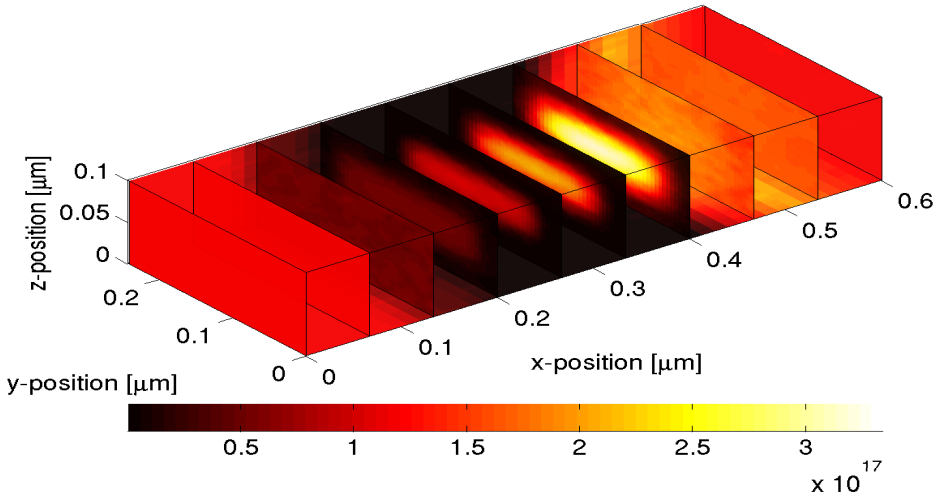
Geometry



Temperature

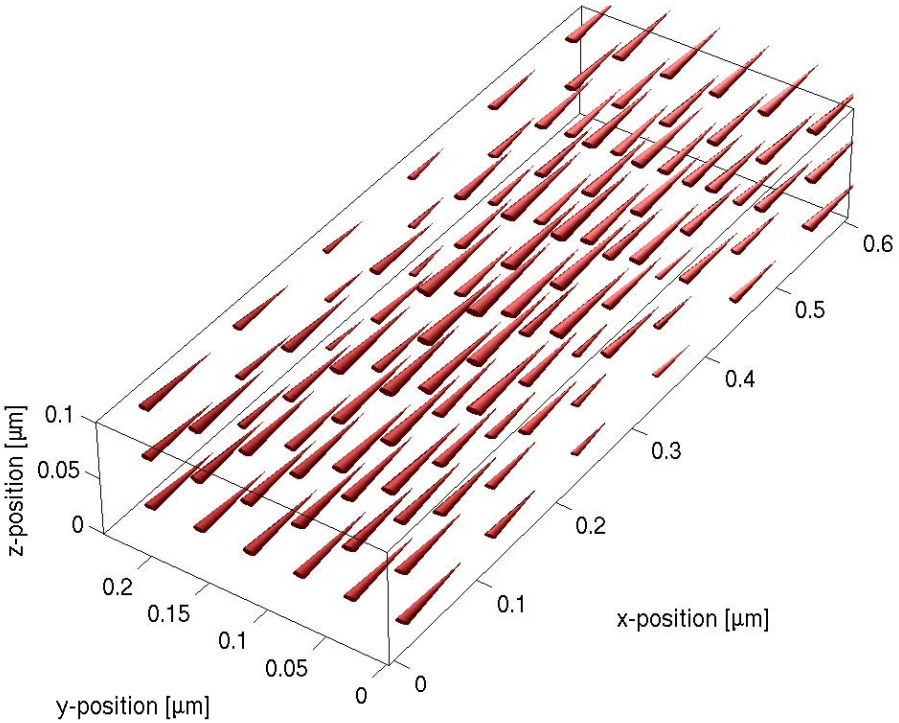


Thermal energy

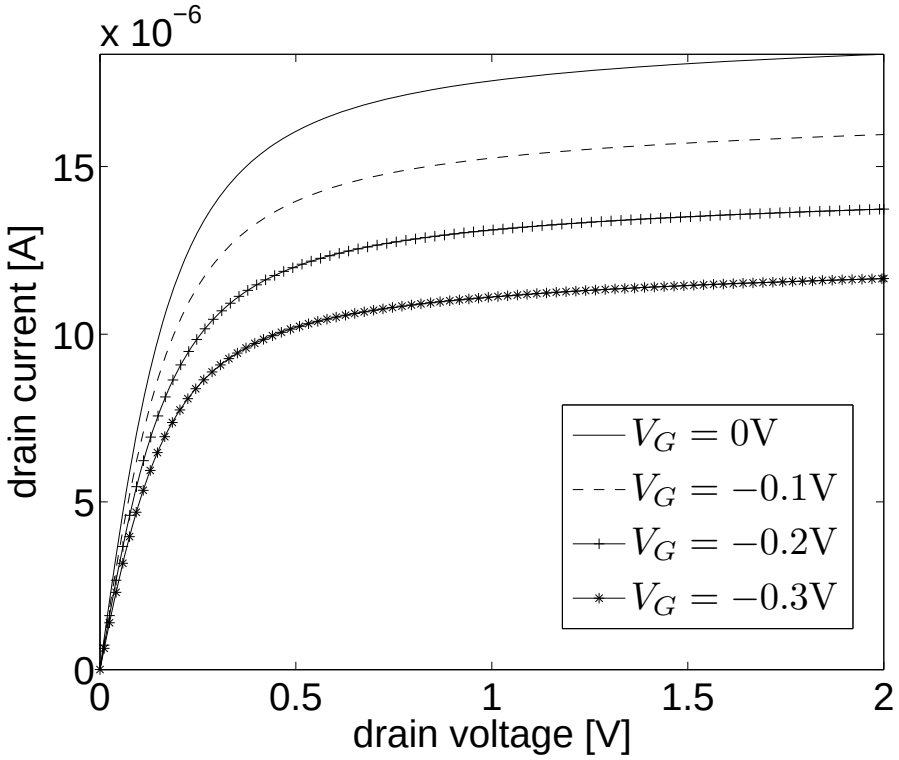


3D Gate-All-Around MESFET

Electron current density



Current-voltage characteristics



Summary

Energy-transport equations (Chen)

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(\tfrac{3}{2}nT) - \operatorname{div} J_1 + J_0 \cdot \nabla V = W(n,T)$$
$$J_0 = \mu^*\left(\nabla n - \frac{n}{T}\nabla V\right), \quad J_1 = \frac{3}{2}\mu^*\left(\nabla(nT) - n\nabla V\right)$$

- Energy-transport model for general energy bands formulated
- Primal entropy variables μ/T, $-1/T$ related to $n = NT^{3/2}e^{\mu/T}$ $\longrightarrow$ relation to nonequilibrium thermodynamics
- Dual entropy variables $(\mu - V)/T$, $-1/T$ allow to symmetrize the system
- Drift-diffusion variables $g_0 = D_{00}$, $g_1 = D_{10}$ allow for efficient numerical discretization
- Mixed finite-element simulations of 2D and 3D transistors

Overview

1. Semiconductor modeling
   - Basics of semiconductor physics
   - Kinetic models
2. Semi-classical macroscopic models
   - General strategy
   - Drift-diffusion models
   - Energy-transport models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Quantum kinetic models
   - Quantum Maxwellians
   - Quantum drift-diffusion models
   - Quantum hydrodynamic models
4. New and future devices
5. Summary

Assumptions

Boltzmann equation in hydrodynamic scaling:

$$\alpha\partial_t f + \alpha\big(v(k)\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f\big) = Q_0(f) + \alpha Q_1(f)$$

Assumptions:

- Parabolic band approximation: $E(k) = \frac{1}{2}|k|^2$, $k\in\mathbb{R}^3$
- Weight functions: $\kappa(k) = (1, k, \frac{1}{2}|k|^2)$
- Conservation property: $\langle\kappa_i Q_0(f)\rangle = 0$, $i = 0,1,2$
- Kernel of Q_0 spanned by Maxwellians
  $f = M[f] = M = \exp(\lambda_0 + k\cdot\lambda_1 + \frac{1}{2}|k|^2\lambda_2)$
- Mass conservation: $\langle Q_1(f)\rangle = 0$

Maxwellians: electron density n, temperature T, mean velocity u

$$n = \langle M\rangle,\ \lambda_2 = -\frac{1}{T},\ \lambda_1 = \frac{u}{T} \quad\Rightarrow\quad M(k) = \frac{1}{2}\left(\frac{2\pi}{T}\right)^{3/2} n e^{-|u-k|^2/2T}$$

Derivation

$$\alpha\partial_t f_\alpha + \alpha\big(k\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_k f_\alpha\big) = Q_0(f_\alpha) + \alpha Q_1(f_\alpha)$$

Moment equations:

$$\partial_t\langle\kappa_i f_\alpha\rangle + \mathrm{div}_x\langle k\kappa_i f_\alpha\rangle - \nabla_x V\cdot\langle\nabla_k\kappa_i f_\alpha\rangle = \alpha^{-1}\underbrace{\langle\kappa_i Q_0(f)\rangle}_{=0} + \langle\kappa_i Q_1(f)\rangle$$

Step 1: limit $\alpha\to 0$ in Boltzmann equation

$$Q_0(f)=0, \quad \text{where } f=\lim_{\alpha\to 0} f_\alpha \quad\Rightarrow\quad f = M \text{ for some } n,u,T$$

Step 2: limit $\alpha\to 0$ in moment equations

$$\partial_t\langle\kappa_i M\rangle + \mathrm{div}_x\langle k\kappa_i M\rangle - \nabla_x V\cdot\langle\nabla_k\kappa_i M\rangle = \langle\kappa_i Q_1(M)\rangle$$

$\to$ compute moments of M

Derivation

Lemma

$$\langle kM\rangle = nu, \quad \langle k\otimes kM\rangle = n(u\otimes u)+nT\,\mathrm{Id}, \quad \langle \tfrac{1}{2}k|k|^2M\rangle = \tfrac{1}{2}nu(|u|^2+5T).$$

Hydrodynamic equations:

$$\partial_t n - \operatorname{div} J_n = 0, \quad \lambda_D^2\Delta V = n - C(x)$$
$$\partial_t J_n - \operatorname{div}\left(\frac{J_n\otimes J_n}{n}\right) - \nabla(nT) + n\nabla V = -\langle kQ_1(M)\rangle$$
$$\partial_t(ne) - \operatorname{div}\big(J_n(e+T)\big) + J_n\cdot\nabla V = \langle \tfrac{1}{2}|k|^2Q_1(M)\rangle$$

where energy density $ne = \frac{1}{2}n|u|^2 + \frac{3}{2}nT$

Relaxation-time model for Q_1: constant scattering rate $\sigma = 1/\tau$

$$\langle kQ_1(M)\rangle = \frac{J_n}{\tau}, \quad \langle \tfrac{1}{2}|k|^2Q_1(M)\rangle = -\frac{1}{\tau}\left(ne - \frac{3}{2}n\right)$$

Remarks

Hydrodynamic model

$$\partial_t n - \operatorname{div} J_n = 0, \quad \lambda_D^2 \Delta V = n - C(x)$$
$$\partial_t J_n - \operatorname{div}\left(\frac{J_n \otimes J_n}{n}\right) - \nabla(nT) + n\nabla V = -\frac{J_n}{\tau}$$
$$\partial_t(ne) - \operatorname{div}\left(J_n(e+T)\right) + J_n \cdot \nabla V = -\frac{1}{\tau}\left(ne - \frac{3}{2}n\right)$$

- First derivations: Bløtekjær 1970, Baccarani/Wordeman 1985
- Heat flux: Bløtekjær defines $q = -\kappa^* \nabla T$, Anile/Romano 2000 define

$$q = -\frac{5}{2}T\nabla T + \frac{5}{2}nTu\left(\frac{1}{\tau_p} - \frac{1}{\tau_e}\right)\tau_e,$$

  where τ_p: momentum relaxation time, τ_e: energy relaxation time
- No external forces, homogeneous case: $J_n(t) \to 0$, $(ne)(t) - \frac{3}{2}e \to 0$ as $t \to \infty$

Remarks

Euler equations of gas dynamics: no electric field, no scattering

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t J_n - \operatorname{div}\left(\frac{J_n \otimes J_n}{n}\right) - \nabla(nT) = 0$$
$$\partial_t(ne) - \operatorname{div}\big(J_n(e+T)\big) = 0$$

- Rigorous derivation from Boltzmann equation: Caflisch 1980, Lachowicz 1987, Nishida 1987, Ukai/Asano 1983
- Hyperbolic conservation laws: shock waves possible
- Numerical discretization (also for semiconductor model): Anile, Jerome, Osher, Russo etc. (since 1990s)

Relations between the macroscopic models

Rescaled hydrodynamic equations:

$$\partial_t n - \operatorname{div} J_n = 0, \quad \alpha\partial_t J_n - \alpha\operatorname{div}\left(\frac{J_n \otimes J_n}{n}\right) - \nabla(nT) + n\nabla V = -J_n$$

$$\partial_t(ne) - \operatorname{div}\left(J_n(e+T)\right) + \nabla V \cdot J_n - \operatorname{div}\left(\kappa\nabla T\right) = -\frac{n}{\beta}\left(e - \frac{3}{2}\right)$$

$$e = \beta\frac{|J_n|^2}{2n^2} + \frac{3}{2}T, \quad \kappa = \kappa_0 nT$$

where $\alpha = \tau_p/\tau$, $\beta = \tau_e/\tau$ (τ: reference time)

- $\alpha \to 0$ and $\beta \to 0$: drift-diffusion equations

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla(nT) - n\nabla V, \quad e = \frac{3}{2} \;\Rightarrow\; T = 1$$

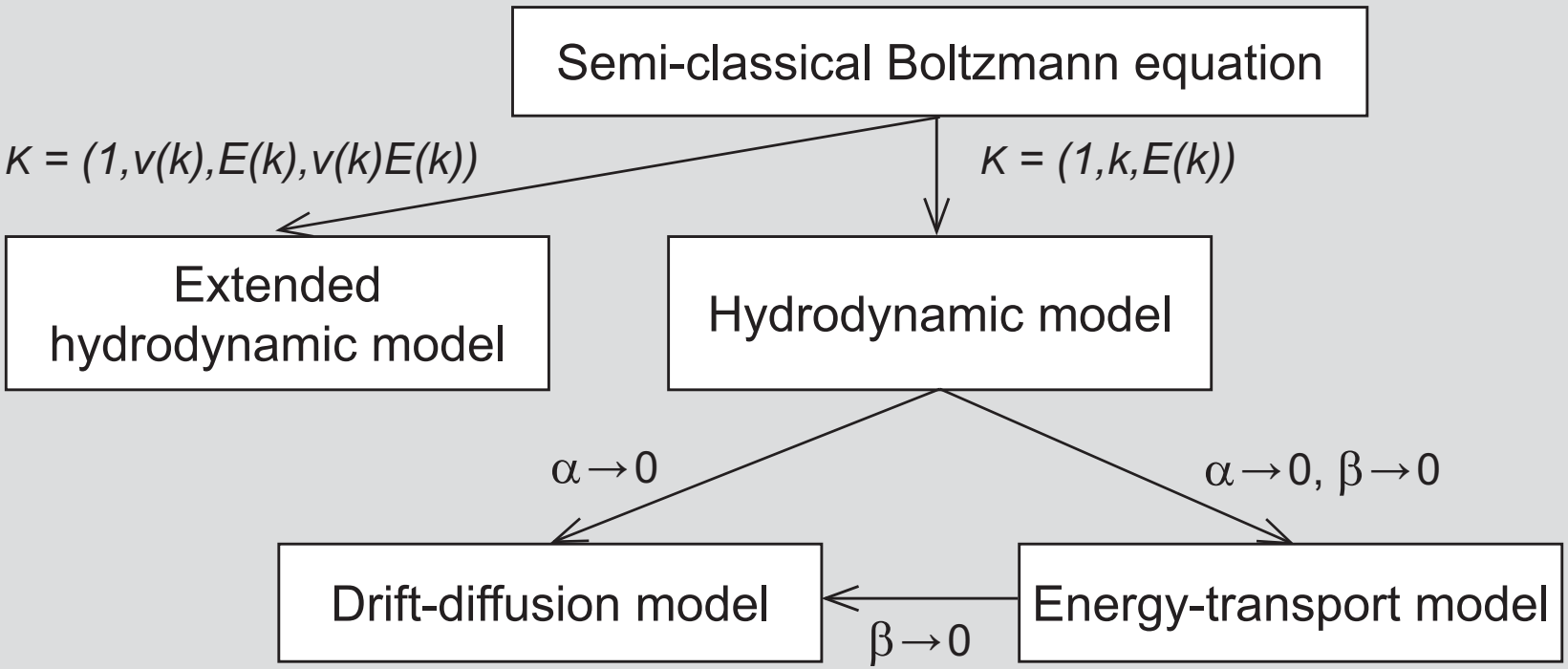
- $\alpha \to 0$: energy-transport equations

$$\partial_t\left(\tfrac{3}{2}nT\right) - \operatorname{div}\left(\tfrac{5}{2}J_n T + \kappa\nabla T\right) + J_n \cdot \nabla V = -\frac{3}{2}\frac{n}{\beta}(T-1)$$

