A non-local Fokker-Planck equation related to the Becker-Döring model

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arXiv: 1711.00782

Interplay of Analysis and Probability, Oberwolfach

February 14, 2018

Lehrstuhl I für Mathematik | RWTH AACHEN UNIVERSITY

Outline

1. Thermodynamics and modeling
2. Well-posedness and regularity
3. Energy-dissipation, gradient structure and longtime behaviour
4. Rate of convergence to equilibrium (subcritical)

Motivation

Water droplet nucleation from H2O vapor by a molecular dynamics simulations.

[K. K. Tanaka, A. Kawano & H.Tanaka, J. Chem. Phys. 2014]

1. Thermodynamics and modeling

Model: thermodynamic modeling of nucleation

Goal: A dynamic model of condensation/dissolution of droplets

Ingredients:

- $c : [0,T] \times \mathbb{R}^+ \to \mathbb{R}^+$ cluster volume distribution
- $W : \mathbb{R}^+ \to \mathbb{R}^+$ bulk energy per volume $\approx 1 + x$
- $V : \mathbb{R}^+ \to \mathbb{R}^+$ surface energy per volume $\approx (1+x)^{2/3}$
- $a : \mathbb{R}^+ \to \mathbb{R}^+$ reactivity per volume $\approx (1+x)^{2/3}$
- $\theta : [0,T] \to \mathbb{R}$ affinity of phase transformation ($\theta = 0$ equilibrium)

Assumptions: θ is proportional to gaseous phase

conservation of energy: $\theta + \int W c = \rho$

local Gibbs distribution: $c_\theta(x) = a(x)^{-1} \exp(-V(x) + \theta\, W(x))$

Stationary affinity: Critical volume density: $\rho_s := \int c_{\theta=0} = \int W a^{-1} e^{-V} < \infty$

For $\rho \in (-\infty, \rho_s]$ let $\theta_{\mathrm{eq}}(\rho)$ be defined by $\theta_{\mathrm{eq}} + \int W c_{\theta_{\mathrm{eq}}} = \rho$

For $\rho > \rho_s$ set $\theta_{\mathrm{eq}}(\rho) = 0 \;\Rightarrow\;$ no stationary state conserving energy

Two regimes: $\rho \leq \rho_s$ subcritical and $\rho > \rho_s$ coarsening and nucleation.

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Fokker-Planck model

Dynamic evolution of cluster size distribution relative to local Gibbs distribution

$$\begin{cases} \partial_t c(x,t) = \partial_x \left(a(x)\, c(x,t)\, \partial_x \log \dfrac{c(x,t)}{c_{\theta(t)}(x)} \right) & \text{with} \quad c(x,0) = c^0(x) \\ c(0,t) = c_{\theta(t)}(0) & \text{thermodynamic consistent b.c.} \\ \rho = \theta(t) + \int_{\mathbb{R}^+} W(x) c(x,t)\, \mathrm{d}x & \text{mass conservation} \end{cases}$$

$$c_\theta(x) = a(x)^{-1} \exp(-V(x) + \theta\, W(x)) \qquad \text{local Gibbs distribution}$$

Expanded (Itô) form

$$\partial_t c(x,t) = \partial_x \Big(\partial_x \big(a(x) c(x,t)\big) + \overbrace{a(x)\big(V'(x) - \theta(t) W'(x)\big)}^{=:-b(x,t)} c(x,t) \Big).$$

Assumptions on potentials

- $a(\cdot),\ V(\cdot),\ W(\cdot)$ are C^2 with uniformly bounded second derivatives.
- $W(\cdot)$ is strictly increasing with $W(0) > 0$
- $\inf_{x\in\mathbb{R}^+} a(x) \geq c_0 > 0$
- V', $(\log a)'$ and V'', W'', $(\log a)''$ are dominated by W' and $(W')^2$, respectively
- The function $\frac{W}{a}\exp(-V)$ is integrable on $\mathbb{R}^+$

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Well-posedness, regularity, convergence to equilibrium

Theorem

Assume a, V, W *satisfy the above assumptions and let* $c(x,0),\ x>0,$ *be such that*

$$\int_0^\infty W(x)c(x,0)\,\mathrm{d}x \;<\; \infty\,.$$

Then there exists a unique solution $c(\cdot,t),\ t>0,$ *to the Cauchy problem.*

$\forall t>0: c(\cdot,t)\in C^1([0,\infty))$ *and* $\theta\in C^1([0,\infty))$.

