# Quantum Semiconductor Modeling

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# Contents

# Literature

**Main reference**

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- Physics of semiconductors:
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- Microscopic semiconductor models:
  - A. Arnold and A. Jüngel. Multi-scale modeling of quantum semiconductor devices. In: A. Mielke (ed.), *Analysis, Modeling and Simulation of Multiscale Problems*, pp. 331-363, Springer, Berlin, 2006.
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  - P. Degond. Mathematical modelling of microelectronics semiconductor devices. Providence, 2000.
  - P. Markowich, C. Ringhofer, and C. Schmeiser. *Semiconductor Equations.* Vienna, 1990.

# History of Intel processors

1971

4004

108 KHz, 2250 transistors,
channel length: $10\mu$m ($1\mu$m$= 10^{-6}$m)

1982

80286

12 MHz, 134,000 transistors,
channel length: $1.5\mu$m

1993

Pentium 1

66 MHz, 7,500,000 transistors,
channel length: $0.35\mu$m

2008

Core 2

3 GHz, 410,000,000 transistors,
channel length: $0.045\mu$m$=$ 45nm

# Transistor feature size

# Challenges in semiconductor simulation

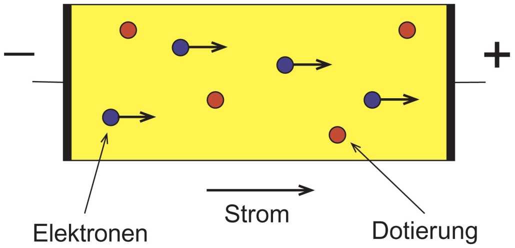
Future processors (2011):

- Number of transistors $> 1{,}000{,}000{,}000$
- Transistor channel length $22\,\text{nm}$
- Highly-integrated circuits:
  power density $> 100\,\text{W}/\text{cm}^2$

Key problems:

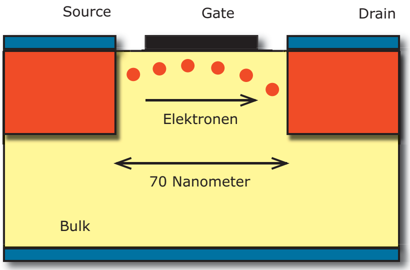
| | | |
|---|---|---|
| Decreasing power supply | $\longrightarrow$ | noise effects |
| Increasing frequencies | $\longrightarrow$ | multi-scale problems |
| Increasing design variety | $\longrightarrow$ | need of fast and accurate simulations |
| Increasing power density | $\longrightarrow$ | parasitic 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 materials: 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

- Describe quantum transport in semiconductors
- Formulate microscopic quantum models
- Model macroscopic electron transport (numerically cheaper than microscopic models)
- Describe simple quantum collision mechanisms and quantum diffusion
- Numerical approximation of quantum models

# Overview

1. Semiconductor modeling
2. Microscopic quantum models
   - Density matrices
   - Schrödinger models
   - Wigner models
3. Macroscopic quantum models
   - Quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Actual and emerging directions
   - Quantum transistor
   - Spintronics
   - New materials and devices
5. Summary and open problems

# Classical particle transport

- Given particle ensemble with mass $m$ moving in a vacuum
- Trajectory $(x(t), v(t))$ computed from Newton 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* $\dot{x} = X(x,v)$, $\dot{v} = U(x,v)$. *If*

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

$\longrightarrow$ 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:

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

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

$$\text{Particle density:} \quad n(x,t) = \int_{\mathbb{R}^3} f(x,v,t)dv$$

$$\text{Current density:} \quad J(x,t) = \int_{\mathbb{R}^3} vf(x,v,t)dv$$

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

- 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 $\psi$
- 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.)
- Goal: exploit periodicity of lattice potential

# 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)*

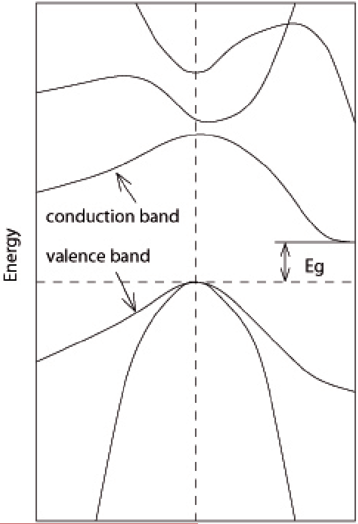
$$-\frac{\hbar^2}{2m}\Delta\psi - qV_L(x)\psi = E\psi, \quad \psi(x+y) = e^{ik\cdot x}\psi(x), \ y \in \textit{lattice}$$

- *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*

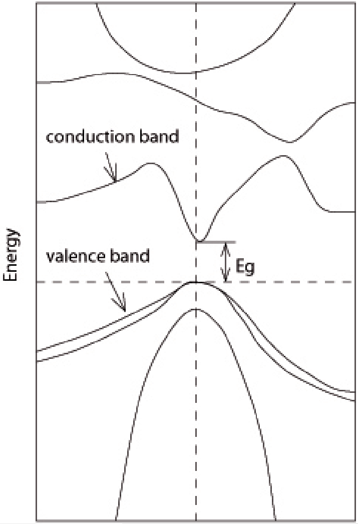
- $E_n(k) = n$-th energy band
- energy gap = all $E^*$ for which there is no $k$ with $E_n(k) = E^*$

# Energy bands

Silicon



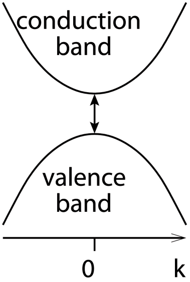

Gallium Arsenide



# Parabolic band approximation

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

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




- Diagonalization:

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

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

"Proof" of theorem:

- Insert $\psi_{n,k}(x) = e^{ik\cdot x}u_{n,k}(x)$ in Schrödinger equation $\Rightarrow$ first eq.
- $P\psi = \hbar k\psi$ if $\psi = e^{ik\cdot x}$: $\hbar k$ = 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 $m^*$:

$$p = m^* v_n, \quad \text{where } p = \hbar k$$

- 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:

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

# 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

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

- 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 $E = E_{\rm ext} + E_{\rm mean}$
- Mean-field approximation of electric field:

$$E_{\rm mean}(x,t) = \int_{\mathbb{R}^3} n(y,t)E_c(x,y)dy$$

- Electric force given by Coulomb field:

$$E_c(x,y) = -\frac{q}{4\pi\varepsilon_s}\frac{x-y}{|x-y|^3} \quad \Rightarrow \quad {\rm div}\, E_{\rm mean} = -\frac{q}{\varepsilon_s}n$$

- External electric field generated by doping atoms:

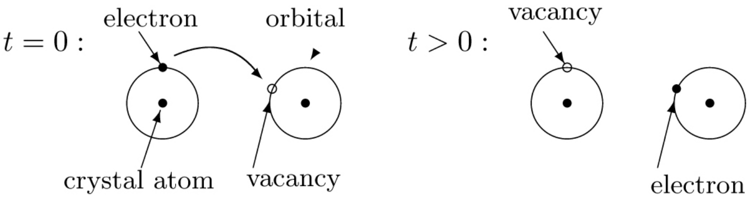
$$E_{\rm ext}(x,t) = \frac{q}{4\pi\varepsilon_s}\int_{\mathbb{R}^3} C(y)\frac{x-y}{|x-y|^3}dy \quad \Rightarrow \quad {\rm div}\, E_{\rm ext} = \frac{q}{\varepsilon_s}C(x)$$

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

**Poisson equation**

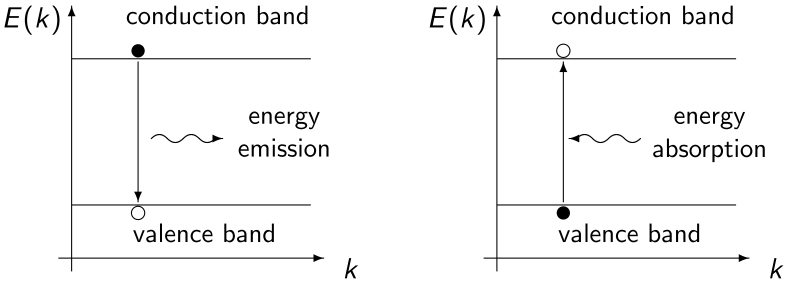
$$\varepsilon_s \Delta V = -\varepsilon_s {\rm div}\,(E_{\rm mean} + E_{\rm ext}) = q(n - C(x))$$

# 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:

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

# 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 $k \in B \sim (-\pi,\pi)^3$)
- Total number of quantum states (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 $dk$:

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

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

# Collisions

- 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 $\delta$: delta distribution, $E' = E(k')$
- If phonon scattering is elastic: $s(x,k,k') = \sigma(x,k,k')\delta(E' - E)$

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

- Mass and energy conservation:

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

# 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: $s(k,k',k_1,k_1') = \sigma\delta(E'+E_1'-E-E_1)$
- Collision operator:

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

- 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:

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

# Overview

# Liouville-von Neumann equation

Formulations of quantum mechanical motion of electrons:

- Schrödinger formulation
- Density-matrix formulation
- Kinetic Wigner formulation

Schrödinger equation:

$$i\hbar\partial_t\psi = H_x\psi = \Big(-\frac{\hbar^2}{2m}\Delta_x - V(x,t)\Big)\psi, \quad \psi(\cdot,0)=\psi_I$$

Motivation for density matrix formulation:

- Define density matrix $\rho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}$
- 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:

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

# Density matrix

General quantum state is represented by density matrix operator $\widehat{\rho}$

Liouville-von Neumann equation:

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

- 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)
- There exists density matrix $\rho(x, y, t)$ such that

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

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

# Density matrix

- $\widehat{\rho}$: self-adjoint compact solution of Liouville-von Neumann equation
- $\rho(x,y,t)$: corresponding density matrix
- $(\psi_j,\lambda_j)$: eigenfunction-eigenvalue pairs of $\widehat{\rho}$

## Proposition (Properties of density matrix)

- *$\rho$ solves Liouville-von Neumann "matrix" equation*

$$i\hbar\partial_t\rho(x,y,t) = (H_x - H_y)\rho(x,y,t), \quad t>0, \quad \rho(x,y,0)=\rho_I(x,y),$$

*where $H_x$, $H_y$ act on $x$, $y$, respectively, and $\rho_I$ is given by*

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

- *$\rho$ can be expanded in terms of $(\psi_j)$:*

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

# Relation between density matrix and Schrödinger equation

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

**Theorem (Mixed-state Schrödinger equation)**

*Eigenfunction $\psi_j$ 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 $(\psi_j, \lambda_j)$ 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 states:

- Sequence of solutions $\psi_j$ to

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

- Sequence of numbers $\lambda_j$: gives particle density

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

## Single 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: $J = -(\hbar q/m)\mathrm{Im}(\overline{\psi}\nabla_x\psi)$

# Overview

# Schrödinger equation

- Suitable for ballistic transport (no collisions)
- Closed quantum systems: no interactions with environment
- Open quantum systems: interactions with environment

Stationary Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\Delta\psi - qV(x)\psi = E\psi \quad \text{in } \Omega$$

- Scaling: $x = Lx_s$, $V = (k_B T_L/q)V_s$, $E = (k_B T_L)E_s$
- Scaled Schrödinger equation:

$$-\frac{\varepsilon^2}{2}\Delta\psi - V(x)\psi = E\psi, \quad \varepsilon = \frac{\hbar}{\sqrt{m^* k_B T_L L^2}}$$

Macroscopic quantities:

- Electron density: $n(x,t) = |\psi(x,t)|^2$
- Electron current density: $J(x,t) = -\varepsilon \mathrm{Im}(\overline{\psi}\nabla\psi)$

# Transparent boundary conditions

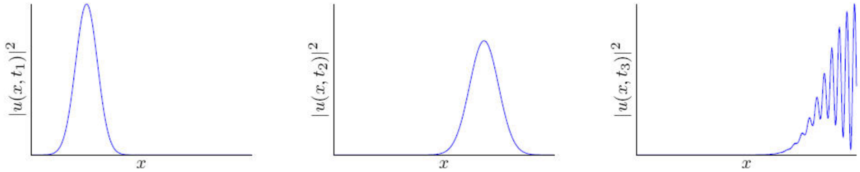
Objective: solve Schrödinger equation in $\mathbb{R}$

Idea: solve Schrödinger equation in bounded interval

Problem: how to choose (transparent) boundary conditions

What can go wrong?