- $\beta \to 0$ in energy-transport model: drift-diffusion equations

Relations between the macroscopic models

Hydrodynamic models and relaxation-time limits



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Quantum mechanics

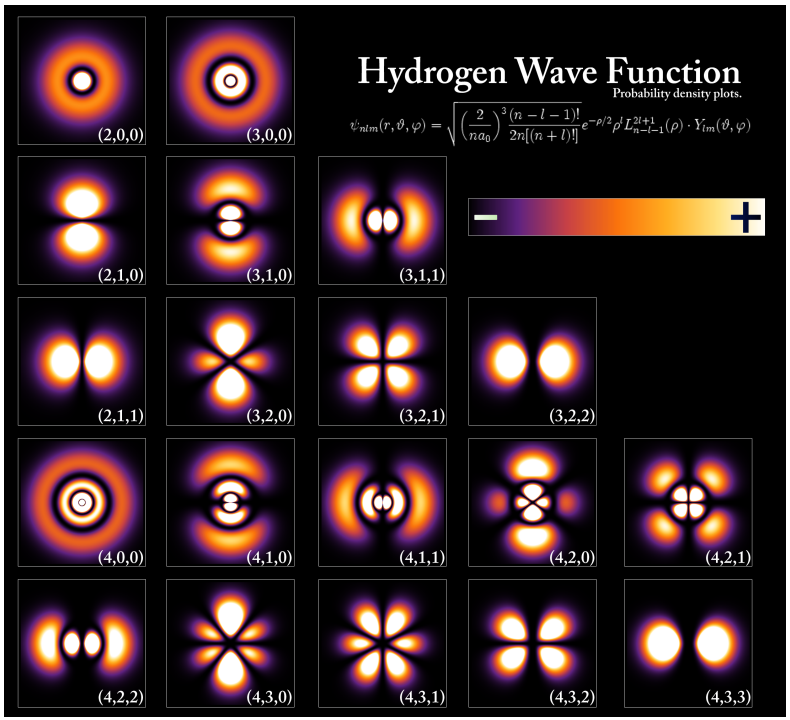
Pure state:

Can be described by a wave function ψ solving the Schrödinger equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi - V(x,t)\psi \quad \text{in } \mathbb{R}^3$$

Mixed state:

- Statistical ensemble of pure states
- Cannot be described by wave function but by density matrix operator $\widehat{\rho}$
- Countable mixed state given by $\widehat{\rho} = \sum_k p_k \psi_k \psi_k^* = \sum_k p_k |\psi_k\rangle\langle\psi_k|$



Source: Wikipedia

Liouville–von Neumann equation

Question: Which evolution equation satisfies $\widehat{\rho}$?

Answer: Liouville–von Neumann equation

Motivation:

- Write Schrödinger equation as $i\hbar\partial_t\psi = H_x\psi$ with $H_x = -(\hbar^2/2m)\Delta_x - V(x)$
- There exists density matrix $\rho(x,y,t)$ such that

$$(\widehat{\rho}\psi)(x,t) = \int_{\mathbb{R}^3} \rho(x,y,t)\psi(y,t)dy$$

- Pure state: $\rho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}$
- Evolution equation for $\rho(x,y,t)$:

$$\begin{aligned} i\hbar\partial_t\rho &= i\hbar\big(\partial_t\psi(x,t)\overline{\psi(y,t)} + \psi(x,t)\overline{\partial_t\psi(y,t)}\big) \\ &= H_x\psi(x,t)\overline{\psi(y,t)} - \psi(x,t)H_y\overline{\psi(y,t)} = H_x\rho - H_y\rho =: [H,\rho] \end{aligned}$$

- Motivates Liouville-von Neumann "matrix" equation:

$$i\hbar\rho = [H,\rho]$$

Liouville–von Neumann equation

- Evolution equation for density matrix operator $\widehat{\rho}$:

$$i\hbar\partial_t\widehat{\rho} = [H, \widehat{\rho}], \quad t > 0, \quad \widehat{\rho}(0) = \widehat{\rho}_I$$

- Commutator $[H, \widehat{\rho}] = H\widehat{\rho} - \widehat{\rho}H$
- Formal solution: $\widehat{\rho}(t) = e^{-iHt/\hbar}\widehat{\rho}_I e^{iHt/\hbar}$ (if H time-independent)
- $\widehat{\rho}$ is self-adjoint compact operator
- Density matrix $\rho(x, y, t)$ satisfies

$$(\widehat{\rho}\psi)(x, t) = \int_{\mathbb{R}^3} \rho(x, y, t)\psi(y, t)dy$$

- Particle density: $n(x, t) = 2\rho(x, x, t) \geq 0$
- Particle current density: $J(x, t) = \frac{i\hbar q}{m}(\nabla_r - \nabla_q)\rho(r, q, t)|_{r=q=x}$

Relation between density matrix and Schrödinger equation

- $\widehat{\rho}$: solution of Liouville-von Neumann equation
- (ψ_j, λ_j): eigenfunction-eigenvalue pairs of $\widehat{\rho}$
- ψ_j^0: eigenfunctions of initial datum $\widehat{\rho}_I$

Theorem (Mixed-state Schrödinger equation)

Eigenfunction ψ_j solves

$$i\hbar\partial_t\psi_j = H\psi_j, \quad t > 0, \quad \psi_j(\cdot, 0) = \psi_j^0$$

and particle density can be written as

$$n(x,t) = \sum_{j=1}^{\infty} \lambda_j |\psi_j(x,t)|^2$$

Conversely, let (ψ_j, λ_j) be solutions to the Schrödinger equation. Then

$$\rho(x,y,t) = \sum_{j=1}^{\infty} \lambda_j \psi_j(x,t)\overline{\psi_j(y,t)}$$

solves Liouville-von Neumann equation.

Mixed states and single state

Mixed state:

- Sequence of solutions ψ_j to

$$i\hbar\partial_t\psi_j = H\psi_j, \quad t > 0, \quad \psi_j(\cdot, 0) = \psi_j^0$$

- Sequence of numbers λ_j: gives particle density

$$n(x,t) = \sum_{j=1}^{\infty} \lambda_j |\psi_j(x,t)|^2$$

Pure state:

- If $\rho_I(x,y) = \psi_I(x)\overline{\psi_I(y)}$ then $\rho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}$, where

$$i\hbar\partial_t\psi = H\psi, \quad t > 0, \quad \psi(\cdot, 0) = \psi_I$$

- Particle density: $n(x,t) = 2\rho(x,x,t) = 2|\psi(x,t)|^2$
- Current density: $J = -(\hbar q/m)\mathrm{Im}(\overline{\psi}\nabla_x\psi)$

Quantum kinetic formulation

Question: Does there exist a kinetic formulation for quantum systems?
Answer: Yes, Wigner formalism
Reminder: Semi-classical Vlasov equation

$$\partial_t f + \frac{\hbar k}{m} \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = 0, \quad x \in \mathbb{R}^3, \ k \in \mathbb{R}^3$$

- Pseudo-wave vector: $k \in \mathbb{R}^3$
- Parabolic band structure: $E(k) = \hbar^2 |k|^2 / 2m$, $v(k) = \hbar k / m$
- Electric potential V computed from Poisson equation

$$\varepsilon_s \Delta V = q(n - C(x)), \quad C(x): \text{ doping profile}$$

- Electron density:

$$n(x,t) = \int_{\mathbb{R}^3} f(x,k,t) \frac{dk}{4\pi^3} \geq 0$$

Formulate equation in terms of crystal momentum $p = \hbar k$

Quantum kinetic formulation

Question: Does there exist a kinetic formulation for quantum systems?
Answer: Yes, Wigner formalism
Reminder: semi-classical Vlasov equation

$$\partial_t f + \frac{p}{m}\cdot\nabla_x f + q\nabla_x V\cdot\nabla_p f = 0, \quad x\in\mathbb{R}^3,\ p\in\mathbb{R}^3$$

- Crystal momentum: $p=\hbar k\in\mathbb{R}^3$
- Parabolic band structure: $E(k)=\hbar^2|k|^2/2m$, $v(k)=\hbar k/m = p/m$
- Electric potential V computed from Poisson equation

$$\varepsilon_s\Delta V = q(n-C(x)), \quad C(x):\ \text{doping profile}$$

- Electron density:

$$n(x,t)=\int_{\mathbb{R}^3} f(x,p,t)\frac{dp}{4(\hbar\pi)^3}\geq 0$$

Objective: formulate quantum kinetic equation

Wigner transform

- Liouville-von Neumann "matrix" equation:

$$i\hbar\partial_t\rho(r,s,t) = (H_r - H_s)\rho(r,s,t), \quad \rho(r,s,0) = \rho_I(r,s)$$

- Fourier transform and its inverse:

$$(\mathcal{F}(f))(p) = \int_{\mathbb{R}^3} f(y)e^{-iy\cdot p/\hbar}dy$$

$$(\mathcal{F}^{-1}(g))(y) = (2\pi\hbar)^{-3}\int_{\mathbb{R}^3} g(p)e^{iy\cdot p/\hbar}dp$$

- Wigner transform (Wigner 1932):

$$W[\rho](x,p,t) = (\mathcal{F}(u))(x,p,t), \quad u(x,y,t) = \rho\left(x+\frac{y}{2}, x-\frac{y}{2}, t\right)$$

- Wigner-Weyl transform = inverse of Wigner transform

Wigner equation

Proposition (Quantum Vlasov or Wigner equation)

Let ρ be solution to Liouville-von Neumann equation. Then $W[\rho]$ solves

$$\partial_t w + \frac{p}{m^*}\cdot\nabla_x w + q\theta[V]w = 0, \quad t>0, \quad w(x,p,0) = w_I(x,p),$$

where

$$w_I(x,p) = \int_{\mathbb{R}^3} \rho_I\left(x+\frac{y}{2}, x-\frac{y}{2}, t\right) e^{-iy\cdot p/\hbar} dy$$

Proof: write Liouville eq. in (x,y) variables, apply Fourier transform

- Pseudo-differential operator $\theta[V]$:

$$(\theta[V]w)(x,p,t) = (2\pi\hbar)^{-3}\int_{\mathbb{R}^6} \delta V(x,y,t) w(x,p',t) e^{iy\cdot(p-p')/\hbar} dp'\, dy$$

- Symbol of $\theta[V]$:

$$\delta V(x,y,t) = \frac{i}{\hbar}\left(V\left(x+\frac{y}{2},t\right) - V\left(x-\frac{y}{2},t\right)\right)$$

Potential operator

$$(\theta[V]w)(x,p,t) = (2\pi\hbar)^{-3}\int_{\mathbb{R}^3} \delta V(x,y,t) w(x,p',t) e^{iy\cdot(p-p')/\hbar} dp'\,dy$$

$$\delta V(x,y,t) = \frac{i}{\hbar}\left(V\left(x+\frac{y}{2},t\right) - V\left(x-\frac{y}{2},t\right)\right)$$

- Symbol δV = discrete directional derivative:

$$\delta V(x,\hbar y,t) \to i\nabla_x V(x,t)\cdot y \quad \text{as } \text{“}\hbar\to 0''$$

- Relation to classical Liouville equation: $\theta[|x|^2/2] = x\cdot\nabla_p w$

$$\partial_t w + \frac{p}{m^*}\cdot\nabla_x w + q\nabla_x\left(\frac{|x|^2}{2}\right)\cdot\nabla_p w = 0$$

Relation between Wigner and Schrödinger equation

- Given density matrix operator $\widehat{\rho}$ with eigenfunction-eigenvalue pairs (ψ_j, λ_j)
- Define the Wigner function

$$w(x,p,t) = (2\pi)^{-3} \sum_{j=1}^{\infty} \lambda_j \int_{\mathbb{R}^3} \psi_j\left(x + \frac{\hbar\eta}{2m}\right) \overline{\psi_j}\left(x - \frac{\hbar\eta}{2m}\right) e^{-ip\cdot\eta} d\eta$$

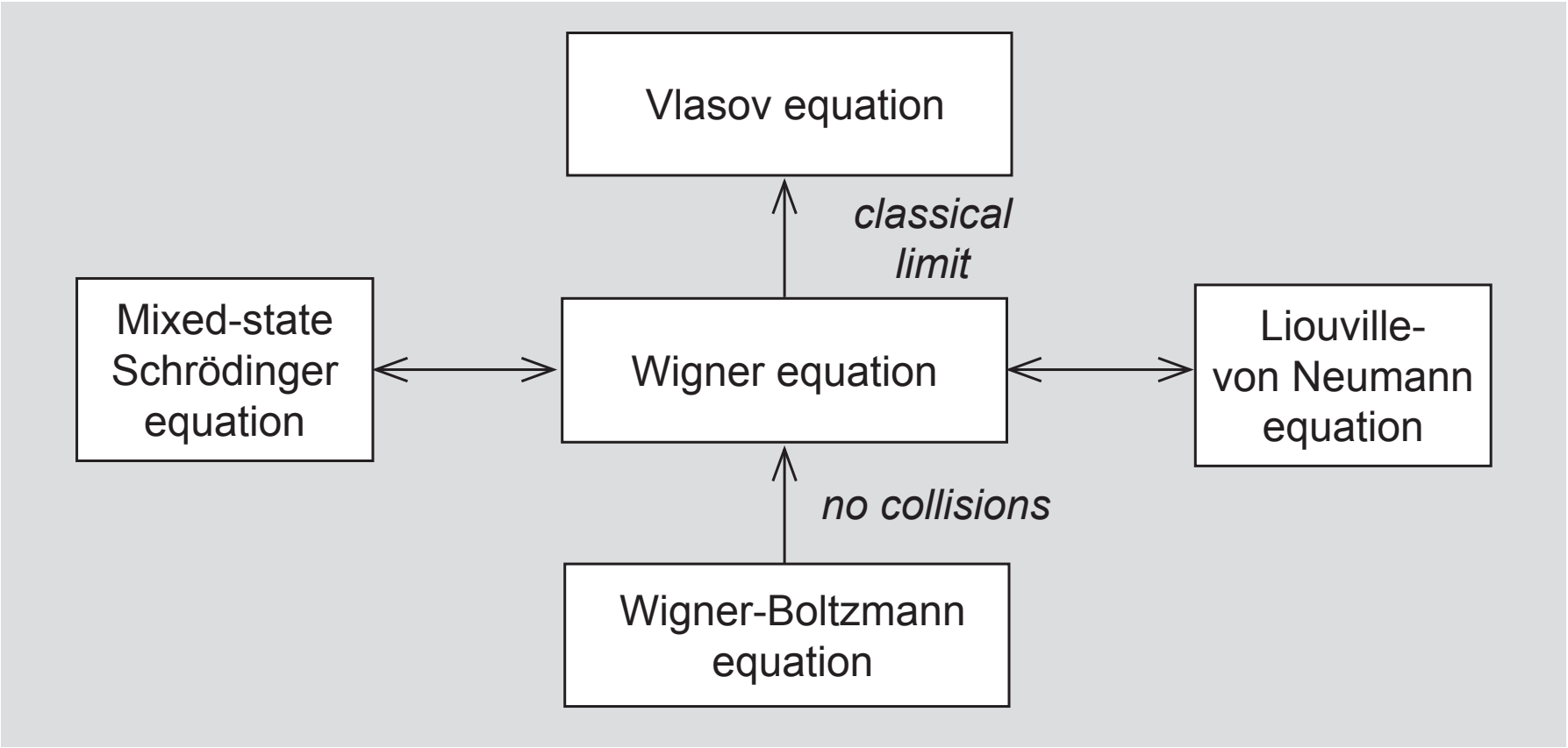
- Then w solves the Wigner equation

$$\partial_t w + \frac{p}{m} \cdot \nabla_x w + q\theta[V]w = 0$$

- Quantum mechanical formulations:
  Schrödinger – density matrix – Wigner

Summary

Relation between density matrix – Schrödinger – Wigner formulation



Wigner equation: scaling

$$\partial_t w + \frac{p}{m^*} \cdot \nabla_x w + q\theta[V]w = 0, \quad t > 0, \quad w(x,p,0) = w_I(x,p)$$

