

A non-local Fokker-Planck equation related to nucleation

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joint work with José Cañizo and Joseph Conlon

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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

Goal: A dynamic model of condensation/dissolution of droplets

Modeling ingredients:

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

Modeling assumptions: θ is proportional to gaseous phase

total conservation of mass $\theta + \int Wc = \rho$

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

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

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

For $\rho > \rho_s$ set $\theta_{\text{eq}}(\rho) = 0$.

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

$$\left\{ \begin{array}{l} \partial_t c(x, t) = \partial_x \left(a(x) c(x, t) \partial_x \log \frac{c(x, t)}{c_{\theta(t)}(x)} \right) \\ c_{\theta}(x) = a(x)^{-1} \exp(-V(x) + \theta W(x)) \\ c(0, t) = c_{\theta(t)}(0) \\ \rho = \theta(t) + \int W(x) c(x, t) dx \end{array} \right. \quad \begin{array}{l} \text{with } c(x, 0) = c^0(x) \\ \text{local Gibbs distribution} \\ \text{thermodynamic consistent} \\ \text{mass conservation} \end{array} \quad (\text{FP})$$

Expanded (Itô) form

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

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
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2. Well-posedness

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

Adjoint problem

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

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

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

$$\int w_0(x) c(x, T) dx = \int w(x, 0) c^0(x) dx + \int_0^T \partial_x w(0, t) e^{-V(0) + \theta(t)W(0)} dt. \quad (\text{weak})$$

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Well-posedness: Fixed point argument

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

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

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

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

Fixed point map

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

From the weak formulation follows the identity

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

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

⇒ **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 $\theta(t) > -\infty$

⇒ **Global existence** by iteration of local existence argument

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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):

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

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

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

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

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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$$\begin{aligned} \dot{\theta}(t) &= - \int W \partial_t c \, dx = W(0) \partial_x \log \frac{c}{c_{\theta(t)}} \Big|_{x=0} + \text{bulk} \\ &= W(0) \partial_x c(0, t) - (W(0)b(0, t) + W'(0)) c_{\theta(t)}(0) + \text{bulk} \\ &\Rightarrow \text{formally } |\dot{\theta}(t) - W(0) \partial_x c(0, t)| \leq C. \end{aligned}$$

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

Regularity results allow to establish the **energy-dissipation-identity**:

$$\frac{d}{dt} \mathcal{F}(c(t)) \leq -\mathcal{D}(c(t), \theta(t)) \quad (\text{EDI})$$

with

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

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

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 (EDI) and equation in the form

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

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State space including **constraint**

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

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

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

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

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

Then K is linear, nonnegative definite and defines metric

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

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

$$\partial_t c(x,t) = -K[c(\cdot, t)]D\mathcal{F}(c) = \partial_x \left(a(\cdot)c(\cdot, t) \partial_x \log \frac{c(\cdot, t)}{c_\theta(t)(\cdot)} \right).$$

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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 $t \rightarrow \infty$ to the equilibrium $c_\theta(\cdot)$ with $\theta = \theta_{\text{eq}}(\rho)$. If $\rho \leq \rho_s$ then also

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

Proof (Sketch):

- EDI $\dot{\mathcal{F}} \leq -\mathcal{D}$ and lower semicontinuity of \mathcal{F} and \mathcal{D}
 \Rightarrow LaSalle's invariance principle: $c \rightarrow c_{\theta_\infty}$ for some $\theta_\infty \leq 0$
- Global existence: $\inf_{t>0} \mathcal{F}(c(t)) \geq \mathcal{F}(c_{\theta_{\text{eq}}(\rho)})$
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4. Rate of convergence to equilibrium (subcritical)

For $\rho < \rho_s$ the minimizer of

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

is attained.

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

Relative entropy identities

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

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

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 $\theta + \int Wc = \rho$

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

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Weighted log-Sobolev inequalities

Let $\delta > 0$. Then, there exists a constant $C_{\text{LSI}} = C_{\text{LSI}}(V, W, a, \delta)$, such that for all c with $\theta + \int Wc = \rho$ 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

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

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

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Free energy-dissipation-estimate

Via interpolation for $k > 0$

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

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

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Quantified rate of convergence

Further ingredients:

- Lower dissipation bound: $\mathcal{D}(c, \theta) \geq \varepsilon > 0$, whenever $\theta \geq \theta_{\text{eq}} + \delta$
- Propagation of moment bound:

Whenever $\int \frac{W^{k+1}}{a^k} c(0, x) dx \leq C_0$ for $k > 0$, then for any $t_0 > 0$ and $t_0 \leq t_1 < t_2$ holds

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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 $k > 0$

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

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 $\int W(x)c(x, 0) dx < \infty$ there exists $C > 0$ and $\lambda > 0$ such that $\mathcal{F}_{\rho}(c(t)) \leq Ce^{-\lambda t}$.

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Summary

- 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 Sobolev inequalities and interpolation

Open questions

- supercritical behaviour: description by coarsening equations (LSW) similar to the Becker-Döring equation [Niethammer '03, S. '16]
- nucleation: timescales of (dynamic) metastable states
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