A hierarchy of diffusive higher-order moment models for semiconductors

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- Introduction
- Derivation of the moment models
- Properties and examples
- Drift-diffusion and entropy formulations

Derivation of macroscopic models

Semiclassical Boltzmann equation:

$$\partial_t f + u(p) \cdot \nabla_x f + \nabla_x V \cdot \nabla_p f = Q(f)$$

$f(x,p,t)$	: distribution function, p: crystal momentum
$u = \nabla_p \varepsilon$	: velocity, ε: energy band
$V(x,t)$	: electric potential
$Q(f)$	: collision operator

Moment equations: weight functions $\kappa_i(p)$

Define $\langle g \rangle = \int_B g(p)dp$, B: Brillouin zone

$$\partial_t \langle f \kappa_i \rangle + \mathrm{div}_x \langle u f \kappa_i \rangle - \nabla_x V \cdot \langle f \nabla_p \kappa_i \rangle = \langle Q(f) \kappa_i \rangle$$

Objective: derive evolution equations for moments $\langle f \kappa_i \rangle$

Moment equations

$$\partial_t\langle f\kappa_i\rangle + \mathsf{div}_x\langle u f\kappa_i\rangle - \nabla_x V\cdot\langle f\nabla_p\kappa_i\rangle = \langle Q(f)\kappa_i\rangle$$

Nonparabolic energy band : $\varepsilon(p) = |p|^2(1+\sqrt{1+2\delta|p|^2})^{-1}$

Weight functions: $\kappa_i(p) = \varepsilon(p)^i$, $i = 0, 1, \ldots$

Moments:	$\langle f\rangle$	: electron density
	$\langle f\varepsilon\rangle$	: energy density
Fluxes:	$\langle fu\rangle$	: electron current density
	$\langle fu\varepsilon\rangle$	: energy current density

Mass and energy equations:

$$i = 0: \quad \partial_t\langle f\rangle + \mathsf{div}_x\langle fu\rangle = \langle Q(f)\rangle = 0$$

$$i = 1: \quad \partial_t\langle f\varepsilon\rangle + \mathrm{div}_x\langle fu\varepsilon\rangle - \nabla_x V\cdot\langle fu\rangle = \langle Q(f)\varepsilon\rangle$$

Closure problem: $\langle fu\varepsilon\rangle$ cannot be expressed by $\langle f\rangle$, $\langle f\varepsilon\rangle$

Moment equations

Diffusive models	*Hydrodynamic models*	*# Variables*
Drift-diffusion equations *Van Roosbroeck 1950*		1
	Isothermal hydro-dynamic equations	4
Energy-transport equations *Stratton 1962*		2
	Full hydrodynamic equations *Blotekjaer 1970*	6
Fourth-order moment equations *Grasser et al. 2001*		3
	Extended hydro-dynamic equations *Anile 1995*	13
Higher-order moment equations *A.J./Krause/Pietra 2007*		
	Higher-order hydro-dynamic equations *Struchtrup 1999*	

Goal:
derive hierarchy for diffusive models

Advantages:

- numerical effort less than Boltzmann
- less variables than hydrodynamic models

Solution of closure problem

① Generalized Maxwellians: Given f, let $M_f = \exp(\lambda \cdot \kappa)$ be defined as maximizer of the "entropy"

$$H(g) = -\int_B g(\log g - 1 + \varepsilon)dp \text{ subject to } \langle g\kappa_i \rangle = \langle f\kappa_i \rangle$$

Maximization problem may be delicate!
(Junk 1998, Dreyer/Junk/Kunik 2001)

② Diffusive scaling: Introduce Knudsen No. α (Levermore)

$$\alpha^2 \partial_t \langle f\kappa_i \rangle + \alpha(\text{div}_x \langle uf\kappa_i \rangle - \nabla_x V \cdot \langle f \nabla_p \kappa_i \rangle) = \langle Q(f)\kappa_i \rangle$$

③ Assumptions on collision operator:

- $Q(f) = Q_1(f) + \alpha^2 Q_2(f)$
- $Q_1(f) = 0 \Leftrightarrow f = M_f$, conservation: $\langle Q_1(f)\kappa_i \rangle = 0 \ \forall\ i$
- mass conservation: $\langle Q_2(f) \rangle = 0$