- Reference length λ, reference time τ, reference momentum $m^*\lambda/\tau$, reference voltage $k_B T_L/q$
- Assumption: wave energy $\ll$ thermal/kinetic energies

$$\frac{\hbar/\tau}{k_B T_L} = \frac{\hbar/\tau}{m(\lambda/\tau)^2} = \varepsilon \ll 1$$

- Scaled Wigner equation:

$$\partial_t w + p \cdot \nabla_x w + \theta[V]w = 0$$

$$(\theta[V]w)(x,p,t) = (2\pi)^{-3} \int_{\mathbb{R}^3} \delta V(x,\eta,t) w(x,p',t) e^{i\eta\cdot(p-p')} dp'\, d\eta$$

$$\delta V(x,\eta,t) = \frac{i}{\varepsilon}\left(V\left(x + \frac{\varepsilon}{2}\eta, t\right) - V\left(x - \frac{\varepsilon}{2}\eta, t\right)\right)$$

Wigner equation: semi-classical limit

$$\partial_t w + p\cdot\nabla_x w + \theta_\varepsilon[V]w = 0$$

$$(\theta_\varepsilon[V]w)(x,p,t) = (2\pi)^{-3}\int_{\mathbb{R}^3} \delta V(x,\eta,t) w(x,p',t) e^{i\eta\cdot(p-p')}dp'\,d\eta$$

$$\delta V(x,\eta,t) = \frac{i}{\varepsilon}\left(V\left(x+\frac{\varepsilon}{2}\eta,t\right) - V\left(x-\frac{\varepsilon}{2}\eta,t\right)\right)$$

- Recall that $\delta V(x,\eta,t) \to i\nabla_x V(x,t)\cdot\eta$ as $\varepsilon\to 0$
- Limit in potential operator: $\theta_\varepsilon[V]w \to \nabla_x V\cdot\nabla_p w$ as $\varepsilon\to 0$
- Classical limit of Wigner equation = Vlasov equation

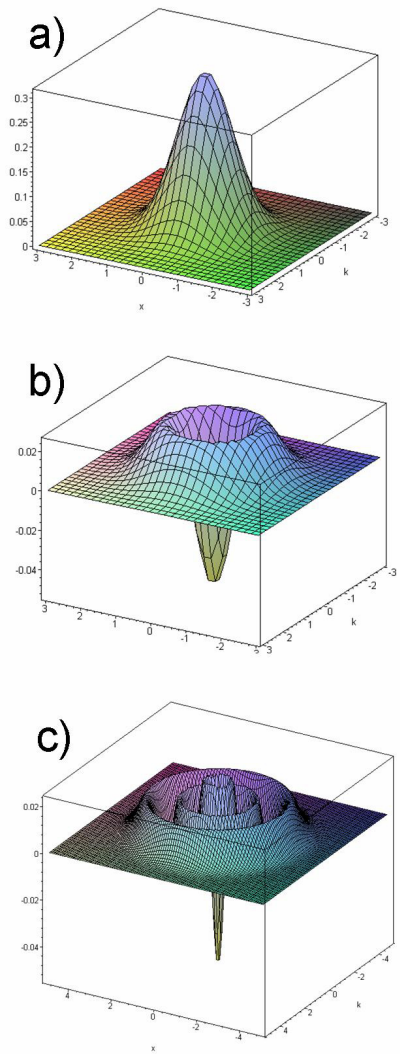
$$\partial_t w + p\cdot\nabla_x w + \nabla_x V\cdot\nabla_p w = 0$$

Wigner equation: nonnegativity of Wigner function

- Solution of Liouville equation preserves nonnegativity
- This is not true for Wigner equation
- But it holds $n(x,t) = \int w(x,p,t)dp/(4\pi^3) \geq 0$
- Hudson 1974:

$$w(x,p,t) = \int_{\mathbb{R}^3} \psi(x+\tfrac{\varepsilon y}{2},t)\overline{\psi}(x+\tfrac{\varepsilon y}{2},t)e^{-iy\cdot p}dy$$

nonnegative if and only if
$\psi = \exp(-x^\top A(t)x - a(t)\cdot x - b(t))$



Source: Wikipedia

Semi-classical Wigner equation

Objective: Wigner equation for general energy bands $E(k)$, $k \in B$

- Wigner function on lattice L:

$$w(x,k,t) = \sum_{y\in L} \rho\Big(x+\frac{y}{2}, x-\frac{y}{2}, t\Big) e^{-iy\cdot k}$$

- Arnold et al. 1989: α, β, γ parameter

$$\partial_t w + \frac{i}{\alpha}\Big[\beta E\Big(k+\frac{\alpha}{2i}\nabla_x\Big) - \beta E\Big(k-\frac{\alpha}{2i}\nabla_x\Big) + \gamma V\Big(x+\frac{\alpha}{2i}\nabla_k\Big) - \gamma V\Big(x-\frac{\alpha}{2i}\nabla_k\Big)\Big] w = 0,$$

  where $E(\cdots)$, $V(\cdots)$ are pseudo-differential operators
- α = ratio of characteristic wave vector and device length
- Simplification: let $\alpha \to 0$ in lattice $L = \alpha L_0$, $L_0 = O(1)$, but not in potential operator (to maintain quantum effects)

$$\partial_t w + \beta \nabla_k E(k) \cdot \nabla_x w + \theta[V] w = 0$$

- Reference: Ringhofer 1997

Wigner-Boltzmann equation

$$\partial_t w + p \cdot \nabla_x w + \theta[V]w = Q(w)$$

Caldeira-Leggett model:

$$Q(w) = D_{pp}\Delta_p w + 2\gamma \mathrm{div}_p(pw)$$

- Problem: Does not satisfy Lindblad condition which is generic to preserve complete positivity of density matrix
- Caldeira-Leggett model quantum mechanically not correct

Quantum Fokker-Planck model:

$$Q(w) = \underbrace{D_{pp}\Delta_p w}_{\text{class. diff.}} + \underbrace{2\gamma \mathrm{div}_p(pw)}_{\text{friction}} + \underbrace{D_{qq}\Delta_x w + 2D_{pq}\mathrm{div}_x(\nabla_p w)}_{\text{quantum diffusion}}$$

- Satisfies Lindblad condition $D_{pp}D_{qq} - D_{pq}^2 \geq \gamma^2/4$ (diffusion dominates friction) $\Rightarrow$ Preservation of positivity of density matrix
- Analysis of Wigner-Fokker-Planck models: Arnold et al. 2002-2008

Wigner-Boltzmann equation

BGK (Bhatnagar-Gross-Krook) model:

$$Q(w) = \frac{1}{\tau}\left(\frac{n}{n_0}w_0 - w\right)$$

- Particle densities:

$$n(x,t) = \frac{2}{(2\pi\hbar)^3}\int_{\mathbb{R}^3} w(x,p,t)dp,\ n_0(x,t) = \frac{2}{(2\pi\hbar)^3}\int_{\mathbb{R}^3} w_0(x,p,t)dp$$

- w_0 = Wigner function of quantum thermal equilibrium, defined by

$$\rho_{\mathrm{eq}}(r,s) = \sum_j f(E_j)\psi_j(r)\overline{\psi_j(s)}, \quad \psi_j \text{ Schrödinger eigenfunctions}$$

- Used in tunneling diode simulations (Frensley 1987, Kluksdahl et al. 1989)

Other models:

- Semi-classical Boltzmann operator $\rightarrow$ quantum mech. not correct
- Degond/Ringhofer 2003: derived collision operator which conserves set of moments and dissipates quantum entropy $\rightarrow$ highly nonlocal

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Classical Maxwellian

Classical thermal equilibrium:

$$M(p) = n \exp\left(-\frac{|p-u|^2}{2T}\right)$$

Derived from maximization of kinetic entropy

$$S(f) = -\int_{\mathbb{R}^3}\int_B f(\log f - 1 + E(p))dxdp$$

under the constraints of given moments m_i:

$$\int_B \kappa_i(p) f \frac{dp}{4\pi^3} = m_i, \quad \kappa(p) = (1, p, |p|^2/2)$$

Quantum thermal equilibrium: maximize quantum entropy

Quantum exponential/logarithm: (Degond/Ringhofer 2001)

$$\mathrm{Exp}(f) = W(\exp W^{-1}(f)), \quad \mathrm{Log}(f) = W(\log W^{-1}(f))$$

Properties: $\frac{d}{dw}\mathrm{Log}\, w = 1/w$, $\frac{d}{dw}\mathrm{Exp}\, w = \mathrm{Exp}\, w$

Quantum Maxwellian

- Relative quantum entropy:

$$S(w) = -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} w\left(\operatorname{Log} w - 1 + \frac{|p|^2}{2} - V\right)dx\,dp$$

- Weight functions $\kappa(p) = (\kappa_0(p), \ldots, \kappa_N(p))$ given with $\kappa_0(p) = 1$, $\kappa_2(p) = \frac{1}{2}|p|^2$
- Moments of $w(x, p, t)$:

$$m_j(x,t) = \langle w(x,p,t)\kappa_j(p)\rangle = \frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} w(x,p,t)\kappa_j(p)dp$$

- Constrained maximization problem: given w, solve

$$\max\{S(f) : \langle f(x,p,t)\kappa(p)\rangle = \langle w(x,p,t)\kappa(p)\rangle \text{ for all } x,t\}$$

Formal solution:

$$M[w] = \operatorname{Exp}(\lambda\cdot\kappa), \quad \lambda = \text{Lagrange multiplier}$$

Quantum Maxwellian

- Define, for given w, electron density n, mean velocity u, energy density ne,

$$\begin{pmatrix} n \\ nu \\ ne \end{pmatrix}(x,t) = \frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3} w(x,p,t)\begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix} dp$$

- One moment (n) prescribed:

$$M_1[w](x,p,t) = \mathrm{Exp}\Big(A(x,t) - \frac{|p|^2}{2}\Big),$$

- Two moments (n, ne) prescribed:

$$M_2[w] = \mathrm{Exp}\Big(A(x,t) - \frac{|p|^2}{2T(x,t)}\Big),$$

- Three moments (n, nu, ne) prescribed:

$$M_3[w] = \mathrm{Exp}\Big(A(x,t) - \frac{|p-v(x,t)|^2}{2T(x,t)}\Big),$$

Quantum Maxwellian

Expansion of quantum Maxwellian in powers of ε^2:

$$M_1[w] = \mathrm{Exp}\left(A(x,t) - \frac{|p|^2}{2}\right) = \exp\left(A(x,t) - \frac{|p|^2}{2}\right)$$
$$\times\left[1 + \frac{\varepsilon^2}{8}\left(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Ap\right)\right] + O(\varepsilon^4)$$

$$M_2[w] = \mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right) = \exp\left(A - \frac{|p|^2}{2T}\right)$$
$$\times\left[1 + \frac{\varepsilon^2}{8T}\left(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Ap\right.\right.$$
$$+ \frac{|p|^2}{2}\Delta\beta + T(p\cdot\nabla\beta)^2 + \frac{|p|^2}{3T}p^\top(\nabla\otimes\nabla)\beta p$$
$$+ \frac{2}{3}(p\cdot\nabla\beta)(p\cdot\nabla A) - \frac{|p|^2}{3}(p\cdot\nabla\beta)^2 - \frac{|p|^2}{3}\nabla A\cdot\nabla\beta$$
$$\left.\left. + \frac{|p|^4}{3}|\nabla\beta|^2\right)\right] + O(\varepsilon^4), \quad \beta = 1/T$$

Quantum Maxwellian

- Maximization of quantum entropy *without* constraints ($T = \text{const.}$)

$$M_0 = \text{Exp}(V - \tfrac{1}{2}|p|^2)$$

- Expansion in powers of ε^2:

$$M_0 = e^{V-|p|^2/2}\left[1 + \frac{\varepsilon^2}{8}\left(\Delta V + \frac{1}{3}|\nabla V|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Vp\right)\right] + O(\varepsilon^4)$$

  $\longrightarrow$ first derived by Wigner 1932

- Compare to Maxwellian of constrained problem:

$$M[w] = e^{A-|p|^2/2}\left[1 + \frac{\varepsilon^2}{8}\left(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Ap\right)\right] + O(\varepsilon^4)$$

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Derivation

- Diffusion-scaled Wigner-Boltzmann equation:

$$\alpha^2 \partial_t w_\alpha + \alpha\big(p \cdot \nabla_x w_\alpha + \theta[V] w_\alpha\big) = Q(w_\alpha)$$

- BGK-type collision operator: $Q(w) = M[w] - w$,
  $M[w] = \mathrm{Exp}(A - \frac{1}{2}|p|^2)$ (one moment prescribed)
- Properties of collision operator: (reminder: $\langle g \rangle = \int_{\mathbb{R}^3} g(p)dp/4\pi^3$)

$$\langle Q(w) \rangle = 0, \quad Q(w) = 0 \ \Leftrightarrow \ w = M[w]$$

- Properties of potential operator:

$$\langle \theta[V] w \rangle = 0, \quad \langle p\theta[V] w \rangle = -\langle w \rangle \nabla_x V$$

- Derivation performed in three steps

Step 1: limit $\alpha \to 0$ in Wigner-BGK equation $\Rightarrow Q(w) = 0$, where
$w = \lim_{\alpha \to 0} w_\alpha \Rightarrow w = M[w] = \mathrm{Exp}(A - \frac{1}{2}|p|^2)$

Derivation

$$\alpha^2\partial_t w_\alpha + \alpha\big(p\cdot\nabla_x w_\alpha + \theta[V]w_\alpha\big) = M[w_\alpha] - w_\alpha$$

Step 2: Chapman-Enskog expansion

- Insert $w_\alpha = M[w_\alpha] + \alpha g_\alpha$ into collision operator:

$$\alpha\partial_t w_\alpha + \big(p\cdot\nabla_x w_\alpha + \theta[V]w_\alpha\big) = \alpha^{-1}(M[w_\alpha] - w_\alpha) = -g_\alpha$$

- Limit $\alpha\to 0$:

$$g = \lim_{\alpha\to 0} g_\alpha = -\big(p\cdot\nabla_x M[w] + \theta[V]M[w]\big)$$

Step 3: limit $\alpha\to 0$ in moment equation

- Moment equation:

$$\partial_t\langle w_\alpha\rangle + \alpha^{-1}\mathrm{div}_x\underbrace{\langle pM[w_\alpha]\rangle}_{=0} + \mathrm{div}_x\langle pg_\alpha\rangle$$
$$+\alpha^{-1}\underbrace{\langle\theta[V]M[w_\alpha]\rangle}_{=0} + \underbrace{\langle\theta[V]g_\alpha\rangle}_{=0} = \underbrace{\langle Q(w_\alpha)\rangle}_{=0}$$

Derivation

- Moment equation: $\partial_t \langle w_\alpha \rangle + \mathrm{div}_x \langle p g_\alpha \rangle = 0$
- Limit $\alpha \to 0$:

$$\partial_t \langle M[w] \rangle + \mathrm{div}_x \langle p g \rangle = 0$$

- Computation of current density J_n:

$$\begin{aligned} J_n &= -\langle p g \rangle = \langle p(p \cdot \nabla_x M[w] + \theta[V] M[w]) \rangle \\ &= \mathrm{div}_x \langle p \otimes p M[w] \rangle - \langle M[w] \rangle \nabla_x V \end{aligned}$$

Theorem (Nonlocal quantum drift-diffusion model)

$$\partial_t n - \mathrm{div}\, J_n = 0, \quad J_n = \mathrm{div}\, P - n \nabla V, \quad \lambda_D^2 \Delta V = n - C(x)$$

where the electron density and quantum stress tensor are defined by

$$n = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \mathrm{Exp}\left(A - \frac{|p|^2}{2}\right) dp, \quad P = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} p \otimes p \mathrm{Exp}\left(A - \frac{|p|^2}{2}\right) dp$$

Expansion in powers of ε^2

- Nonlocal relations:

$$n = \frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3}\mathrm{Exp}\left(A-\frac{|p|^2}{2}\right)dp,\ P = \frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^3}p\otimes p\,\mathrm{Exp}\left(A-\frac{|p|^2}{2}\right)dp$$

- Expansion of quantum exponential:

$$\mathrm{Exp}\left(A-\frac{|p|^2}{2}\right) = \exp\left(A(x,t)-\frac{|p|^2}{2}\right) \times\left[1+\frac{\varepsilon^2}{8}\left(\Delta A+\frac{1}{3}|\nabla A|^2-\frac{1}{3}p^\top(\nabla\otimes\nabla)Ap\right)\right]+O(\varepsilon^4)$$