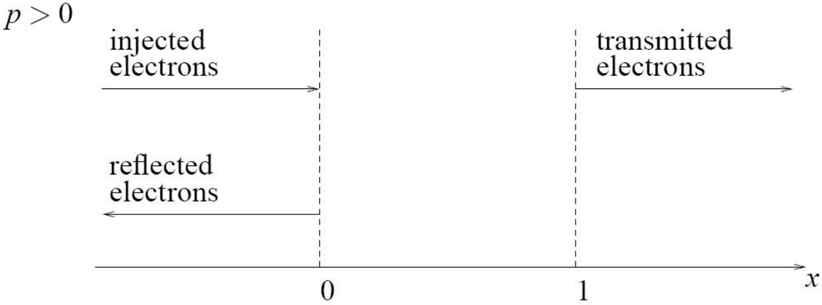
- Example: transient Schrödinger equation in $\mathbb{R}$
- Solve Schrödinger equation in bounded interval $I$ with boundary conditions $\psi = 0$ on $\partial I$
- Problem: spurious oscillations when wave hits the boundary
- Solution: construct transparent boundary conditions



# One-dimensional transparent boundary conditions

- One-dimensional stationary equation: $-\frac{\varepsilon^2}{2}\Delta\psi - V(x)\psi = E\psi$ in $\mathbb{R}$
- Active region: $(0,1)$, wave guides: $(-\infty,0)$ and $(1,\infty)$
- Electric potential: $V(x) = V(0)$ for $x<0$, $V(x)=V(1)$ for $x>1$

Objective: construct exact transparent boundary conditions (Lent/Kirkner 1990, Ben Abdallah/Degond/Markowich 1997)



# One-dimensional transparent boundary conditions

- Ansatz for explicit solution if $p > 0$:

$$\psi_p(x) = \begin{cases} \exp(ipx/\varepsilon) + r(p)\exp(-ipx/\varepsilon) & \text{for } x < 0 \\ t(p)\exp(ip_+(p)(x-1)/\varepsilon) & \text{for } x > 1 \end{cases}$$

- $r(p)$ and $t(p)$ can be determined from Schrödinger equation
- Insert ansatz into Schrödinger equation:

$$E = \frac{p^2}{2} - V(0), \quad p_+(p) = \sqrt{2(E + V(1))} = \sqrt{p^2 + 2(V(1) - V(0))}$$

- Boundary conditions at $x = 0$ and $x = 1$: employ ansatz and eliminate $r(p)$:

$$\varepsilon\psi_p'(0) + ip\psi_p(0) = 2ip, \quad \varepsilon\psi_p'(1) = ip_+(p)\psi_p(1)$$

- Similar results for $p < 0$ with $p_-(p) = \sqrt{p^2 + 2(V(1) - V(0))}$

# One-dimensional transparent boundary conditions

**Theorem (Lent-Kirkner boundary conditions)**

*The solution* $(\psi_p, E_p)$ *of the eigenvalue problem*

$$-\frac{\varepsilon^2}{2}\psi_p'' - V(x)\psi_p = E_p\psi_p, \quad x \in \mathbb{R},$$

*solves the Schrödinger equation on* $(0,1)$ *with boundary conditions*

$$\begin{aligned} \varepsilon\psi_p'(0) + ip\psi_p(0) &= 2ip, \quad \varepsilon\psi_p'(1) = ip_+(p)\psi_p(1), \quad p > 0 \\ -\varepsilon\psi_p'(1) + ip\psi_p(1) &= 2ip, \quad \varepsilon\psi_p'(1) = -ip_-(p)\psi_p(1), \quad p < 0 \end{aligned}$$

*where* $E_p = p^2/2 - V(0)$ *if* $p > 0$ *and* $E_p = p^2/2 - V(1)$ *if* $p < 0$.

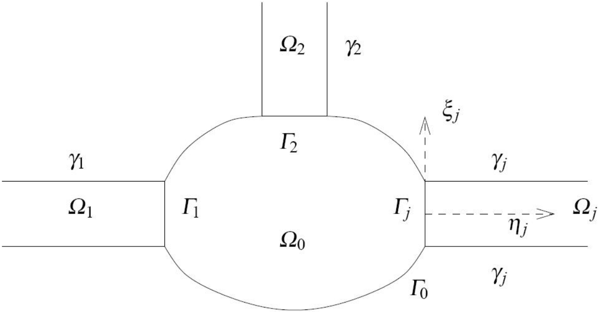
- $r(p)$ and $t(p)$ are given in terms of $\psi_p(x)$, $\psi_p'(x)$ for $x = 0, 1$
- Electron density: $n(x) = \int_{\mathbb{R}} f(p)|\psi_p(x)|^2 dp$, $f(p)$: statistics
- Current density: $J(x) = \frac{q\hbar}{m^*}\int_{\mathbb{R}} f(p)\mathrm{Im}(\overline{\psi_p(x)}\nabla\psi_p(x))dp$

# Multi-dimensional transparent boundary conditions

$$-\frac{\varepsilon^2}{2}\Delta\psi - V(x)\psi = E\psi \text{ in } \Omega, \quad \psi = 0 \text{ on } \partial\Omega$$

- Generalization due to Ben Abdallah 2000, BenAbdallah/Méhats/Pinaud 2005
- Semiconductor domain $\Omega = \Omega_0 \cup \Omega_1 \cup \cdots \cup \Omega_N$
- Active region: $\Omega_0$, wave-guide zones (cylinders): $\Omega_j$

Objective: formulate Schrödinger problem on $\Omega_0$ only



# Multi-dimensional transparent boundary conditions

$$-\frac{\varepsilon^2}{2}\Delta\psi - V(x)\psi = E\psi \text{ in } \Omega, \quad \psi = 0 \text{ on } \partial\Omega$$

- Boundary between active region and wave guides: $\Gamma_j$
- Assumption: $V$ depends only on transversal directions $\xi_j$ in $\Omega_j$
- Let $(\psi_m^j, E_m^j)$ be solution to the transversal Schrödinger problem

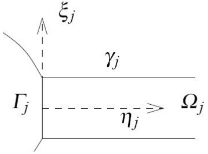
$$-\frac{\varepsilon^2}{2}\Delta\psi - V(\xi_j)\psi = E\psi \quad \text{in } \Gamma_j, \quad \psi = 0 \quad \text{on } \partial\Gamma_j$$

- Solution in waveguide $\Omega_j$:

$$\psi(\xi_j, \eta_j) = \sum_{j=1}^{\infty} \psi_m^j(\xi_j)\lambda_m^j(\eta_j), \quad \lambda_m^j = \text{longitudinal plane waves}$$

Result: boundary condition on $\partial\Omega_0$:

$$\psi|_{\Gamma_0} = 0, \quad \varepsilon\frac{\partial\psi}{\partial\eta_j}\Big|_{\Gamma_j} = \sum_{m=1}^{\infty} f_m(\psi, \psi_m^j)$$



# Transient transparent boundary conditions

$$i\varepsilon\partial_t\psi_m = -\frac{\varepsilon^2}{2}\Delta\psi_m - V(x,t)\psi_m \quad \text{in } \Omega,\ t>0, \quad \psi_m(\cdot,0)=\psi_m^0$$

- Homogeneous boundary conditions: Arnold 1998, Antoine/Besse 2001
- Inhomogeneous boundary cond.: BenAbdallah/Méhats/Pinaud 2005
- Let $\psi_m^0$ be waveguide solutions in $\Omega_j$
- Let $\psi_m^{\rm pw}$ be plane waves in $\Omega_j$
- Reduction to Schrödinger problem on $\Omega_0$ possible with boundary condition (in 1D approximation)

$$\frac{\partial}{\partial\eta_j}(\psi_m - \psi_j^{\rm pw}) = -\sqrt{\frac{2m}{\hbar}}e^{-i\pi/4}\sqrt{\partial_t}(\psi_m - \psi_j^{\rm pw}) \quad \text{on } \Gamma_j$$

- Fractional derivative:

$$\sqrt{\partial_t}f = \pi^{-1/2}\frac{d}{dt}\int_0^t \frac{f(s)}{\sqrt{t-s}}ds$$

- Implementation of $\sqrt{\partial_t}$ delicate: review Arnold/Ehrhardt et al. 2008

# Transient transparent boundary conditions

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - V(x,t)\psi \quad \text{in } \Omega,\ t>0$$

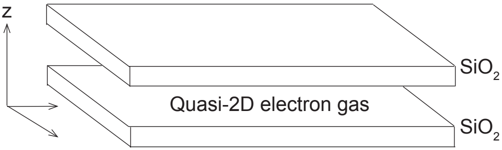
Second approach: Imaginary potential

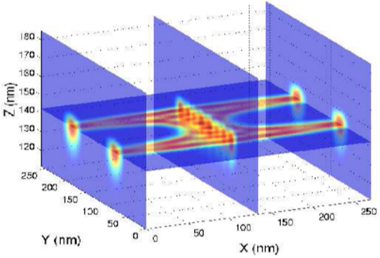
- Idea: add to Schrödinger the imaginary potential $iW(x)$

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - (V(x,t)+iW(x))\psi \quad \text{in } \Omega\cup\Omega_1,\ t>0$$

  where $W=0$ in $\Omega$ (active region) and $W>0$ in $\Omega_1$ (comput. region)
- For $\varepsilon\partial_t|\psi|^2 = -W(x)|\psi|^2$, $|\psi(x,t)|^2$ decays to zero
- Advantages: easy implementation, fast computation
- Drawbacks: computational domain larger, need to adapt values of $W$
- Discussion of form of $W$: Neuhauser/Baer 1989, Ge/Zhang 1998

