W I A S

Weierstraß-Institut für Angewandte Analysis und Stochastik

A Drift-Diffusion Model with
Fully Nonlocal State Equation for
Heterogeneous Semiconductor Materials

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1   Stochastic processes "far" from equilibrium

Closed system of interacting particles occupying a bounded spatial domain Ω.

BUTTA, LEBOWITZ: The free energy of such a system is – in the macroscopic picture – a density functional of the form

$$E(n) = \Phi^*(n) + \Psi(n). \tag{1}$$

The short-range interaction energy

$$\Phi^*(n) = \int_\Omega \varphi^*(n(x))\, dx \tag{2}$$

is a strictly convex functional, and the long-range interaction energy

$$\Psi(n) = \frac{1}{2} \int_\Omega \int_\Omega k(x,y) n(y) n(x)\, dy\, dx + \int_\Omega k_0(y) n(y)\, dy, \tag{3}$$

is a quadratic functional, where k is a symmetric integral kernel.

Minimization of the free energy

Minimizing E under the constraint of particle number conservation. Lagrange functional:

$$E_\zeta(n) \stackrel{\text{def}}{=} E(n) + \int_\Omega (n_0(x) - n(x))\zeta(x)\,dx$$
$$= \Phi^*(n) + \Psi(n) + \int_\Omega (n_0(x) - n(x))\zeta(x)\,dx$$

$$\begin{aligned}
\zeta &= v + w & \text{Lagrange parameter} \\
v &= \partial\Phi^*(n) & \text{chemical potential} \\
w &= \partial\Psi(n) & \text{(long-range) interaction potential}
\end{aligned}$$

Evolution of the density

Lebowitz et al.: Applying diffusive hydrodynamic scaling to the microscopic dynamics one obtains in the limit a drift-diffusion-type transport equation describing the evolution of the density n:

$$\begin{aligned}
n' + \nabla \cdot j &= 0 & \text{in } (0,t) \times \Omega, && \text{(4a)} \\
j \cdot v &= 0 & \text{on } (0,t) \times \partial\Omega, && \text{(4b)} \\
n(0) &= n_0 & \text{on } \Omega. && \text{(4c)}
\end{aligned}$$

Current density:

$$j = -\kappa \nabla \zeta \tag{5}$$

κ is the mobility of the system with only short-range interactions.

Einstein relation

SPOHN, LEBOWITZ:

The diffusivity μ is given in terms of the free energy density φ^*, in such a way that the Einstein relation holds true:

$$\mu(n) = \kappa(n)\, \partial^2 \Phi^*(n), \tag{6}$$

Hence, the current density j can be written as a sum of a semi-linear diffusion and a non-linear, non-local drift part:

$$j = -\mu \nabla n - \kappa \nabla w.$$

2   Drift-diffusion models with local state equations

Thermodynamic design of semiconductor models

VAN ROOSBROECK [1950]: macroscopic model describing drift, diffusion, and reaction processes of charge carriers in a semiconductor

GAJEWSKI, GRÖGER [1989, 1996]: van Roosbroeck's system has free energy of type

$$E(n) = \Phi^*(n) + \Psi(n)$$

as a Lyapunov functional

GLITZKY, HÜNLICH [1997]: thermodynamic approach to more general electro-reaction-diffusion systems

ALBINUS, GAJEWSKI, HÜNLICH [1999]: thermodynamic design of energy models of semiconductor devices

Van Roosbroeck's system I

Evolution equation (unipolar case, no reactions)
$$n' + \nabla \cdot j = 0 \quad \text{in } (0, t) \times \Omega$$
$$j \cdot \nu = 0 \quad \text{on } (0, t) \times \partial\Omega$$
$$n(0) = n_0 \quad \text{on } \Omega$$

Structure of current and Einstein relation
$$j = -\kappa \nabla \zeta, \qquad \mu(n) = \kappa(n) \, \partial^2 \Phi^*(n)$$

State equation
$$n(x) = \begin{cases} \bar{n}(x) \, \exp(v(x)) & \text{Boltzmann statistics} \\ \bar{n}(x) \, \mathcal{F}_{1/2}(v(x)) & \text{Fermi–Dirac statistics} \end{cases}$$

$\bar{n} \in L^\infty(\Omega; \mathbb{R}^+)$ represents a given density of states.