$\forall L>0: c(\cdot,t)$ *converges uniformly on the interval* $[0,L]$ *as* $t\to\infty$ *to the equilibrium* $c_\theta^{\mathrm{eq}}(\cdot)$ *with* $\theta=\theta_{\mathrm{eq}}(\rho)$. *If* $\rho\le\rho_s$ *then also*

$$\lim_{t\to\infty}\int_0^\infty W(x)|c(x,t)-c_\theta^{\mathrm{eq}}(x)|\,\mathrm{d}x \;=\; 0\,.$$

In the case $\rho>\rho_s$ the excess mass $\rho-\rho_s$ vanishes as $t\to\infty$.

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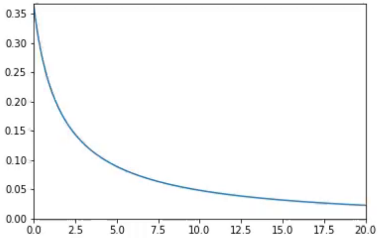
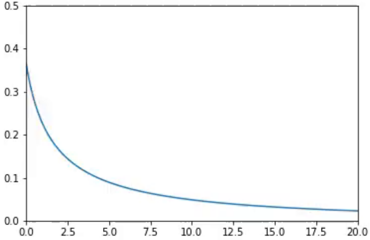
Simulations



Subcritical evolution $\varrho < \varrho_s$



Supercritical evolution $\varrho > \varrho_s$

2. Well-posedness and regularity

Well-posedness: Adjoint problem and weak formulation

W.l.o.g. $a \equiv 1$ by a change of variable $x \mapsto \int_0^x \frac{\mathrm{d}x'}{\sqrt{a(x')}}$

Kolmogorov backward equation

$$\begin{cases} \partial_t w(x,t) + \partial_{xx} w(x,t) + b(x,t)\partial_x w(x,t) = 0 \\ w(x,T) = w_0(x) \\ w(0,t) = 0 \end{cases} \qquad \text{(Adj)}$$

$\Rightarrow$ classical solutions $w \in C^{1,2}_{t,x}(\mathbb{R}^+ \times \mathbb{R}^+)$ for $b \in C^{0,2}_{t,x}(\mathbb{R}^+ \times \mathbb{R}^+)$.

Testing and integrating by w yields formulation for measure valued solutions.

Definition (weak formulation)

The pair (c,θ) with $c(t,\cdot) \in \mathcal{M}_{ac}(\mathbb{R}^+)$ and $\theta \in C([0,T];\mathbb{R})$ is a solution to (FP) if for all w, solution to (Adj), with $w_0 \in C_b(\mathbb{R}^+)$ and $T > 0$ holds

$$\int_{\mathbb{R}^+} w_0(x) c(x,T)\,\mathrm{d}x = \int_{\mathbb{R}^+} w(x,0)\, c^0(x)\,\mathrm{d}x + \int_0^T \partial_x w(0,t)\, \underbrace{e^{-V(0)+\theta(t)W(0)}}_{=c_{\theta(t)}(0)}\,\mathrm{d}t.$$

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Well-posedness: Fixed point argument

Basic properties of adjoint problem for a continuous function θ with $\|\theta\|_\infty \le \theta_\infty$:

- Let $w_0(x) = W(x)$ then for any $T < T_0$

$$w(x,0) \le C(T_0,\theta_\infty)W(x) \qquad \text{and} \qquad 0 \le \partial_x w(0,t) \le \frac{C(T_0,\theta_\infty)}{\sqrt{T-t}}$$

- Let w^0 and w^1 two such solutions for θ^0 and θ^1, respectively, then

$$\begin{aligned} \left|w^1(x,t) - w^0(x,t)\right| &\le C(\theta_\infty)\|\theta^1 - \theta^0\|_\infty \sqrt{T-t}\, W(x) \\ \left|\partial_x w^1(x,t) - \partial_x w^0(x,t)\right| &\le C(\theta_\infty)\|\theta^1 - \theta^0\|_\infty . \end{aligned}$$

