Semi-classical and Quantum Macroscopic Semiconductor Models and Electric Circuits

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Literature

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History of Intel processors

1971

4004
108 KHz, 2250 transistors,
channel length: 10μm (1μm$= 10^{-6}$m)

1982

80286
12 MHz, 134,000 transistors,
channel length: 1.5μm

1993

Pentium 1
66 MHz, 7,500,000 transistors,
channel length: 0.35μm

2007

Core Duo
3 GHz, 410,000,000 transistors,
channel length: 0.045μm$=$ 45nm

Channel lengths 2000–2016

Challenges in semiconductor simulation

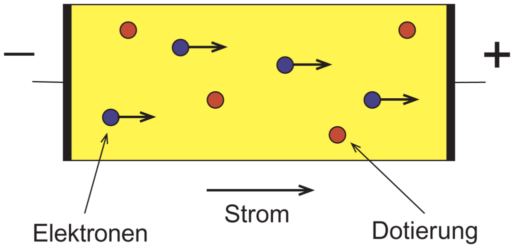
Future processors (2010):

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

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 material: Silicon, Germanium, GaAs etc.
- Doping of the basis material with other atoms, gives higher conductivity
- Modeled by doping concentration $C(x)$

Objectives

- Modeling of macroscopic electron transport (numerically cheaper than kinetic models)
- Modeling of quantum transport and quantum diffusion effects
- Numerical approximation of macroscopic models (finite-element and finite-difference methods)
- Modeling and numerical simulation of electric circuits
- Coupling of electron temperature, lattice temperature, and circuit temperature

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

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

$\longrightarrow$ 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 ψ
- Schrödinger eigenvalue problem:

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

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

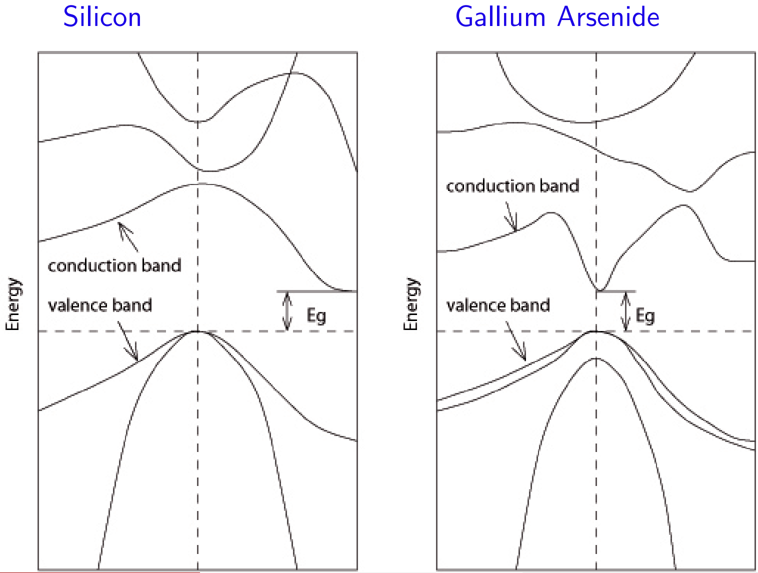
Schrödinger eigenvalue problem in $\mathbb{R}^3$ can be reduced to Schrödinger problem on lattice cell, indexed by $k \in B$ (B: dual cell or Brillouin zone)

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

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

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

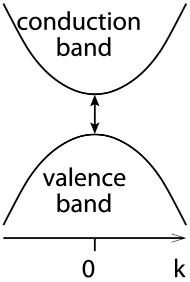
Energy bands



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

"Derivation":

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

Effective mass

- Semi-classical equations of motion:

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

- Definition of effective mass m^*:

$$p = m^* v_n$$

- Consequence:

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

- Effective mass equation:

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

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:

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

- External electric field generated by doping atoms:

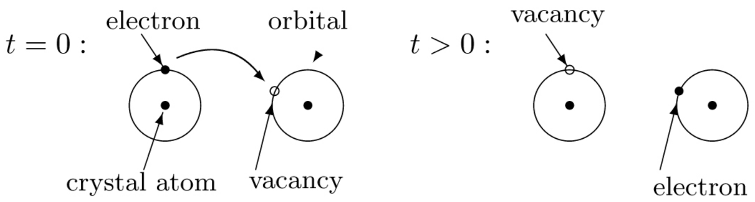
$$E_{\rm ext}(x,t) = \frac{q}{4\pi\varepsilon_s}\int_{\mathbb{R}^3} C(y)\frac{x-y}{|x-y|^3}dy \quad \Rightarrow \quad \operatorname{div} E_{\rm ext} = \frac{q}{\varepsilon_s} C(x)$$

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

Poisson equation

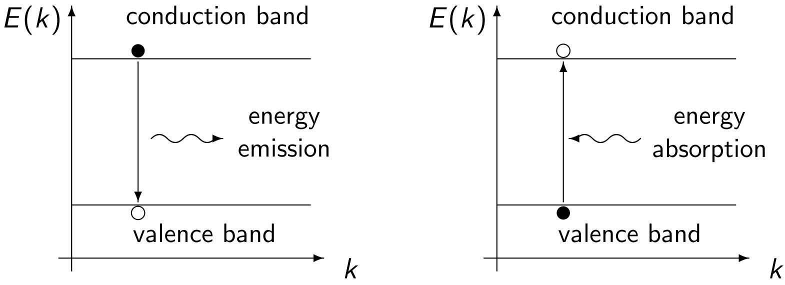
$$\varepsilon_s \Delta V = -\varepsilon_s \operatorname{div}(E_{\rm mean} + E_{\rm ext}) = q(n - C(x))$$

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):

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

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

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

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

Collision models

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

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

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

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

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

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

Scattering rates

Electron-phonon scattering:

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

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

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

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

- 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:

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

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Scaling of Boltzmann equation

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

- Introduce reference values for

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

- Scaled Boltzmann equation:

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

- Scaled Poisson equation:

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

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

Moment method

Boltzmann equation with parabolic band:

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

- Integrate over $k \in B$:

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

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

- Multiply by k and integrate by parts:

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

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

Moment method

- Mass balance equation:

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

- Momentum balance equation:

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

- Energy balance equation (assuming energy conservation):

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

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

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

Solution of closure problem

Scaling of Boltzmann equation:

- Collision time $\tau_c = \tau/\alpha$: hydrodynamic scaling

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

- Collision time $\tau_c = \tau/\alpha^2$: diffusion scaling

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

Maxwellian:

- Kinetic entropy: $S(f) = -\int_B f(\log f - 1 + E(k))dk$
- Given f, solve constrained maximization problem with $\kappa = 1, k, \frac{1}{2}|k|^2$:

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

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

Model hierarchy

Model hierarchy depends on ...

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

Hydrodynamic models:

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

Diffusive models:

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

Model hierarchy

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

Warm-up: drift-diffusion equations

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

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

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

- Derivation in three steps

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

Warm-up: drift-diffusion equations

Step 2:

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

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

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

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

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

Step 3:

- Insert Chapman-Enskog expansion in Boltzmann equation:

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

Warm-up: drift-diffusion equations

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

- Limit $\alpha \to 0$:

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

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

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

Theorem (Drift-diffusion equations)

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

Bipolar drift-diffusion equations

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

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

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

  with physical parameter n_i, τ_n, τ_p, n_d, p_d
- Auger recombination-generation term (high carrier densities):

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

  with physical parameter C_n and C_p
- Equilibrium state: $np = n_i^2 =$ intrinsic density

Drift-diffusion equations

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

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

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

Overview

1. Semiconductor modeling
2. Semi-classical macroscopic models
   - General strategy
   - Energy-transport models
   - Higher-order diffusion models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Wigner models and quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Electric circuits
5. Summary and open problems

Semi-classical Boltzmann equation

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

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

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

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

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

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

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

Properties of elastic collision operator

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

Proposition

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

Proof:

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

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

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

Properties of elastic collision operator

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

Proposition

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

Proof:

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

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

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

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

Properties of electron-electron collision operator

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

Proposition

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

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

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

Proof: Show that

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

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

Properties of electron-electron collision operator

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

Averaged collision operator:

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

Proposition

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

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

Proof similar as above

General strategy

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

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

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

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

Strategy of derivation:

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

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

Step 1

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

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

Step 2:

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

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

- Formal limit $\alpha\to 0$ gives

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

- Operator equation solvable iff

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

Step 2

- Solvability condition for operator equation:

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

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

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

- Solvability condition becomes

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

$\Rightarrow F$ = Fermi-Dirac

Step 3

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

$$Q_{\rm el}(g) = v(k)\cdot\nabla_x F_{\mu,T} + \nabla_x V\cdot\nabla_k F_{\mu,T} - Q_{\rm ee}(F_{\mu,T})$$
$$= F_{\mu,T}(1-F_{\mu,T})v(k)\cdot\Big(\nabla_x\frac{\mu}{T} - \frac{\nabla_x V}{T} - E\nabla_x\frac{1}{T}\Big)$$

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

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

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

- Limit $\alpha\to 0$:

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

Step 3: balance equations

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

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

- Moment equation for $j = 1$:

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

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

Balance equations

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

Step 3: current densities

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

where g is solution of

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

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

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

- Insert into expressions for current densities:

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

- Diffusion coefficients:

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

Summary

Energy-transport equations

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

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

- Electron and energy densities:

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

- Diffusion coefficients:

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

- Energy-relaxation term:

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

Literature

Energy-transport equations

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

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

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

Relation to nonequilibrium thermodynamics

Energy-transport equations

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

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

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

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

- Thermodynamic fluxes:

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

- Intensive variables n, ne
- Extensive (entropy) variables μ/T, $-1/T$

Properties of diffusion matrix

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

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

Proposition

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

Proof:

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

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

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

Properties of relaxation-time term

Inelastic (electron-phonon) collision operator:

$$Q_{\rm in}(f) = \int_B \big(s(k',k)f'(1-f) - s(k,k')f(1-f')\big)dk'$$

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

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

Proposition

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

Proof: After some manipulations,

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

Boundary conditions

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

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

- Dirichlet conditions at contacts Γ_D:

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

- Neumann conditions at insulating boundary Γ_N:

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

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

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

(second-order correction from Boltzmann equation)

Open problem: improved boundary conditions for energy-transport

Explicit models: spherical symmetric energy band

Assumptions:

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

Proposition

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

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

Proof: Use coarea formula for, for instance,

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

Parabolic band approximation

Assumptions:

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

Proposition

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

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

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

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

Parabolic band approximation

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

Diffusion matrix: typical choices for β

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

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

Relaxation-time term:

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

Chen model: τ_β constant in T

Nonparabolic band approximation

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

Proposition

$$n = N(T)T^{3/2}e^{\mu/T}, \quad N(T) = \frac{\sqrt{2}}{\pi^2}\int_0^\infty e^{-z}\sqrt{z(1+\alpha Tz)}(1+2\alpha Tz)dz$$

$$ne = \frac{3}{2}Q(T)nT, \quad Q(T) = \frac{2}{3}\frac{\int_0^\infty \sqrt{z(1+\alpha Tz)}(1+2\alpha Tz)zdz}{\int_0^\infty \sqrt{z(1+\alpha Tz)}(1+2\alpha Tz)dz}$$

$$D_{ij} = \mu_{ij}(T)n, \quad \mu_{ij} = \mu_0 T^{i+j+1/2-\beta}\int_0^\infty \frac{z^{i+j+1-\beta}(1+\alpha Tz)}{(1+2\alpha Tz)^2}e^{-z}dz$$

$\longrightarrow$ Numerical comparison parabolic/nonparabolic bands: Degond/A.J./Pietra 2000

Symmetrization and entropy

- Equations:

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

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

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

- Symmetrized equations:

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

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

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

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

Symmetrization and entropy

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

Entropy (free energy):

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

- Entropy inequality:

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

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

Drift-diffusion formulation

Drift-diffusion equations:

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

Theorem

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

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

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

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

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

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

Drift-diffusion formulation

Assumptions: parabolic band and scattering rate with parameter β:

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

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

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

Lyumkis model: $\beta = 0$

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

Nonparabolic bands: $E(1+\alpha E) = \frac{1}{2}|k|^2$

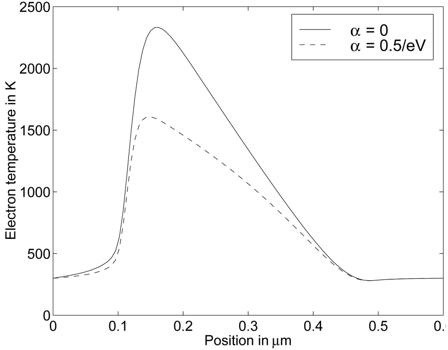
$$J_0 = \nabla(\mu_{0,\alpha}(T)n) - \mu_{0,\alpha}(T)\frac{n}{T}\nabla V, \quad J_1 = \nabla(\mu_{1,\alpha}(T)n) - \mu_{1,\alpha}(T)\frac{n}{T}\nabla V$$

Open problem: existence of solutions in general case

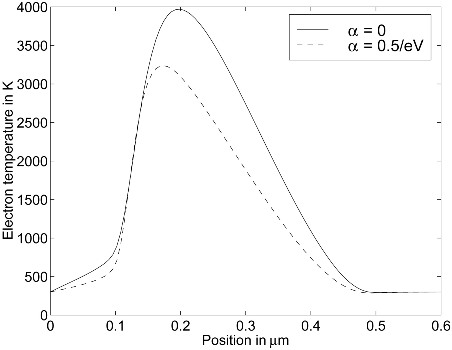
Numerical comparison in ballistic diode

Simulation of temperature:

Chen model



Lyumkis model



Numerical approximation: stationary equations

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

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

Objective:

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

Difficulties:

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

Solution:

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

Discretization of stationary equations

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

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

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

Discretization of stationary equations

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

3. Hybridization and condensation:

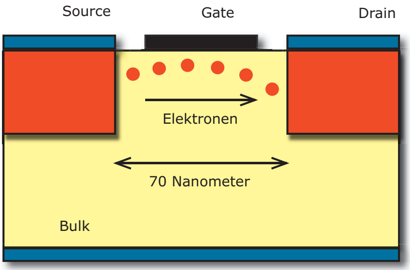
- Mixed finite-element scheme yields indefinite algebraic system $\rightarrow$ hybridization
- Variables $J_h \in H_{\rm loc}(\mathrm{div})$, $u_h \in L^2$ und λ_h on surfaces
- Static condensation: reduce system for (J_h, z_h, λ_h)

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

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

Simulation of field-effect transistors

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



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

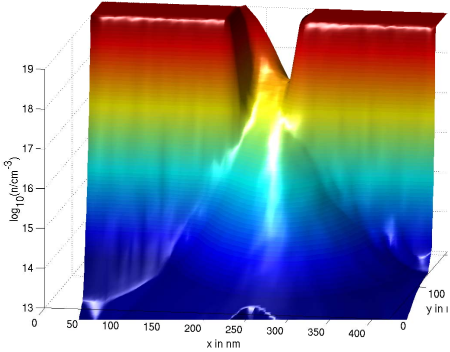
Iteration scheme:

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

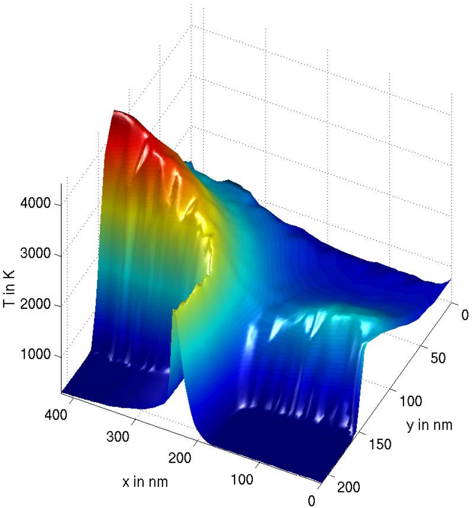
Simulation of 2D MOSFET

(Holst/A.J./Pietra 2003)

Electron density



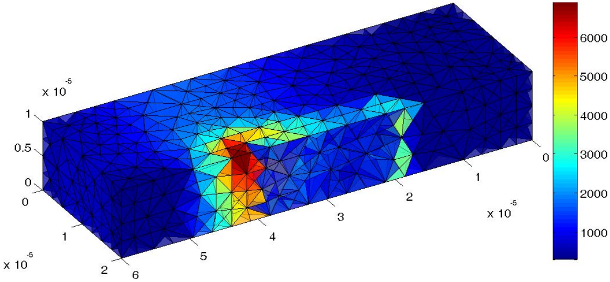
Temperature



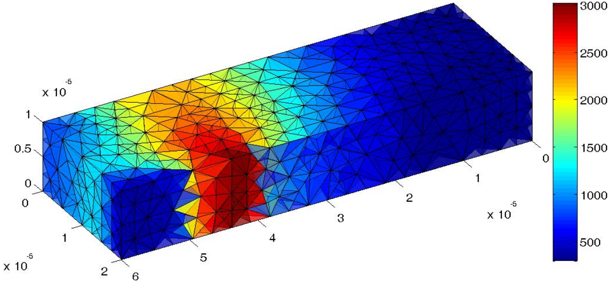
Simulation of 3D single-gate MESFET

(Gadau/A.J. 2007)

Off state

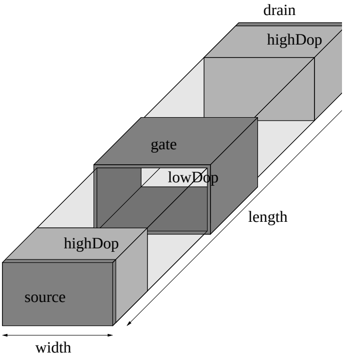


On state

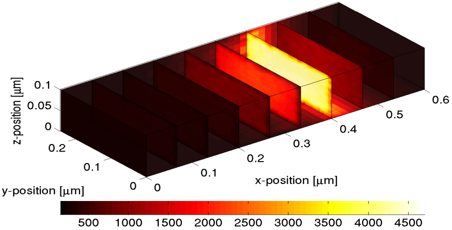


3D Gate-All-Around MESFET

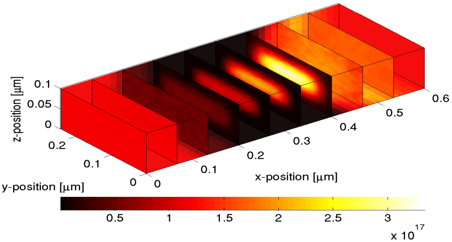
Geometry



Temperature

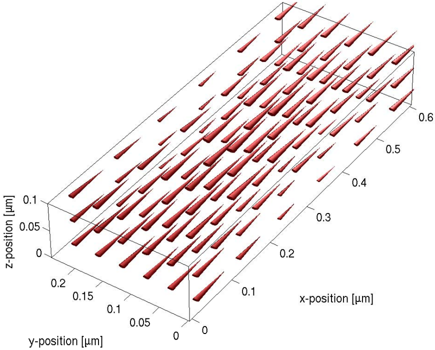


Thermal energy

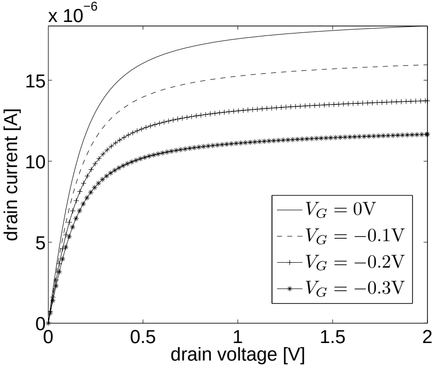


3D Gate-All-Around MESFET

Electron current density



Current-voltage characteristics



Summary

Energy-transport equations (Chen)

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

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

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

Overview

1. Semiconductor modeling
2. Semi-classical macroscopic models
   - General strategy
   - Energy-transport models
   - Higher-order diffusion models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Wigner models and quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Electric circuits
5. Summary and open problems

Semi-classical Boltzmann equation

$$\alpha^2\partial_t f + \alpha\big(v(k)\cdot\nabla_x f + \nabla_x V\cdot\nabla_k f\big) = Q_0(f) + \alpha^2 Q_1(f)$$

- Weight functions: $\kappa_i(k) = E(k)^i$, $i = 0, \ldots, N$
- Moments: $m_i(x,t) = \langle \kappa_i f(x,k,t)\rangle = \int_B \kappa_i f dk/4\pi^3$
- Moment equations:

$$\alpha^2\partial_t m_i + \alpha\big(\mathrm{div}_x\langle v\kappa_i f\rangle - \nabla_x V\cdot\langle\nabla_k\kappa_i f\rangle\big) = \langle\kappa_i Q_0(f)\rangle + \alpha^2\langle\kappa_i Q_1(f)\rangle$$