The Fermi integral to the index $\alpha > -1$ is defined by $\mathcal{F}_\alpha(s) = \frac{1}{\Gamma(\alpha+1)} \int_0^\infty \frac{\tau^\alpha d\tau}{1+\exp(\tau-s)}$

Chemical potential

The convex functional Φ^* is the dual of

$$\Phi(v) \stackrel{\text{def}}{=} \int_\Omega \bar{n}(x) \varphi(v(x)) \, dx$$

where
$$\varphi(x) = \begin{cases} \exp(x) & \text{Boltzmann statistics} \\ \mathcal{F}_{3/2}(x) & \text{Fermi–Dirac statistics} \end{cases}$$

Hence, the state equation can be written as

$$n = \partial \Phi(v)$$

that means
$$n(x) = \bar{n}(x) \varphi'(v(x)) \quad x \in \Omega$$

Van Roosbroeck's system II

Poisson equation

$$-\nabla \cdot (\varepsilon \nabla v_0) = p - n \quad \text{in } (0, t) \times \Omega$$
$$\nu \cdot (\varepsilon \nabla v_0) + \tau v_0 = 0 \qquad \text{on } (0, t) \times \partial \Omega$$

$\varepsilon \in L^\infty(\Omega; \mathbb{R}^+)$ dielectric permittivity, $\dfrac{1}{\varepsilon} \in L^\infty(\Omega; \mathbb{R})$

$\tau \in L^\infty(\partial\Omega; \mathbb{R}^+)$ capacitance of the boundary, $\|\tau\|_{L^1(\partial\Omega;\mathbb{R})} > 0$

p given doping profile

Interaction potential

The (long-range) interaction potential is given by

$$w = v_c - v_0,$$

where

$$v_c \quad \text{band edge offset,}$$
$$v_0 \quad \text{electrostatic potential.}$$

Correspondingly, the (long-range) interaction energy is

$$\Psi(n) = \int_\Omega \frac{\varepsilon}{2} |\nabla v_0|^2 \, dx + \int_{\partial\Omega} \frac{\tau}{2} |v_0|^2 \, d\sigma + \int_\Omega n v_c \, dx,$$

such that indeed,

$$w = \partial \Psi(n).$$

Analysis of drift-diffusion semiconductor models

Weak solutions

Gajewski/Gröger 1989-1996
Glitzky/Hünlich 1997
Albinus/Gajewski/Hünlich 1999

free energy of the system is a convex functional

exponential decay of the free energy along trajectories

energetic estimates

existence and uniqueness of bounded weak solutions of the evolution system which asymptotically converge to an equilibrium state

In order to obtain uniqueness Gajewski introduced the concept of *E*-monotonicity.

Analysis of drift-diffusion semiconductor models

Classical solutions

HCK/Neidhardt/Rehberg 2006

existence and uniqueness of local in time classical solutions of the
drift-diffusion system for semiconductors
(rather general reaction terms)

methods for quasi-linear parabolic equations in Lebesgue spaces

Gajewski/Skrypnik 2006

global in time (unique) classical solutions
(under restricting conditions on the reaction terms)

3   The stationary problem with non-local state equations

Density Functional Theory (DFT)

- aims at ground states of a quantum mechanical system

- is precise for systems in equilibrium

- treats many-particle systems with one-particle equations

- identifies the particles in equilibrium, and

- accounts for the interaction of particles by an additional operator in a one-particle Hamiltonian (the xc-potential)

Fundamental applications of DFT in

- nuclear physics, and physical chemistry

- solid state physics, and in particular semiconductor physics

DFT and Kohn–Sham system

Kohn [1965] (1998 half a Nobel Prize in Chemistry for DFT)

DFT calculations are based on the Kohn–Sham system, and have been performed for a long time.

Mathematical analysis of Kohn–Sham systems started only in the 1990s: HCK/Rehberg [1997], Prodan/Nordlander [2003].

Solutions of the Kohn–Sham system describe the stationary states of the evolution system under consideration here.

The Kohn–Sham system is a stationary Schrödinger–Poisson system with self-consistent effective Kohn–Sham potential.