Fixed point map:

$$\mathcal{B}\theta(t) := \rho - \int_{\mathbb{R}+} W(x)c(x,t)\,\mathrm{d}x$$

From the weak formulation follows the identity

$$\begin{aligned} \mathcal{B}\theta^1(T) - \mathcal{B}\theta^0(T) &= \int_0^\infty [w^1(x,0) - w^0(x,0)]c(x,0)\,dx \\ &+ \int_0^T \left[\partial_x w^1(0,t) - \partial_x w^0(0,t)\right] \exp[-V(0) + \theta^1(t)W(0)]\;\mathrm{d}t \\ &+ \int_0^T \partial_x w^0(0,t)\left(\exp[-V(0)+\theta^1(t)W(0)] - \exp[-V(0)+\theta^0(t)W(0)]\right)\;\mathrm{d}t \end{aligned}$$

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From the weak formulation follows the identity and bound

$$\mathcal{B}\theta_1(T) - \mathcal{B}\theta_2(T) = \quad \dots \quad \le C\sqrt{T}\|\theta^1 - \theta^0\|_\infty.$$

$\Rightarrow$ Local existence for some $T = T(\theta_\infty) > 0$ and $\theta \in C([0,T];\mathbb{R})$

Refined analysis of $\partial_x w(0,t)$ yields uniform lower bound $\theta(t) > -\infty$

$\Rightarrow$ Global existence by iteration of local existence argument

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Regularity: Smoothness of order parameter

Fixed point argument yields $\theta \in C([0,T];\mathbb{R})$, want to show $\theta \in C^1([0,T];\mathbb{R})$

Two observations: Local analysis close to boundary

1. Dirichlet-to-Neumann map gains $\frac{1}{2}^{-}$ Hölder regularity (Schauder estimate):

$$\theta \in C^{0,\alpha}([0,T];\mathbb{R}) \quad \Rightarrow \quad t \mapsto \int_0^t \partial_x c(0,s)\,\mathrm{d}s \in C^{0,\alpha+1/2^-}([0,T];\mathbb{R})$$

2. $\dot{\theta}$ and $\partial_x c(0,\cdot)$ have the same regularity:

$$\dot{\theta}(t) = -\int W \partial_t c \ \mathrm{d}x = W(0) \ \ \partial_x \log \frac{c}{c_{\theta(t)}}\bigg|_{x=0} + \text{bulk}$$

$$= W(0)\partial_x c(0,t) - \big(W(0)b(0,t) + W'(0)\big)c_{\theta(t)}(0) + \text{bulk}$$

$\Rightarrow$ formally $|\dot{\theta}(t) - W(0)\partial_x c(0,t)| \le C$.

Iterate three times: $\theta \in C^1([0,T],\mathbb{R})$

By parabolic regularity also $c(t,\cdot) \in C^1(\mathbb{R}^+,\mathbb{R}^+)$.

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3. Energy-dissipation, gradient structure and longtime behaviour

Energy-dissipation-identity

The equatoin satisfies energy–energy-dissipation inequality:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(c(t),\theta(t)) \leq -\mathcal{D}(c(t),\theta(t)) \qquad \text{(EED)}$$

with

$$\mathcal{F}(c,\theta) := \int (\log c - 1)c + \int (V + \log a)c + \frac{1}{2}\theta^2 \qquad \text{with} \qquad \theta := \rho - \int W c$$

$$\mathcal{D}(c,\theta) := \int a \left(\partial_x \log \frac{c}{c_\theta}\right)^2 c \qquad \text{with} \qquad c_\theta(x) := a(x)^{-1} \exp(-V(x) + \theta\, W(x))$$

The term $\frac{1}{2}\theta^2$ is typical for free energies of interaction type (McKean-Vlasov):

$$\frac{1}{2}\theta^2 = \frac{1}{2}\iint W(x)W(y)c(x)c(y) + \rho(\rho-\theta) + \frac{1}{2}\rho^2$$

The (EED) and equation in the form

$$\partial_t c(x,t) = \partial_x\left(a(x)\, c(x,t)\, \partial_x \log \frac{c(x,t)}{c_{\theta(t)}(x)}\right) \qquad \text{and} \qquad \log \frac{c(0,t)}{c_{\theta(t)}(0)} = 0$$

$\Rightarrow$ gradient flow wrt. a-weighted transportation metric with Dirichlet b.c.