Solution of closure problem

$$\alpha^2 \partial_t \langle f\kappa \rangle + \alpha(\mathrm{div}_x \langle u f \kappa \rangle - \nabla_x V \cdot \langle f \nabla_p \kappa \rangle) = \langle Q(f)\kappa \rangle$$

④ Balance equations for moments $m_i = \langle M_f \kappa_i \rangle$:

Chapman-Enskog: insert $f = M_f + \alpha g$ and let $\alpha \to 0$

⑤ Constitutive equations for fluxes $J_i = \langle g u \kappa_i \rangle$:

- Assumptions on $DQ_1(M_f)$ (for Fredholm alternative)
- To simplify: $\kappa_i = \varepsilon^i$

$$\partial_t m_i + \mathrm{div}_x J_i - i \nabla_x V \cdot J_{i-1} = \langle Q_2(f)\kappa_i \rangle$$

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

where D_{ij} solves operator equation related to $DQ_1(M_f)$ and $m_i(\lambda) = \langle M_f \kappa_i \rangle = \langle e^{\lambda \cdot \kappa} \kappa_i \rangle$

Higher-order moment model

$$\partial_t m_i + \operatorname{div} J_i - i\nabla V \cdot J_{i-1} = W_i$$

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

Properties:

- Moments $m_i(\lambda) = \langle e^{\lambda\cdot\kappa}\kappa_i\rangle$ monotone w.r.t. λ
- Diffusion matrix (D_{ij}) is symmetric
- Matrix (D_{ij}) positive definite (if $-DQ_1(M_f)$ coercive)
- Entropy density $h(m) = m \cdot \lambda - m_0$ (Albinus 1995)
- Extensive variables $\lambda_i = \frac{\partial h}{\partial m_i}$

Example: parabolic band and Q_1 = relaxation operator

$$D_{ij} = \int_0^\infty \varepsilon^{i+j+3/2} \exp(\lambda_0 + \cdots + \lambda_N \varepsilon^N) d\varepsilon$$

$$m_i = \int_0^\infty \varepsilon^{i+1/2} \exp(\lambda_0 + \cdots + \lambda_N \varepsilon^N) d\varepsilon$$

Examples of moment models

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

$$\partial_t m_0 + \operatorname{div} J_0 = 0, \quad J_0 = -D_{00}\nabla(\lambda_0 - V)$$

$m_0 = Ae^{\lambda_0}$: electron density, $\lambda_0 - V$: quasi Fermi potential

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

$$\partial_t m_0 + \operatorname{div} J_0 = 0$$

$$\partial_t m_1 + \operatorname{div} J_1 - \nabla V \cdot J_0 = W_1$$

$$J_i = -D_{i0}(\nabla\lambda_0 + \nabla V \lambda_1) - D_{i1}\nabla\lambda_1, \quad i = 0, 1$$

Parabolic band and energy-depending relaxation time:

$$m_0 = T^{3/2}e^{\lambda_0}, \quad m_1 = \frac{3}{2}m_0 T, \quad T = -\frac{1}{\lambda_1}$$

$$(D_{ij}) = c_\beta m_0 T^{1-\beta}\begin{pmatrix} 1 & \frac{5}{2}T \\ \frac{5}{2}T & \frac{35}{4}T^2 \end{pmatrix}, \quad \beta \geq 0$$

Examples of moment models

Higher-order model ($N = 2$):

$$\partial_t m_0 + \operatorname{div} J_0 = 0$$

$$\partial_t m_1 + \operatorname{div} J_1 - \nabla V \cdot J_0 = W_1$$

$$\partial_t m_2 + \operatorname{div} J_2 - 2\nabla V \cdot J_1 = W_2$$

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

Parabolic band:

$$m_i = e^{\lambda_0} \int_0^\infty \varepsilon^{i+1/2} e^{\lambda_1\varepsilon + \lambda_2\varepsilon^2} d\varepsilon$$

$$D_{ij} = e^{\lambda_0} \int_0^\infty \varepsilon^{i+j+3/2} e^{\lambda_1\varepsilon + \lambda_2\varepsilon^2} d\varepsilon$$

$\longrightarrow$ No analytical formulas

$\longrightarrow$ Similar model: Grasser 2001

Drift-diffusion formulation

Theorem: Current densities can be written as

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

where λ_j given by $d_i(\lambda)$ through solution of operator equation

Advantage: numerical decoupling of stationary system

Given $\widetilde{d}_i$ from previous iteration step, solve decoupled system

$$\operatorname{div} J_i(d) = i \nabla V \cdot J_{i-1}(d) + W_i(\widetilde{d})$$

$$J_i(d) = -\nabla d_i - F_i(\widetilde{d}) d_i \nabla V$$

- Gives system of linear equations for d_i
- "Symmetrization" by local Slotboom variables possible
- Approximation by mixed finite elements: work in progress