Kohn–Sham equations

for a heterogeneous semiconductor material:

$$-\tfrac{\hbar^2}{2}\nabla \cdot \left(m^{-1}\nabla\psi_\ell\right) + (v_\mathrm{c} + v_\mathrm{xc} - v_0)\psi_\ell = E_\ell\psi_\ell$$
$$-\nabla \cdot (\varepsilon\nabla v_0) = p - n$$
$$n = \sum_{\ell\in\mathbb{N}} f(E_\ell - \zeta)\,|\psi_\ell|^2$$

m	position-dependent effective mass tensor
$v_\mathrm{xc} = v_\mathrm{xc}(n)$	exchange-correlation potential
ε	dielectric permittivity
p	given doping profile
$\zeta = \zeta(n)$	normalizing shift which fixes the number of particles

f describes the distribution of the particles on the energy scale;
in the three-dimensional case f is the Fermi function.

Analysis of the Kohn–Sham system

Without xc-potential:

unique solution depending boundedly Lipschitz continuous on the reference potential v_c in the Schrödinger operator

System is a non-linear Poisson eq. with fully non-local state eqs.

Non-linear Poisson operator is strongly monotone and boundedly Lipschitz continuous

With xc-potential:

Kohn–Sham system has at least one solution (Schauder)

Sufficient conditions on the xc-potential for unique solution

4   Von Neumann-type trace functionals

The analysis for the Kohn–Sham system rests upon the following property:

The quantum mechanical carrier density operator depending on the potential of the defining Schrödinger operator is anti-monotone and boundedly Lipschitz continuous.

Caussignac, Nier, HCK/Rehberg [1990–1997]

All these results are special cases of a general result on the convexity and differentiability of von Neumann-type trace functionals.

HCK/Neidhardt/Rehberg [2003]

Von Neumann-type trace functionals

Notations

$\mathcal{H}$	separable, infinite-dimensional Hilbert space
$\mathcal{B}$	space of bounded linear operators on $\mathcal{H}$
$\mathcal{B}_1$	subspace of trace class operators
$\mathcal{B}^s$	subspace of self-adjoint operators from $\mathcal{B}$
$\mathcal{B}_1^s$	subspace of self-adjoint operators from $\mathcal{B}_1$
$\mathcal{B}_1^+$	the cone of self-adjoint non-negative trace class operators

Von Neumann-type trace functionals

Convexity

Proposition (VON NEUMANN [1932], LIEB / PEDERSEN [2002])

If H is a self-adjoint operator with compact resolvent which is semi-bounded from below, and
$G : \mathbb{R} \to \mathbb{R}^+$ is continuous, decreasing, convex, and such that
$G(H + \gamma)$ is nuclear for each $\gamma \in \mathbb{R}$,
then the functional

$$\mathcal{B}^s \ni U \longmapsto \operatorname{tr}\big(G(H + U)\big)$$

is convex.

Von Neumann-type trace functionals

Differentiability

Proposition (BIRMAN AND SOLMYAK [1973])

If H is a self-adjoint operator with compact resolvent which is semi-bounded from below, and
$G : \mathbb{R} \to \mathbb{R}$ is continuously differentiable, and such that
G' is bounded, integrable, and Hölder continuous on all (γ, ∞),
then for each $W \in \mathcal{B}_1^s$ the function

$$\mathbb{R} \ni s \longmapsto G(H + sW) \in \mathcal{B}_1$$

is continuously differentiable, and

$$\frac{\mathrm{d}}{\mathrm{d}s} \operatorname{tr}\big(G(H + sW)\big)\big|_{s=t} = \operatorname{tr}\big(G'(H + tW)W\big) \quad \text{for all } t \in \mathbb{R}.$$

Von Neumann-type trace functionals

Gradient

Proposition (HCK/Neidhardt/Rehberg [2003])

If H is a self-adjoint operator with compact resolvent which is semi-bounded from below, and

$G : \mathbb{R} \to \mathbb{R}^+$ is continuously differentiable, decreasing, convex, and such that $G(H + \gamma)$ is nuclear for each $\gamma \in \mathbb{R}$,

then the functional

$$\mathcal{B}^s \ni U \longmapsto \Phi(U) \stackrel{\text{def}}{=} \text{tr}\left(G(H + U)\right)$$

is Fréchet differentiable, and its gradient

$$\partial\Phi \,:\, \mathcal{B}^s \to \mathcal{B}_1^s \subseteq (\mathcal{B}^s)^*, \qquad \partial\Phi(U) = G'(H + U) \quad \text{is monotone.}$$

5   The model with fully non-local state equation

We aim at a drift-diffusion model of semiconductor heterostructures.