- Electron density:

$$n = \frac{2}{(2\pi\varepsilon)^{3/2}}e^A\left(1+\frac{\varepsilon^2}{12}\left(\Delta A+\frac{1}{2}|\nabla A|^2\right)\right)+O(\varepsilon^4)$$

Expansion in powers of ε^2

- Electron density:

$$n = \frac{2}{(2\pi\varepsilon)^{3/2}} e^A \left(1 + \frac{\varepsilon^2}{12}\left(\Delta A + \frac{1}{2}|\nabla A|^2\right)\right) + O(\varepsilon^4)$$

- Quantum stress tensor:

$$\begin{aligned} P_{j\ell} &= \frac{2}{(2\pi\varepsilon)^{3/2}} e^A \left(1 + \frac{\varepsilon^2}{12}\left(\Delta A + \frac{1}{2}|\nabla A|^2\right)\right)\delta_{j\ell} \\ &\quad - \frac{\varepsilon^2}{6(2\pi\varepsilon)^{3/2}} e^A \frac{\partial^2 A}{\partial x_j \partial x_\ell} + O(\varepsilon^4) \\ &= n\delta_{j\ell} - \frac{\varepsilon^2}{12} n \frac{\partial^2 A}{\partial x_j \partial x_\ell} + O(\varepsilon^4) \end{aligned}$$

$$\operatorname{div} P = \nabla n - \frac{\varepsilon^2}{12} n \nabla\left(\Delta A + \frac{1}{2}|\nabla A|^2\right) + O(\varepsilon^4)$$

- Express A in terms of n

Expansion in powers of ε^2

- Express A in terms of n: Since $n = 2(2\pi\varepsilon)^{-3/2}e^A + O(\varepsilon^2)$ and $\nabla A = \nabla n/n + O(\varepsilon^2)$,

$$\Delta A + \frac{1}{2}|\nabla A|^2 = 2\frac{\Delta\sqrt{n}}{\sqrt{n}} + O(\varepsilon^2)$$

- Recall formula:

$$\operatorname{div} P = \nabla n - \frac{\varepsilon^2}{12} n\nabla\left(\Delta A + \frac{1}{2}|\nabla A|^2\right) + O(\varepsilon^4)$$

- Current density:

$$J_n = \operatorname{div} P - n\nabla V = \nabla n - n\nabla V - \frac{\varepsilon^2}{6}\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + O(\varepsilon^4)$$

Theorem (Local quantum drift-diffusion equations)

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$$

Local quantum drift-diffusion equations

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right), \quad x \in \Omega$$

- Mathematically fourth-order parabolic equation
- Expression $\Delta\sqrt{n}/\sqrt{n}$: quantum Bohm potential
- Ancona 1987: strong inversion layers near oxide of MOS transistor
- Notation in engineering literature: density-gradient model
- Boundary conditions: $\partial\Omega = \Gamma_D \cup \Gamma_N$

$$n = n_D, \ V = V_D \quad \text{on } \Gamma_D, \quad J_n \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N$$

$$\underbrace{\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) \cdot \nu = 0 \quad \text{on } \Gamma_N}_{\text{no quantum current}}, \qquad \underbrace{\Delta\sqrt{n} = 0 \quad \text{on } \Gamma_D}_{\text{no quantum effects on } \Gamma_D}$$

Local quantum drift-diffusion equations

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right), \quad x \in \Omega$$

$$n = n_D, \ V = V_D \quad \text{on } \Gamma_D, \quad J_n \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N$$

- Alternative boundary condition for quantum quasi-Fermi potential $F = \log n - V - (\varepsilon^2/6)\Delta\sqrt{n}/\sqrt{n}$:

$$\nabla F \cdot \nu = 0 \quad \text{on } \Gamma_N, \quad F = F_D \quad \text{on } \Gamma_D$$

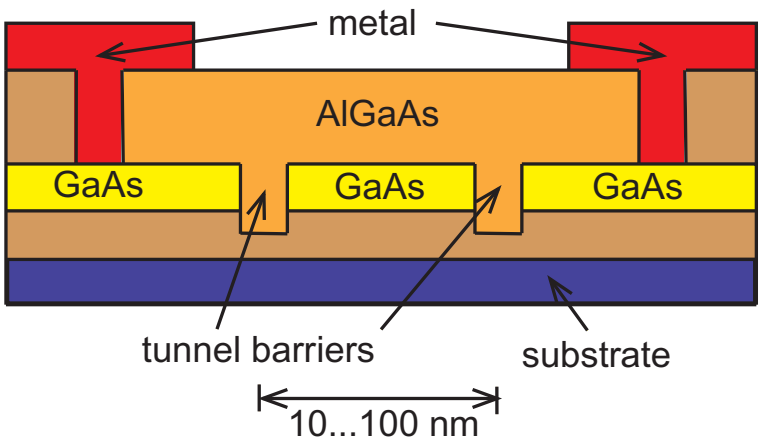
Mathematical results:

- 1D, $V = 0$: local existence of solutions (Bleher et al. 1994)
- 1D, $V = 0$: global existence of solutions (A.J./Pinnau 2000)
- 1D, $V \neq 0$: global existence of solutions (A.J./Violet 2007)
- 3D, $V = 0$: global existence of solutions (A.J./Matthes 2008, Gianazza/Savaré/Toscani 2008)

Resonant tunneling diode

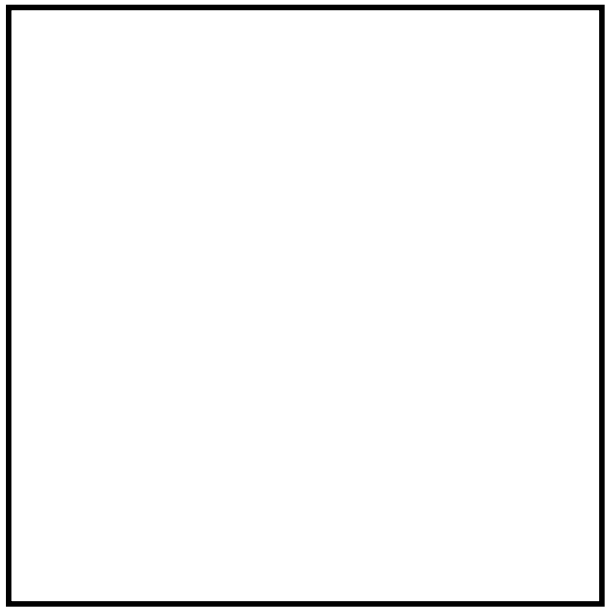
Geometry:

- AlGaAs layer width: 5 nm
- device length: 75 nm
- doping: n^+nn^+ structure
- barrier height: 0.4 eV



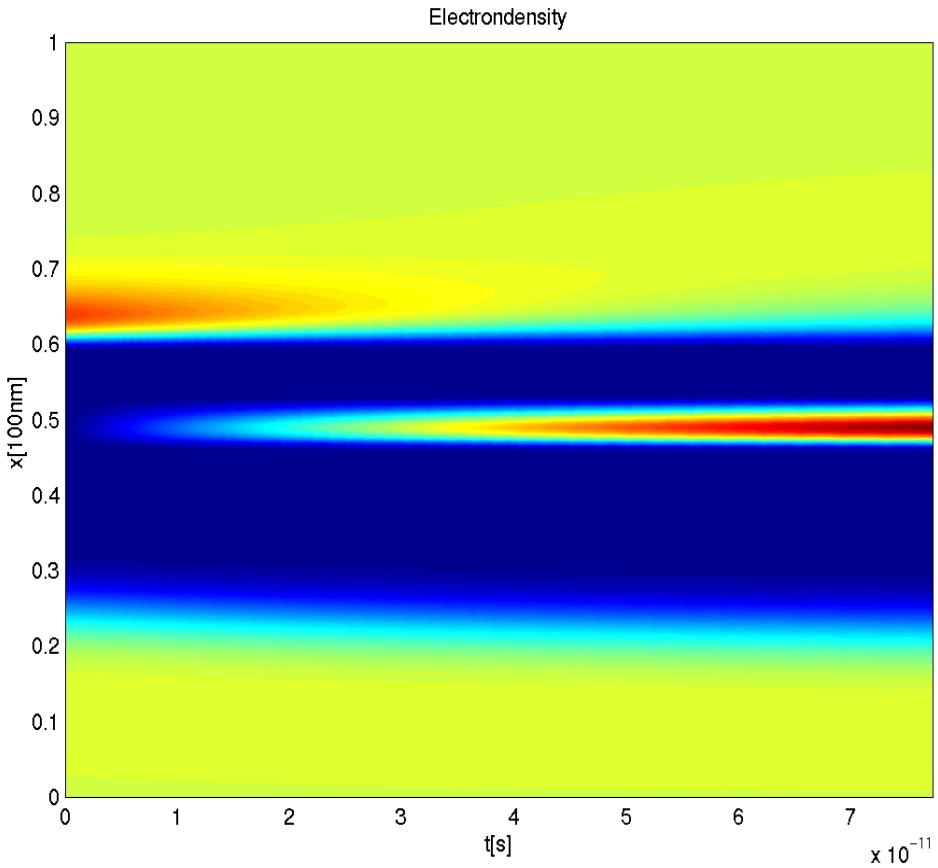
Numerical method:

- semi-discretization in time
- finite differences in space (one-dimensional)
- Newton iterations

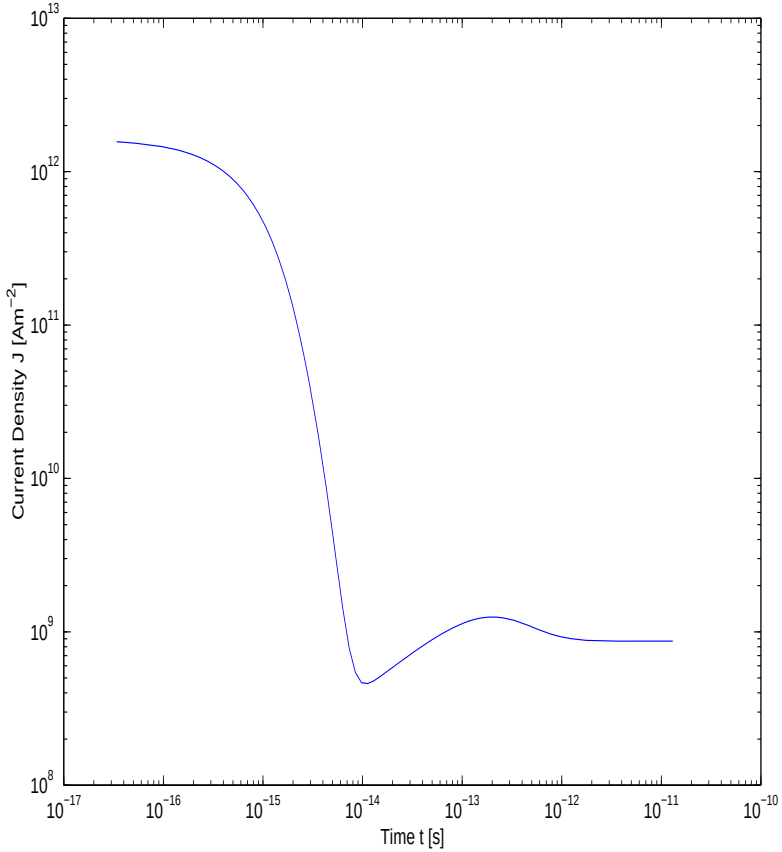


Time-dependent simulations of tunneling diode

Electron density $n(t)$

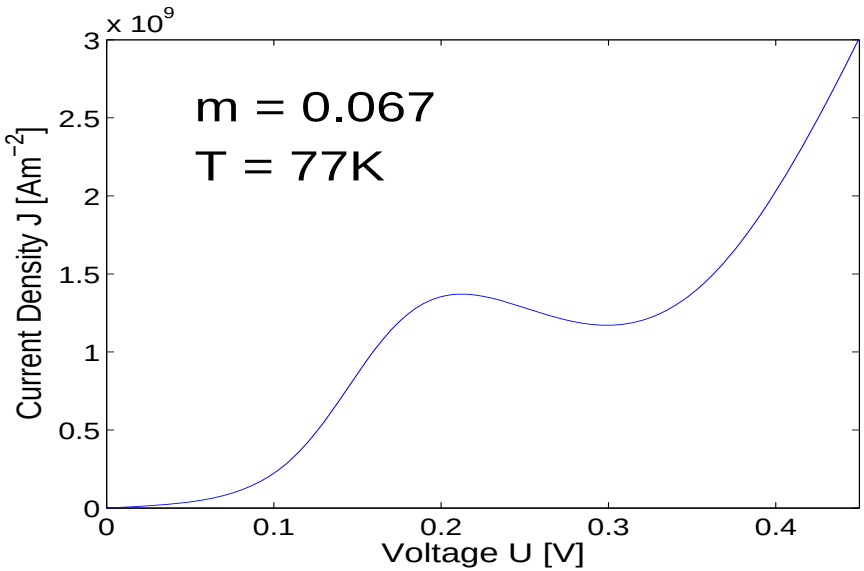


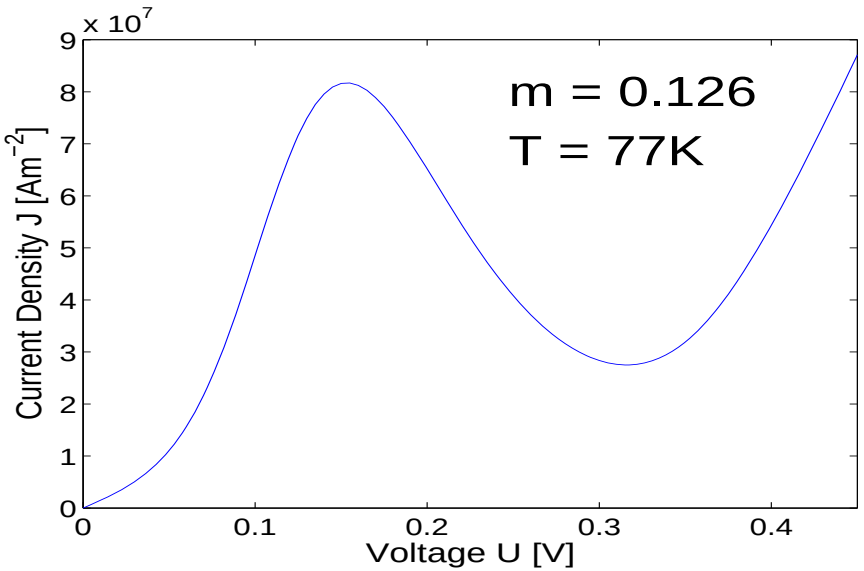
Current density $J(t)$

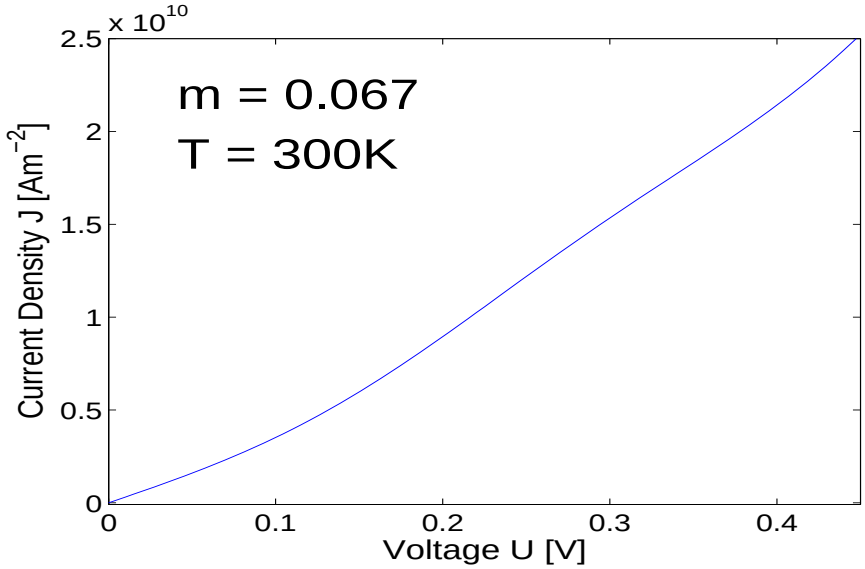


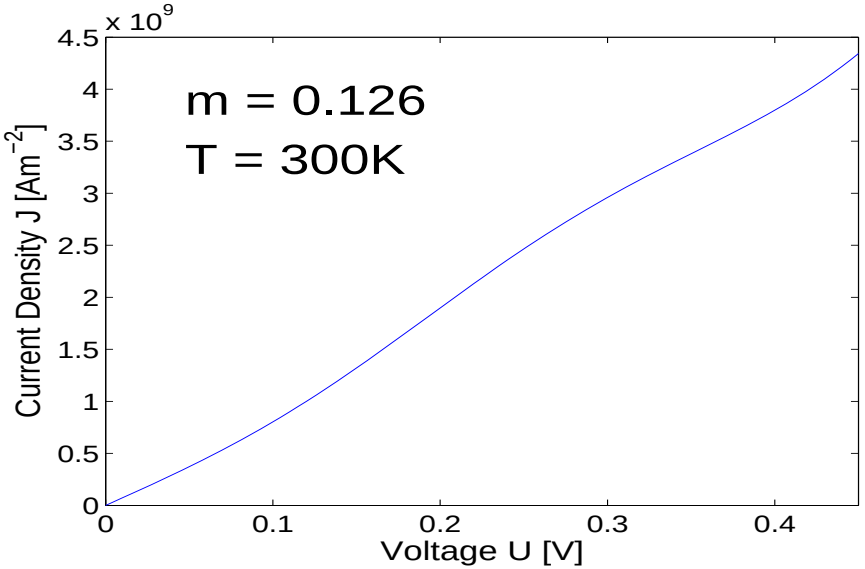
$\longrightarrow$ stabilization after $\sim 10^{-11}$ sec. (100 GHz)

