

Macroscopic limit of the Becker-Döring equation via gradient flows

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State space $u \in \mathcal{M} \subseteq \{\mathbb{R}^n, \text{functions, measures}\}$ with conservation laws

Velocity $\mathcal{T}_u \mathcal{M} = \{\dot{\gamma}|_{t=0} : \gamma(0) = u, \gamma \in C^1((-\varepsilon, \varepsilon), \mathcal{M})\}$

Energy $\mathcal{F} : \mathcal{M} \rightarrow \mathbb{R}$

Force differential $D\mathcal{F}(u) : \mathcal{T}_u \mathcal{M} \rightarrow \mathbb{R} \in \mathcal{T}_u^* \mathcal{M}$ **covector**

Metric Identify covector and vector $\mathcal{K}(u) : \mathcal{T}_u^* \mathcal{M} \rightarrow \mathcal{T}_u \mathcal{M}$ linear, definite

Gradient flow $\partial_t u_t = -\mathcal{K}(u_t) D\mathcal{F}(u_t). \quad (\diamond)$

Variational characterization [De Giorgi '80]

A couple $[0, T] \ni t \mapsto (u_t, \psi_t) \in \mathcal{M} \times \mathcal{T}_{u_t}^* \mathcal{M}$ solves the continuity equation if

$$\forall t \in [0, T] : \quad \partial_t u_t = \mathcal{K}(u_t) \psi_t \quad \text{denoted by} \quad (u, \psi) \in \text{CE}_T.$$

Then, each $(u, \psi) \in \text{CE}_T$ satisfies $\mathcal{J}(u) \geq 0$ where

$$\mathcal{J}(u) := \mathcal{F}(u_T) - \mathcal{F}(u_0) + \frac{1}{2} \int_0^T \langle D\mathcal{F}(u_t), \mathcal{K}(u_t) D\mathcal{F}(u_t) \rangle dt + \frac{1}{2} \int_0^T \langle \psi_t, \mathcal{K}(u_t) \psi_t \rangle dt.$$

Moreover, $\mathcal{J}(u) = 0$ if and only if u satisfies (\diamond) .

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Definition: action $\mathcal{A}(u, \psi) := \langle \psi, \mathcal{K}(u)\psi \rangle$
 dissipation $\mathcal{D}(u) := \langle D\mathcal{F}(u), \mathcal{K}(u)D\mathcal{F}(u) \rangle.$

Remark: Gradient flow solutions $\partial_t u_t = -\mathcal{K}(u_t)D\mathcal{F}(u_t)$ satisfy the
energy–dissipation identity $\mathcal{F}(u_T) + \int_0^T \mathcal{D}(u_t) dt = \mathcal{F}(u_0)$

Technical ingredients:

- Strong upper gradient property: $\forall (u, \psi) \in \text{CE}_T, 0 \leq s < t \leq T$

$$|\mathcal{F}(u_t) - \mathcal{F}(u_s)| \leq \int_s^t \sqrt{\mathcal{A}(u_r, \psi_r)} \sqrt{\mathcal{D}(u_r)} dr.$$

- Compactness and lower semicontinuity of \mathcal{J} :

Let $(u^n, \psi^n) \in \text{CE}_T$ starting from u_0 such that $\mathcal{J}(u^n) \leq C < \infty$, then there exists a limit $(u, \psi) \in \text{CE}_T$ such that

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Sufficient to prove lower semicontinuity for the energy, action and dissipation, separately.

