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

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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)

1. Thermodynamics and modeling

Model: thermodynamic modeling of nucleation

Goal: A dynamic model of condensation/dissolution of droplets

Modeling ingredients:

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

Modeling assumptions: θ is proportional to gaseous phase

total conservation of mass $\quad \theta + \int W c = \rho$

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

Stationary affinity: Critical equilibrium volume density: $\rho_s := \int W a^{-1} e^{-V} < \infty$
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 $\theta_{\mathrm{eq}}(\rho) = 0$.

Two regimes: $\rho \le \rho_s$ 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

$$\begin{cases} \partial_t c(x,t) = \partial_x \Big(a(x)\, c(x,t)\, \partial_x \log \dfrac{c(x,t)}{c_{\theta(t)}(x)} \Big) & \text{with} \quad c(x,0) = c^0(x) \\ c_\theta(x) = a(x)^{-1} \exp(-V(x) + \theta\, W(x)) & \text{local Gibbs distribution} \\ c(0,t) = c_{\theta(t)}(0) & \text{thermodynamic consistent} \\ \rho = \theta(t) + \int W(x) c(x,t)\, \mathrm{d}x & \text{mass conservation} \end{cases} \qquad \text{(FP)}$$

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 increasing with $W(0) > 0$ and at least linear growth at ∞
- $\inf_{x \in \mathbb{R}^+} a(x) \geq c_0 > 0$
- 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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2. Well-posedness

Well-posedness: Adjoint problem and weak formulation

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

Adjoint problem

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

$\Rightarrow$ 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 (FP) 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

$$\int w_0(x) c(x,T)\,\mathrm{d}x = \int w(x,0)\, c^0(x)\,\mathrm{d}x + \int_0^T \partial_x w(0,t)\, e^{-V(0)+\theta(t)W(0)}\,\mathrm{d}t. \tag{weak}$$

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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

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

Fixed point map

$$\mathcal{B}\theta(t) := \rho - \int_0^\infty W(x) c(x,t) \, \mathrm{d}x$$

From the weak formulation follows the identity

$$\mathcal{B}\theta^1(T) - \mathcal{B}\theta^0(T) = \int_0^\infty [w^1(x,0) - w^0(x,0)] c(x,0) \, dx$$
$$+ \int_0^T \left[\partial_x w^1(0,t) - \partial_x w^0(0,t)\right] \exp[-V(0) + \theta^1(t) W(0)] \, \mathrm{d}t$$
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$\Rightarrow$ 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 $\theta \in C([0,T];\mathbb{R})$

Two observations:

1. Dirichlet-to-Neumann map gains $1/2$ 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:

$$\begin{aligned}\dot\theta(t) &= -\int W \partial_t c \;\mathrm{d}x = W(0)\partial_x \log \frac{c}{c_{\theta(t)}}\bigg|_{x=0} + \text{bulk} \\ &= W(0)\partial_x c(0,t) - \big(W(0)b(0,t) + W'(0)\big)c_{\theta(t)}(0) + \text{bulk}\end{aligned}$$

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

Iterate three times: $\theta \in C^1([0,T],\mathbb{R})$ and $c(t,\cdot) \in C^1(\mathbb{R}_+,\mathbb{R}_+)$.

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1. Dirichlet-to-Neumann map gains $1/2$ 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:

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

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

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

Iterate three times: $\theta \in C^1([0,T],\mathbb{R})$ and $c(t,\cdot) \in C^1(\mathbb{R}_+,\mathbb{R}_+)$.

3. Energy-dissipation, gradient structure and longtime behaviour

Energy-dissipation-identity

Regularity results allow to establish the energy–energy-dissipation inequality:

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

with

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

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

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

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

The (EED) and equation in the form

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

suggest a gradient flow formulation wrt. a-weighted transportation metric.

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Gradient flow formulation with boundary condition (formal)

State space including constraint

$$\mathcal{M} = \left\{ (c, \theta) : \int W(x) c(x) \, \mathrm{d}x = \rho - \theta, c(0) = c_\theta(0) \right\}$$

Define Sobolev space $H_0^1(\nu)$ as closure of $\varphi \in C^\infty(\mathbb{R}^+; \mathbb{R})$: $\varphi(0) = 0$

with respect to $\quad \|\varphi\|^2_{H^1(\nu)} = \int a(x) |\partial_x \varphi|^2 \, \mathrm{d}\nu$

Define operator $K[\nu] : H_0^1(\nu) \to (H_0^1(\nu))^*$ by

$$K[\nu]\varphi = -\partial_x (a \, c \, \partial_x \varphi)$$

Then K is linear, nonnegative definite and defines metric

$$\psi, \varphi \in H_0^1(\nu) : \qquad \langle \psi, K[\nu]\varphi \rangle = \int a \, \partial_x \psi \, \partial_x \varphi \, \mathrm{d}\nu.$$

First variation of $\mathcal{F}(c)$: $x \mapsto \log \frac{c(x,t)}{c_\theta(x)}$ satisfies boundary condition and hence

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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 $\theta = \theta_{\mathrm{eq}}(\rho)$. 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: $\inf_{t>0} \mathcal{F}(c(t)) \ge \mathcal{F}(c_{\theta_{\mathrm{eq}}(\rho)})$
  and monotonicity of $\theta \mapsto \mathcal{F}(c_\theta)$ yields $\theta_\infty \le \theta_{\mathrm{eq}}(\rho)$
- “Tightness” argument to pass to the limit in

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Qualitative convergence to equilibrium

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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.

$\Rightarrow$ normalized free energy: $\mathcal{F}_\rho(c) := \mathcal{F}(c) - \mathcal{F}_0(\rho)$

Relative entropy identities

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

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

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 $\theta + \int Wc = \rho$

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

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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

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

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

Then, $B/4 \leq A \leq B$ 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

Via interpolation for $k > 0$

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

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

In particular, if a has the same growth as W at ∞, then there exists a constant $C_{\mathrm{LSI}} = C_{\mathrm{LSI}}(V, W, a, \delta)$ such that $\mathcal{F}_\rho(c) \le C_0 \, C_{\mathrm{LSI}} \, \mathcal{D}(c, \theta)$.

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Quantified rate of convergence

Further ingredients:

- Lower dissipation bound: $\mathcal{D}(c,\theta) \geq \varepsilon > 0$, whenever $\theta \geq \theta_{\mathrm{eq}} + \delta$
- Propagation of moment bound:
  Whenever $\int \frac{W^{k+1}}{a^k} c(0,x)\,\mathrm{d}x \leq C_0$ for $k > 0$, then for any $t_0 > 0$ and $t_0 \leq t_1 < t_2$ holds

$$\sup_{t\in[t_1,t_2]} \left(\|c(t,\cdot)\|_\infty + \int \frac{W^{k+1}}{a^k} c(t,x)\,\mathrm{d}x \right) \leq C,$$

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Theorem (Rate of convergence in subcritical regime)

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

$$\mathcal{F}_\rho(c) \leq C_0 \qquad \text{and} \qquad \left(\int \frac{W^{k+1}}{a^k} c(x,0) \right) \mathrm{d}x \leq C_0$$

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

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Summary

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- dynamic model of condensation/dissolution of droplets
- non-local Fokker-Planck equation including boundary conditions
- local existence via fixed point argument
- improved regularity by Schauder estimate
- Gradient flow structure with boundary condition
- qualitative convergence to equilibrium via entropy-dissipation-identity
- rate of convergence (subcritical) via modified entropy method based on weighted logarithmic Sobolve inequalities and interpolation

Open questions

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