Current-voltage characteristics of tunneling diode



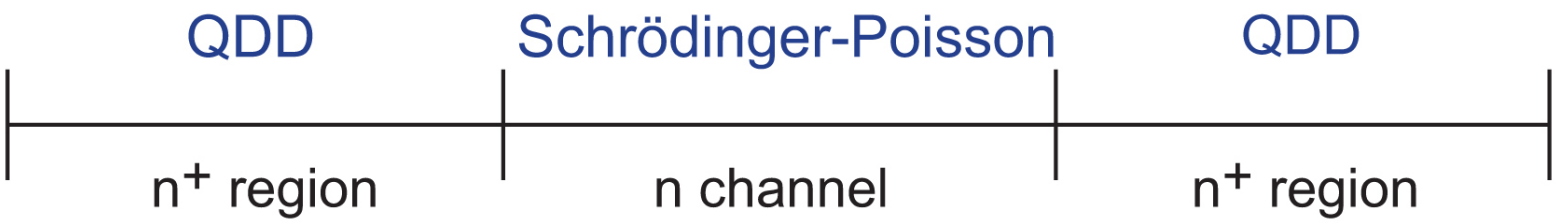






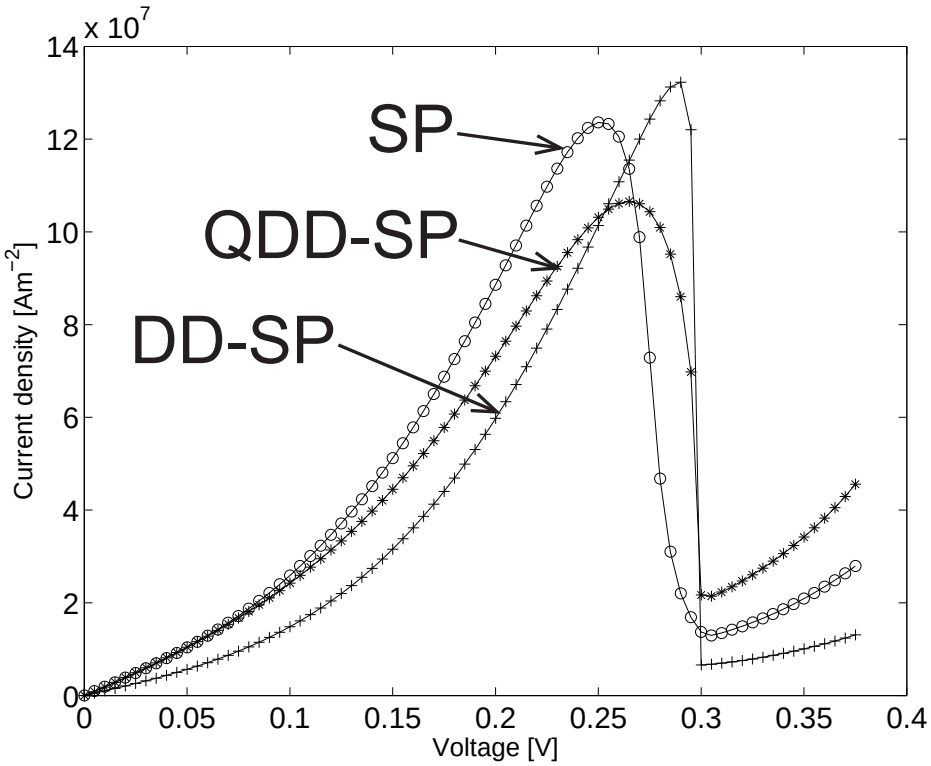
Coupled QDD-Schrödinger-Poisson model

(El Ayyadi/A.J. 2005)



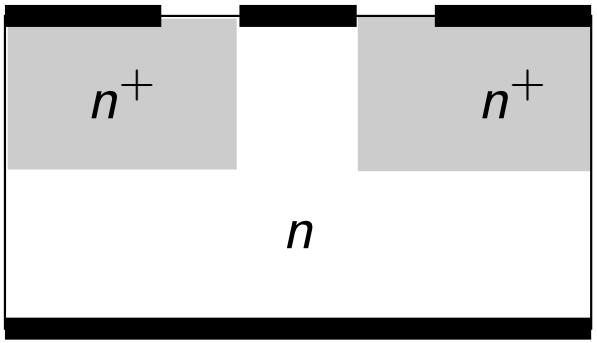
Numerical comparison:

- Schrödinger-Poisson (SP)
- QDD-Schrödinger-Poisson
- Drift-Diffusion-Schrödinger-Poisson (Degond/El Ayyadi 2002)



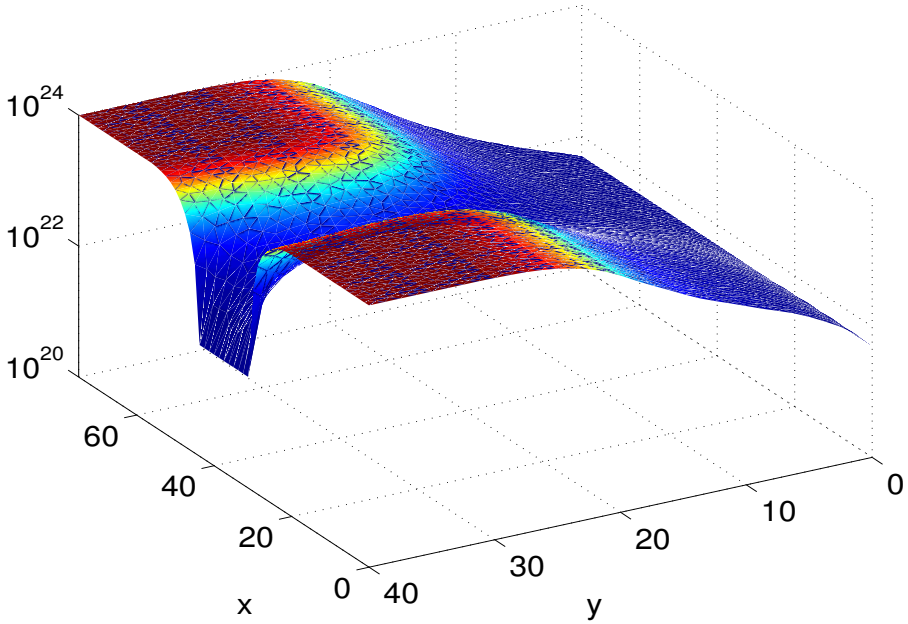
Simulation of a 2D nanoscale MESFET

(Chainais/Gisclon/A.J. *Numer. Meth. PDE* 2010)

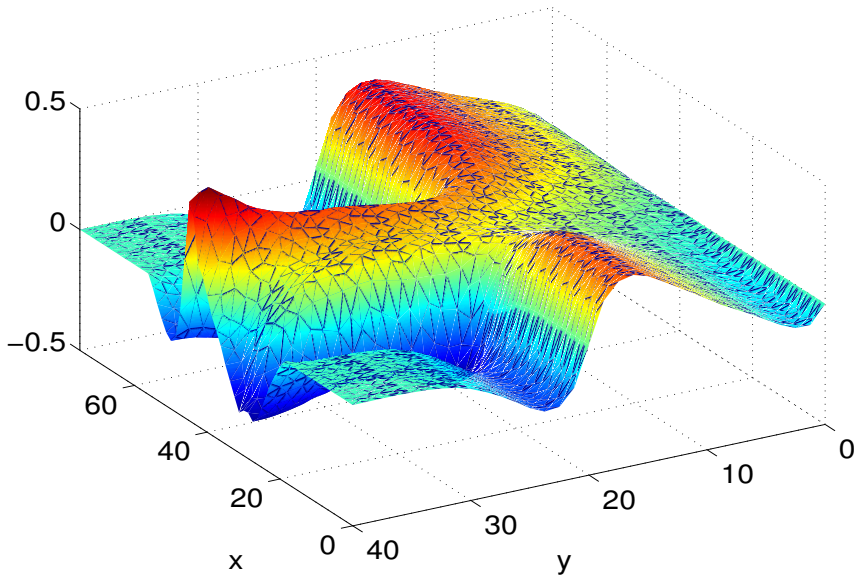


- Channel length: 15nm
- Inversion layer at gate
- Bohm potential $\frac{\varepsilon^2}{2}\frac{\Delta\sqrt{n}}{\sqrt{n}}$ vanishes at contacts

Electron density:



Bohm potential:



Quantum entropy

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$$

- Quantum kinetic entropy (or free energy):

$$S(w) = -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} w\left(\operatorname{Log} w - 1 + \frac{|p|^2}{2} - V\right)dx\,dp$$

- Quantum fluid entropy: insert $w_0 = \operatorname{Exp}(A - |p|^2/2)$

$$S(w_0) = -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} w_0(A - 1 - V)dx\,dp = -\int_{\mathbb{R}^3} n(A - 1 - V)dx,$$

- Entropy inequality (Degond/Ringhofer 2003):

$$\frac{dS}{dt}(w_0) \geq \int_{\mathbb{R}^3} n\partial_t V dx, \quad n \text{ solves nonlocal model}$$

- Expansion of quantum entropy: $\log n \approx A + \frac{\varepsilon^2}{12}(\Delta A + \frac{1}{2}|\nabla A|^2)$

$$S_0 = -\int_{\mathbb{R}^3}\left(n(\log n - 1) + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 - nV\right)dx + O(\varepsilon^4)$$

Quantum entropy

$$S_0 = -\int_{\mathbb{R}^3} \left(n(\log n - 1) + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 - nV \right) dx$$

Proposition (Entropy inequality)

Let n solve local quantum drift-diffusion model. Then

$$\frac{dS_0}{dt} - \int_{\mathbb{R}^3} n\left|\nabla\left(\log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right|^2 dx = \int_{\mathbb{R}^3} n\partial_t V dx$$

Proof:

- Reformulate quantum drift-diffusion equation:

$$\partial_t n = \operatorname{div}\left(n\nabla\left(\log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right)$$

- Differentiate S_0, insert equation for $\partial_t n$, and straight-forward computations

Summary

Local quantum drift-difusion model (QDD)

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V - \frac{\varepsilon^2}{6}\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right), \quad \lambda_D^2 \Delta V = n - C(x)$$

- Derivation from Wigner-BGK equation by moment method and $O(\varepsilon^4)$-expansion
- Simulation of resonant tunneling diode: negative differential resistance for small temperature or large effective mass
- Coupled QDD-Schrödinger models give qualitatively good results
- Mathematical theory well developed
- Quantum entropy provides estimates

Overview

1. Semiconductor modeling
   - Basics of semiconductor physics
   - Kinetic models
2. Semi-classical macroscopic models
   - General strategy
   - Drift-diffusion models
   - Energy-transport models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Quantum kinetic models
   - Quantum Maxwellians
   - Quantum drift-diffusion models
   - Quantum hydrodynamic models
4. New and future devices
5. Summary

Single-state Schrödinger equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi - qV(x,t)\psi, \quad x\in\mathbb{R}^3,\ t>0$$

- Scaling: reference length λ, reference time τ, reference voltage U, and assume that $m(\lambda/\tau)^2 = qU$

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - V(x,t)\psi, \quad \varepsilon = \frac{\hbar/\tau}{m(\lambda/\tau)^2} = \frac{\text{wave energy}}{\text{kinetic energy}}$$

- Madelung transform: $\psi = \sqrt{n}\exp(iS/\varepsilon)$, where n: particle density, S: phase function
- Quantum hydrodynamic equations for $n = |\psi|^2$ and $J = -\varepsilon\mathrm{Im}(\overline{\psi}\nabla\psi)$:

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t J_n - \operatorname{div}\left(\frac{J_n\otimes J_n}{n}\right) + n\nabla V + \frac{\varepsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 0$$

- Schrödinger $\to$ QHD if initial datum well-prepared, $\psi(\cdot,0) = \sqrt{n_I}\exp(iS_I/\varepsilon)$

Zero-temperature quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t J_n - \operatorname{div}\left(\frac{J_n \otimes J_n}{n}\right) + n\nabla V + \frac{\varepsilon^2}{2} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = 0$$

- Single state equation $\Rightarrow$ no temperature or pressure term
- Mathematically third-order differential equations
- Analytical and numerical difficulties: highly nonlinear, vacuum points (x,t) at which $n(x,t)=0$
- Quantum Bohm potential $\Delta\sqrt{n}/\sqrt{n}$ appears naturally
- Nondiagonal quantum stress tensor: $P = (\varepsilon^2/4) n(\nabla\otimes\nabla)\log n$

$$\frac{\varepsilon^2}{2} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = \frac{\varepsilon^2}{4}\operatorname{div}\left(n(\nabla\otimes\nabla)\log n\right),$$

- Applications: description of quantum trajectories, superfluidity models, photodissociation problems etc.