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Limits of gradient flows [Sandier, Serfaty '04]

A sequence $(\mathcal{M}^\varepsilon, \mathcal{F}^\varepsilon, \mathcal{K}^\varepsilon)$ of gradient structures converges to a gradient structure $(\mathcal{M}, \mathcal{F}, \mathcal{K})$ provided that there exists $\Pi^\varepsilon : \mathcal{M}^\varepsilon \times \mathcal{T}^* \mathcal{M}^\varepsilon \rightarrow \mathcal{M} \times \mathcal{T}^* \mathcal{M}$ such that for all $(u^\varepsilon, \psi^\varepsilon) \in \text{CE}_T^\varepsilon$ with $J^\varepsilon(u^\varepsilon) \leq C$, there exists a subsequence with $\Pi^\varepsilon(u^\varepsilon, \psi^\varepsilon) \rightarrow (u, \psi) \in \text{CE}_T$ satisfying the following lim inf-estimates

$$\forall t \in [0, T] : \liminf_{\varepsilon \rightarrow 0} \mathcal{F}^\varepsilon(u^\varepsilon) \geq \mathcal{F}(u)$$

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Corollary (Convergence of solutions)

Suppose the sequence $(\mathcal{M}^\varepsilon, \mathcal{F}^\varepsilon, \mathcal{K}^\varepsilon)$ of gradient structures converges to $(\mathcal{M}, \mathcal{F}, \mathcal{K})$ and assume the initial data u_0^ε is **well-prepared** $\mathcal{F}^\varepsilon(u_0^\varepsilon) \rightarrow \mathcal{F}(u_0)$, then the sequence of gradient flow solutions converge to a gradient flow solution.

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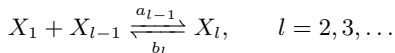
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Becker-Döring equation – derivation

Model [Becker–Döring '35] for **coagulation** and **fragmentation** of clusters consisting of identical monomers



under the assumption of **conservation of the total mass density**

$$\varrho(t) := \sum_{l=1}^{\infty} l n_l(t) = \sum_{l=1}^{\infty} l n_l(0) = \varrho_0.$$

Let J_l be the **net-flux** from $l - 1$ to l -clusters

$$\dot{n}_l(t) = J_{l-1}(t) - J_l(t) \quad l = 2, 3, \dots$$

Mass conservation implies

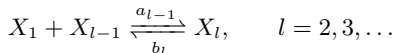
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The flux is determined from **mass-action-kinetics**

$$J_l(t) = a_l n_1(t) n_l(t) - b_{l+1} n_{l+1}(t), \quad l = 1, 2, \dots$$

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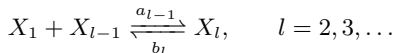
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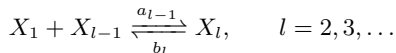
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Stationary states are characterized by the **detailed balance condition**

$$J_l = 0 \quad \Rightarrow \quad a_l \omega_l \omega_l = b_{l+1} \omega_{l+1} \quad \Rightarrow \quad \omega_l(z) = z^l Q_l \quad \text{with } Q_l := \frac{a_{l-1} \cdots a_1}{b_l \cdots b_2}.$$

Has $\omega(z)$ finite mass?

Assumption: Series $z \mapsto \sum_{l=1}^{\infty} l \omega_l(z)$ finite radius of convergence $z_s < \infty$ with finite value $\rho_s := \sum_{l=1}^{\infty} l \omega_l(z_s) < \infty$.

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$$\omega_l(z) \sim \exp\left(l \log\left(\frac{z}{z_s}\right) - \frac{q}{1-\gamma} l^{1-\gamma}\right) \quad l \gg 1.$$

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Stationary states are characterized by the [detailed balance condition](#)

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$$\mathcal{F}(n) := \mathcal{H}(n|\omega(z)) := \sum_{l=1}^{\infty} \omega_l \eta\left(\frac{n_l}{\omega_l}\right) \quad \text{with} \quad \eta(x) = x \log x - x + 1.$$

Long-time behavior [Ball, Carr, Penrose '89]

- For $z = z(\varrho_0)$ as before holds $\mathcal{F}(n) \rightarrow 0$ as $t \rightarrow \infty$.
- In the case $\varrho_0 > \varrho_s$ holds $n(t) \xrightarrow{*} \omega(z_s)$ in L^1 as $t \rightarrow \infty$.
- In particular for $\varrho_0 > \varrho_s$ the infimum

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Interpret as chemical reaction $X_1 + X_l \xrightleftharpoons[b_{l+1}]{a_l} X_{l+1}$ and formalism by [Mielke '11].