# Confined electron transport




Ben Abdallah/Polizzi 2002

- Quantum waveguides rely on formation of quasi 2D electron gas
- Objective: derive 2D Schrödinger model
- Confinement of electrons in $z$ direction, transport in other directions
- Assumption: $z$ length scale is of order of de Broglie wave length

# Partially quantized Schrödinger models

## Scaled Schrödinger equation:

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta_x\psi - \frac{1}{2}\partial_z^2\psi - V(x,z,t)\psi, \quad \psi(\cdot,0) = \psi_I$$

- Solve for $(x,z) \in \mathbb{R}^m \times (0,1)$, $t > 0$, $V$ given
- Hard-wall boundary conditions: $\psi(x,z,t) = 0$ for $z = 0$ and $z = 1$
- $\varepsilon$: ratio between length scale in transversal/longitudinal directions
- Objective: $\varepsilon \to 0$ (Ben Abdallah/Méhats 2005)

## Subbands:

- Transversal Hamiltonian $-\frac{1}{2}\partial_z^2 - V$ has discrete spectrum
- Eigenfunction-eigenvalue pairs $(\chi_p^\varepsilon, E_p^\varepsilon)$ of

$$-\frac{1}{2}\partial_z^2\chi_p^\varepsilon - V\chi_p^\varepsilon = E_p^\varepsilon\chi_p^\varepsilon, \quad \chi_p^\varepsilon(x,z,t) = 0 \quad \text{for } z = 0,1$$

- Definition of subband: $L^2(\mathbb{R}^m) \otimes \mathrm{span}(\chi_p^\varepsilon)$
- Effects as $\varepsilon \to 0$: adiabatic decoupling of subbands and semi-classical transport within each subband

# Partially quantized Schrödinger models

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta_x\psi - \frac{1}{2}\partial_z^2\psi - V(x,z,t)\psi, \quad \psi(\cdot,0) = \psi_I$$

- Electron and current densities: $n_\varepsilon = |\psi^\varepsilon|^2$, $J_\varepsilon = \varepsilon \mathrm{Im}(\overline{\psi}_\varepsilon \nabla\psi_\varepsilon)$
- Surface electron and current densities: $n_\varepsilon^s = \int_0^1 n_\varepsilon dz$, $J_\varepsilon^s = \int_0^1 J_\varepsilon dz$

**Theorem (Ben Abdallah/Méhats 2005)**

*As $\varepsilon \to 0$, $(n_\varepsilon, J_\varepsilon)$ converges (in the sense of distributions) to*

$$n(x,z,t) = \sum_p \Big( \int_{\mathbb{R}^m} f_p(x,v,t)dv \Big) |\chi_p(x,z,t)|^2$$

$$J(x,z,t) = \sum_p \Big( \int_{\mathbb{R}^m} f_p(x,v,t)vdv \Big) |\chi_p(x,z,t)|^2,$$

*where $f_p$ solves a Vlasov equation.*

# Partially quantized Schrödinger models

$$n(x,z,t) = \sum_p \Big( \int_{\mathbb{R}^m} f_p(x,v,t)dv \Big) |\chi_p(x,z,t)|^2$$

$$J(x,z,t) = \sum_p \Big( \int_{\mathbb{R}^m} f_p(x,v,t)vdv \Big) |\chi_p(x,z,t)|^2,$$

- Vlasov equation for $f_p$:

$$\partial_t f_p + v \cdot \nabla_x f_p - \nabla_x E_p \cdot \nabla_v f_p = 0, \quad f_p(\cdot,\cdot,0) = f_{p,I}(x,v),$$

- Initial datum $f_{p,I}$ given by Wigner transform of $\psi_I$ (see below)
- $(n_\varepsilon^s, J_\varepsilon^s)$ converges to $(n^s, J^s) = \int_0^1 (n,J)dz$ with

$$\partial_t n^s - \mathrm{div}\, J^s = 0$$

- Transport in subband driven by $\nabla_x E_p$, where $E_p = \lim_{\varepsilon\to 0} E_p^\varepsilon$
- Advantage: dimension reduction, cheaper numerical cost
- Inclusion of Poisson equation: Ben Abdallah/Méhats/Pinaud 2006

# Overview

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   - Quantum Maxwellian
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   - New materials and devices
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# 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: $E(k) = \hbar^2 |k|^2 / 2m^*$, $v(k) = \nabla_k E(k)/\hbar = \hbar k / m^*$
- 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 $p = \hbar k$

# 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: $E(k) = \hbar^2|k|^2/2m^*$, $v(k) = \nabla_k E(k)/\hbar = \hbar k/m^* = p/m^*$
- 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):

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

- Wigner-Weyl transform = inverse of Wigner transform

# Wigner equation

## Proposition (Quantum Vlasov or Wigner equation)

*Let $\rho$ 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*

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

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

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

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

- Symbol of $\theta[V]$:

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

# Potential operator

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

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

- Acts in the Fourier space as multiplication operator:

$$(\theta[V]w)(x,p,t) = (2\pi\hbar)^3\mathcal{F}(\delta V(x,y,t)u(x,-y,t))$$

- Symbol $\delta V$ = discrete directional derivative:

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

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

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

# 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 $\lambda$, reference time $\tau$, 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:

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

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

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

# Wigner equation: properties

$$\partial_t w + p \cdot \nabla_x w + \theta_\varepsilon[V]w = 0, \quad t > 0, \quad w(x,p,0) = w_I(x,p),$$

Semi-classical limit:

- 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 $\varepsilon \to 0$
- Semi-classical limit of Wigner equation = Vlasov equation

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

Nonnegativity of Wigner function:

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

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

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

# 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: $\alpha$, $\beta$, $\gamma$ 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
- $\alpha$ = 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:

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

- 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

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

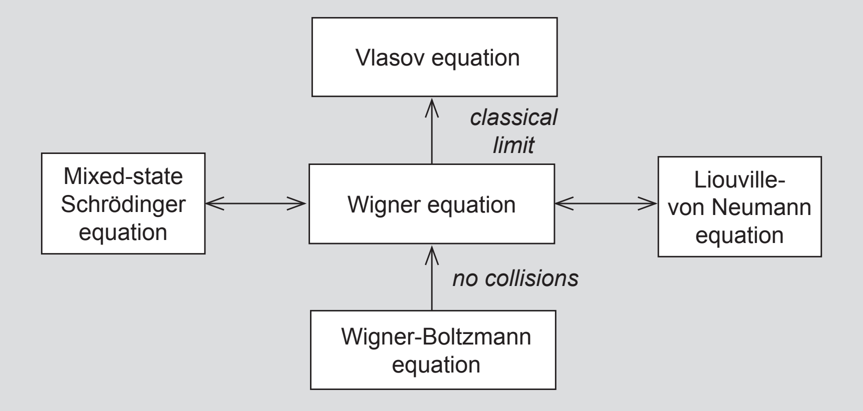
- Used in tunneling diode simulations (Frensley 1987, Kluksdahl et al. 1989)

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

# Summary

## Relation between density matrix – Schrödinger – Wigner formulation



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# Wigner equation

$$\partial_t w + \frac{p}{m^*} \cdot \nabla_x w + q\theta[V]w = 0, \quad x, p \in \mathbb{R}^3$$

Scaling:

| | |
|---|---|
| reference length $\lambda$ | reference time $\tau$ |
| reference momentum $m^*\lambda/\tau$ | reference voltage $k_B T_L/q$ |

- Assume that

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

- Scaled Wigner equation:

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

$$\theta[V]w(x,p,t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^6} \delta V(x,y,t) w(x,p',t) e^{iy\cdot(p-p')} dp'\, dy$$

$$\delta V(x,y,t) = \frac{i}{\varepsilon}\Big(V\Big(x + \frac{\varepsilon}{2}y, t\Big) - V\Big(x - \frac{\varepsilon}{2}y, t\Big)\Big)$$

# Classical Maxwellian

Classical thermal equilibrium:

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

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:

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

- Weight functions $\kappa(p) = (\kappa_0(p), \dots, \kappa_N(p))$ 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:

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

# 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:

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

- Two moments ($n$, $ne$) prescribed:

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

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

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

# Quantum Maxwellian

Expansion of quantum Maxwellian in powers of $\varepsilon^2$:

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

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

# Quantum Maxwellian

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

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

- Expansion in powers of $\varepsilon^2$:

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

$\longrightarrow$ first derived by Wigner 1932

- Compare to Maxwellian of constrained problem:

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

# Overview

1. Semiconductor modeling
2. Microscopic quantum models
   - Density matrices
   - Schrödinger models
   - Wigner models
3. Macroscopic quantum models
   - Quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Actual and emerging directions
   - Quantum transistor
   - Spintronics
   - New materials and devices
5. Summary and open problems

# Derivation

- Diffusion-scaled Wigner-Boltzmann equation: $t \to t/\alpha$, $Q(w) \to Q(w)/\alpha$

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

- 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:

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

- Properties of potential operator:

$$\langle \theta[V]w \rangle = 0, \quad \langle p\theta[V]w \rangle = -\langle w \rangle \nabla_x V \quad \text{for all } w$$

- 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 $\alpha \to 0$:

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

- Computation of current density $J_n$:

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

**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*

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

# Expansion in powers of $\varepsilon^2$

- Nonlocal relations:

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

- Expansion of quantum exponential:

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

- Electron density:

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

# Expansion in powers of $\varepsilon^2$

- Electron density:

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

- Quantum stress tensor:

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

- Express $A$ in terms of $n$

# Expansion in powers of $\varepsilon^2$

- 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:

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

- Current density:

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

**Theorem (Local quantum drift-diffusion equations)**

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

# Local quantum drift-diffusion equations

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

- 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: $\partial\Omega = \Gamma_D \cup \Gamma_N$

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

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

# Local quantum drift-diffusion equations

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

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

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

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

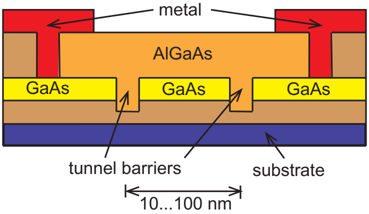
Mathematical results:

- 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

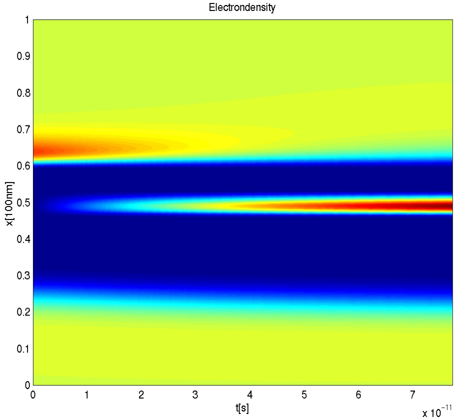



## Numerical method:

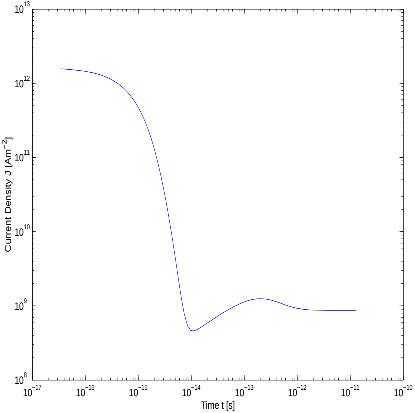
- semi-discretization in time
- finite differences in space (one-dimensional)
- Newton iterations