Wigner equation and quantum hydrodynamics

- Wigner-Boltzmann equation in hydrodynamic scaling:

$$\alpha\partial_t w + \alpha\big(p\cdot\nabla_x w + \theta[V]w\big) = Q_0(w) + \alpha Q_1(w)$$

- Advantages of approach:
  - Scattering can be included
  - Closure obtained through limiting process
- Assumptions on scattering: Q_0 conserves mass, momentum, energy, Q_1 conserves mass

$$\langle Q_0(w)\rangle = \langle Q_1(w)\rangle = 0, \quad \langle pQ_0(w)\rangle = 0, \quad \langle \tfrac{1}{2}|p|^2 Q_0(w)\rangle = 0$$

  and $Q_0(w) = 0$ iff $w =$ quantum Maxwellian
- Quantum entropy: $S(w) = -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} w(\operatorname{Log} w - 1 + \frac{|p|^2}{2} - V)dx\,dp$
- Quantum Maxwellian: Let w be given and $M[w]$ be solution of

$$S(w^*) = \max_v S(v) \text{ under constraints } \langle \kappa_j v\rangle = \langle \kappa_j w\rangle$$

  where $\kappa = (1, p, \frac{1}{2}|p|^2) \Rightarrow M[w] = \operatorname{Exp}(A - |p-v|^2/2T)$

Derivation

$$\partial_t w_\alpha + \left(p \cdot \nabla_x w_\alpha + \theta[V] w_\alpha\right) = \alpha^{-1} Q_0(w_\alpha) + Q_1(w_\alpha)$$

Step 1: Limit $\alpha \to 0$ in Wigner-Boltzmann equation $\Rightarrow Q_0(w) = 0$, where $w = \lim_{\alpha\to 0} w_\alpha \Rightarrow w = M[w]$

Step 2: Limit in moment equations

- Moment equations:

$$\partial_t \langle \kappa_j w_\alpha \rangle + \mathrm{div}_x \langle p \kappa_j w_\alpha \rangle + \langle \kappa_j \theta[V] w_\alpha \rangle = \langle \kappa_j Q_1(w_\alpha) \rangle$$

- Limit $\alpha \to 0$:

$$\partial_t \langle \kappa_j M[w] \rangle + \mathrm{div}_x \langle p \kappa_j M[w] \rangle + \langle \kappa_j \theta[V] M[w] \rangle = \langle \kappa_j Q_1(M[w]) \rangle$$

- Moments: $(n, nu, ne) = \langle (1, p, \frac{1}{2}|p|^2) M[w] \rangle$, $J = -nu$
- Use properties

$$\langle \theta[V] M[w] \rangle = 0,\ \langle p\theta[V] M[w] \rangle = -n\nabla V,\ \langle \tfrac{1}{2}|p|^2 \theta[V] M[w] \rangle = J \cdot \nabla V$$

Derivation

- Balance equation for electron density n:

$$\partial_t \underbrace{\langle M[w]\rangle}_{=n} + \mathrm{div}_x \underbrace{\langle pM[w]\rangle}_{=-J} + \underbrace{\langle \theta[V]M[w]\rangle}_{=0} = \underbrace{\langle Q_1(M[w])\rangle}_{=0}$$

- Balance equation for current density J:

$$\partial_t \underbrace{\langle pM[w]\rangle}_{=-J} + \mathrm{div}_x \langle p\otimes pM[w]\rangle + \underbrace{\langle p\theta[V]M[w]\rangle}_{=-n\nabla V} = \langle pQ_1(M[w])\rangle$$

- Balance equation for energy density ne:

$$\partial_t \underbrace{\langle \tfrac{1}{2}|p|^2 M[w]\rangle}_{=ne} + \mathrm{div}_x \langle \tfrac{1}{2}p|p|^2 M[w]\rangle + \underbrace{\langle \tfrac{1}{2}|p|^2\theta[V]M[w]\rangle}_{=J\cdot\nabla V} = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

- Define quantum stress tensor and quantum heat flux

$$P = \langle (p-u)\otimes(p-u)M[w]\rangle, \quad q = \langle \tfrac{1}{2}(p-u)|p-u|^2 M[w]\rangle$$

Derivation

Theorem (Nonlocal quantum hydrodynamic model)

$$\partial_t n - \operatorname{div} J = 0,\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n} + P\right) + n\nabla V = -\langle pQ_1(w)\rangle$$
$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J - q\right) + J\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

where

$$P = \langle (p-u)\otimes(p-u)M[w]\rangle, \quad q = \langle \tfrac{1}{2}(p-u)|p-u|^2 M[w]\rangle$$

Simplifications:

- Isothermal model: $M[w] = \mathrm{Exp}(A - |p-v|^2/2)$
- $O(\varepsilon^4)$-expansion

Conserved quantities

$$\partial_t n - \operatorname{div} J = 0, \quad \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n} + P\right) + n\nabla V = 0$$

$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J - q\right) + J\cdot\nabla V = 0$$

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 + \varepsilon^2\text{-quantum correction}$$

$$P = nT\,\mathrm{Id} + \varepsilon^2\text{-quantum correction}$$

$$q = -\frac{\varepsilon^2}{24}n\Big(5R\nabla\log T + 2\operatorname{div} R + \Delta u + 2\nabla\operatorname{div} u\Big), \quad R = \nabla u - \nabla u^\top$$

Proposition

The energy is conserved, $dE/dt = 0$, where

$$E(t) = \int_{\mathbb{R}^3}\left(ne + \frac{\lambda_D^2}{2}|\nabla V|^2\right)dx = \int_{\mathbb{R}^3}\left(\frac{3}{2}nT + \frac{1}{2}n|u|^2 + \frac{\lambda_D^2}{2}|\nabla V|^2 + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + \frac{\varepsilon 2}{16}n|\nabla\log T|^2 + \frac{\varepsilon^2}{24T}n\mathrm{Tr}(R^\top R)\right)dx \geq 0$$

Local quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J = 0,\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n} + P\right) + n\nabla V = -\langle pQ_1(w)\rangle$$
$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J - q\right) + J\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

First simplification: small temperature $\nabla \log T = O(\varepsilon^2)$

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\left(\Delta\log n - \frac{1}{T}\mathrm{Tr}(R^\top R)\right)$$
$$P = nT\,\mathrm{Id} - \frac{\varepsilon^2}{12}n\left((\nabla\otimes\nabla)\log n - \frac{1}{T}R^\top R\right)$$
$$q = -\frac{\varepsilon^2}{24}n(2\operatorname{div} R + \Delta u + 2\nabla\operatorname{div} u)$$

$\longrightarrow$ Gives closed set of equations

Second simplification: $R = \nabla u - \nabla u^\top = O(\varepsilon^2)$

Local quantum hydrodynamic model

Theorem (Local quantum hydrodynamic model)

$$\partial_t n - \operatorname{div} J = 0$$

$$\partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\langle pQ_1(w)\rangle$$

$$\partial_t(ne) - \operatorname{div}\big((P+ne\,\mathrm{Id})J\big) - \frac{\varepsilon^2}{24}\operatorname{div}\left(n\Delta u + 2n\nabla\operatorname{div} u\right) + J\cdot\nabla V = \left\langle \tfrac{1}{2}|p|^2 Q_1(w)\right\rangle$$

where

$$P = nT\,\mathrm{Id} - \frac{\varepsilon^2}{12} n(\nabla\otimes\nabla)\log n, \quad ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Delta\log n$$

Quantum heat flux $q = -(\varepsilon^2/24)n(\Delta u + 2\nabla\operatorname{div} u)$:

- Also derived by Gardner 1995 from mixed-state Wigner model
- Appears in "smooth" QHD model (Gardner/Ringhofer 2000)
- Seems to stabilize system numerically (A.J./Matthes/Milisic 2006)

Dissipative QHD models

$$\partial_t n - \operatorname{div} J = 0, \quad q = \frac{\varepsilon^2}{24} n(\Delta u + 2\nabla \operatorname{div} u)$$

$$\partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\langle p Q_1(w)\rangle$$

$$\partial_t(ne) - \operatorname{div}\big((P + ne\,\mathrm{Id})J\big) - \operatorname{div} q + J \cdot \nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

Caldeira-Leggett operator: $Q_1(w) = \frac{1}{\tau}(\Delta_p w + \operatorname{div}_p(pw))$

- Averaged quantities:

$$-\langle p Q_1(w)\rangle = -\frac{J}{\tau}, \quad \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

- Relaxation-time model: $J(t) \to 0$, $(ne)(t) - \frac{3}{2}n(t) \to 0$ as $t \to \infty$

Dissipative QHD models

Caldeira-Leggett operator:

$$\partial_t n - \operatorname{div} J = 0, \quad q = \frac{\varepsilon^2}{24} n(\Delta u + 2\nabla \operatorname{div} u)$$

$$\partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\frac{J}{\tau}$$

$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J\right) - \operatorname{div} q + J \cdot \nabla V = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

- Does not satisfy Lindblatt cond. (positivity-preserving density matrix)
- Rescaled time and current density: $t \to t/\tau$, $J \to \tau J$

$$\tau\partial_t n - \tau \operatorname{div} J = 0$$

$$\tau^2\partial_t J - \tau^2 \operatorname{div}\left(\tfrac{J\otimes J}{n}\right) - \nabla n + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\left(\tfrac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\tau\frac{J}{\tau}$$

- Limit $\tau \to 0$ gives quantum drift-diffusion model:

$$\partial_t n - \operatorname{div} J = 0, \quad J = \nabla n - n\nabla V - \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$$

Dissipative QHD models

Caldeira-Leggett operator:

$$\partial_t n - \operatorname{div} J = 0, \quad q = \frac{\varepsilon^2}{24} n(\Delta u + 2\nabla \operatorname{div} u)$$

$$\partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\frac{J}{\tau}$$

$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J\right) - \operatorname{div} q + J \cdot \nabla V = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

- Existence of stationary "subsonic" solutions with $T = 1$ and $|J/n|$ "small" (A.J. 1998)
- Nonexistence of solutions with $T = 1$ and special boundary conditions (A.J./Gamba 2001)
- Existence of transient solutions with $T = 1$ (Antonelli/Marcati 2008)
- Numerical solution: upwind finite differences (Gardner 1994), central finite differences (A.J./Milisic 2007)

Dissipative QHD models

$$\partial_t n - \operatorname{div} J = \langle Q_1(w)\rangle$$

$$\partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\langle pQ_1(w)\rangle$$

$$\partial_t(ne) - \operatorname{div}\big((P+ne\,\mathrm{Id})J\big) - \operatorname{div}\, q + J\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

Fokker-Planck operator:

$$Q_1(w) = D_{pp}\Delta_p w + 2\gamma \operatorname{div}_p(pw) + D_{qq}\Delta_x w + 2D_{pq}\operatorname{div}_x(\nabla_p w)$$

- Lindblatt condition satisfied if $D_{pp}D_{qq} - D_{pq}^2 \geq \gamma^2/4$
- Averaged quantities:

$$\langle Q_1(w)\rangle = D_{qq}\Delta_x n, \quad -\langle pQ_1(w)\rangle = -2\gamma J + 2D_{pq}\nabla_x n + D_{qq}\Delta_x J$$

$$\langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle = -2\left(2\gamma ne - \frac{3}{2}D_{pp}n\right) + 2D_{pq}\operatorname{div}_x J + D_{qq}\Delta_x(ne)$$

- Gives viscous quantum hydrodynamic model

Viscous quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J = D_{qq}\Delta n$$

$$\partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n}\right) - \nabla(nT) + n\nabla V + \frac{\varepsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$$
$$= D_{qq}\Delta J - 2\gamma J + 2D_{pq}\nabla_x n$$

$$\partial_t(ne) - \operatorname{div}\big((P+ne\,\mathrm{Id})J\big) - \operatorname{div}\, q + J\cdot\nabla V$$
$$= D_{qq}\Delta_x(ne) - 2\left(2\gamma ne - \frac{3}{2}D_{pp}n\right) + 2D_{pq}\operatorname{div}_x J$$

- D_{qq} provides diffusive terms
- Effective current density $J_{\mathrm{eff}} = J - D_{qq}\nabla n$: $\partial_t n - \operatorname{div} J_{\mathrm{eff}} = 0$
- Existence of 1D stationary solutions with $T = 1$ (A.J./Milisic 2007)
- Lobal existence of transient solutions (Chen/Dreher 2006)
- Global existence of 3D transient solutions (A.J. 2009)

Quantum Navier-Stokes equations

Objective: Derive Navier-Stokes correction (Brull/Méhats 2009)

Wigner-BGK equation:

- Hydrodynamic scaling:

$$\alpha\partial_t w + \alpha\big(p\cdot\nabla_x w + \theta[V]w\big) = M[w] - w$$

- Quantum Maxwellian: $M[w] = \mathrm{Exp}(A - |p-v|^2/2)$ (isothermal case)

Step 1: Moment equations

- Balance equation for electron density n:

$$\partial_t \underbrace{\langle w\rangle}_{=n} + \mathrm{div}_x \underbrace{\langle pw\rangle}_{=nu} + \underbrace{\langle\theta[V]w\rangle}_{=0} = \alpha^{-1}\underbrace{\langle M[w]-w\rangle}_{=0}$$

- Balance equation for current density $-nu$:

$$\partial_t \underbrace{\langle pw\rangle}_{=nu} + \mathrm{div}_x\langle p\otimes pw\rangle + \underbrace{\langle p\theta[V]w\rangle}_{=-n\nabla V} = \alpha^{-1}\underbrace{\langle p(M[w]-w)\rangle}_{=0}$$

Quantum Navier-Stokes equations

$$\partial_t n + \operatorname{div}(nu) = 0, \quad \partial_t(nu) + \langle p \otimes pw \rangle - n\nabla V = 0$$

Step 2: Chapman-Enskog expansion $w = M[w] + \alpha g$

- Computation of g: insert expansion into Wigner-BGK equation

$$\begin{aligned} g &= \alpha^{-1}(M[w] - w) = -\partial_t w - (p \cdot \nabla_x w + \theta[V]w) \\ &= -\partial_t M[w] - (p \cdot \nabla_x M[w] + \theta[V]M[w]) + O(\alpha) \end{aligned}$$

- Second-order moment: insert Chapman-Enskog expansion

$$\begin{aligned} \langle p \otimes pw \rangle &= \langle p \otimes pM[w] \rangle - \alpha S \\ S &= \langle p \otimes p(\partial_t M[w] + p \cdot \nabla_x M[w] + \theta[V]M[w]) \rangle \end{aligned}$$

- Stress tensor:

$$P = \langle (p-u) \otimes (p-u) M[w] \rangle = \langle p \otimes pM[w] \rangle - nu \otimes u$$

- Second-order moment: $\langle p \otimes pw \rangle = P + nu \otimes u - \alpha S$

Quantum Navier-Stokes equations

$$\partial_t n + \operatorname{div}(nu) = 0, \quad \partial_t(nu) + \operatorname{div}(nu \otimes u + P) - n\nabla V = \alpha S$$

- Correction S depends on n, nu, A, v, and P
- $O(\varepsilon^4)$ expansion under small vorticity assumption $\nabla u - \nabla u^\top = O(\varepsilon^2)$:

$$P = n\,\mathrm{Id} - \frac{\varepsilon^2}{12} n\nabla^2 \log n + O(\varepsilon^4)$$

$$\alpha S = 2\alpha \operatorname{div}(nD(u)) + O(\alpha\varepsilon^2) + O(\alpha^2), \quad D(u) = \tfrac{1}{2}(\nabla u + \nabla u^\top)$$

- Compare to classical Navier-Stokes correction:

$$S = 2\operatorname{div}(\mu(n)D(u)) + \nabla(\lambda(n)\operatorname{div} u)$$

- Extension to non-isothermal model: A.J./Milisic 2011

Quantum Navier-Stokes equations

Reformulation of quantum Navier-Stokes model:

$$\partial_t n + \operatorname{div}(nu) = 0$$

$$\partial_t(nu) + \operatorname{div}(nu\otimes u) + \nabla n - \frac{\varepsilon^2}{6} n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) - n\nabla V = 2\alpha\operatorname{div}(nD(u))$$

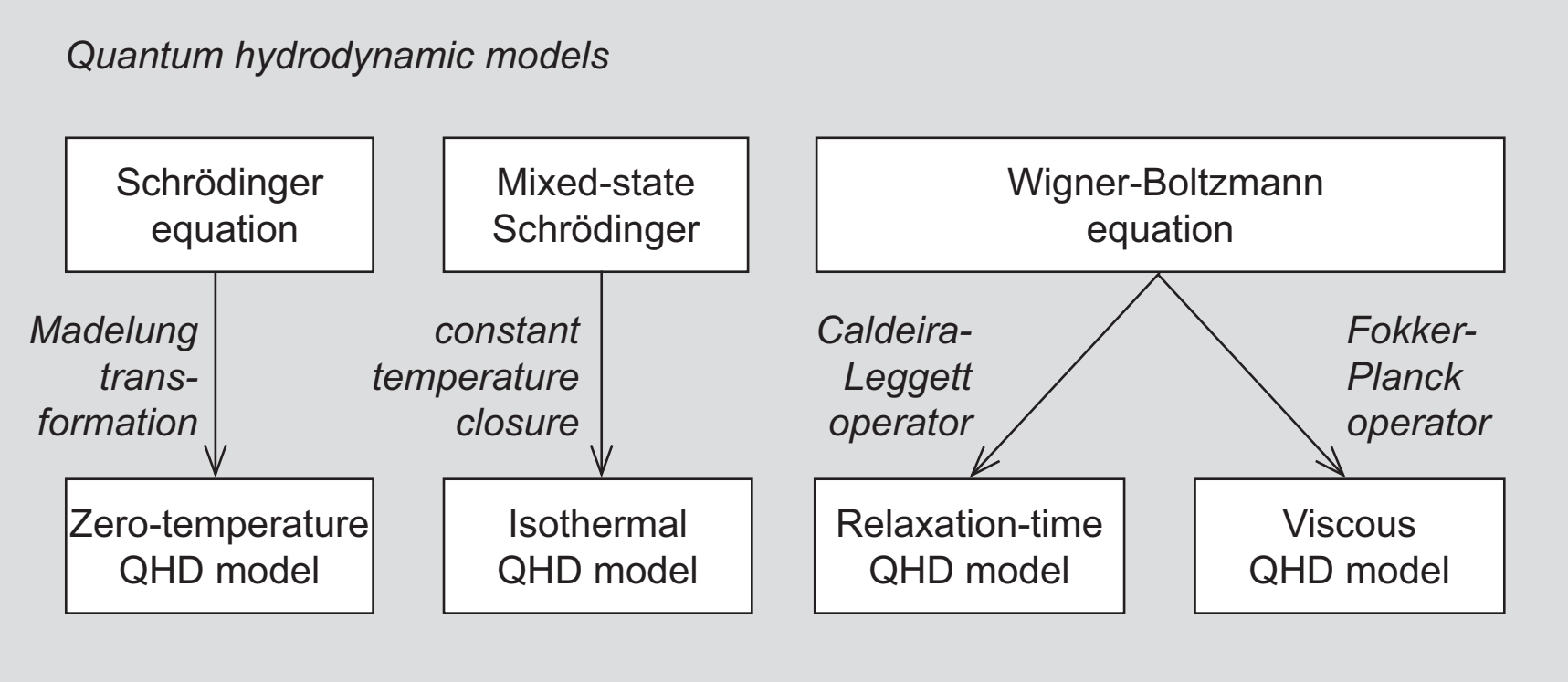
- Assumption: $\alpha = \varepsilon^2/6$
- Effective velocity: $w = u + \sqrt{\alpha}\nabla \log n$
- Quantum Navier-Stokes system is equivalent to viscous Euler system:

$$\partial_t n + \operatorname{div}(nw) = \alpha\Delta n$$

$$\partial_t(nw) + \operatorname{div}(nw\otimes w) + \nabla n - n\nabla V = \alpha\Delta(nw)$$