Strategy:

- Define equilibrium state (generalized Maxwellians)
- Assumptions on collision operators
- Derivation of macroscopic equations by Chapman-Enskog expansion and $\alpha\to 0$

Generalized Maxwellians

- Entropy (free energy): $S(f) = -\int_B f(\log f - 1 + E(k))dk/4\pi^3$
- Given f and moments $m = \langle \kappa f \rangle$, solve constrained maximization problem:

$$\max\{S(g) : \langle \kappa(k) g(x,k,t) \rangle = m(x,t) \text{ for all } x, t\}$$

$\rightarrow$ formal solution: generalized Maxwellian $M[f] = \exp(\kappa(k) \cdot \lambda(x,t))$

- Maximization problem may be delicate (Junk 1998, Dreyer/Junk/Kunik 2001), uniquely solvable if either
  - Brillouin zone B bounded
  - nonparabolic band approximation and $\kappa = (1, E, E^2)$
  - parabolic band approximation and $\kappa = (1, E)$
- Case of Fermi-Dirac statistics: equilibrium $f^* = 1/(1 + \exp(-\kappa \cdot \lambda))$

Examples: parabolic band $E(k) = \frac{1}{2}|k|^2$

$$M[f] = \exp(\lambda_0 + \tfrac{1}{2}\lambda_1 |k|^2), \quad M[f] = \exp(\lambda_0 + \tfrac{1}{2}\lambda_1 |k|^2 + \tfrac{1}{4}\lambda_2 |k|^4)$$

Assumptions on collision operators:

Let f_α be solution to Boltzmann equation and $F = \lim_{\alpha\to 0} f_\alpha$

- Conservation properties: $\langle \kappa_i Q_0(f)\rangle = 0$ for all f, i
- Kernel $N(Q_0)$ = generalized Maxwellians
- Mass conservation property: $\langle Q_1(f)\rangle = 0$
- Derivative $L = DQ_0(M[F])$ symmetric with respect to scalar product $(f,g)_F = \int_B fgdk/(4\pi^3 M[F])$ and kernel spanned by $M[F]$

Example: relaxation-time operator

$$Q_0(f) = \frac{1}{\tau}(M[f] - f)$$

Discussion:

- Mass conservation: $\langle Q_0(f)\rangle = 0$
- Energy conservation: $\langle E(k)Q_0(f)\rangle = 0$
- Also higher-order conservation for Q_0 required
- Last assumption needed for Fredholm alternative

Step 1

$$\alpha^2\partial_t f_\alpha + \alpha\big(v(k)\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_k f_\alpha\big) = Q_0(f_\alpha) + \alpha^2 Q_1(f_\alpha)$$

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

Step 2:

- Chapman-Enskog expansion $f_\alpha = M[f_\alpha] + \alpha g_\alpha$
- Expand collision operator:
  $Q_0(f_\alpha) = Q_0(M[f_\alpha]) + \alpha DQ_0(M[f_\alpha])g_\alpha + O(\alpha^2)$
- Insert expansion in Boltzmann equation:

$$\begin{aligned}\alpha\partial_t f_\alpha &+ \big(v\cdot\nabla_x M[f_\alpha] + \nabla_x V\cdot\nabla_k M[f_\alpha]\big)\\ &+ \alpha\big(v\cdot\nabla_x g_\alpha + \nabla_x V\cdot\nabla_k g_\alpha\big) = DQ_0(g_\alpha) + \alpha Q_1(f_\alpha)\end{aligned}$$

- Formal limit $\alpha \to 0$ gives

$$L(G) = v\cdot\nabla_x M[F] + \nabla_x V\cdot\nabla_k M[F], \quad G = \lim_{\alpha\to 0} g_\alpha$$

Step 2

$$L(G) = v \cdot \nabla_x M[F] + \nabla_x V \cdot \nabla_k M[F]$$
$$= v \cdot (\nabla_x \lambda)\kappa M[f] + \nabla_x V \cdot \nabla_k \kappa\lambda M[f] =: H, \quad \text{since } M[F] = e^{\kappa\cdot\lambda}$$

- Operator equation $LG = H$ solvable iff

$$H \in N(L^*)^\perp \overset{\text{symm.}}{=} N(L)^\perp$$
$$\iff \quad (H, f)_F = 0 \text{ for all } f \in N(L) = \text{span}\{M[F]\}$$
$$\iff \quad 0 = (H, M[F])_F = \int_B H dk/4\pi^3$$

  and since $v\kappa M[F]$ and $\nabla_k \kappa M[F]$ odd in k, $\int_B H dk = 0$

- Solution is given by

$$G = -\sum_{i=0}^{N} \left(\phi_i \cdot \nabla_x \lambda_j + i\nabla_x V \cdot \phi_{i-1}\lambda_i\right)$$

  where ϕ_i solves $L\phi_i = -v\kappa_i M[F]$

Step 3

- Use that $\langle v\kappa M[F]\rangle = 0$ and $\langle \nabla_k \kappa M[F]\rangle = i\langle v\kappa_{i-1} M[F]\rangle = 0$
- Insert $f_\alpha = M[f_\alpha] + \alpha g_\alpha$ in moment equations:

$$\partial_t\langle \kappa_i f_\alpha\rangle + \alpha^{-1}\Big(\mathrm{div}_x \underbrace{\langle v\kappa_i f_\alpha\rangle}_{=\alpha\langle v\kappa_i g_\alpha\rangle} - i\nabla_x V\cdot \underbrace{\langle v\kappa_{i-1} f_\alpha\rangle}_{=\alpha\langle v\kappa_{i-1} g_\alpha\rangle}\Big)$$

$$= \alpha^{-2}\underbrace{\langle \kappa_i Q_0(f_\alpha)\rangle}_{=0} + \langle \kappa_i Q_1(f_\alpha)\rangle$$

- Limit $\alpha \to 0$:

$$\partial_t\langle \kappa_i M[F]\rangle + \mathrm{div}_x\langle v\kappa_i G\rangle - \nabla_x V\cdot\langle v\kappa_{i-1} G\rangle = \langle \kappa_i Q_1(M[F])\rangle$$

- Computation of the fluxes:

$$J_i = -\langle v\kappa_i G\rangle = \Big\langle \sum_{j=0}^{N} v\kappa_i\big(\phi_j\cdot\nabla_x\lambda_j + j\nabla_x V\cdot\phi_{j-1}\lambda_j\big)\Big\rangle$$

$$= \sum_{j=0}^{N}\Big(\underbrace{\langle v\otimes\phi_j\kappa_i\rangle}_{=D_{ij}}\nabla_x\lambda_j + j\underbrace{\langle v\otimes\phi_{j-1}\kappa_i\rangle}_{=D_{i,j-1}}\nabla_x V\lambda_j\Big)$$

Higher-order diffusive moment model

Theorem

$$\partial_t m_i - \operatorname{div} J_i + iJ_{i-1} \cdot \nabla V = W_i, \quad \lambda_D^2 \Delta V = m_0 - C(x)$$
$$J_i = \sum_{j=0} \left(D_{ij} \nabla \lambda + jD_{i,j-1} \nabla V \lambda_j \right), \quad i = 0, \ldots, N$$

- Moments and right-hand side:

$$m_i = \int_B e^{\kappa \cdot \lambda} E(k)^i \frac{dk}{4\pi^3}, \quad W_i = \int_B Q_1(e^{\kappa \cdot \lambda}) E(k)^i \frac{dk}{4\pi^3}$$

- Diffusion coefficients:

$$D_{ij} = \int_B v(k) \otimes \phi_j E(k)^i \frac{dk}{4\pi^3}, \quad \phi_j \text{ solves } L\phi_j = -vE^i e^{\kappa \cdot \lambda}$$

Properties of diffusion matrix

$$D_{ij} = \int_B v(k) \otimes \phi_j E(k)^i \frac{dk}{4\pi^3}, \quad \phi_j \text{ solves } L\phi_j = -vE^i e^{\kappa\cdot\lambda}$$

Proposition

- *Symmetry:* $D_{ij}^\top = D_{ji}$
- *If* $-L$ *coercive on* $N(L)^\perp$ *and* $(v_i E^j)$ *linearly independent then* (D_{ij}) *positive definite*

Proof: similar as for energy-transport model

- Parabolic or nonparabolic bands $\Rightarrow$ $(v_i E^j)$ linearly independent
- Q_0 relaxation-time operator and (E^j) linearly independent $\Rightarrow -L$ coercive

Examples

Drift-diffusion equations ($N = 0$):

- Equations:

$$\partial_t m_0 - \mathrm{div}\, J_0 = 0, \quad J_0 = D_{00}\nabla(\lambda_0 - V), \quad D_{00} = \langle v \otimes \phi_0 \rangle$$

- Since $m_0 = \langle e^{\lambda_0 - E} \rangle \Rightarrow \nabla\lambda_0 = \nabla m_0 / m_0$,

$$J_0 = \mu_0(\nabla m_0 - m_0 \nabla V), \quad \mu_0 = \frac{1}{m_0}\int_B v \otimes d_0 \frac{dk}{4\pi^3}$$

Energy-transport equations ($N = 1$):

$$\partial_t m_0 - \mathrm{div}\, J_0 = 0, \quad \partial_t m_1 - \mathrm{div}\, J_1 + J_0 \cdot \nabla V = W_1$$
$$J_i = D_{i0}(\nabla\lambda_0 + \lambda_1 \nabla V) + D_{i1}\nabla\lambda_1$$

Examples

Fourth-order moment model ($N = 2$):

- Balance equations:

$$\partial_t m_0 - \mathrm{div}\, J_0 = 0, \quad \partial_t m_1 - \mathrm{div}\, J_1 + J_0 \cdot \nabla V = W_1$$
$$\partial_t m_2 - \mathrm{div}\, J_2 + 2J_1 \cdot \nabla V = W_2$$

- Current densities:

$$J_i = D_{i0}(\nabla \lambda_0 + \nabla V \lambda_1) + D_{i1}(\nabla \lambda_1 + 2\nabla V \lambda_2) + D_{i2}\nabla \lambda_2$$