# Time-dependent simulations of tunneling diode

## Electron density $n(t)$

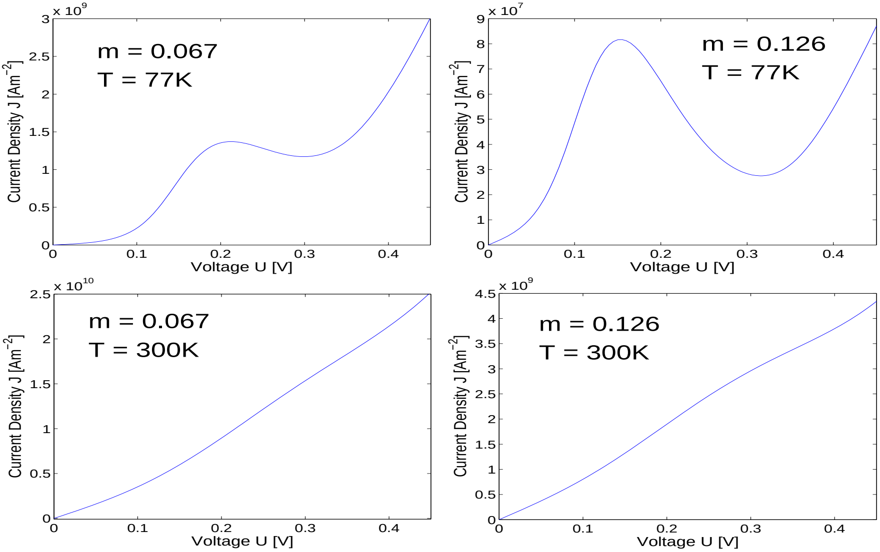



## Current density $J(t)$



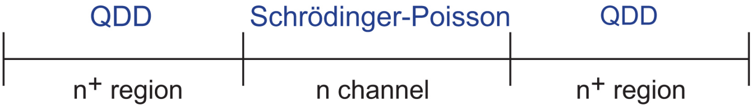

$\longrightarrow$ stabilization after $\sim 10^{-11}$ sec. (100 GHz)

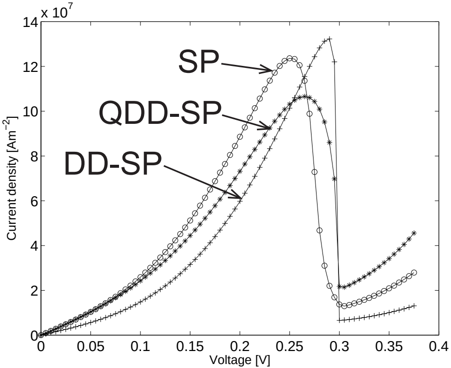
# Current-voltage characteristics of tunneling diode



# 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)

# Quantum entropy

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

- Quantum kinetic entropy (or free energy):

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

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

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

- Entropy inequality (Degond/Ringhofer 2003):

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

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

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

# 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:

- 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 $S_0$:

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

# Quantum entropy

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

**Proposition (Entropy inequality)**

*Let n solve local quantum drift-diffusion model. Then*

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

- Differentiate $S_0$:

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

# Quantum entropy

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

- Let $(n, V)$ solve quantum drift-diffusion model with Poisson equation $\lambda_D^2 \Delta V = n - C(x)$
- Quantum entropy:

$$\begin{aligned} S_1 &= -\int_{\mathbb{R}^3} \Big( n(\log n - 1) + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 - \frac{1}{2}(n-C)V \Big) dx \\ &= -\int_{\mathbb{R}^3} \Big( n(\log n - 1) + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + \frac{\lambda_D^2}{2}|\nabla V|^2 \Big) dx. \end{aligned}$$

- Entropy inequality:

$$-\frac{dS_1}{dt} + \int_{\mathbb{R}^3} n \Big| \nabla \Big( \log n - V - \frac{\varepsilon^2}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}} \Big) \Big|^2 dx \le 0$$

# Summary

**Local quantum drift-diffusion 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 model gives qualitatively good results
- Mathematical theory well developed
- Quantum entropy provides a priori estimates

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# Wigner-BGK equation

- Wigner-BGK equation in diffusion scaling:

$$\alpha^2\partial_t w_\alpha + \alpha\big(p\cdot\nabla_x w_\alpha + \theta[V]w_\alpha\big) = Q(w_\alpha), \quad x,p\in\mathbb{R}^3,\ t>0$$

- Collision operator:

$$Q(w) = Q_0(w) + \alpha^2 Q_1(w), \quad Q_0(w) = M[w] - w$$

- Quantum Maxwellian: $M[w] = \operatorname{Exp}(\kappa\cdot\lambda)$ for given weight functions $\kappa = (\kappa_0,\ldots,\kappa_N)$
- Quantum Maxwellian for two prescribed moments:

$$M[w] = \operatorname{Exp}\Big(A - \frac{|p|^2}{2T}\Big)$$

- Moment equations: set $\langle g(p)\rangle = 2(2\pi\varepsilon)^{-3}\int_{\mathbb{R}^3} g(p)dp$

$$\partial_t\langle\kappa w_\alpha\rangle + \alpha^{-1}\big(\operatorname{div}_x\langle\kappa p w_\alpha\rangle + \langle\kappa\theta[V]w_\alpha\rangle\big) = \langle\kappa Q_1(w_\alpha)\rangle$$

# Derivation

$$\alpha^2\partial_t w_\alpha + \alpha\big(p\cdot\nabla_x w_\alpha + \theta[V]w_\alpha\big) = Q_0(w_\alpha) + \alpha^2 Q_1(w_\alpha)$$

Step 1: limit $\alpha\to 0$ in Wigner-BGK equation $\Rightarrow Q_0(w)=0$,
$w=\lim_{\alpha\to 0} w_\alpha \Rightarrow w = M[w] = \mathrm{Exp}(A-|p|^2/2T)$

Step 2: Chapman-Enskog expansion $w_\alpha = M[w_\alpha]+\alpha g_\alpha$

- Insert into Wigner-BGK equation:

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

- Limit $\alpha\to 0$: $g=\lim_{\alpha\to 0} g_\alpha = -p\cdot\nabla_x M[w]-\theta[V]M[w]$

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

- Insert $w_\alpha = M[w_\alpha]+\alpha g_\alpha$

$$\partial_t\langle\kappa w_\alpha\rangle + \alpha^{-1}\mathrm{div}_x \underbrace{\langle\kappa p M[w_\alpha]\rangle}_{=0} + \alpha^{-1}\underbrace{\langle\kappa\theta[V]M[w_\alpha]\rangle}_{=0}$$
$$+\,\mathrm{div}_x\langle\kappa p g_\alpha\rangle + \langle\kappa\theta[V]g_\alpha\rangle = \langle\kappa Q_1(w_\alpha)\rangle$$

# Derivation

- Moment equations:

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

- Limit $\alpha \to 0$:

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

where $g = -p \cdot \nabla_x M[w] - \theta[V] M[w]$

**Lemma**

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

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

$$\langle \tfrac{1}{2} p |p|^2 \theta[V] w \rangle = -\big( \langle p \otimes p w \rangle + \langle \tfrac{1}{2} |p|^2 w \rangle \, \mathrm{Id} \big) \nabla V + \frac{\varepsilon^2}{8} \langle w \rangle \nabla \Delta V$$

# Derivation

**Lemma**

$$\langle\theta[V]w\rangle = 0, \quad \langle p\theta[V]w\rangle = -\langle w\rangle\nabla V, \quad \langle\tfrac{1}{2}|p|^2\theta[V]w\rangle = -\langle pw\rangle\cdot\nabla V,$$
$$\langle\tfrac{1}{2}p|p|^2\theta[V]w\rangle = -\big(\langle p\otimes pw\rangle + \langle\tfrac{1}{2}|p|^2 w\rangle\,\mathrm{Id}\big)\nabla V + \tfrac{\varepsilon^2}{8}\langle w\rangle\nabla\Delta V$$

- Moment equation with $\kappa_0(p) = 1$ (if $Q_1$ conserves mass):

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

$$\Rightarrow \quad \partial_t n - \mathrm{div}\, J_n = 0$$

- Moment equation with $\kappa_2(p) = \frac{1}{2}|p|^2$:

$$\partial_t \underbrace{\langle\tfrac{1}{2}|p|^2 M[w]\rangle}_{=ne} + \mathrm{div}_x \underbrace{\langle\tfrac{1}{2}|p|^2 pg\rangle}_{=-J_e} + \underbrace{\langle\tfrac{1}{2}|p|^2\theta[V]g\rangle}_{=-\langle pg\rangle\cdot\nabla_x V} = \underbrace{\langle\tfrac{1}{2}|p|^2 Q_1(M[w])\rangle}_{=W}$$

$$\Rightarrow \quad \partial_t(ne) - \mathrm{div}\, J_e + J_n\cdot\nabla V = W$$

# Derivation

## Lemma

$$\langle \theta[V]w \rangle = 0, \quad \langle p\theta[V]w \rangle = -\langle w \rangle \nabla V, \quad \langle \tfrac{1}{2}|p|^2\theta[V]w \rangle = -\langle pw \rangle \cdot \nabla V,$$
$$\langle \tfrac{1}{2}p|p|^2\theta[V]w \rangle = -\big(\langle p \otimes pw \rangle + \langle \tfrac{1}{2}|p|^2 w \rangle \,\mathrm{Id}\big)\nabla V + \tfrac{\varepsilon^2}{8}\langle w \rangle \nabla \Delta V$$

**Current densities:**

$$J_n = \langle p(p \cdot \nabla_x M[w] + \theta[V]M[w]) \rangle = \mathrm{div}_x \underbrace{\langle p \otimes pM[w] \rangle}_{=P} + \underbrace{\langle p\theta[V]M[w] \rangle}_{=-\langle M[w] \rangle \nabla_x V}$$
$$= \mathrm{div}\, P - n\nabla V$$

$$J_e = \langle \tfrac{1}{2}|p|^2(p \cdot \nabla_x M[w] + \theta[V]M[w]) \rangle$$
$$= \mathrm{div}_x \underbrace{\langle \tfrac{1}{2}p \otimes p|p|^2 M[w] \rangle}_{=U} + \langle \tfrac{1}{2}p|p|^2\theta[V]M[w] \rangle$$
$$= \mathrm{div}\, U - \big(\langle p \otimes pM[w] \rangle + \langle \tfrac{1}{2}|p|^2 M[w] \rangle \mathrm{Id}\big)\nabla V + \tfrac{\varepsilon^2}{8}\langle M[w] \rangle \nabla \Delta V$$
$$= \mathrm{div}\, U - (P + ne\,\mathrm{Id})\nabla V + \tfrac{\varepsilon^2}{8} n \nabla \Delta V$$