- Same viscous terms in viscous quantum hydrodynamic model!
- Osmotic velocity: $\sqrt{\alpha}\nabla \log n$ (Nelson 1966)
- Velocity w used in viscous Korteweg models (Bresch/Desjardins); can be obtained from gauge transform $\psi' = e^{i\theta}\psi$, $\theta = \sqrt{\alpha}\nabla \log n/\hbar$

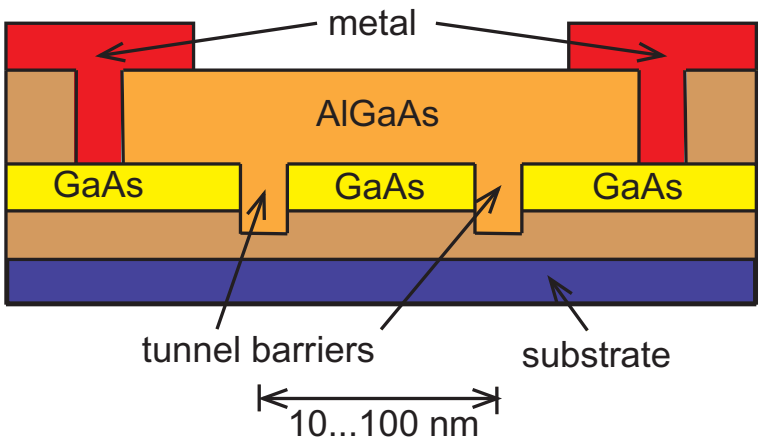
Hierarchy of quantum hydrodynamic models



Resonant tunneling diode

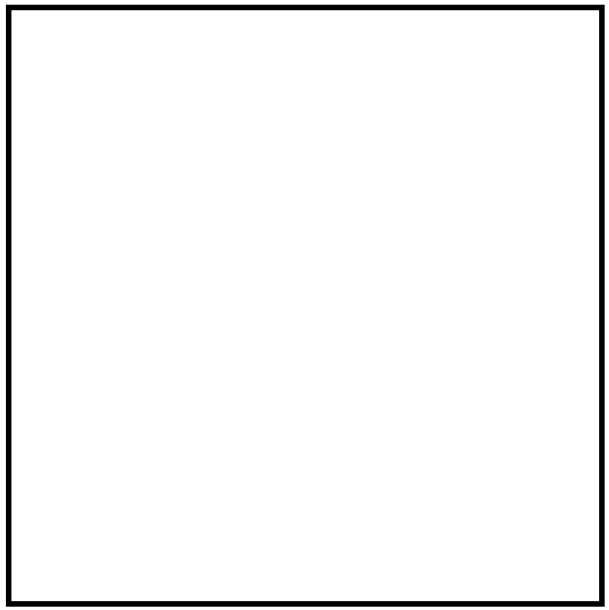
Geometry:

- AlGaAs layer width: 5 nm
- channel length: 25 nm
- doping: n^+nn^+ structure
- barrier height: 0.4 eV



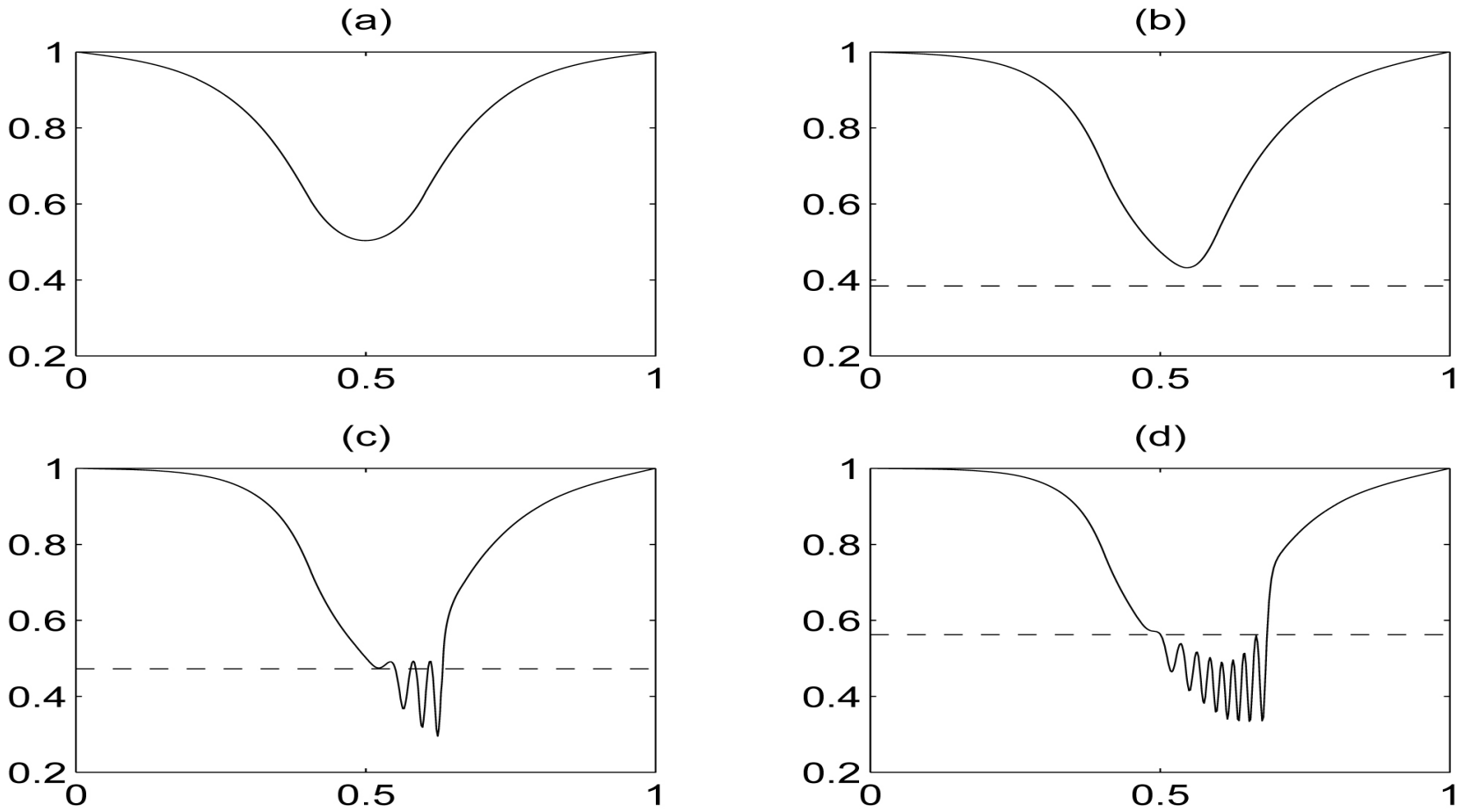
Numerical method:

- Relaxation scheme (QHD)
- Central finite differences (viscous QHD)
- Newton iterations

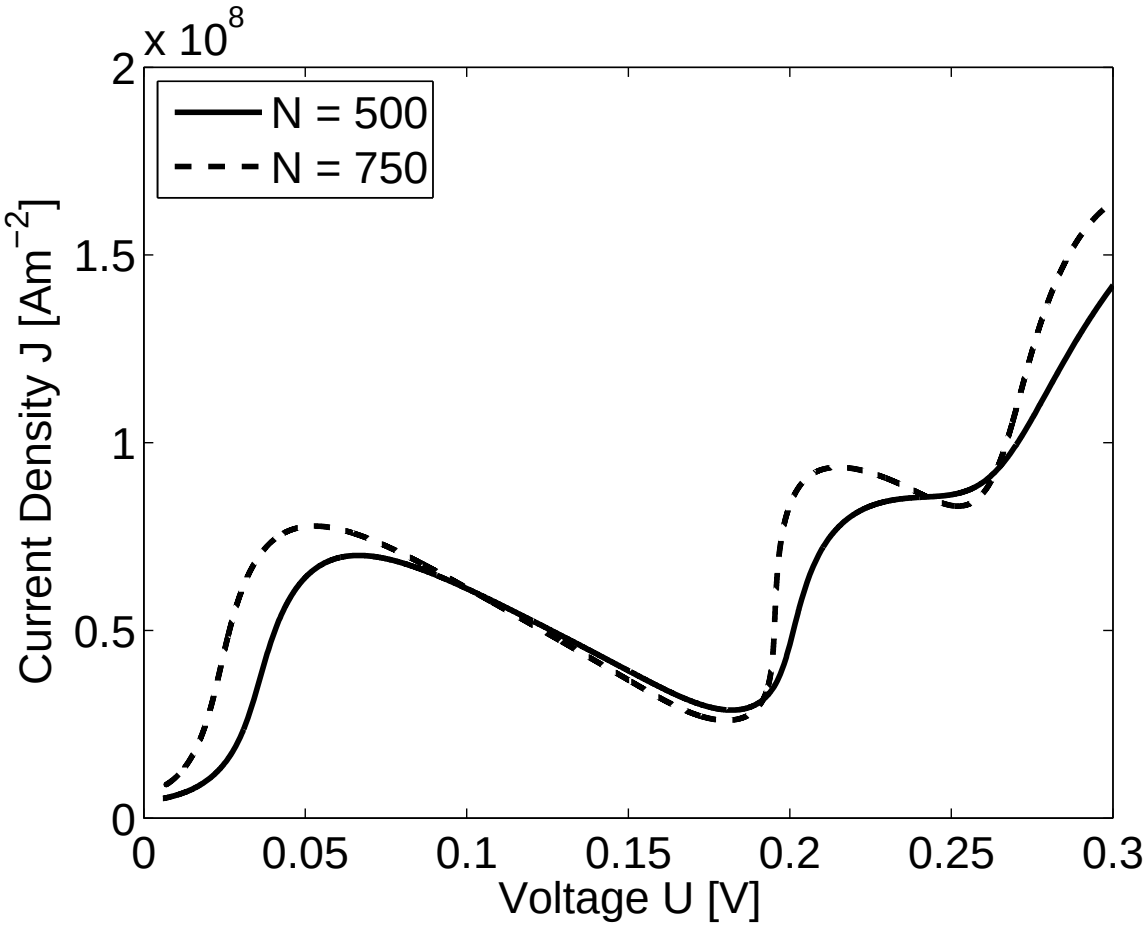


Simulation of quantum hydrodynamic model

- Classical gas dynamics: subsonic means $J/n < \sqrt{T}$
- Quantum hydrodynamics: dashed line separates sub- and supersonic
- From (a) to (d): increasing applied voltage



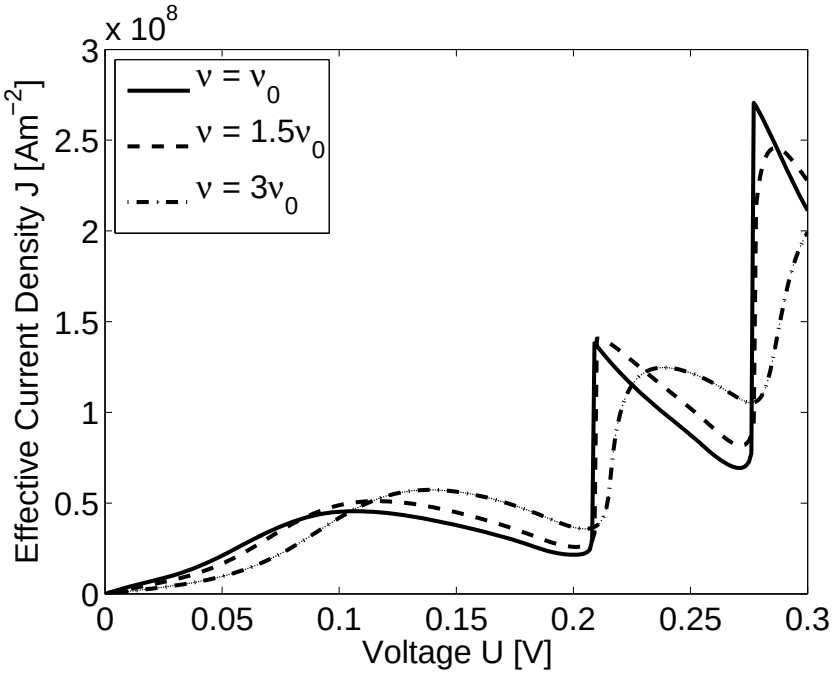
Upwind finite differences for quantum hydrodynamics



- Scheme strongly mesh dependent
- Central finite difference scheme unstable
- Central finite differences for viscous QHD stable

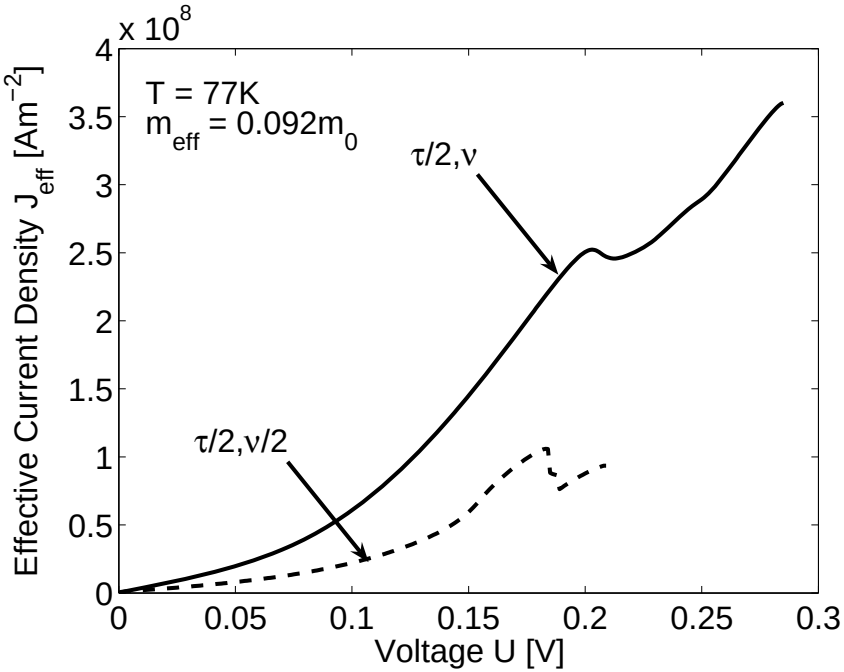
Viscous quantum hydrodynamic model

Isothermal viscous QHD:



- Curve not physical (wrong jump)
- Use full viscous quantum hydrodynamic model

Full viscous QHD:



- Effective mass larger than physical mass $m^* = 0.067 m_0$
- Weak negative differential resistance $\longrightarrow$ viscosity too strong

Summary

Quantum hydrodynamic (QHD) equations

$$\partial_t n - \operatorname{div} J = 0,\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n} + P\right) + n\nabla V = -\langle pQ_1(w)\rangle$$
$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J - q\right) + J\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