- Assume parabolic band and $Q_0 =$ relaxation-time operator:

$$m_i = \frac{\sqrt{2}}{\pi^2} e^{\lambda_0} \int_B \varepsilon^{i+1/2} e^{\lambda_1 \varepsilon + \lambda_2 \varepsilon^2} d\varepsilon$$
$$D_{ij} = \frac{\sqrt{8}\tau}{3\pi^2} e^{\lambda_0} \int_B \varepsilon^{i+j+3/2} e^{\lambda_1 \varepsilon + \lambda_2 \varepsilon^2} d\varepsilon$$

Drift-diffusion formulation

Proposition

- *Current densities:*

$$J_i = \underbrace{\nabla d_i}_{\textit{diffusion}} + \underbrace{F_i(d) d_i \nabla V}_{\textit{drift}}, \quad F_i(d) = \sum_{j=1}^{N} \frac{j D_{i,j-1}}{D_{i0}} \lambda_j$$

where $d_i = \langle E^i v \otimes \phi_0 \rangle$, $L\phi_0 = -v e^{\kappa \cdot \lambda}$

- *The mapping* $d = d(\lambda)$ *is invertible since* $d'(\lambda) = \det(D_{ij}) > 0$

Fourth-order model:

- Current densities:

$$J_i = \frac{2}{3}\tau \left(\nabla m_{i+1} - \frac{2i+3}{2} m_i \nabla V \right), \quad i = 0, 1, 2$$

- System for unknown m_0, m_1, m_2, where $m_3 = -\frac{1}{2\lambda_2}(\frac{5}{2} m_1 + \lambda_1 m_2)$
- Relation $m = m(\lambda)$ can be inverted since $m'(\lambda)$ positive definite

Model of Grasser et al. 2001

$$\begin{aligned}
&\partial_t m_0 - \mathrm{div}\, J_0 = 0 \\
&\partial_t m_1 - \mathrm{div}\, J_1 + J_0 \cdot \nabla V = W_1 \\
&\partial_t m_2 - \mathrm{div}\, J_2 + 2J_1 \cdot \nabla V = W_2 \\
&J_i = \frac{2}{3}\tau\Big(\nabla m_{i+1} - \frac{2i+3}{2} m_i \nabla V\Big), \quad i = 0,1,2 \\
&m_i = \frac{\sqrt{2}}{\pi^2} e^{\lambda_0} \int_0^\infty e^{\lambda_1\varepsilon + \lambda_2\varepsilon} d\varepsilon
\end{aligned}$$

- Equations as above with $m_0 = n$, $m_1 = \frac{3}{2}nT$, $m_2 = \frac{15}{4}nT^2\beta_n$ (new variables n, T, β_n)
- Kurtosis $\beta_n = 3m_0m_2/5m_1^2$: Cauchy-Schwarz inequality $\Rightarrow \beta_n \geq \frac{3}{5}$
- Function m_3 heuristically given by $m_3 = \frac{105}{8}nT^2\beta_n^c$, c computed from Monte-Carlo simulations
- Grasser's model contained in model hierarchy if $\lambda_2 = -(1-\beta_n)/7T\beta_n^c$
- Integral m_i exists only if $\lambda_2 < 0 \Rightarrow \beta_n \leq 1 \Rightarrow \frac{3}{5} \leq \beta_n \leq 1$

Symmetrization and entropy

- Definitions:

$$\text{Dual entropy variables } \nu_i : \quad \lambda = P\nu$$
$$\text{Transformed moments } \rho_i : \quad \rho = P^\top m$$
$$\text{Thermodynamic fluxes } F_i : \quad F = P^\top J$$

- Transformation matrix:

$$P_{ij} = (-1)^{i+j} \binom{j}{i} a_{ij} V^{j-i}, \quad a_{ij} = \begin{cases} 1 & \text{if } i \le j \\ 0 & \text{if } i > j \end{cases}$$

Theorem

$$\partial_t \rho_i - \operatorname{div} F_i = (P^\top W + V^{-1} \partial_t V R m)_i \quad F_i = \sum_{j=0}^{N} C_{ij} \nabla \nu_j$$

where $R_{ij} = (i-j)P_{ij}$, and $C = P^\top DP$ symmetric positive definite

Symmetrization and entropy

- Thermal equilibrium: $\bar\lambda = (V, -1, 0, \ldots)$
- Relative macroscopic entropy:

$$S(t) = -\int_{\mathbb{R}^3} \big(m \cdot (\lambda - \bar\lambda) - m_0(\lambda) + m_0(\bar\lambda)\big)\,dx \le 0$$

- Example: energy-transport model:

$$S(t) = -\int_{\mathbb{R}^3} \Big(n \log \frac{n}{T^{3/2}} - nV\Big)\,dx$$

Theorem

If relaxation terms are dissipating, $\int_{\mathbb{R}^3} W \cdot (\lambda - \bar\lambda)dx \le 0$ then

$$-\frac{dS}{dt} + \sum_{i,j=0}^{N} C_{ij} \nabla \nu_i \cdot \nabla \nu_j dx \le 0$$

$\longrightarrow$ entropy nondecreasing in time and gradient estimates for ν_i

Summary

Higher-order diffusive moment model

$$\partial_t m_i - \operatorname{div} J_i + iJ_{i-1} \cdot \nabla V = W_i, \quad \lambda_D^2 \Delta V = m_0 - C(x)$$

$$J_i = \sum_{j=0} \big(D_{ij} \nabla \lambda + jD_{i,j-1} \nabla V \lambda_j \big), \quad i = 0, \ldots, N$$

- Diffusion matrix symmetric and positive definite
- Model formulated for general band structure
- Dual entropy variables allow symmetrization of equations
- Drift-diffusion formulation possible
- Generalization of Grasser's model

Open problems:

- Formulation for Fermi-Dirac statistics (work in progress with Krause)
- Numerical solution and comparison with energy-transport model

Overview

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   - Higher-order diffusion models
   - Hydrodynamic models
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   - Quantum drift-diffusion models
   - Quantum energy-transport models
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4. Electric circuits
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Assumptions

Boltzmann equation in hydrodynamic scaling:

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

Assumptions:

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

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

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

Derivation

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

Moment equations:

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

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

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

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

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

$\longrightarrow$ compute moments of M

Derivation

Lemma

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

Hydrodynamic equations:

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

$$\partial_t J_n - \mathrm{div}\left(\frac{J_n\otimes J_n}{n}\right) - \nabla(nT) + n\nabla V = -\langle kQ_1(M)\rangle$$

$$\partial_t(ne) - \mathrm{div}\,\big(J_n(e+T)\big) + J_n\cdot\nabla V = \langle \tfrac{1}{2}|k|^2Q_1(M)\rangle$$

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

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

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

Remarks

Hydrodynamic model

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

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

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

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

Remarks

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

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

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

Extended hydrodynamic model

- Reference: Anile/Romano 2000
- Weight functions: $\kappa = (1, v(k), E(k), v(k)E(k))$, moments: $m_i = \langle \kappa_i M \rangle$
- Maxwellian: $M = \exp(\lambda_0 + \lambda_1 \cdot v + \lambda_2 E + \lambda_3 \cdot vE)$
- Moment equations:

$$\partial_t m_i - \operatorname{div} J_i + \nabla V \cdot I_i = 0$$
$$J_i = -\langle v\kappa_i M \rangle, \quad I_i = -\langle \nabla_k \kappa_i M \rangle$$

- Mapping $\lambda \mapsto m$ cannot be explicitly inverted: approximate
- Assumptions: $E(k)$ isotropic, anisotropy of M small $\Rightarrow$

$$\lambda_0 = \lambda_0^{(0)} + \delta^2 \lambda_0^{(2)}, \ \lambda_1 = \delta \lambda_1^{(1)}, \ \lambda_2 = \lambda_2^{(0)} + \delta^2 \lambda_2^{(2)}, \ \lambda_3 = \delta \lambda_3^{(1)}$$

$\rightarrow$ if $\delta = 0$ then equilibrium values

- Approximate Maxwellian up to $O(\delta^3)$:

$$M = \exp\left(\lambda_0^{(0)} + \lambda_2^{(0)} E\right)\Big(1 + \delta v \cdot A_1 + \delta^2 A_2 + \frac{\delta^2}{2}|v \cdot A_1|^2\Big)$$

Extended hydrodynamic model

- Approximated Maxwellian:

$$M = \exp\left(\lambda_0^{(0)} + \lambda_2^{(0)} E\right)\left(1 + \delta v \cdot A_1 + \delta^2 A_2 + \frac{\delta^2}{2}|v \cdot A_1|^2\right)$$

where $A_1 = \lambda_1^{(1)} + \lambda_3^{(1)} E(k)$ and $A_2 = \lambda_0^{(2)} + \lambda_2^{(2)} E(k)$

- Insert in moment definition and identify equal powers of δ:

$$\frac{m_2}{m_0} = \frac{\langle e^{\lambda_2^{(0)} E}\rangle}{\langle e^{\lambda_2^{(0)}}\rangle} \;\Rightarrow\; \lambda_2^{(0)} \text{ (numerically)}$$

$$m_0 = e^{\lambda_0^{(0)}} \int_B e^{\lambda_2^{(0)} E} \frac{dk}{4\pi^3} \;\Rightarrow\; \text{for given } m_0, \text{ compute } \lambda_0^{(0)}$$

$$m_1 = e^{\lambda_0^{(0)}} \int_B e^{\lambda_2^{(0)} E} v(v \cdot A_1) \frac{dk}{4\pi^3} \text{ and}$$

$$m_3 = e^{\lambda_0^{(0)}} \int_B e^{\lambda_2^{(0)} E} vE(v \cdot A_1) \frac{dk}{4\pi^3} \;\Rightarrow\; (\lambda_1^{(1)}, \lambda_3^{(1)})$$

Extended hydrodynamic model

- Recall that $A_1 = \lambda_1^{(1)} + \lambda_3^{(1)} E(k)$ and $A_2 = \lambda_0^{(2)} + \lambda_2^{(2)} E(k)$
- Insert in moment definition and identify equal powers of δ:

$$0 = \int_B e^{\lambda_2^{(0)} E} \Big(A_2 + \frac{1}{2}|v \cdot A_1|^2 \Big) \frac{dk}{4\pi^3} \quad \text{and}$$
$$0 = \int_B e^{\lambda_2^{(0)} E} \Big(A_2 + \frac{1}{2}|v \cdot A_1|^2 \Big) E \frac{dk}{4\pi^3} \quad \Rightarrow \quad (\lambda_0^{(2)}, \lambda_2^{(2)})$$