# Quantum energy-transport model

## Theorem (Nonlocal quantum energy-transport equations)

*Assume that $Q_1$ conserves mass. Then*

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t(ne) - \operatorname{div} J_e + J_n \cdot \nabla V = W$$

$$J_n = \operatorname{div} P - n\nabla V, \quad J_e = \operatorname{div} U - (P + ne\,\mathrm{Id})\nabla V + \frac{\varepsilon^2}{8} n\nabla\Delta V$$

*where*

$$n = \left\langle \mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right)\right\rangle, \quad ne = \left\langle \frac{1}{2}|p|^2 \mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right)\right\rangle$$

$$P = \left\langle p \otimes p \mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right)\right\rangle, \quad U = \left\langle \frac{1}{2} p \otimes p |p|^2 \mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right)\right\rangle$$

$$W = \left\langle \frac{1}{2}|p|^2 Q_1\left(\mathrm{Exp}\left(A - \frac{|p|^2}{2T}\right)\right)\right\rangle$$

# Nonlocal quantum energy-transport model

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t(ne) - \operatorname{div} J_e + J_n \cdot \nabla V = W$$

$$J_n = \operatorname{div} P - n\nabla V, \quad J_e = \operatorname{div} U - (P + ne\,\mathrm{Id})\nabla V + \frac{\varepsilon^2}{8} n\nabla\Delta V$$

- Evolution system for $n$ and $ne$, nonlocally dependent on $A$ and $T$
- Classical interpretation: $A$ = chemical potential, $T$ = temperature
- Quantum entropy:

$$\begin{aligned} S &= -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} M[w](\operatorname{Log} M[w] - 1)\,dp\,dx \\ &= -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} \operatorname{Exp}\Big(A - \frac{|p|^2}{2T}\Big)\Big(A - \frac{|p|^2}{2T} - 1\Big)\,dp\,dx \\ &= -\int_{\mathbb{R}^3}\Big(An + \frac{ne}{T} - n\Big)\,dx \end{aligned}$$

- Entropy inequality: $-dS/dt \le 0$
  (Proof uses Liouville-von Neumann formalism)

# Local quantum energy-transport model

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t(ne) - \operatorname{div} J_e + J_n \cdot \nabla V = W$$

$$J_n = \operatorname{div} P - n\nabla V, \quad J_e = \operatorname{div} U - (P + ne\,\mathrm{Id})\nabla V + \frac{\varepsilon^2}{8} n\nabla\Delta V$$

$O(\varepsilon^4)$ expansion:

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

$$ne = \frac{3}{2}nT - \frac{\varepsilon^2}{24} n\Delta\log n + O(\varepsilon^4)$$

$$U = \frac{5}{2}nT^2\,\mathrm{Id} - \frac{\varepsilon^2}{24} nT\big(\Delta\log n\,\mathrm{Id} + 7(\nabla\otimes\nabla)\log n\big) + O(\varepsilon^4)$$

Open problems:

- Fourth-order differential equations
- Mathematical structure still unknown
- Entropic structure? Entropy inequality?

# Summary

## Local quantum energy transport equations

$$\partial_t n - \operatorname{div} J_n = 0, \quad \partial_t(ne) - \operatorname{div} J_e + J_n \cdot \nabla V = W$$

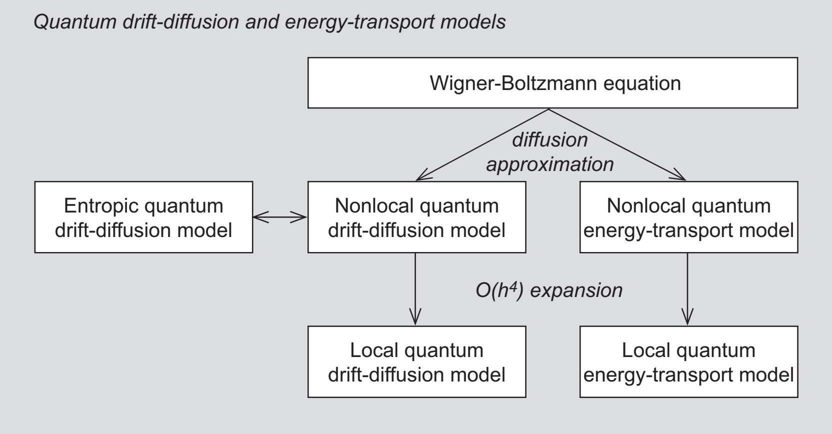
$$J_n = \operatorname{div} P - n\nabla V, \quad J_e = \operatorname{div} U - (P + ne\,\mathrm{Id})\nabla V + \frac{\varepsilon^2}{8} n\nabla\Delta V$$

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

$$U = \frac{5}{2}nT^2\,\mathrm{Id} - \frac{\varepsilon^2}{24} nT\big(\Delta \log n\,\mathrm{Id} + 7(\nabla \otimes \nabla)\log n\big)$$

- Derivation from Wigner-BGK equation using moment method
- Procedure can in principle be generalized to higher-order quantum diffusive models
- Mathematical structure unclear

# Model hierarchy




Entropic QDD = nonlocal QDD

# Overview

1. Semiconductor modeling
2. Microscopic quantum models
   - Density matrices
   - Schrödinger models
   - Wigner models
3. Macroscopic quantum models
   - Quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Actual and emerging directions
   - Quantum transistor
   - Spintronics
   - New materials and devices
5. Summary and open problems

# 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 $\lambda$, reference time $\tau$, 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

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

- 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: $P = (\varepsilon^2/4)n(\nabla \otimes \nabla)\log n$

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

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

# Schrödinger equation and quantum hydrodynamics

## Liouville-von Neumann and mixed-state Schrödinger

- Given density matrix operator $\hat\rho$, solving Liouville-von Neumann equation

$$i\hbar\partial_t\hat\rho = [H,\hat\rho], \quad t>0$$

- Eigenfunction-eigenvalue pairs $(\psi_j,\lambda_j)$ of $\hat\rho$
- $\psi_j$ solves mixed-state Schrödinger system $i\hbar\partial_t\psi_j = H\psi_j$, $j\in\mathbb{N}$, with particle density

$$n=\sum_{j=1}^\infty \lambda_j|\psi_j|^2, \quad \lambda_j\ge 0:\ \text{occupation probability}$$

## Mixed-state Schrödinger and quantum hydrodynamics

- Let $(\psi_j,\lambda_j)$ be solution of mixed-state Schrödinger system
- Define electron and current density:

$$n=\sum_{j=1}^\infty n_j = \sum_{j=1}^\infty \lambda_j|\psi_j|^2, \quad J=\sum_{j=1}^\infty J_j = -\varepsilon\sum_{j=1}^\infty \lambda_j\,\mathrm{Im}(\overline{\psi}_j\nabla\psi_j)$$

# Schrödinger equation and quantum hydrodynamics

$$n=\sum_{j=1}^{\infty} n_j=\sum_{j=1}^{\infty}\lambda_j|\psi_j|^2,\quad J=\sum_{j=1}^{\infty}J_j=-\varepsilon\sum_{j=1}^{\infty}\lambda_j\,\mathrm{Im}(\overline{\psi}_j\nabla\psi_j)$$

- Then $(n,J)$ solves

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

$$\theta=\sum_{j=1}^{\infty}\lambda_j\frac{n_j}{n}\Big[\underbrace{\left(\frac{J_j}{n_j}-\frac{J}{n}\right)\otimes\left(\frac{J_j}{n_j}-\frac{J}{n}\right)}_{\text{current temperature}}+\underbrace{\frac{\varepsilon^2}{4}\nabla\log\frac{n_j}{n}\otimes\nabla\log\frac{n_j}{n}}_{\text{osmotic temperature}}\Big]$$

- Closure condition 1: $\theta=T\,\mathrm{Id}$, $T>0$ (isothermal model)
- Closure condition 2 (Gasser/Markowich/Ringhofer 1996): small temperature and small $\varepsilon$ gives equation for energy tensor

$$E=\frac{1}{2}\left(\frac{J\otimes J}{n}+n\theta-\frac{\varepsilon^2}{4}n(\nabla\otimes\nabla)\log n\right)$$

# 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 $Q_0(w) = 0$ if and only if $w =$ 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

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

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: $(n, nu, ne) = \langle(1, p, \frac12|p|^2)M[w]\rangle$, $J=-nu$
- Use properties

$$\langle\theta[V]M[w]\rangle = 0,\ \langle p\theta[V]M[w]\rangle = -n\nabla V,\ \langle\tfrac12|p|^2\theta[V]M[w]\rangle = J\cdot\nabla V$$

# 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 $ne$:

$$\partial_t \underbrace{\langle \tfrac12|p|^2M[w]\rangle}_{=ne} + \mathrm{div}_x \langle \tfrac12 p|p|^2M[w]\rangle + \underbrace{\langle \tfrac12|p|^2\theta[V]M[w]\rangle}_{=J\cdot\nabla V} = \langle \tfrac12|p|^2Q_1(w)\rangle$$

- Define quantum stress tensor and quantum heat flux

$$P = \langle (p-u)\otimes(p-u)M[w]\rangle, \quad q = \langle \tfrac12(p-u)|p-u|^2M[w]\rangle$$

# Derivation

**Theorem (Nonlocal quantum hydrodynamic model)**

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

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

# Isothermal quantum hydrodynamic model

- Derived by Degond/Gallego/Méhats 2007
- Quantum Maxwellian: $M[w] = \mathrm{Exp}(A - |p-v|^2/2)$
- Isothermal model equations:

$$\partial_t n - \operatorname{div} J = 0, \quad \partial_t J + \operatorname{div}(J \otimes v) + (\nabla v)(J + nv) + n\nabla(V - A) = 0$$

- Relation between $(n, J)$ and $(A, v)$:

$$n = \left\langle \mathrm{Exp}\Big(A - \frac{1}{2}|p-v|^2\Big)\right\rangle, \quad J = -\left\langle p\mathrm{Exp}\Big(A - \frac{1}{2}|p-v|^2\Big)\right\rangle$$

Relation between velocity $u = -J/n$ and $v$: $nu = nv + O(\varepsilon^2)$

- Local isothermal model (A.J./Matthes 2005):

$$\partial_t n - \operatorname{div} J = 0, \quad U_{j\ell} = \sum_{m=1}^{3}\Big(\frac{\partial u_m}{\partial x_j} - \frac{\partial u_j}{\partial x_m}\Big)\Big(\frac{\partial u_m}{\partial x_\ell} - \frac{\partial u_\ell}{\partial x_m}\Big)$$

$$\partial_t J - \operatorname{div}\Big(\frac{J \otimes J}{n}\Big) - \nabla n + n\nabla V + \frac{\varepsilon^2}{6} n \nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = \frac{\varepsilon^2}{12}\operatorname{div}(nU)$$