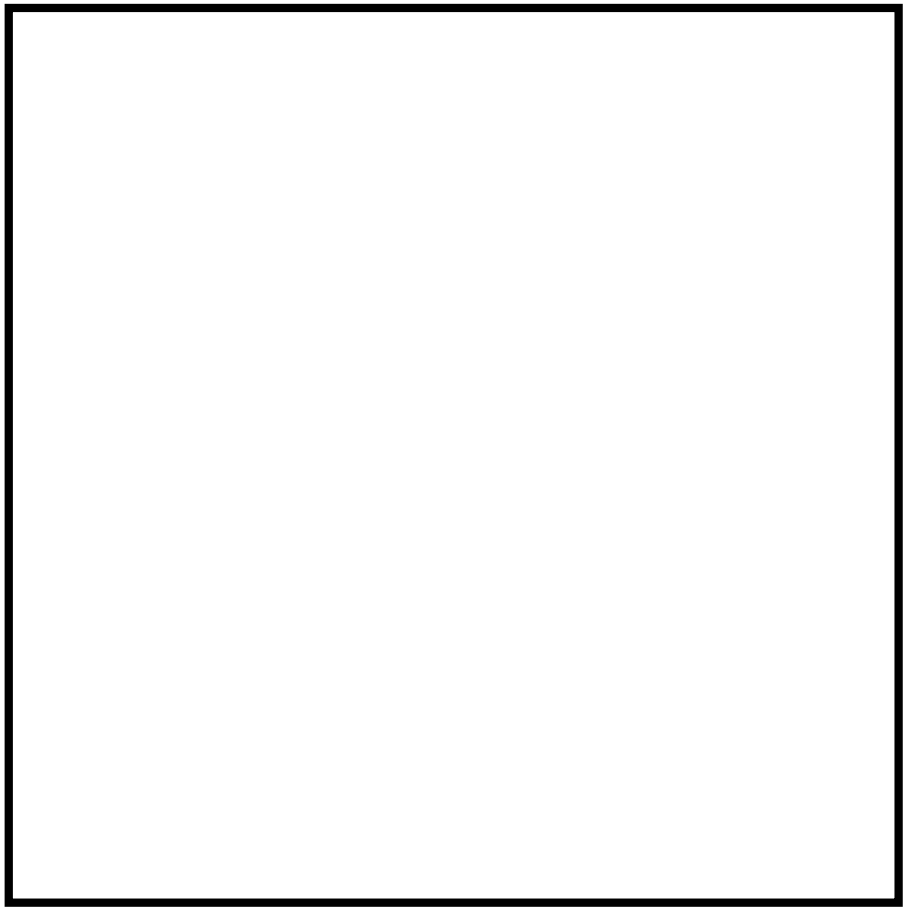
- Single-state Schrödinger $\longrightarrow$ zero-temperature QHD
- Diffusion approximation of Wigner equation $\longrightarrow$ full QHD
- $O(\varepsilon^4)$-expansion gives local QHD model with vorticity-type terms
- Scattering models: Caldeira-Leggett and Fokker-Planck
- Viscous QHD model: influences (too) strongly quantum effects
- Quantum Navier-Stokes model: viscous correction related to viscous QHD

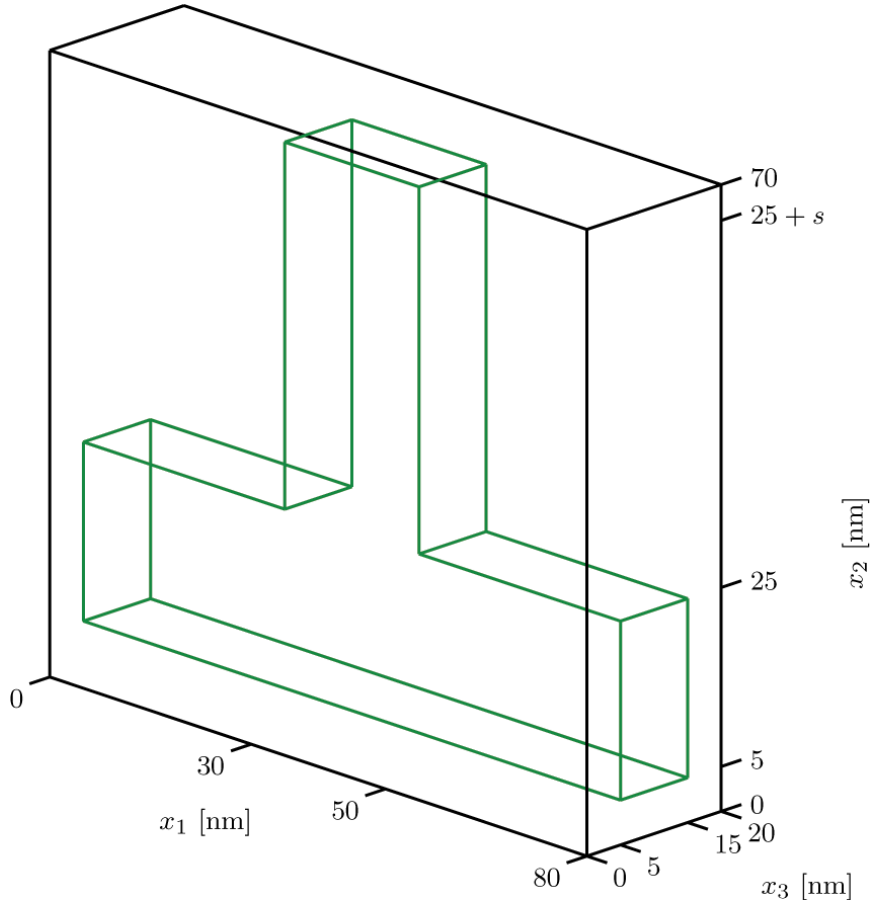
Overview

1. Semiconductor modeling
   - Basics of semiconductor physics
   - Kinetic models
2. Semi-classical macroscopic models
   - General strategy
   - Drift-diffusion models
   - Energy-transport models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Quantum kinetic models
   - Quantum Maxwellians
   - Quantum drift-diffusion models
   - Quantum hydrodynamic models
4. New and future devices
5. Summary

Quantum transistor

- Controls electron current by potential variation in stub
- Transistor has two states: on-state and off-state
- Typical size: 10...25 nm





Quantum transistor: evolution of density

The video can be found at http://www.jungel.at.vu → Simulations

Spintronics

- Up to now, only electron charge used in semiconductors
- Electrons can be distinguished by their spin: "up" or "down"

Applications:

- Densely-packed storage in hard drives
- Spin-polarized transport in transistors

Giant magnetoresistance:

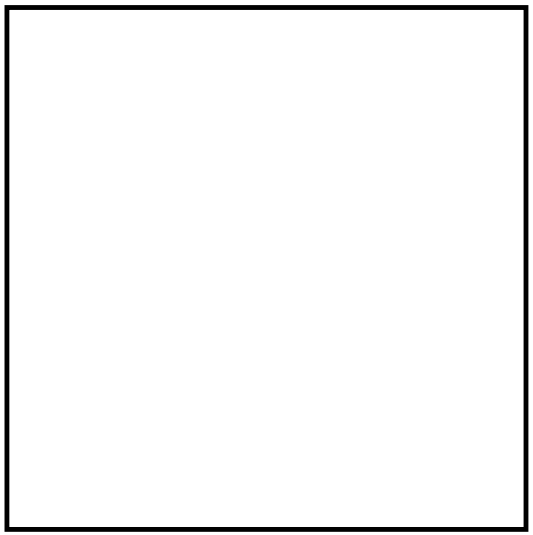
- 2007 Nobel Prize in Physics for Fert and Grünberg
- Hard disc with layers of different ferromagnetic material
- Magnetization influences electrical resistance
- Allows for increased sensitivity of hard-drive read head

Spin transistor:

- Source: gives spin-polarized electrons
- Drain: works as spin analyzer
- Gate voltage: changes spin of electrons to control the current

Beyond silicon

- Silicon may be used up to 22 nm technology (expected 2012) but devices are extremely sensitive to fabrication spreads
- New materials allow for higher speed and less power:
  - Gallium arsenide used 1993 in Cray 3 design
  - Indium-antimonide-based transistor (Intel 2006): 1.5 times the speed of silicon-based transistors and 1/10 the power
  - Blend of silicon and indium antimonide (Intel 2008): runs as fast as 140 GHz
  - Hafnium-based 45nm devices (IBM, Intel 2008): reduce leak current
  - Drawbacks: smaller wafers, expensive production
- Silicon-based nanowires: very small, easy handling, but high power consumption



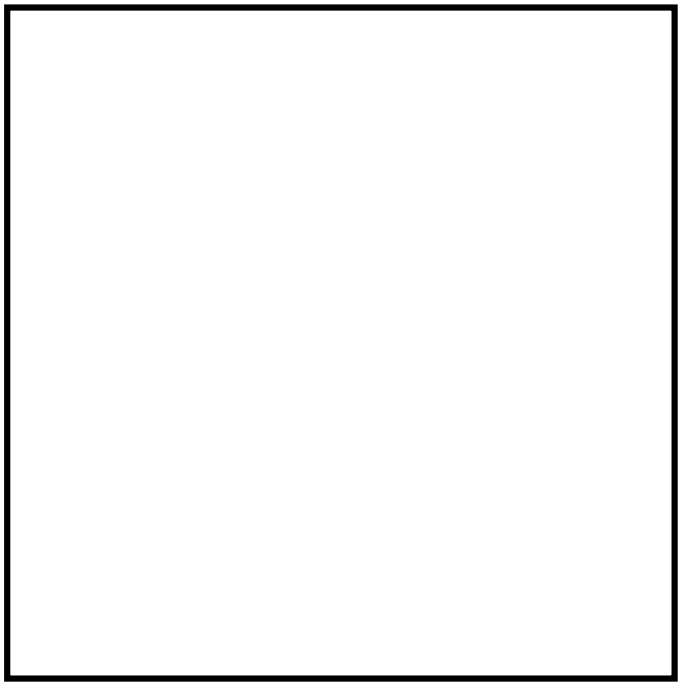
Beyond silicon

Carbon nanotubes:

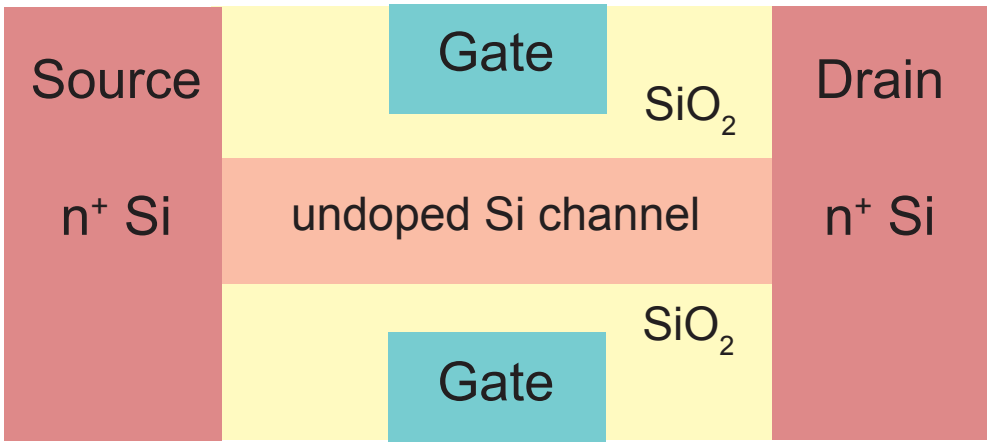
- Advantages: extremely small (diameter 1 nm), potential for ultra high-speed, fast cooling
- Difficulty: to place nanotubes precisely, mass production

Graphen:

- Advantage: high conductivity $\longrightarrow$ noise reduction and 100 GHz clock speed (IBM 2010)
- Difficulty: metal-like properties, mass production



New transistors



- Double-gate field-effect transistor
  - Allows for a very efficient control of carrier transport
  - Fabrication more complex than standard MOS transistors
  - Suitable for sub-10 nm silicon transistors?
- Single-electron transistor
  - Like MOS transistor with channel replaced by quantum dot limited by two tunnel barriers
  - Difficulties: Sensitivity to random background charges and to fabrication spreads

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Summary

Kinetic models:

- Allow for a statistical description of transport phenomena
- Important: modeling of collisions

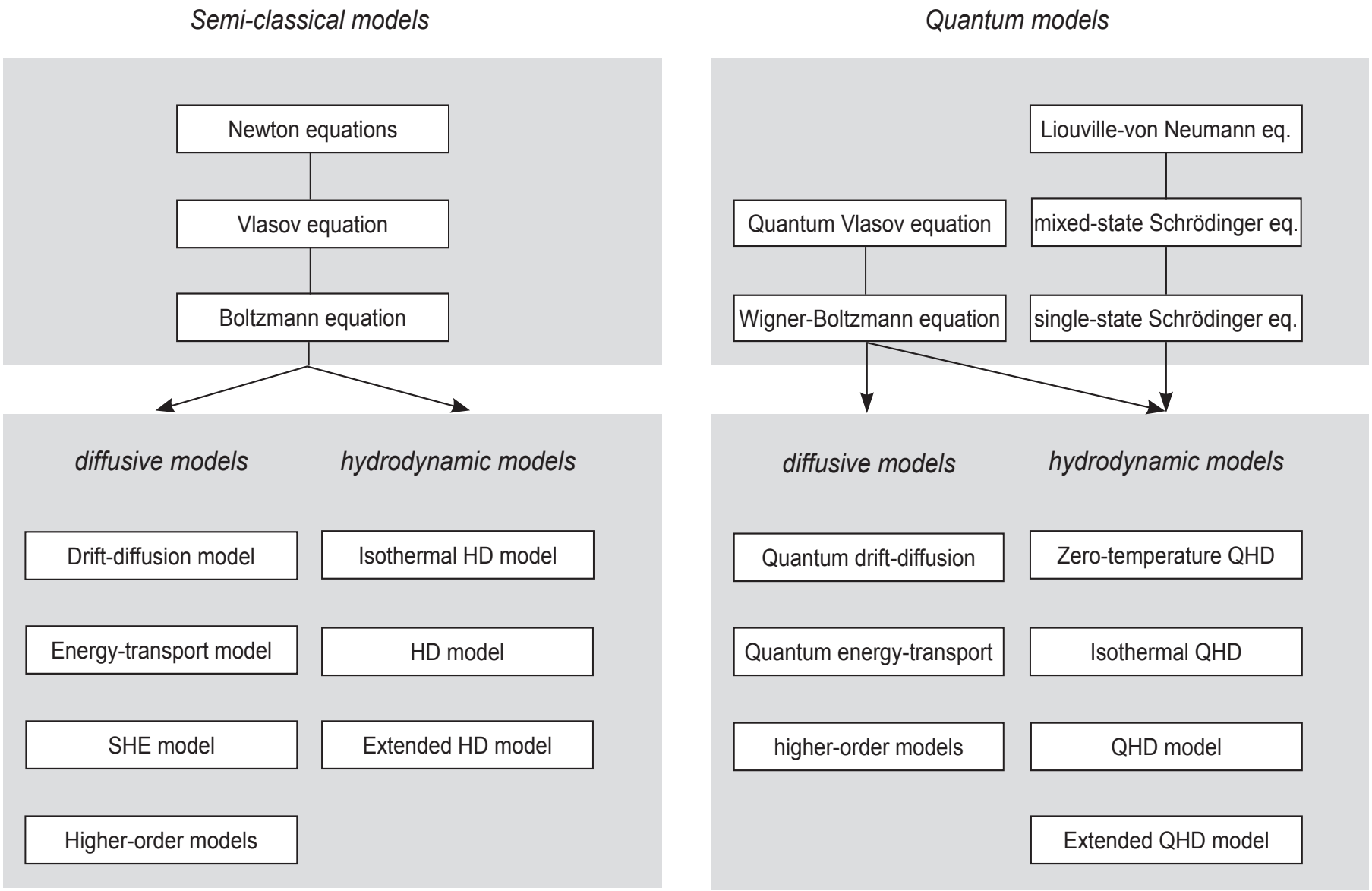
Semi-classical macroscopic models:

- Numerically cheaper than kinetic models
- Derivation from kinetic model by moment method
- Diffusive models derived by 3-step method (Chapman-Enskog expansion)
- Hydrodynamic models derived by 2-step method

Quantum macroscopic models:

- Relaxation-time collision operator with quantum Maxwellian
- Derivation by 2-step or 3-step method
- Local models derived by expansion in scaled Planck constant

Summary


Semi-classical models
Quantum models
Newton equations
Vlasov equation
Boltzmann equation
Liouville-von Neumann eq.
Quantum Vlasov equation
mixed-state Schrödinger eq.
Wigner-Boltzmann equation
single-state Schrödinger eq.
Microscopic models
diffusive models
hydrodynamic models
diffusive models
hydrodynamic models
Drift-diffusion model
Isothermal HD model
Energy-transport model
HD model
SHE model
Extended HD model
Higher-order models
Quantum drift-diffusion
Zero-temperature QHD
Quantum energy-transport
Isothermal QHD
higher-order models
QHD model
Extended QHD model
Macroscopic models