Bulk material:

averaging over a fundamental cell of the translational lattice yields

$$n(x) = \bar{n}\, \mathcal{F}_{1/2}\big(\zeta(x) - v_{\text{c}} + v_0(x)\big).$$

At the interface of different semiconductor materials this averaging is not justified anymore!

We propose a drift-diffusion model for heterogeneous semiconductor materials with the non-locally defined particle density from DFT. This regularizes the discontinuities of the band edge offset v_{c}.

5.1 The free energy of the system

We assume that the *free energy* of the system is a *density functional* $E : (\mathcal{B}^s)^* \to \mathbb{R}$ of the following form

$$E(N) \stackrel{\text{def}}{=} \Phi^*(N) + \Psi(N) + \Lambda(N) \quad \text{for } N \in \text{dom}(E),$$

Φ^*	dual of a von Neumann functional
Ψ	a quadratic functional
Λ	xc-energy functional

$\Lambda : (\mathcal{B}^s)^* \to \mathbb{R}$ is the so-called *exchange-correlation energy* which makes good for passing from a multi-particle picture to a one-particle representation in Density Functional Theory.

Assumption: Λ is Fréchet differentiable on $\partial\Phi[\mathcal{B}^s]$.

Notations

$\mathcal{H}$	separable, infinite-dimensional Hilbert space
$\mathcal{B}$	space of bounded linear operators on $\mathcal{H}$
$\mathcal{B}_1$	subspace of trace class operators
$\mathcal{B}^s$	subspace of self-adjoint operators from $\mathcal{B}$
$\mathcal{B}_1^s$	subspace of self-adjoint operators from $\mathcal{B}_1$
$\mathcal{B}_1^+$	cone of self-adjoint non-negative trace class operators
H	self-adjoint, compact resolvent, semi-bounded from below
f	thermodynamic equilibrium distribution function

$$F(s) \stackrel{\text{def}}{=} \int_s^\infty f(\tau)\,d\tau$$

Generically, f is the Fermi function $f(s) = \frac{1}{1+\exp(s)}$.

The generalized von Neumann functional

If $F(H + \gamma) \in \mathcal{B}_1$ for each $\gamma \in \mathbb{R}$, then the *von Neumann functional* $\Phi : \mathcal{B}^s \to \mathbb{R}$ is well-defined by

$$\Phi(V) \overset{\text{def}}{=} \operatorname{tr}\left(\bar{N}F(H - V)\right) \quad \text{for } V \in \mathcal{B}^s. \tag{7}$$

$\bar{N}$ is fixed such that $\bar{N}F(H - V)$ becomes a statistical operator (up to normalization).

Looking for minimal assumptions on F and H such that...

The von Neumann functional Φ is convex and Fréchet differentiable.

$\partial\Phi : \mathcal{B}^s \to \mathcal{B}_1^s \subset (\mathcal{B}^s)^*$ is given by

$$\partial\Phi(V) = -\bar{N}F'(H - V) = \bar{N}f(H - V) \quad \text{for } V \in \mathcal{B}^s \tag{8}$$

$\partial\Phi$ is monotone, takes its values in $\mathcal{B}_1^+$ — essentially is a statistical operator, namely the *particle density* $N = \partial\Phi(V)$.

The dual of the von Neumann functional

$$\Phi^*(N) \overset{\text{def}}{=} \sup_{U \in \mathcal{B}^s} \left(\langle N, U\rangle_{\mathcal{B}} - \Phi(U)\right) \quad \text{for } N \in (\mathcal{B}^s)^*. \tag{9}$$

Φ and Φ^* are convex and Fréchet differentiable.

$\partial\Phi^* : (\mathcal{B}^s)^* \to \mathcal{B}^s$ is given by

$$\partial\Phi^* = \partial\Phi^{-1} \quad \text{on } \partial\Phi[\mathcal{B}^s] \subset \mathcal{B}_1^+ \subset (\mathcal{B}^s)^*.$$

Moreover,

$$\Phi^*(N) + \Phi(V) = \langle N, V\rangle_{\mathcal{B}} = \operatorname{tr}(NV)$$

where

$$N = \partial\Phi(V), \quad V \in \mathcal{B}^s$$

The 2nd derivative of the von Neumann functional

If the function F is twice continuously differentiable,
then the operator function

$$\mathcal{B}^s \ni V \mapsto \bar{N}F(H - V) \in \mathcal{B}_1$$

is twice Fréchet differentiable (Hansen [2006]).