Higher-order model

$$\partial_t m_0 + \operatorname{div} J_0 = 0$$

$$\partial_t m_1 + \operatorname{div} J_1 - \nabla V \cdot J_0 = W_1$$

$$\partial_t m_2 + \operatorname{div} J_2 - 2\nabla V \cdot J_1 = W_2$$

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

- System in 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 $m'(\lambda)$ pos. def.
- Model of Grasser: he introduces (n, T, β_n) by

$$m_0 = n, \quad m_1 = \tfrac{3}{2}nT, \quad m_2 = \tfrac{15}{4}nT^2\beta_n, \quad m_3 = \tfrac{105}{8}nT^2\beta_n^c$$

$\longrightarrow$ Value of c computed heuristically from MC simulations

$\longrightarrow$ Our model: $m_3 = m_3(n, T, \beta_n)$,
Grasser's model obtained if $m_3 = \frac{105}{8}nT^2\beta_n^c$

Entropy formulation

Definitions:

dual-entropy variables ν_i: $\lambda = P\nu$

transformed moments ρ_i: $\rho = P^\top m$

thermodynamic fluxes F_i: $F = P^\top J$

with the 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: The moment model can be written as

$$\partial_t \rho_i + \operatorname{div} F_i = (P^\top W + V^{-1} \partial_t V R m)_i$$

$$F_i = -\sum_{j=0}^{N} C_{ij} \nabla \nu_j$$

where $R_{ij} = (i-j)P_{ij}$, $C = P^\top D P$ symm. positive definite

Advantage: system is symmetrized

Higher-order model is of parabolic type

$$\partial_t \rho_i(\nu) - \operatorname{div} \sum_j C_{ij} \nabla \nu_j = \widetilde{W}_i$$

Existence of solutions: Alt/Luckhaus 1983 ($V = 0$), Degond/Génieys/A.J. 1997 (unif. elliptic)

Energy-transport equations:

- Define chemical potential μ and temperature T by $\lambda_0 = \frac{\mu}{T}$, $\lambda_1 = -\frac{1}{T}$
- Dual-entropy variables: $\nu_0 = \frac{\mu - V}{T}$, $\nu_1 = -\frac{1}{T}$

Higher-order model:

- Define second-order temperature θ by $\lambda_2 = -\frac{1}{\theta T}$
- Dual-entropy variables:

$$\nu_0 = \frac{\mu - V}{T} - \frac{V^2}{\theta T}, \quad \nu_1 = -\frac{1}{T} - \frac{2V}{\theta T}, \quad \nu_2 = -\frac{1}{T}$$

Entropy dissipation

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

$$H(t) = -\int_{\mathbb{R}^3} (m \cdot (\lambda - \bar{\lambda}) - m_0(\lambda) + m_0(\bar{\lambda}))dx \leq 0$$

- Energy-transport model: $H = -\int (n \log(nT^{-3/2}) - nV)dx$

Theorem: If $\int W \cdot (\lambda - \bar{\lambda})dx \leq 0$ then

$$-\frac{dH}{dt} + \sum_{i,j=1}^{N} \int_{\mathbb{R}^3} C_{ij} \nabla \nu_i \cdot \nabla \nu_j dx \leq 0$$

$\longrightarrow$ entropy is nondecreasing in time

$\longrightarrow$ if (C_{ij}) unif. positive definite: gradient estimates for ν_j

Summary

Main features:

- General assumptions on collision operator
- Gives hierarchy of diffusive moment models
- Drift-diffusion formulation allows for numerical decoupling
- Entropy formulation allows for symmetrization
- Thermodynamic interpretation possible

Limitations:

- Maxwell-Boltzmann statistics assumed
  $\longrightarrow$ Can be generalized to Fermi-Dirac (in progress)
- Conservation of all moments of Q_1 questionable
  $\longrightarrow$ Generalization possible?
- $M_f = e^{\lambda_0 + \lambda_1 \varepsilon + \lambda_2 \varepsilon^2}$ good approximation?
  $\longrightarrow$ Distinguish hot and cold electrons? (in progress)