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Theorem (Convergence to equilibrium)

For any $L > 0$ the solution $c(\cdot, t)$ converges uniformly on the interval $[0, L]$ as $t \to \infty$ to the equilibrium $c_\theta(\cdot)$ with $\theta = \theta_{\text{eq}}(\rho)$. If $\rho \le \rho_s$ then also

$$\lim_{t\to\infty} \int_0^\infty W(x)|c(x,t) - c_\theta(x)|\, dx \;=\; 0\,.$$

Proof (Sketch):

- EED $\dot{\mathcal{F}} \le -\mathcal{D}$ and lower semicontinuity of $\mathcal{F}$ and $\mathcal{D}$ $\Rightarrow$ LaSalle's invariance principle: $c \to c_{\theta_\infty}$ for some $\theta_\infty \le 0$
- Global existence: $\inf_{t>0} \mathcal{F}(c(t), \theta(t)) \ge \mathcal{F}(c_{\theta_{\text{eq}}(\rho)}, \theta_{\text{eq}}(\rho))$ and monotonicity of $\theta \mapsto \mathcal{F}(c_\theta)$ yields $\theta_\infty \le \theta_{\text{eq}}(\rho)$
- "Tightness" argument to pass to the limit in

$$\theta(t) + \int W c_{\theta(t)} \;\overset{t\to\infty}{\to}\; \theta_\infty + \int W c_{\theta_\infty}$$

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4. Rate of convergence to equilibrium (subcritical)

Free energy and relative entropies

For $\rho < \rho_s$ the minimizer of

$$\mathcal{F}_0(\rho) := \inf\left\{\mathcal{F}(c) : \theta + \int Wc = \rho\right\}$$

is attained and equation $c_{\theta_{\mathrm{eq}}}$ with $\theta_{\mathrm{eq}} = \theta_{\mathrm{eq}}(\rho)$.
$\Rightarrow$ normalized free energy: $\mathcal{F}_\rho(c) := \mathcal{F}(c) - \mathcal{F}_0(\rho)$

Relative entropy identities

Let $\rho < \rho_s$, then for all $c \in \mathcal{M}_{ac}(\mathbb{R}^+)$

$$\mathcal{F}_\rho(c,\theta) = \mathcal{H}\left(c|c_{\theta_{\mathrm{eq}}}\right) + \tfrac{1}{2}(\theta - \theta_{\mathrm{eq}})^2 \qquad \text{with} \qquad \theta = \rho - \int Wc,$$

where $\mathcal{H}(f|g) := \int g\,\Psi\left(\frac{f}{g}\right)$ with $\Psi(r) := r\log r - r + 1$.
For any $\theta < 0$ and any $c \in \mathcal{M}_{ac}(\mathbb{R}^+)$ with $\theta + \int Wc = \rho$

$$\mathcal{F}_\rho(c) + \tfrac{1}{2}(\theta - \theta_{\mathrm{eq}})^2 \le \mathcal{H}(c|c_\theta).$$

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$$\mathcal{F}_\rho(c) + \tfrac{1}{2}(\theta - \theta_{\mathrm{eq}})^2 \leq \mathcal{H}(c|c_\theta).$$

Weighted log-Sobolev inequalities

Let $\delta > 0$. Then, there exists a constant $C_{\mathrm{LSI}} = C_{\mathrm{LSI}}(V, W, a, \delta)$, such that for all c with $\theta + \int W c = \rho$ and $-1/\delta \leq \theta \leq -\delta$ as well as $c(0) = c_\theta(0)$ holds

$$\int_{\mathbb{R}+} \frac{1}{\omega}\, c_\theta\, \Psi\left(\frac{c}{c_\theta}\right) \leq C_{\mathrm{LSI}}\, \mathcal{D}(c, \theta) \qquad \text{with weight} \qquad \omega = \frac{W}{a\,(W')^2}.$$

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Proof: Modify argument due to [Bobkov& Götze '99]: Derive log-Sobolev inequality as Poincaré inequality in suitable Orlicz-spaces:

Let $\nu \in \mathcal{P}(\mathbb{R}^+)$ and $\mu \in \mathcal{M}_{ac}(\mathbb{R}^+)$ and let A be the smallest constant such that for any smooth f on $\mathbb{R}^+$ with $f(0) = 1$ holds

$$\mathrm{Ent}_\nu(f) := \int f \log \frac{f}{\int f \,\mathrm{d}\nu}\,\mathrm{d}\nu \le A \int |\partial_x \log f|^2 f \,\mathrm{d}\mu.$$