We aim at the representation

$$\partial^2\Phi(V) = \bar{N}F''(H - V) \in \mathcal{B}_1^+ \quad \text{for all } V \in \mathcal{B}^s \qquad (10)$$

Quadratic interaction energy

$\Psi : (\mathcal{B}^s)^* \to \mathbb{R}$

$$\Psi(N) \stackrel{\text{def}}{=} \tfrac{1}{2}\langle N - P, K(N - P)\rangle_\mathcal{B} \quad \text{for } N \in \text{dom}(K) \qquad (11)$$

$P \in \text{dom}(K)$ is given

$K : (\mathcal{B}^s)^* \to \mathcal{B}^s$ is a bounded linear operator on the linear subset $\text{dom}(K) \subset (\mathcal{B}^s)^*$ such that

$$\langle N, K(M)\rangle_\mathcal{B} = \langle M, K(N)\rangle_\mathcal{B} \quad \text{for all } M, N \in \text{dom}(K).$$

Ψ is Fréchet differentiable on $\text{dom}(K)$:

$$\partial\Psi(N) = K(N - P) \quad \text{for all } N \in \text{dom}(K). \qquad (12)$$

Minimization of the free energy

The free energy of the system is the *density functional* $E : (\mathcal{B}^s)^* \to \mathbb{R}$

$$E(N) \overset{\text{def}}{=} \Phi^*(N) + \Psi(N) + \Lambda(N) \quad \text{for } N \in \text{dom}(E),$$
$$\text{dom}(E) = \partial\Phi[\mathcal{B}^s] \cap \text{dom}(K). \tag{13}$$

In the sense of Density Functional Theory we are looking for the minima of the free energy E subject to the constraint

$$\text{tr}(N - N_0) = 0, \quad \text{where } N_0 \in \mathcal{B}_1^+ \subset (\mathcal{B}^s)^* \text{ is fixed.} \tag{14}$$

Lagrange multiplier $Z \in \mathcal{B}^s$; Lagrange functional $E_Z : (\mathcal{B}^s)^* \to \mathbb{R}$

$$E_Z(N) \overset{\text{def}}{=} E(N) + \langle N_0 - N, Z \rangle_{\mathcal{B}}$$
$$= E(N) + \text{tr}\left((N_0 - N)Z\right) \quad \text{for } N \in \text{dom}(E). \tag{15}$$

The Euler-Lagrange equation $\partial E_Z(N) = 0$ yields

$$Z = \partial E(N) = \partial\Phi^*(N) + \partial\Psi(N) + \partial\Lambda(N). \tag{16}$$

Real-space representation of QM

We illustrate the setting in the real-space representation of quantum mechanics:

$$\mathcal{H} = L^2(\Omega; \mathbb{C})$$

$\Omega \subset \mathbb{R}^d$ bounded Lipschitz domain, $d \le 3$

$H = -\frac{\hbar^2}{2}\nabla \cdot m^{-1}\nabla + v_c$ Schrödinger operator

$L^\infty(\Omega; \mathbb{R})$ space of potentials

Each element u from the space $L^\infty(\Omega; \mathbb{C})$ induces a bounded multiplication operator on $L^2(\Omega; \mathbb{C})$.

In this sense $L^\infty(\Omega; \mathbb{R})$ embeds into $\mathcal{B}^s$.

Lemma:

(HCK, Neidhardt, Rehberg 2007)
Let $(Y, \mathfrak{S}, \mu)$ be a σ–finite measure space, and let
$$\pi : L^1(\mu)^* \cong L^\infty(\mu) \longrightarrow \mathcal{B}$$
be the natural embedding. Then the dual mapping
$$\pi^* : \mathcal{B}^* \longrightarrow L^\infty(\mu)^* \cong L^1(\mu)^{**}$$
has the following properties:

1. the restriction of π^* to the sub-space $\mathcal{B}_1 \subset \mathcal{B}^*$ maps onto $L^1(\mu)$

2. the restriction of π^* to the sub-space $\mathcal{B}_1^s \subset (\mathcal{B}^s)^*$ maps onto $L^1_{\mathbb{R}}(\mu)$