# Isothermal quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J = 0, \quad U_{j\ell} = \sum_{m=1}^{3} \Big(\frac{\partial u_m}{\partial x_j} - \frac{\partial u_j}{\partial x_m}\Big)\Big(\frac{\partial u_m}{\partial x_\ell} - \frac{\partial u_\ell}{\partial x_m}\Big)$$

$$\partial_t J - \operatorname{div}\Big(\frac{J \otimes J}{n}\Big) - \nabla n + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) = \frac{\varepsilon^2}{12}\operatorname{div}(nU)$$

Interpretation of $U$:

- Vorticity $\omega = \operatorname{curl} u$ satisfies

$$\partial_t \omega + \operatorname{curl}(\omega \times v) = 0,$$

- Relation between $U$ and vorticity:

$$\operatorname{div}(nU) = \omega \times (\operatorname{curl}(n\omega)) + \frac{1}{2} n\nabla(|\omega|^2).$$

# Local quantum hydrodynamic model

$$\partial_t n - \operatorname{div} J = 0, \ \partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n} + P\right) + n\nabla V = -\langle p Q_1(w)\rangle$$

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

Expansion of $ne$, $P$, and $q$: $R_{j\ell} = \partial u_j/\partial x_\ell - \partial u_\ell/\partial x_j$

$$ne = \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n\Big(\Delta\log n - \frac{1}{T}\mathrm{Tr}(R^\top R) - \frac{3}{2}|\nabla\log T|^2 - \Delta\log T - \nabla\log T\cdot\nabla\log n\Big) + O(\varepsilon^4)$$

$$P = nT\,\mathrm{Id} + \frac{\varepsilon^2}{12}n\Big(\frac{5}{2}\nabla\log T\otimes\nabla\log T - \nabla\log T\otimes\nabla\log n - \nabla\log n\otimes\nabla\log T - (\nabla\otimes\nabla)\log(nT^2) + \frac{1}{T}R^\top R\Big) + \frac{\varepsilon^2}{12}T\operatorname{div}\left(\frac{n}{T}\nabla\log T\right) + O(\varepsilon^4)$$

$$q = -\frac{\varepsilon^2}{24}n\Big(5R\nabla\log T + 2\operatorname{div}R + 3\Delta u\Big) + O(\varepsilon^4)$$

# Conserved quantities

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

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

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

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

$$q = -\frac{\varepsilon^2}{24}n\Big(5R\nabla\log T + 2\operatorname{div} R + 3\Delta u\Big)$$

## Proposition

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

$$E(t) = \int_{\mathbb{R}^3}\left(ne + \frac{\lambda_D^2}{2}|\nabla V|^2\right)dx = \int_{\mathbb{R}^3}\Big(\frac{3}{2}nT + \frac{1}{2}n|u|^2 + \frac{\lambda_D^2}{2}|\nabla V|^2$$

$$+ \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + \frac{\varepsilon^2}{16}n|\nabla\log T|^2 + \frac{\varepsilon^2}{24T}n\mathrm{Tr}(R^\top R)\Big)dx \ge 0$$

# Local quantum hydrodynamic model

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

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

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

$\longrightarrow$ Gives closed set of equations

Second simplification: $R = O(\varepsilon^2)$

# Local quantum hydrodynamic model

**Theorem (Local quantum hydrodynamic model)**

$$\partial_t n - \mathrm{div}\, J = 0$$

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

$$\partial_t(ne) - \mathrm{div}\left((P + ne\,\mathrm{Id})J\right) - \frac{\varepsilon^2}{8}\mathrm{div}\,(n\Delta u) + J \cdot \nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

*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 $q = -(\varepsilon^2/8)n\Delta u$:

- 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)

# Other quantum hydrodynamic models

- Quantum hydrodynamic model with energy equation first derived by Ferry/Zhou 1993
- Derivation from Wigner equation by Gardner 1994:

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

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

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

- Gardner uses unconstrained quantum equilibrium :

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

and substitutes $\nabla V = T\nabla \log n + O(\varepsilon^2)$

# Other quantum hydrodynamic models

- Gardner uses unconstrained quantum equilibrium:

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

and substitutes $\nabla V = T\nabla \log n + O(\varepsilon^2)$

- Quantum Maxwellian:

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

and, if $T = \text{const.}$, $\nabla A = \nabla \log n + O(\varepsilon^2) \Rightarrow w_Q = M[w] + O(\varepsilon^2)$

- "Smooth" quantum hydrodynamic model (Gardner/Ringhofer 1996):

$$\text{expressions}\quad \frac{\varepsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\quad\text{and}\quad\frac{\varepsilon^2}{12}(\nabla\otimes\nabla)\ln n$$

$$\text{are replaced by}\quad \frac{\varepsilon^2}{4}\operatorname{div}\left(n(\nabla\otimes\nabla)\overline{V}\right)\quad\text{and}\quad\frac{\varepsilon^2}{4}(\nabla\otimes\nabla)\overline{V}$$

and $\overline{V} = \overline{V}(x, T)$ depends nonlocally on $x$ and $T$

# Dissipative QHD models

$$\partial_t n - \mathrm{div}\, J = 0$$

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

$$\partial_t(ne) - \mathrm{div}\left((P + ne\,\mathrm{Id})J\right) - \frac{\varepsilon^2}{8}\mathrm{div}\,(n\Delta u) + J\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

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

- Averaged quantities:

$$-\langle pQ_1(w)\rangle = -\frac{J}{\tau}, \quad \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

- Relaxation-time model: $J(t) \to 0$, $(ne)(t) - \frac{3}{2}n(t) \to 0$ as $t \to \infty$
- Formal equivalence to Schrödinger-Langevin equation if $T = 1$:

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - V\psi + \log(|\psi|^2)\psi - \frac{i\varepsilon}{\tau}\log\frac{\psi}{\overline{\psi}}, \quad \psi = \sqrt{n}e^{iS/\varepsilon}$$

# Dissipative QHD models

Caldeira-Leggett operator:

$$\partial_t n - \mathrm{div}\, J = 0$$

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

$$\partial_t(ne) - \mathrm{div}\left((P + ne\,\mathrm{Id})J\right) - \frac{\varepsilon^2}{8}\mathrm{div}\,(n\Delta u) + J \cdot \nabla V = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

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

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

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

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

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

# Dissipative QHD models

Caldeira-Leggett operator:

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

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

$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J\right) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) + J \cdot \nabla V = -\frac{2}{\tau}\left(ne - \frac{3}{2}n\right)$$

- 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

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

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

$$\partial_t(ne) - \operatorname{div}\left((P + ne\,\mathrm{Id})J\right) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) + J \cdot \nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w) \rangle$$

Fokker-Planck operator:

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

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

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

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

- Gives viscous quantum hydrodynamic model

# Viscous quantum hydrodynamic model

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

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

$$= D_{qq}\Delta J - 2\gamma J + 2D_{pq}\nabla_x n$$

$$\partial_t(ne) - \operatorname{div}\big((P + ne\,\mathrm{Id})J\big) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) + J\cdot\nabla V$$

$$= D_{qq}\Delta_x(ne) - 2\left(2\gamma ne - \frac{3}{2}D_{pp}n\right) + 2D_{pq}\mathrm{div}_x J$$

- $D_{qq}$ provides diffusive terms
- Effective current density $J_{\text{eff}} = J - D_{qq}\nabla n$: $\partial_t n - \operatorname{div} J_{\text{eff}} = 0$
- Existence of 1D stationary solutions with $T = 1$ (A.J./Milisic 2007)
- Lobal existence of 3D transient solutions (Chen/Dreher 2006), global existence of 1D transient solutions (Gamba/A.J./Vasseur 2009)
- Open problem: global existence of solutions for full system

# 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 $-nu$:

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

# 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

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

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

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

$$\begin{aligned} S_i &= \sum_{j,k} \left(\partial_j(\partial_j u_k P_{ij} + \partial_j(\partial_i u_k P_{jk}) + \partial^2_{jk}(u_k P_{ij})\right) \\ &\quad - n\partial_i(\partial_t A) + \sum_k \partial_k(nu_k)\partial_i A - \frac{\varepsilon^2}{4}\sum_{j,k} \partial^2_{jk}(n\partial^2_{ij} u_k) + O(\alpha) \\ &= \partial_j(n(\partial_i u_j + \partial_j u_i)) + O(\varepsilon^2) + O(\alpha), \quad \text{where } \partial_j = \partial/\partial x_j \text{ etc.} \end{aligned}$$

- Correction term:

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

# Quantum Navier-Stokes equations

**Theorem (Local quantum Navier-Stokes equations)**

*Neglecting $O(\alpha\varepsilon^2) + O(\alpha^2)$ term in $\alpha S$ gives*

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

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

- Classical Navier-Stokes correction:

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

- Viscosity coefficients: $\mu(n)$, $\lambda(n)$
- Monoatomic gases: $\lambda = \frac{2}{3}\mu$
- Quantum Navier-Stokes correction: $\mu(n) = \alpha n$ and $\lambda(n) = 0$

# Quantum Navier-Stokes equations

Reformulation of quantum Navier-Stokes model:

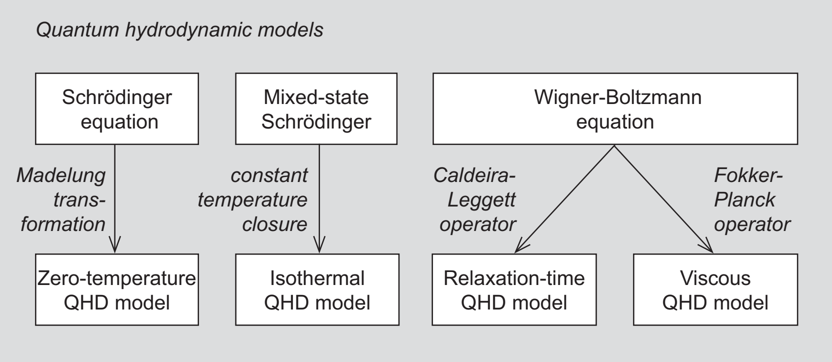
$$\partial_t n + \operatorname{div}(nu) = 0$$
$$\partial_t(nu) + \operatorname{div}(nu \otimes u) + \nabla n - \frac{\varepsilon^2}{6} n \nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) - n\nabla V = 2\alpha \operatorname{div}(nD(u))$$

- 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!
- Velocity $w$ also used in viscous Korteweg-type models (Bresch/Desjardins) and fluid mixtures (Joseph/Huang/Hu 1996)

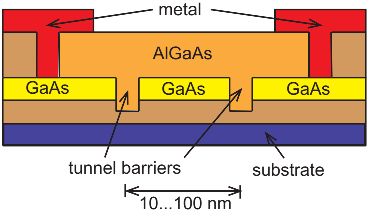
# Hierarchy of quantum hydrodynamic models



# Resonant tunneling diode

Geometry:

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

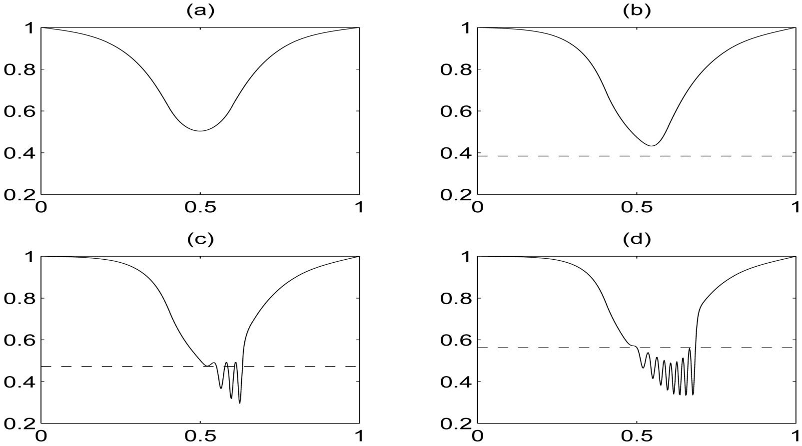



Numerical method:

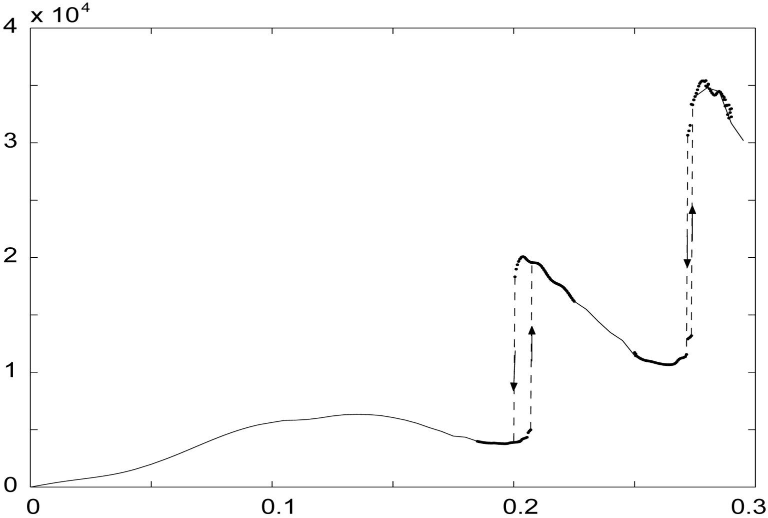
- Relaxation scheme (QHD)
- Central finite differences (viscous QHD)
- Newton iterations

# Zero external potential

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

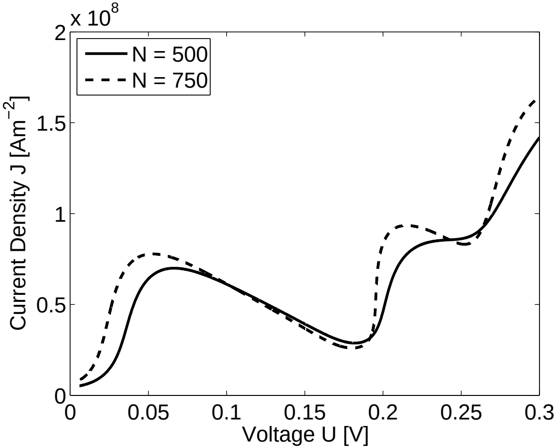


# Resonant tunneling diode: current-voltage characteristics




$\longrightarrow$ hysteresis phenomenum

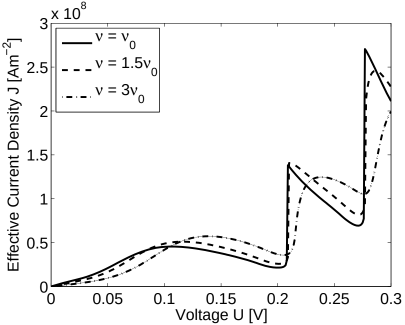
# Upwind finite differences




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

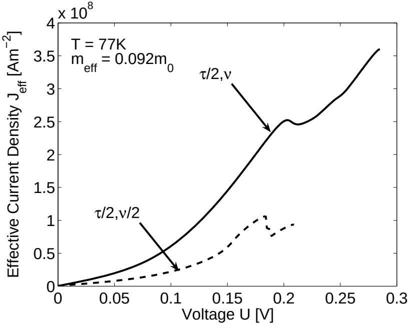
# Viscous quantum hydrodynamic model

## 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 $\to$ viscosity too strong

# Summary

## Quantum hydrodynamic equations

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

- Single-state Schrödinger → zero-temperature quantum hydrodynamics
- Mixed-state Schrödinger → isothermal quantum hydrodynamics
- Diffusion approximation of Wigner equation → full quantum hydrodynamics
- $O(\varepsilon^4)$ expansion gives local quantum hydrodynamic model with vorticity-type terms
- Scattering models: Caldeira-Leggett and Fokker-Planck
- Viscous quantum hydrodynamic model: influences (too) strongly quantum effects

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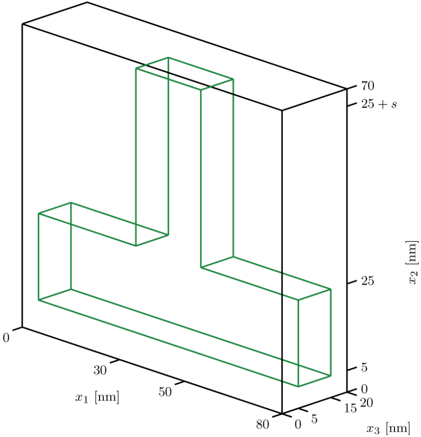
   - Quantum hydrodynamic models
4. Actual and emerging directions
   - Quantum transistor
   - Spintronics
   - New materials and devices
5. Summary and open problems

# Quantum transistor: principle

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



# Quantum transistor: numerical approximation

Time-splitting method: (Bao/Jin/Markowich 2002)

- Trotter splitting: approximate solution $e^{i\varepsilon\Delta/2+V(x)/\varepsilon}$ by $e^{i\varepsilon\Delta/2}e^{V(x)/\varepsilon}$

$$i\varepsilon\partial_t\psi_1 = -\frac{\varepsilon^2}{2}\Delta\psi_1 \quad \text{in } [t_j, t_{j+1}], \quad \psi_1(t_j) = \psi_0,$$
$$i\varepsilon\partial_t\psi_2 = -V(x)\psi_2 \quad \text{in } [t_j, t_{j+1}], \quad \psi_2(t_j) = \psi_1(t_{j+1})$$

- Equation for $\psi_2$: explicit solution $\psi_2(t_{j+1}) = e^{-iV/\varepsilon}\psi_1(t_{j+1})$
- Equation for $\psi_1$: use spectral method (write equation in discrete Fourier space)

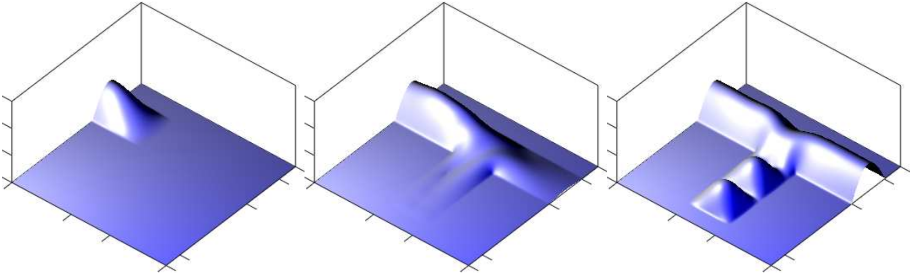
Algorithm:

- Compute discrete Fourier transform of $\psi_0$
- Solve equation for $\psi_1$ in discrete Fourier space
- Multiply solution by $e^{-iV/\varepsilon}$

Use discrete FFT for Fourier transformations: complexity $O(N\log N)$

# Quantum transistor: numerical details

- Transparent boundary conditions: imaginary potential method
- Incoming plane waves: $e^{ik\cdot x - i\omega t}$ describes plane wave with energy $E = |\hbar k|^2/2m$, frequency $\omega$, construct additive incoming wave
- Boundary of transistor realized by smoothed external potential
- Initial condition: stationary solution from Numerov method
- Implementation: Matlab, FFT package; visualization: POV-Ray
- Computing time: 4 hours on quad-core processor for 3D



# Quantum transistor: evolution of density

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# Spin-based devices

- Up to now, only electron charge used in semiconductors
- Electrons can be distinguished by their spin: "up" or "down"
- What is spintronics? "Teaching electrons new tricks." (Patrick Bruno, Germany)

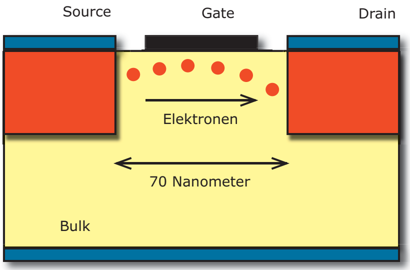
Applications:

- 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




- Spin field-effect transistor due to Datta/Das 1990
- Source and drain made of ferromagnetic materials
- Source: gives spin-polarized electrons
- Drain: works as spin analyzer
- Gate voltage: changes spin of electrons to control the current

Objective: Derive spintronics models

# Schrödinger spin models

- Vector-valued Schrödinger equation:

$$i\hbar\partial_t\psi = H\psi + H_s\psi, \quad x \in \mathbb{R}^3,\ \psi \in \mathbb{C}^2$$

- Energy Hamiltonian:

$$H = \Big(-\frac{\hbar^2}{2m^*}\Delta_x + V(x,t)\Big)\mathbb{I}_2, \quad \mathbb{I}_2: \text{ identity matrix in } \mathbb{C}^{2\times 2}$$

- Spin-orbit Hamiltonian:

$$H_s = \alpha\hbar\vec{\Omega}(x,t,i\hbar\nabla_x)\cdot\vec{\sigma}$$

  where $\alpha$: coupling constant, $\vec{\Omega}$: effective field (pseudo-differential operator), $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$

- Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

# Schrödinger spin models

$$i\hbar\partial_t\psi = H\psi + H_s\psi, \quad x \in \mathbb{R}^3,\ \psi \in \mathbb{C}^2$$

- Example: Rashba spin-orbit Hamiltonian (for 2D electron gas):

$$H_s = \alpha i\hbar(\sigma_1\partial_y - \sigma_2\partial_x)$$

- Electron density and current density:

$$N(x,t) = \psi(x,t) \otimes \overline{\psi(x,t)} \in \mathbb{C}^{2\times 2}$$
$$J(x,t) = \frac{\hbar}{2i}\big(\nabla\psi(x,t) \otimes \overline{\psi(x,t)} - \psi(x,t) \otimes \nabla\overline{\psi(x,t)}\big)$$

Semi-classical limit:

- Scaled Schrödinger model:

$$i\varepsilon\partial_t\psi_\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\psi_\varepsilon + V\psi_\varepsilon + \alpha\vec{\Omega}(x,t,i\varepsilon\nabla_x)\cdot\vec{\sigma}\psi_\varepsilon$$