Then, $B/4 \le A \le B$ with $B := \sup_{x>0} \nu([x,\infty]) \log\left(1 + \frac{e^2}{\nu([x,\infty])}\right) \int_0^x \frac{\mathrm{d}y}{\mu(y)}$

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Free energy-dissipation-estimate

For $-1/\delta \leq \theta \leq -\delta$ use interpolation for $k > 0$

$$\mathcal{F}_\rho(c) \leq \mathcal{H}(c|c_\theta) = \int c_\theta \Psi\left(\frac{c}{c_\theta}\right) \leq \underbrace{\left(\int \frac{1}{\omega} c_\theta \Psi\left(\frac{c}{c_\theta}\right)\right)}_{\text{weighted LSI}}^{\frac{k}{k+1}} \underbrace{\left(\int \omega^k c_\theta \Psi\left(\frac{c}{c_\theta}\right)\right)}_{\text{assume}}^{\frac{1}{k+1}}$$

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$$\mathcal{F}_\rho(c)^{\frac{1+k}{k}} \leq C_0 \, C_{\mathrm{LSI}} \, \mathcal{D}(c, \theta).$$

In particular, if $\sup_{x>0} \omega(x) \leq C_0$, then there exists $C_{\mathrm{LSI}} = C_{\mathrm{LSI}}(V, W, a, \delta)$ with

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Rate of convergence

- Lower dissipation bound: $\mathcal{D}(c,\theta) \geq \varepsilon > 0$, whenever $\theta \geq \theta_{\mathrm{eq}} + \delta$
  $\Rightarrow$ Total amount of time, for which $\theta(t) \geq \theta_{\mathrm{eq}} + \delta$ is bounded.
- Propagation of moment bound: Enough to proof for $t \in \{t : \theta(t) \leq \theta_{\mathrm{eq}} + \delta\}$
  Whenever $\int \omega(x)^k W(x) c(0,x)\,\mathrm{d}x \leq C_0$ for $k > 0$, then for any $t_0 > 0$ and $t_0 \leq t_1 < t_2$ holds

$$\sup_{t\in[t_1,t_2]} \left(\|c(t,\cdot)\|_\infty + \int \omega(x)^k W(x) c(t,x)\,\mathrm{d}x \right) \leq C,$$

where C is uniform for $t \in \{t : \theta(t) \leq \theta_{\mathrm{eq}} + \delta\}$.

Theorem (Rate of convergence in subcritical regime)

Let $\rho < \rho_s$ and let the initial condition $c(\cdot,0)$ satisfy for some $k > 0$

$$\mathcal{F}_\rho(c) \leq C_0 \qquad \text{and} \qquad \left(\int \omega(x)^k W(x)\, c(x,0) \right) \mathrm{d}x \leq C_0$$

then there exists λ and C such that $\mathcal{F}_\rho(c(t)) \leq \frac{1}{(C+\lambda t)^k}$.
Moreover, if $\sup_{x\in\mathbb{R}+} \omega(x) \leq C_0$, then for any initial data $\int W(x)c(x,0)\,\mathrm{d}x < \infty$ there exists $C > 0$ and $\lambda > 0$ such that $\mathcal{F}_\rho(c(t)) \leq Ce^{-\lambda t}$.

- Lower dissipation bound: $\mathcal{D}(c,\theta) \geq \varepsilon > 0$, whenever $\theta \geq \theta_{\text{eq}} + \delta$
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Thank you for your attention!

Summary

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- dynamic model of condensation/dissolution of droplets
- non-local non-linear Fokker-Planck equation with boundary conditions
- local existence via fixed point argument, improved regularity
- Gradient flow structure with boundary condition
- qualitative convergence to equilibrium via entropy-dissipation-identity
- algebraic and exponential rate of convergence via modified entropy method based on weighted logarithmic Sobolve inequalities

Open questions

- supercritical behaviour: description by coarsening equations (LSW) For the Becker-Döring equation [Niethammer '03, S. '16]

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For the Becker-Döring equation [Niethammer '03, S. '16]

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Thank you for your attention!