3. the restriction of π^* to the self-adjoint, non-negative trace-class operators maps onto the real-valued, non-negative functions from $L^1(\mu)$

Density and chemical potential

Let $\bar{N} = \pi(\bar{n})$ be given by a positive function $\bar{n} \in L^\infty(\Omega; \mathbb{R})$, and
$$n \stackrel{\text{def}}{=} \pi^* \circ \partial\Phi \circ \pi(v) = \pi^*\big(-\bar{N}F'(H - \pi(v))\big) = \bar{n}\,\pi^*\big(f(H - \pi(v))\big).$$
If v is a chemical potential from the space $L^\infty(\Omega; \mathbb{R})$ then, n belongs to the non-negative cone of $L^1(\Omega; \mathbb{R})$.

Fenchel–Moreau identity:
$$\Phi^*(N) + \Phi(V) = \int_\Omega nv\,dx$$
$$n = \pi^*(N), N = \partial\Phi(V), V = \pi(v), v \in L^\infty(\Omega; \mathbb{R}).$$

$\kappa_0 : L^\infty(\Omega; \mathbb{R}) \to L^\infty(\Omega; \mathbb{R})^*$
$$\kappa_0(v) \stackrel{\text{def}}{=} \pi^* \circ \partial^2\Phi \circ \pi(v) = \bar{n}\,\pi^*\big(F''(H - \pi(v))\big),$$
takes its values in the non-negative cone of $L^1(\Omega; \mathbb{R})\ [L^\infty(\Omega; \mathbb{R})]$.

Quadratic interaction energy

$K \overset{\text{def}}{=} \pi \circ A \circ \pi^*$ with the solution operator

$$A : L^\infty(\Omega; \mathbb{R}) \to H^1(\Omega; \mathbb{R}) \cap L^\infty(\Omega; \mathbb{R})$$

of the Poisson equation

$$\int_\Omega \varepsilon \nabla v_0 \cdot \nabla \psi \, dx + \int_{\partial \Omega} \tau v_0 \psi \, d\sigma = \int_\Omega \varrho \psi \, dx \quad \text{for all } \psi \in H^1(\Omega; \mathbb{R}),$$

where $v_0 = A(\varrho)$.

A is bounded and symmetric, and these properties pass over to K, where

$$\text{dom}(K) = \left\{ N \in (\mathcal{B}^s)^* : \pi^*(N) \in L^\infty(\Omega; \mathbb{R}) \right\}.$$

$p \in L^\infty(\Omega; \mathbb{R})$ fixed background charge density in the volume, then $P = \pi(p)$.

Electrostatic interaction energy and potential

Electrostatic interaction energy:

$$\Psi(N) = \int_\Omega \frac{\varepsilon}{2} |\nabla v_0|^2 \, dx + \int_{\partial \Omega} \frac{\tau}{2} |v_0|^2 \, d\sigma$$
$$\text{with } v_0 = A(p - \pi^*(N)) \in H^1(\Omega; \mathbb{R}), N \in \text{dom}(K).$$

Electrostatic potential: $v_0 = A(p - \pi^*(N)) \in L^\infty(\Omega; \mathbb{R})$

$$\partial \Psi(N) = \pi\big(- A(p - \pi^*(N)) \big) = \pi(-v_0), \quad N \in \text{dom}(K).$$

Exchange-correlation energy and potential

For each $N \in \partial\Phi[\mathcal{B}^s] \subset \mathcal{B}_1^+$ there is a $v_{\text{xc}} \in L^\infty(\Omega; \mathbb{R})$ with

$$\partial\Lambda(N) = \pi(v_{\text{xc}}).$$

Electrochemical potential and current

In the real-space representation of quantum mechanics the Lagrange parameter (16) can be represented by an electrochemical potential ζ:

$$Z = \pi(\zeta), \quad \zeta = v - v_0 + v_{\text{xc}}. \tag{17}$$

Thermodynamic principles: The driving force to equilibrium is the antigradient of the electrochemical potential ζ.

$$j = -\kappa \nabla \zeta \tag{18}$$

The mobility κ can be modeled by the Einstein relation

$$\kappa(v) = \mu \kappa_0(v), \quad \mu \in L^{\infty}(\Omega; \mathbb{R}), \quad \mu \geq \mu_0 > 0, \tag{19}$$

with a diffusivity μ, SPOHN, LEBOWITZ.