- Objective: $\varepsilon \to 0$ (Ben Abdallah/El Hajj 2008)
- Assumption: weak spin-orbit coupling, $\alpha = O(\varepsilon)$

# Schrödinger spin models

$$i\varepsilon\partial_t\psi_\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x\psi_\varepsilon + V\psi_\varepsilon + \varepsilon\vec{\Omega}(x,t,i\varepsilon\nabla_x)\cdot\vec{\sigma}\psi_\varepsilon$$

**Theorem (Spinor Vlasov equation)**

*Wigner function*

$$F_\varepsilon(x,p,t) = 2(2\pi)^{-3}\int_{\mathbb{R}^3}\psi_\varepsilon(x-\varepsilon\eta/2,t)\otimes\overline{\psi}_\varepsilon(x+\varepsilon\eta/2,t)d\eta$$

*converges (in the sense of distributions) to a solution to*

$$\partial_t F + p\cdot\nabla_x F + \nabla_x V\cdot\nabla_p F = i[\vec{\Omega}\cdot\vec{\sigma}, F]$$

- Commutator: $[A,B] = AB - BA$
- Electron and current densities:

$$N(x,t) = \int_{\mathbb{R}^3} F(x,p,t)dp, \quad J(x,t) = \int_{\mathbb{R}^3} F(x,p,t)p\,dp$$

- Strong spin-orbit coupling $\alpha = O(1)$: $F$ decomposes into $F_{\mathrm{up}}$ and $F_{\mathrm{down}}$ solving two Vlasov equations

# Spinor Boltzmann model

$$\partial_t F + p\cdot\nabla_x F + \nabla_x V\cdot\nabla_p F = Q(F) + \frac{\alpha i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F] + Q_s(F)$$

- $Q(F)$: Semi-classical collision operator without spin interactions
- Spin-flip interactions: $Q_s(F) = \frac{1}{\tau_s}(\mathrm{tr}(F)\mathbb{I}_2 - F)$
- Basis in class of $\mathbb{C}^{2\times 2}$ Hermitian matrices: $\mathbb{I}_2$, $\sigma_1$, $\sigma_2$, $\sigma_3$
- Decompose distribution function in this basis:

$$F(x,p,t) = \tfrac{1}{2} f_c(x,p,t)\mathbb{I}_2 + \vec{f}_s(x,p,t)\cdot\vec{\sigma}$$

  where $f_c$: charge distributions function, $\vec{f}_s$: spin distribution function
- System of spinor Boltzmann equations:

$$\partial_t f_c + p\cdot\nabla_x f_c + \nabla_x V\cdot\nabla_p f_c = 0$$
$$\partial_t \vec{f}_s + p\cdot\nabla_x \vec{f}_s + \nabla_x V\cdot\nabla_p \vec{f}_s = -\alpha\vec{\Omega}\times\vec{f}_s$$

# Macroscopic spinor models

- Diffusion-scaled spinor Boltzmann equation:

$$\varepsilon^2\partial_t F_\varepsilon + \varepsilon\big(p\cdot\nabla_x F_\varepsilon + \nabla_x V\cdot\nabla_p F_\varepsilon\big) = Q(F_\varepsilon) + \alpha\varepsilon\frac{i}{2}[\vec{\Omega}\cdot\vec{\sigma}, F_\varepsilon] + \varepsilon^2 Q_s(F)$$

- Objective: Limit $\varepsilon \to 0$ for various regimes of $\alpha$

Weak spin-orbit coupling: $\alpha = O(\varepsilon)$

- El Hajj 2008: As $\varepsilon \to 0$, $F_\varepsilon \to F = N(x,t)M(p)$, where $M(p)$: Maxwellian and

$$\partial_t N + \operatorname{div}\big(D(\nabla N - N\nabla V)\big) = \frac{i}{2}[\vec{H}\cdot\vec{\sigma}, N] + Q_s(N)$$

- Diffusion matrix $D$: symmetric, positive definite
- Effective field: $\vec{H}(x,t) = \int_{\mathbb{R}^3}\vec{\Omega}(x,p,t)M(p)dp$

# Macroscopic spinor models

Strong spin-orbit coupling: $\alpha = O(\varepsilon^{-1})$

- Diffusion-scaled spinor Boltzmann equation:

$$\varepsilon^2 \partial_t F_\varepsilon + \varepsilon \big( p \cdot \nabla_x F_\varepsilon + \nabla_x V \cdot \nabla_p F_\varepsilon \big) = Q(F_\varepsilon) + \frac{i}{2}[\vec{\Omega} \cdot \vec{\sigma}, F_\varepsilon] + \varepsilon^2 Q_s(F)$$

- Assumption: direction of $\vec{\Omega}$ independent of $i\varepsilon\nabla_x$
- As $\varepsilon \to 0$, $F_\varepsilon \to F$, where $F(x,p,t) = N(x,t)M(p)$, $N = \frac{1}{2} n_c \mathbb{I}_2 + n_s \cdot \vec{\sigma}$
- Spin-up/down densities $n_{\rm up} = n_c + n_s$, $n_{\rm down} = n_c - n_s$ solve

$$\partial_t n_{\rm up} - \operatorname{div}\left(D_1(\nabla n_{\rm up} - n_{\rm up}\nabla V)\right) = \frac{1}{\tau}(n_{\rm down} - n_{\rm up})$$

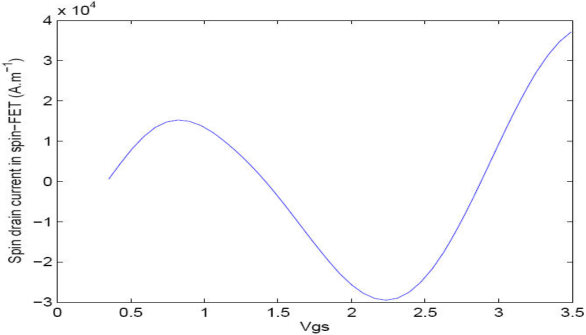
$$\partial_t n_{\rm down} - \operatorname{div}\left(D_2(\nabla n_{\rm down} - n_{\rm down}\nabla V)\right) = \frac{1}{\tau}(n_{\rm up} - n_{\rm down})$$

- Spin relaxation time $\tau$ depends on $\tau_s$, $Q$, and $\vec{\Omega}$

# Numerical example

- Subband quantum/drift-diffusion model: quantum confinement in $x_3$ direction, transport in $x = (x_1, x_2)$ direction
- Schrödinger eigenvalue problem in $x_3$ direction
- Stationary two-component drift-diffusion model for $(n_c, n_s)$
- Rashba effective field (numerical results by El Hajj)

Spin drain current as a function of the gate voltage:



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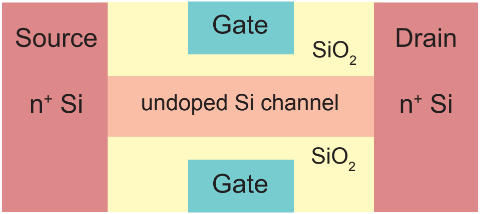
# Beyond silicon

- Silicon may be used up to 22 nm technology (expected 2011) 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

# Carbon nanotubes

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

# 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

# Possible future devices

- Quantum dot arrays (logical devices)
- Single-electron memory cells
- Quantum-based devices (tunneling diodes, spin transistors)
- Polymer thin-film transistors
- Molecular-based devices
- Devices based on self-assembly
- Devices for quantum computing

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   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Actual and emerging directions
   - Quantum transistor
   - Spintronics
   - New materials and devices
5. Summary and open problems

# Summary

Semiconductor modeling:

- Bloch decomposition of wave function
- Semi-classical picture

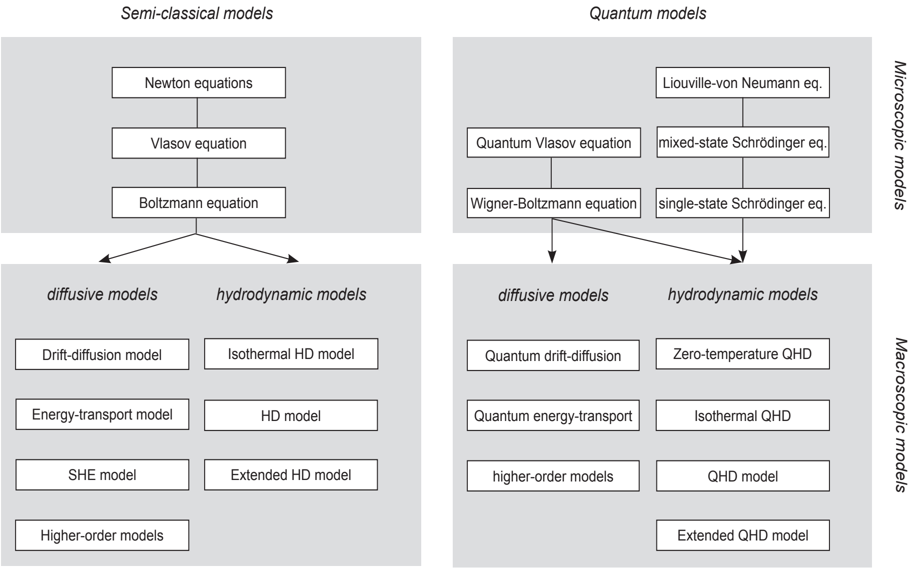
Microscopic quantum models:

- Three formulations: Density matrix – Schrödinger – Wigner
- Density matrix: describes statistical state of quantum system
- Schrödinger equation: describes ballistic carrier transport
- Wigner equation: allows one to include scattering models

Macroscopic quantum models:

- Close moment equations using quantum Maxwellian
- Three- or two-step derivation from Wigner-Boltzmann equation
- Expansion in powers of scaled Planck constant gives local models

# 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
Drift-diffusion model
Isothermal HD model
Energy-transport model
HD model
SHE model
Extended HD model
Higher-order models
diffusive models
hydrodynamic models
Quantum drift-diffusion
Zero-temperature QHD
Quantum energy-transport
Isothermal QHD
higher-order models
QHD model
Extended QHD model
Macroscopic models

# Some open problems

Microscopic quantum models:

- Numerical solution of multi-dimensional Wigner or density matrix models
- Modeling of semiconductor devices in magnetic fields
- Theory for quantum scattering operators
- Entropy methods for the Liouville-von Neumann equation

Quantum drift-diffusion models:

- Existence results for the nonlocal model (entropic structure!)
- Develop a mathematical theory for nonlinear higher-order parabolic equations
- Numerical simulations of 3D quantum devices

Quantum energy-transport models:

- Understand the mathematical structure
- Numerical approximation
- Existence of global-in-time or stationary solutions
- Importance of temperature effects in quantum devices

# Some open problems

Quantum hydrodynamic models:

- Strict positivity of solutions
- Equivalence to Schrödinger equation
- Better numerical approximation schemes
- Existence of global-in-time solutions to multi-dimensional viscous QHD models

Other open problems:

- Derive macroscopic quantum models by variational methods
- Numerical approximation of macroscopic models for spintronics
- Numerical simulation of quantum dot arrays