- For given m_i, compute

$$\lambda_1^{(1)} = a_{11} m_1 + a_{12} m_3, \quad \lambda_0^{(2)} = b_{01} m_1 \cdot m_1 + 2 b_{02} m_1 \cdot m_3 + b_{03} m_3 \cdot m_3,$$
$$\lambda_3^{(1)} = a_{31} m_1 + a_{32} m_3, \quad \lambda_2^{(2)} = b_{21} m_1 \cdot m_1 + 2 b_{22} m_1 \cdot m_3 + b_{23} m_3 \cdot m_3,$$

where a_{ij}, b_{ij} depend on $(\lambda_0^{(0)}, \lambda_2^{(0)})$ or, equivalently, on (m_0, m_2)

Summary

Extended hydrodynamic model

$$\partial_t m_i - \operatorname{div} J_i + \nabla V \cdot I_i = 0, \quad i = 0,1,2,3$$

$$J_i = -\langle v\kappa_i M\rangle, \quad I_i = -\langle \nabla_k \kappa_i M\rangle$$

$$M = \exp\left(\lambda_0^{(0)} + \lambda_2^{(0)} E\right)\left(1 + \delta v \cdot A_1 + \delta^2 A_2 + \frac{\delta^2}{2}|v \cdot A_1|^2\right)$$

where $A_1 = \lambda_1^{(1)} + \lambda_3^{(1)} E(k)$ and $A_2 = \lambda_0^{(2)} + \lambda_2^{(2)} E(k)$

- Relation between m_i and $\lambda_i^{(j)}$ is invertible (numerically)
- M, J_i, and I_i can be formulated as function of moments m_i
- Gives system of hyperbolic equations

Relations between the macroscopic models

Rescaled hydrodynamic equations:

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

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

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

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

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

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

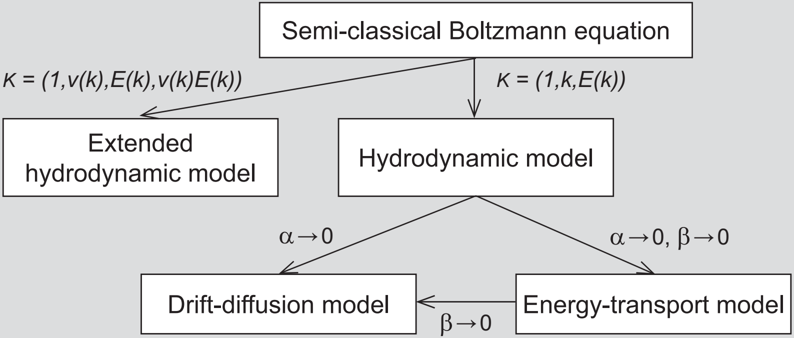
- $\alpha \to 0$: energy-transport equations

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

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

Relations between the macroscopic models

Hydrodynamic models and relaxation-time limits



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Wigner equation

- Quantum ensemble described by Wigner function $w(x,p,t)$, $p=\hbar k$
- Wigner equation (parabolic band):

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

- Potential operator:

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

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

  $\theta[V]$ is pseudo-differential operator, acts on Fourier space as multiplication operator

- Symbol of the operator δV satisfies

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

Wigner equation

- Electron and current density:

$$n(x,t) = \frac{2}{(2\pi\hbar)^3}\int_{\mathbb{R}^3} w(x,p,t)dp, \; J(x,t) = \frac{2q}{(2\pi\hbar)^3 m}\int_{\mathbb{R}^3} w(x,p,t)pdp$$

- Nonnegativity: If initial datum nonnegative then generally *not* $w(x,p,t) \geq 0$ but $n(x,t) \geq 0$
- Scaling:

reference length λ	reference time τ
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:

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

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

Wigner equation

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

Semi-classical limit: Since $\theta[V]w \to \nabla_x V \cdot \nabla_p w$,

$$\partial_t w + p \cdot \nabla_x w + \nabla_x V \cdot \nabla_p w = 0 \quad \Rightarrow \quad \text{Vlasov equation}$$

Scattering models:

- Wigner-Fokker-Planck collision operator:

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

  Lindblad condition $D_{pp}D_{qq} - D_{pd}^2 \geq \gamma^2/4$ for positivity preservation
- Wigner BGK operator (BGK = Bhatagnar-Gross-Krook):

$$Q(w) = \frac{1}{\tau}\Big(\frac{n}{n_0}w_0 - w\Big), \quad w_0: \text{ quantum equilibrium}$$

Liouville-von Heisenberg equation

- Quantum system described by (positive, self-adjoint) density matrix operator $\hat{\rho}$ satisfying

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

where $H =$ Hamiltonian, for instance, $H = -(\hbar^2/2m)\Delta - qV$

- Integral representation by density matrix function $\rho(x,y,t)$:

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

- Electron density: $n(x,t) = \rho(x,x,t)$
- Relation to single-particle Schrödinger equation:

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

density matrix $\rho(x,y,t) = \psi(x,t)\overline{\psi(y,t)}$ solves Liouville-von Neumann equation

Wigner transform

Quantum state representations

Wigner $\longleftrightarrow$ Liouville-von Neumann $\longleftrightarrow$ Schrödinger

- Wigner transform of $\hat{\rho}$:

$$W(\hat{\rho})(x,p) = \int_{\mathbb{R}^3} \rho\Big(x + \frac{\varepsilon}{2}\eta, x - \frac{\varepsilon}{2}\eta\Big) e^{-i\eta\cdot p} d\eta$$

- Weyl quantization:

$$W^{-1}(f)\phi(x) = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^6} f\Big(\frac{x+y}{2}\Big)\phi(y) e^{ip\cdot(x-y)/\varepsilon} dp\, dy$$

- 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:

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

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

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

- Constrained maximization problem: given w, solve

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

Formal solution:

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

Quantum Maxwellian

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

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

- One moment (n) prescribed:

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

- Two moments (n, ne) prescribed:

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

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

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

Quantum Maxwellian

Expansion of quantum Maxwellian in powers of ε^2:

$$
\begin{aligned}
M_1[w] &= \mathrm{Exp}\Big(A(x,t) - \frac{|p|^2}{2}\Big) = \exp\Big(A(x,t) - \frac{|p|^2}{2}\Big) \\
&\quad \times \Big[1 + \frac{\varepsilon^2}{8}\Big(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Ap\Big)\Big] + O(\varepsilon^4) \\
M_2[w] &= \mathrm{Exp}\Big(A - \frac{|p|^2}{2T}\Big) = \exp\Big(A - \frac{|p|^2}{2T}\Big) \\
&\quad \times \Big[1 + \frac{\varepsilon^2}{8T}\Big(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}p^\top(\nabla\otimes\nabla)Ap \\
&\quad + \frac{|p|^2}{2}\Delta\beta + T(p\cdot\nabla\beta)^2 + \frac{|p|^2}{3T}p^\top(\nabla\otimes\nabla)\beta p \\
&\quad + \frac{2}{3}(p\cdot\nabla\beta)(p\cdot\nabla A) - \frac{|p|^2}{3}(p\cdot\nabla\beta)^2 - \frac{|p|^2}{3}\nabla A\cdot\nabla\beta \\
&\quad + \frac{|p|^4}{3}|\nabla\beta|^2\Big)\Big] + O(\varepsilon^4), \quad \beta = 1/T
\end{aligned}
$$

Quantum Maxwellian

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

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

- Expansion in powers of ε^2:

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

$\longrightarrow$ first derived by Wigner 1932

- Compare to Maxwellian of constrained problem:

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

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Derivation

- Diffusion-scaled Wigner-Boltzmann equation:

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

- BGK-type collision operator: $Q(w) = M[w] - w$, $M[w] = \mathrm{Exp}(A - \frac{1}{2}|p|^2)$ (one moment prescribed)
- Properties of collision operator:

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

- Properties of potential operator:

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

- Derivation performed in three steps

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

Derivation

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

Step 2: Chapman-Enskog expansion

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

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

- Limit $\alpha \to 0$:

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

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

- Moment equation:

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

Derivation

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

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

- Computation of current density J_n:

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

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 ε^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 ε^2

- Electron density:

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

- Quantum stress tensor:

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

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

- Express A in terms of n

Expansion in powers of ε^2

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

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

- Recall formula:

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

- 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)

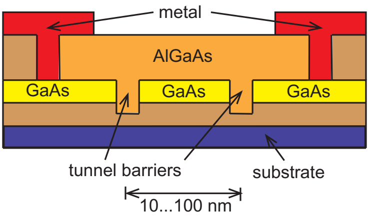
Resonant tunneling diode

Geometry:

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

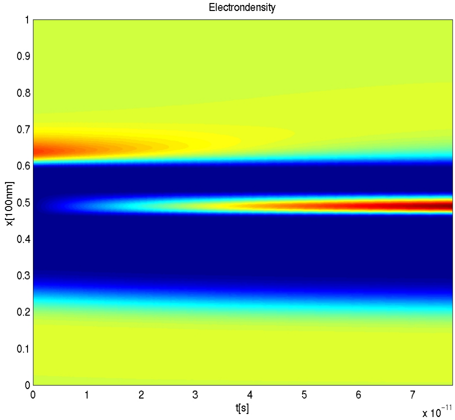
Numerical method:

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

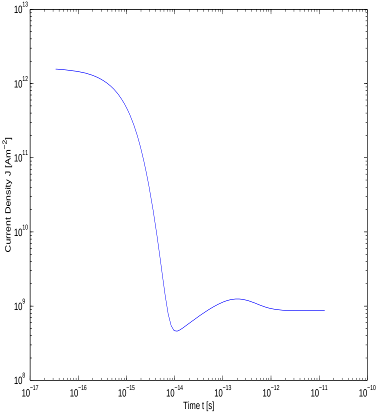


Time-dependent simulations of tunneling diode

Electron density $n(t)$

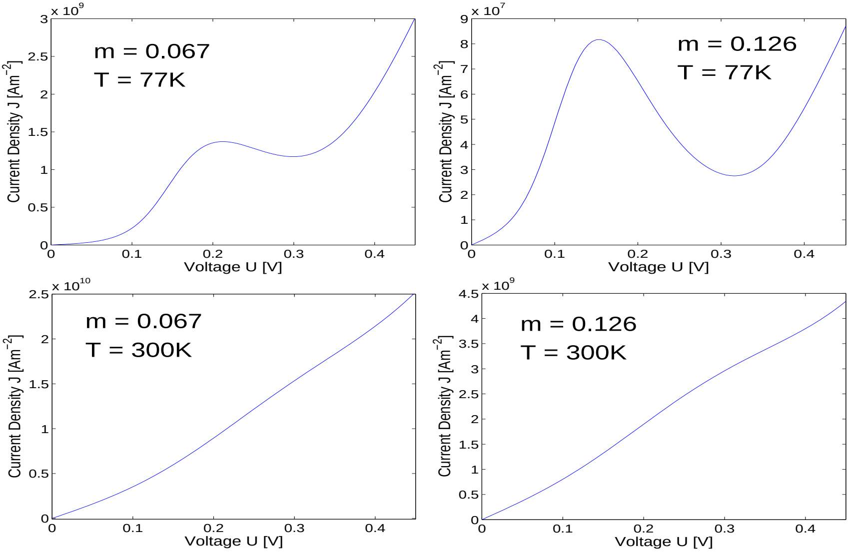


Current density $J(t)$



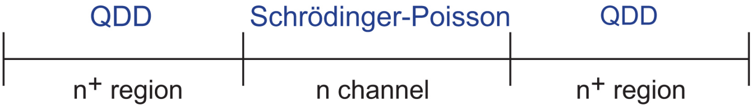
$\longrightarrow$ stabilization after $\sim 10^{-11}$ sec. (100 GHz)

Current-voltage characteristics of tunneling diode



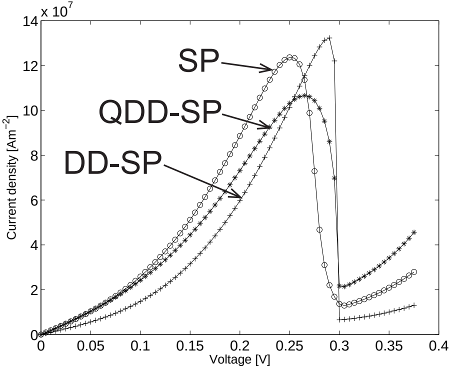
Coupled QDD-Schrödinger-Poisson model

(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):

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

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

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

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:

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

- 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

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

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

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

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

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

- Entropy inequality:

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

Summary

Local quantum drift-difusion model (QDD)

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

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

Overview

1. Semiconductor modeling
2. Semi-classical macroscopic models
   - General strategy
   - Energy-transport models
   - Higher-order diffusion models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Wigner models and quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Electric circuits
5. Summary and open problems

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

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

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

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

Derivation

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

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

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

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

Derivation

- Moment equations:

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

- 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

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

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

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

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: $dS/dt \geq 0$
  (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

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

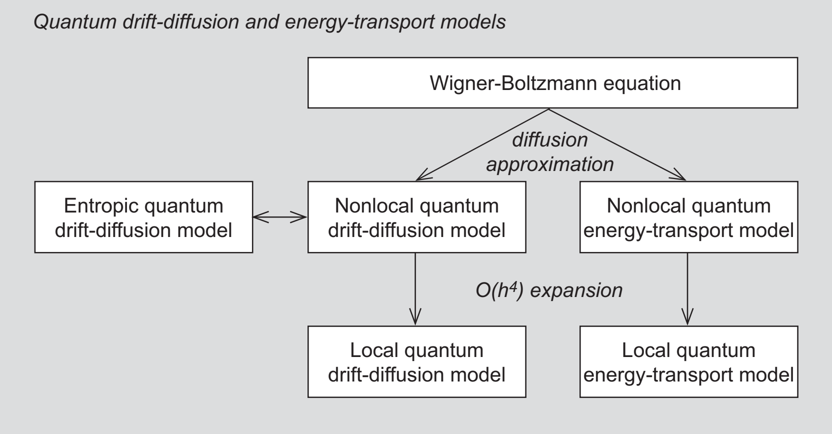
$$J_n = \operatorname{div} P - n\nabla V, \quad J_e = \operatorname{div} U - (P + ne\,\mathrm{Id})\nabla V + \frac{\varepsilon^2}{8} n\nabla\Delta V$$

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

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

- 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



$\longrightarrow$ Entropic QDD = nonlocal QDD

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Single-state Schrödinger equation

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

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

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

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

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

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

Zero-temperature quantum hydrodynamic model

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

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

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

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

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 (ψ_j,λ_j) of $\hat\rho$
- ψ_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 (ψ_j,λ_j) solution of mixed-state Schrödinger system
- Define electron and current density:

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

Schrödinger equation and quantum hydrodynamics

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

- Then (n, J) solves

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

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

- Closure condition 1: $\theta = T\,\mathrm{Id}$, $T > 0$ (isothermal model)
- Closure condition 2 (Gasser/Markowich/Ringhofer 1996): small temperature and small ε 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 $Q_0(w) = 0$ iff $w =$ quantum Maxwellian
- Quantum entropy: $S(w) = -\frac{2}{(2\pi\varepsilon)^3}\int_{\mathbb{R}^6} w(\operatorname{Log} w - 1 + \frac{|p|^2}{2} - V)dx\,dp$
- Quantum Maxwellian: Let w be given and $M[w]$ be solution of

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

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

Derivation

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

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:

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

- Limit $\alpha\to 0$:

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

- 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:

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

- Define quantum stress tensor and quantum heat flux

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

Derivation

Theorem (Nonlocal quantum hydrodynamic model)

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

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: $M[w] = \mathrm{Exp}(A - |p-v|^2/2)$
- $O(\varepsilon^4)$-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 betwenn (n, J) and (A, v):

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

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

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

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

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

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

$$\partial_t n - \operatorname{div} J = 0,\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n} + P\right) + n\nabla V = -\langle pQ_1(w)\rangle$$
$$\partial_t(ne) - \operatorname{div}\big((P + ne\,\mathrm{Id})J - q\big) + J\cdot\nabla V = \langle \tfrac12|p|^2 Q_1(w)\rangle$$

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

$$ne = \frac32 nT + \frac12 n|u|^2 - \frac{\varepsilon^2}{24}n\Big(\Delta\log n - \frac1T \mathrm{Tr}(R^\top R) - \frac32|\nabla\log T|^2 - \Delta\log T - \nabla\log T\cdot\nabla\log n\Big) + O(\varepsilon^4)$$

$$P = nT\,\mathrm{Id} + \frac{\varepsilon^2}{12}n\Big(\frac52\nabla\log T\otimes\nabla\log T - \nabla\log T\otimes\nabla\log n - \nabla\log n\otimes\nabla\log T - (\nabla\otimes\nabla)\log(nT^2) + \frac1T R^\top R\Big) + \frac{\varepsilon^2}{12}T\operatorname{div}\left(\frac nT\nabla\log T\right) + O(\varepsilon^4)$$

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

Conserved quantities

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

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

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

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

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

Proposition

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

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

Local quantum hydrodynamic model

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

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

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

$\longrightarrow$ Gives closed set of equations

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

Local quantum hydrodynamic model

Theorem (Local quantum hydrodynamic model)

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

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

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

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:

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

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

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

- Gardner's 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's 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 $T=$ const., $\nabla A = \nabla \log n + O(\varepsilon^2) \Rightarrow w_Q = M[w]$
- "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

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

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

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

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

- Averaged quantities:

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

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

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

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

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

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

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

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

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

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

Dissipative QHD models

Caldeira-Leggett operator:

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

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

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

- 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

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

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

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

Fokker-Planck operator:

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

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

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

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

- Gives viscous quantum hydrodynamic model

Viscous quantum hydrodynamic model

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

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

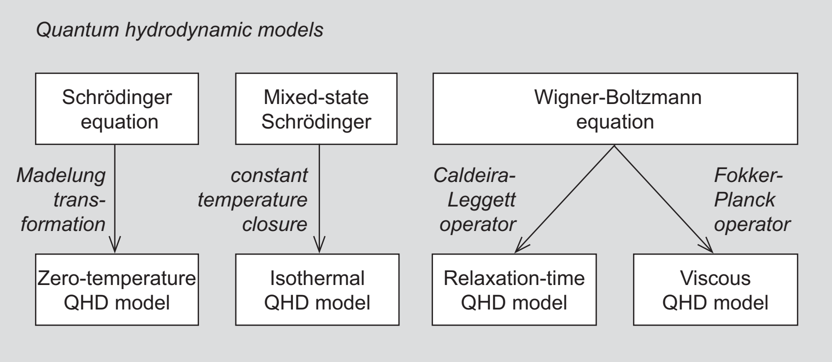
$$= D_{qq}\Delta J - 2\gamma J + 2D_{pq}\nabla_x n$$

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

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

- D_{qq} provides diffusive terms
- Effective current density $J_{\mathrm{eff}} = J - D_{qq}\nabla n$: $\partial_t n - \mathrm{div}\, J_{\mathrm{eff}} = 0$
- Existence of 1D stationary solutions with $T = 1$ (A.J./Milisic 2007)
- Lobal existence of transient solutions (Chen/Dreher 2006), global existence of 1D transient solutions (Gamba/A.J./Vasseur 2008)
- Open problem: global existence of solutions for full system

Hierarchy of quantum hydrodynamic models



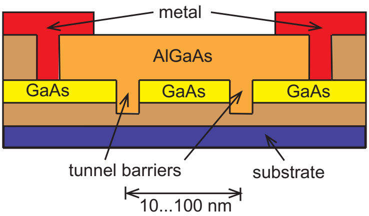
Resonant tunneling diode

Geometry:

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

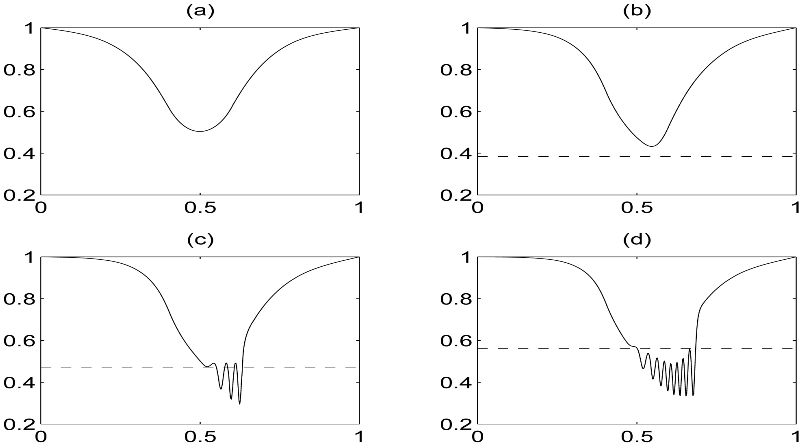
Numerical method:

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

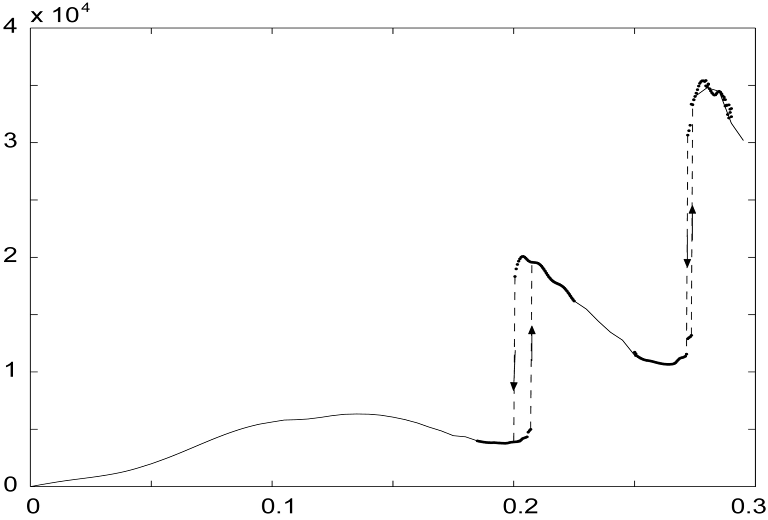


Zero external potential

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

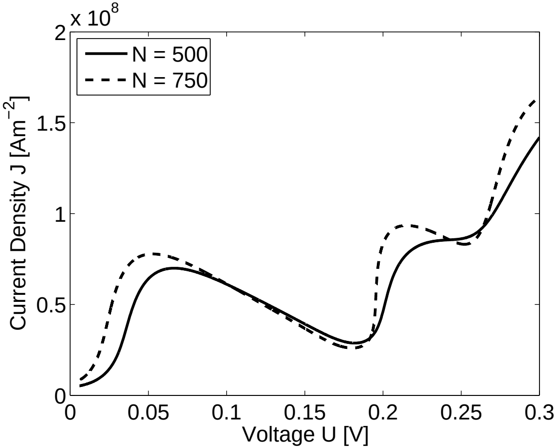


Resonant tunneling diode: current-voltage characteristics



→ hysteresis phenomenum

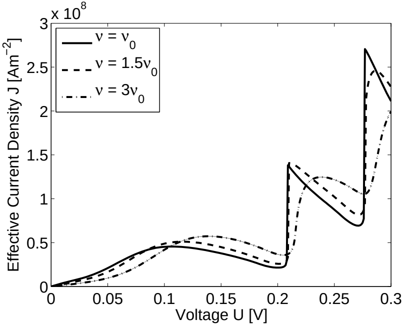
Upwind finite differences



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

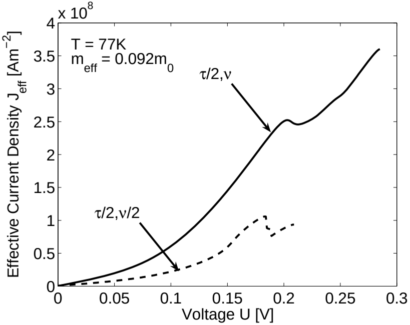
Viscous quantum hydrodynamic model

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 $\rightarrow$ viscosity too strong

Summary

Quantum hydrodynamic equations

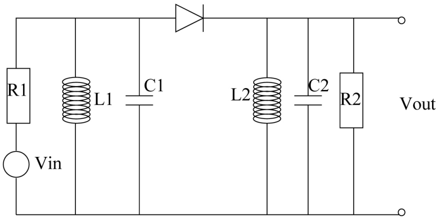
$$\partial_t n - \operatorname{div} J = 0, \;\; \partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n} + P\right) + n\nabla V = -\langle p Q_1(w)\rangle$$
$$\partial_t(ne) - \operatorname{div}\big((P + ne\,\mathrm{Id})J - q\big) + J \cdot \nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(w)\rangle$$

- Single-state Schrödinger $\longrightarrow$ zero-temperature quantum hydrodynamics
- Mixed-state Schrödinger $\longrightarrow$ isothermal quantum hydrodynamics
- Diffusion approximation of Wigner equation $\longrightarrow$ 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

Overview

1. Semiconductor modeling
2. Semi-classical macroscopic models
   - General strategy
   - Energy-transport models
   - Higher-order diffusion models
   - Hydrodynamic models
3. Quantum macroscopic models
   - Wigner models and quantum Maxwellian
   - Quantum drift-diffusion models
   - Quantum energy-transport models
   - Quantum hydrodynamic models
4. Electric circuits
5. Summary and open problems

Semiconductor devices and electric circuits



- Today: compact models in highly-integrated circuits
- Objective: use PDE models for critical devices
- Leads to coupled network-device models: partial differential-algebraic equations (PDAE)

References:

- Günther 2001: PDAE with hyperbolic eqs., models transmission lines
- Bartel/Günther 2002: coupled network and electrothermal model
- Tischendorf et al. 2003: network and drift-diffusion models
- Brunk/A.J. 2007: network and energy-transport models

Circuit modeling

- Circuits contain resistors, capacitors, inductors, voltage sources
- Reduces electric circuits to RCL circuits
- Modal analysis: replace circuit by directed graph (branches & nodes)
- Characterize circuit by incidence matrix $A = (a_{jk})$ describing node-to-node relations (with entries 1, -1, or 0)

Kirchhoff laws:

- Sum of all branch currents entering a node equals zero:

$$Ai = 0, \quad i: \text{ branch currents}$$

- Sum of all branch voltages in a loop equals zero:

$$v = A^\top e$$

v: branch voltages, e: node potentials

Circuit modeling

- Current-voltage characteristics:

$$i_R = g(v_R), \quad i_C = \frac{dq}{dt}(v_C), \quad v_L = \frac{d\Phi}{dt}(i_L)$$

g: conductivity of resistor, q: charge of capacitor, Φ: flux of inductor

- Network branches numbered such that incidence matrix A consists of block matrices A_R, A_C, A_L, A_i, A_v
- Input functions for current and voltages sources: $i_s(t)$, $v_s(t)$

Charge-oriented modified nodal analysis:

- Kirchhoff current law gives:

$$A_C i_C + A_R i_R + A_L i_l + A_v i_v = -A_i i_s$$

- Replace i_C and i_R by current-voltage characteristics:

$$A_C \frac{dq}{dt}(v_C) + A_R g(v_R) + A_L i_l + A_v i_v = -A_i i_s$$

Circuit modeling

$$A_C \frac{dq}{dt}(v_C) + A_R g(v_R) + A_L i_l + A_v i_v = -A_i i_s$$

Differential-algebraic equations for $e(t)$, $i_L(t)$, $i_v(t)$

- Replace v_C and v_R by Kirchhoff voltage law:

$$A_C \frac{dq}{dt}(A_C^\top e) + A_R g(A_R^\top e) + A_L i_L + A_v i_v = -A_i i_s$$

- Kirchhoff voltage laws for v_L and v_s:

$$\frac{d\Phi}{dt}(i_L) - A_L^\top e = 0, \quad A_v^\top e = v_s$$

- Index at most two if circuit contains neither loops of voltage sources only nor cutsets of current sources only
- Index at most one if circuit contains neither LI cutsets nor CV loops with at least one voltage

Coupling of network and energy-transport model

First coupling: semiconductor → circuit

- Semiconductor current density at terminal Γ_k,

$$j_k = \int_{\Gamma_k} J_{\rm tot} \cdot \nu ds, \quad J_{\rm tot} = J_n + J_d$$

$J_d = -\lambda_D^2 \partial_t \nabla V$: displacement current, guarantees charge conservation since $\operatorname{div} J_{\rm tot} = \partial_t n - \lambda_D^2 \partial_t \Delta V = 0$

- Include $j_S = (j_k)_k$ into Kirchhoff current law:

$$A_C \frac{dq}{dt}(A_C^\top e) + A_R g(A_R^\top e) + A_L i_L + A_v i_v + A_S j_S = -A_i i_s$$

Second coupling: circuit → semiconductor

- Let terminal Γ_k of device be connected to circuit node i
- Electric potential in semiconductor device:

$$V(t) = e_i(t) \quad \text{on } \Gamma_k$$

Complete coupled model

Energy-transport and drift-diffusion equations

$$\partial_t n - \operatorname{div} J_0 = -R(n,p), \quad \partial_t(\tfrac{3}{2}nT) - \operatorname{div} J_1 + J_0 \cdot \nabla V = W(n,T) - \tfrac{3}{2}TR(n,p)$$

$$J_0 = \mu^*\Big(\nabla n - \frac{n}{T}\nabla V\Big), \quad J_1 = \frac{3}{2}\mu^*\big(\nabla(nT) - n\nabla V\big), \quad \lambda_D^2 \Delta V = n - C(x)$$

$$\partial_t p + \operatorname{div} J_p = -R(n,p), \qquad J_p = -\nabla p - p\nabla V$$

Network equations

$$A_C \frac{dq}{dt}(A_C^\top e) + A_R g(A_R^\top e) + A_L i_L + A_v i_v + A_S j_S = -A_i i_s$$

$$\frac{d\Phi}{dt}(i_L) - A_L^\top e = 0, \qquad A_v^\top e = v_s$$

Coupling in 1D:

$$j_S(t) = J_n(0,t) + \lambda_D^2 \partial_t V_{xx}, \qquad V(0,t) = e_i, \qquad V(1,t) = e_j$$

Numerical discretization of coupled model

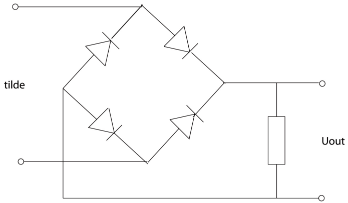
Numerical solution of differential-algebraic equations:

- Implicit Runge-Kutta schemes or backward-difference formulas (BDF)
- Order reduction of Runge-Kutta methods possible
- k-step BDF with $k \leq 6$ feasible and weakly unstable
- Implicit Euler: damping too strong
- Radau IIa: stiffness matrix from semiconductor model not M-matrix
- 2-step BDF provides M-matrix

Numerical solution of energy-transport equations:

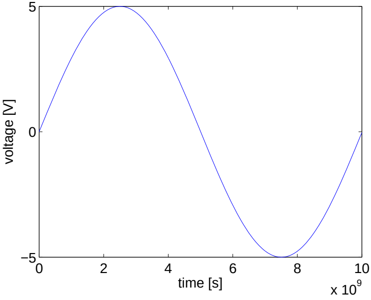
- Time discretization: 2-step BDF
- Space discretization: mixed finite elements

Rectifying circuit

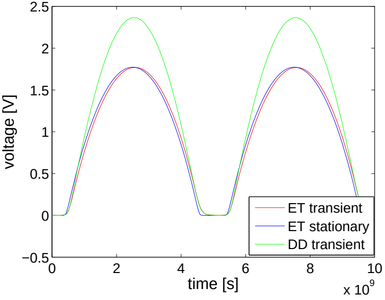


- Contains four *pn* diodes with length 0.1 μm
- Voltage source: $v(t) = U_0 \sin(2\pi\omega t),\ U_0 = 5\ V$
- Input frequency: $\omega = 10\,\mathrm{GHz}$

Input

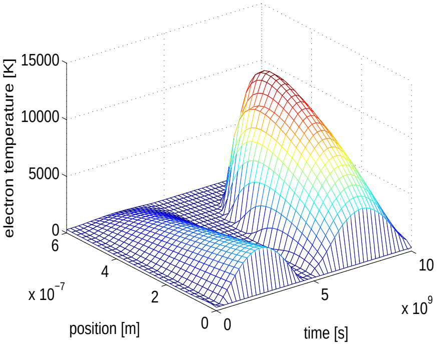


Output

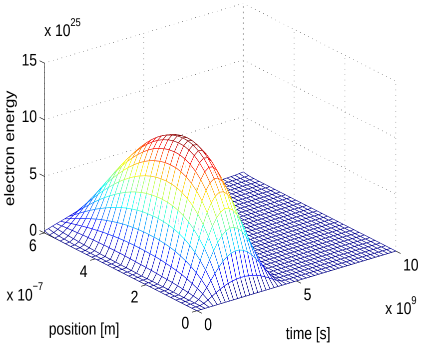


Rectifying circuit

Electron temperature

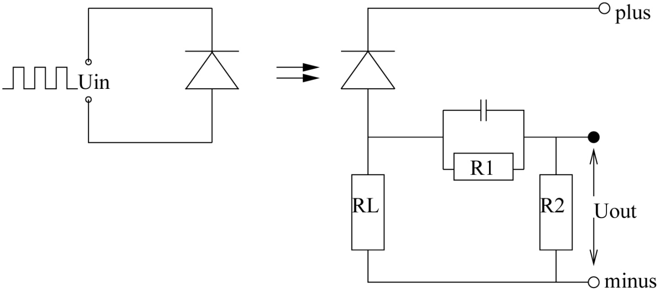


Electron energy



- high temperature in reverse bias
- few electrons in reverse bias → low energy density
- high energy density in forward bias

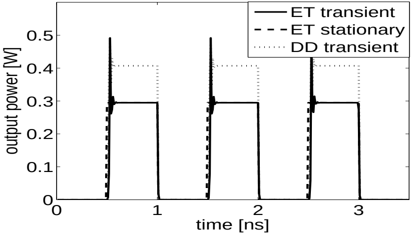
High-pass filter including optoelectronic devices



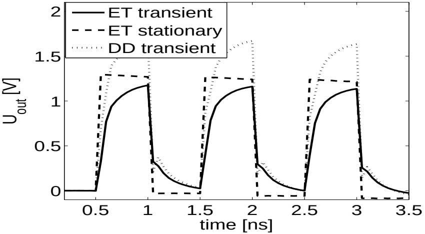
- Laser diode: digital input signal with frequency 1 GHz and 5 GHz
- Photo diode: receives signal and coupled to high-pass filter
- High-pass filter: only passes frequencies larger than cutoff frequency

High-pass filter including optoelectronic devices

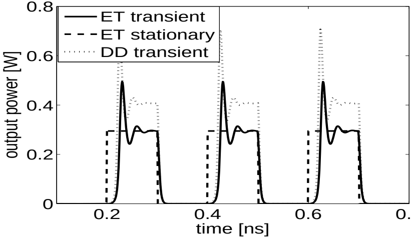
1 GHz: Output of laser diode



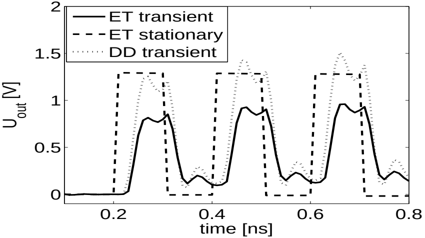
Output of high-pass filter



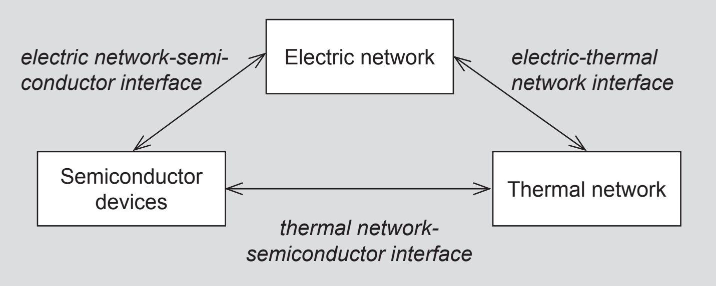
5 GHz: Output of laser diode



Output of high-pass filter

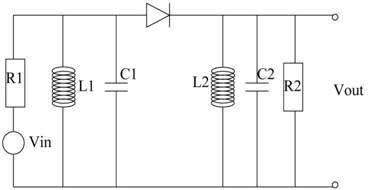


Modeling of device heating



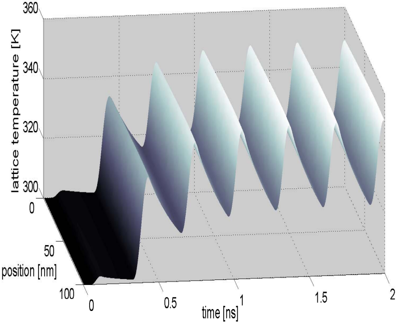
- Electric network modeled by circuit equations (diff.-algebraic eqs.)
- Thermal network modeled by 1D heat equation with power dissipation
- Semiconductor devices modeled by bipolar energy-transport equations
- Lattice temperature modeled by heat equation
- Define coupling conditions: (1) electric–thermal network, (2) electric network–semiconductor devices, (3) thermal network–semiconductor device

Frequency multiplier

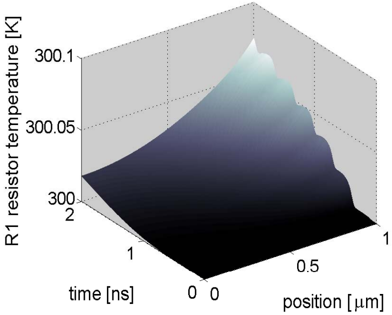


- Diode and resistors thermally relevant
- Input frequency of 3.2 GHz
- Solve PDE + DAE system

Temperature of diode



Temperature of $R1$



Summary

- Electric circuit modeled by differential-algebraic equations obtained from Kirchhoff's laws and modified nodal analysis
- Energy-transport model for semiconductor devives consists of partial differential equations
- Coupled circuit-device model consists of partial differential-algebraic equations
- Time discretization: implicit Ringe-Kutta or BDF schemes
- Space discretization: mixed finite elements
- Numerical examples: rectifying circuit, high-pass filter including laser and photo diode

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Summary

Semiconductor modeling:

- Bloch decomposition of wave function
- Semi-classical picture

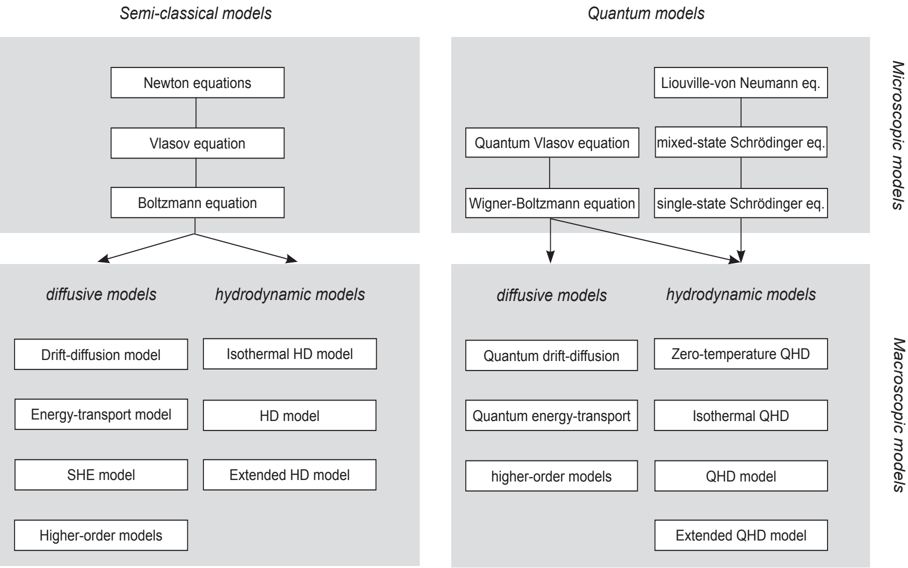
Semi-classical macroscopic models:

- Three- or two-step derivation from semi-classical Boltzmann equation
- Step 1: knowledge about kernel of scattering operator (Maxwellian)
- Step 2: Chapman-Enskog expansion for diffusion correction (only needed for diffusive models)
- Step 3: limit of vanishing Knudsen number in moment equations

Quantum macroscopic models:

- Three- or two-step derivation from Wigner-Boltzmann equation
- Definition of quantum Maxwellian
- 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

Energy-transport models:

- Improved boundary conditions (derived from kinetic conditions)
- Existence of solutions under general assumptions
- Coupling with lattice temperature in 3D (Kristöfel, in progress)

Higher-order diffusive models:

- Numerical approximation and comparison to Grasser's model
- Including Fermi-Dirac statistics (Krause, in progress)
- Existence of solutions, rigorous derivation

Quantum drift-diffusion models:

- Existence results for nonlocal model (entropic structure!)

Some open problems

Quantum energy-transport models:

- Understand mathematical structure
- Numerical approximation
- Existence of solutions

Quantum hydrodynamic models:

- Positivity of solutions
- Equivalence to Schrödinger equation
- Better numerical approximation schemes