5.2 The evolution system

Analogous to the (unipolar) van Roosbroeck system the closed system is described by the following initial-boundary value problem:

$$
\begin{align}
n' - \nabla \cdot (\kappa \nabla \zeta) &= 0 & &\text{in } (0, t) \times \Omega, & \text{(20a)} \\
\nu \cdot (\kappa \nabla \zeta) &= 0 & &\text{on } (0, t) \times \partial\Omega, & \text{(20b)} \\
n(0) &= n_0 & &\text{on } \Omega, & \text{(20c)} \\
-\nabla \cdot (\varepsilon \nabla v_0) &= p - n & &\text{in } (0, t) \times \Omega, & \text{(20d)} \\
\nu \cdot (\varepsilon \nabla v_0) + \tau v_0 &= 0 & &\text{on } (0, t) \times \partial\Omega, & \text{(20e)}
\end{align}
$$

supplemented by the non-local state equation

$$n = \bar{n} \, \pi^* \big(f(H - \pi(v)) \big)$$

and the Einstein relation

$$\kappa(v) = \mu \kappa_0(v) = \mu \bar{n} \, \pi^* \big(F''(H - \pi(v)) \big).$$

Solutions of the evolution system

We expect solutions from the class:

$$n \in C\big([0,t]; L^\infty(\Omega; \mathbb{R})\big)$$

$$n' \in L^2\big((0,t); H^1(\Omega; \mathbb{R})^*\big)$$

$$\zeta \in L^2\big((0,t); H^1(\Omega; \mathbb{R})\big) \cap C\big([0,t]; L^\infty(\Omega; \mathbb{R})\big)$$

$$v_0 \in C\big([0,t]; H^1(\Omega; \mathbb{R})\big) \cap C\big([0,t]; L^\infty(\Omega; \mathbb{R})\big)$$

Conservation of the number of particles along trajectories

Let $t \mapsto N(t)$ be a trajectory in $\mathcal{B}_1^+$ such that $\pi^*(N(t)) = n(t)$ for a solution (n, ζ, v_0) of the evolution system. (20a) and (20b) yield $\int_\Omega n(t,x)\,dx = \int_\Omega n_0(x)\,dx$ for $t \in \mathbb{R}^+$.

Decay of the free energy along trajectories

Let $t \mapsto N(t)$ be a trajectory in $\mathcal{B}_1^+$ such that $\pi^*(N(t)) = n(t)$ for a solution (n, ζ, v_0) of the evolution system. The chain rule yields

$$E(N(t)) - E(N_0) = \int_0^t \mathrm{tr}\,\big(N'(s)\,\partial E(N(s))\big)\,ds$$

$$= \int_0^t \langle n'(s), \zeta(s)\rangle_{H^1(\Omega)}\,ds,$$

and employing (20a) and (20b) gives

$$E(N(t)) - E(N_0) = -\int_0^t \int_\Omega \kappa\,|\nabla\zeta(s)|^2\,dx\,ds \leq 0 \quad \text{for } t \in \mathbb{R}^+,$$

that means, the free energy decays along trajectories.

Links

Stochastic processes "far" from equilibrium:
Lebowitz, Spohn, Varadhan,...

Thermodynamic design of DD models of semiconductor devices:
Albinus, Gajewski, Gröger, Hünlich

Phase separation processes:
Gajewski, Gärtner, Griepentrog, Zacharias

Quantum corrected drift-diffusion models:
Arnold, Ben Abdallah, Degond, Jüngel, Méhats, Vogl,...

Time-dependent Density Functional Theory: Gross, Marques,...

Reaction-diffusion equations for electrically charged species:
Gajewski, Gröger; Glitzky, Hünlich; Gajewski, Skrypnik

Schrödinger–Poisson systems: Nier, HCK, Rehberg,...

Von Neumann trace functionals:
Lieb, Hansen, HCK, Neidhardt, Rehberg

Nonsmooth elliptic and parabolic problems:
Elschner, HCK, Knees, Maz'ya, Rehberg, Schmidt,...

...in particular in Sobolev–Morrey spaces: Griepentrog, Recke

Doubly non-linear evolution equations: Mielke, Otto, Savaré,...