Stoichiometric coefficients $\alpha_i^l := \delta_i^1 + \delta_i^l$ and $\beta_i^l := \delta_i^{l+1}$.

Rewrite evolution with stationary rate $k^l := a_l \omega_1 \omega_l \stackrel{\text{DBC}}{=} b_{l+1} \omega_{l+1}$

$$\dot{n} = - \sum_{l=1}^{\infty} \underbrace{(a_l n_1(t) n_l(t) - b_{l+1} n_{l+1}(t))}_{=J_l} (\alpha^l - \beta^l) = - \sum_{l=1}^{\infty} k^l \left(\frac{n^{\alpha^l}}{\omega^{\alpha^l}} - \frac{n^{\beta^l}}{\omega^{\beta^l}} \right) (\alpha^l - \beta^l).$$

Differential of the free energy: $D\mathcal{F}(n) = \left(\log \frac{n_l}{\omega_l} \right)_{l=1}^{\infty}$.

Metric defined by Onsager matrix

$$\mathcal{K}(n) := \sum_{l=1}^{\infty} k^l \Lambda \left(\frac{n^{\alpha^l}}{\omega^{\alpha^l}}, \frac{n^{\beta^l}}{\omega^{\beta^l}} \right) (\alpha^l - \beta^l) \otimes (\alpha^l - \beta^l) \quad \text{with} \quad \Lambda(a, b) := \frac{a - b}{\log a - \log b}.$$

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Consider large clusters with **cut-off** $l_0 \sim \varepsilon^{-x}$ for some $x \in (0, 1/2)$ and $\varepsilon > 0$.

Define **empirical macroscopic cluster distribution**

$$\nu^\varepsilon(d\lambda) := (\Pi_{\text{mac}}^\varepsilon n)(d\lambda) := \varepsilon \sum_{l \geq l_0} \delta_{\varepsilon l}(\lambda) \frac{n_l}{\varepsilon^2} \quad \Rightarrow \quad \int \lambda \nu^\varepsilon(d\lambda) = \sum_{l \geq l_0} l n_l.$$

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Dissipation $\mathcal{D}^\varepsilon(n) := \frac{1}{\varepsilon^{1-\alpha+2\gamma}} \mathcal{A}(n, -D\mathcal{F}(n))$.

Curves of finite action and variational characterization

A weak solution $[0, T] \ni t \mapsto (n^\varepsilon(t), w^\varepsilon(t))$ to the rescaled continuity equation $\dot{n}^\varepsilon(t) = \mathcal{K}^\varepsilon(n^\varepsilon(t)w^\varepsilon(t))$, denoted by $(n^\varepsilon, w^\varepsilon) \in \mathcal{CE}_T^\varepsilon$, is called a rescaled curve of finite action if

$$\sup_{t \in [0, T]} \mathcal{F}^\varepsilon(n_t^\varepsilon) < \infty, \quad \int_0^T \mathcal{A}^\varepsilon(n^\varepsilon(t), w^\varepsilon(t)) dt < \infty \quad \text{and} \quad \int_0^T \mathcal{D}^\varepsilon(n^\varepsilon(t)) dt < \infty.$$

Moreover, for such a curve the functional

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is non-negative with $\mathcal{J}^\varepsilon(n^\varepsilon) = 0$ if and only if n^ε is a solution to the rescaled Becker–Döring equation.

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The [Lifshitz–Slyozov, Wagner '61] (LSW) equation models the coarsening of large clusters and solves the **nonlocal conservation law**

$$\partial_t \nu_t + \partial_\lambda (\lambda^\alpha (u(\nu_t) - q\lambda^{-\gamma}) \nu_t) = 0 \quad \text{with} \quad u(\nu_t) = \frac{q \int \lambda^{\alpha-\gamma} \nu_t(d\lambda)}{\int \lambda^\alpha \nu_t(d\lambda)}$$

Formal gradient structure [Niethammer '04]

State space $M := \{\nu \in C_c^0(\mathbb{R}_+)^* \mid \int \lambda \nu(d\lambda) = \rho_0 - \rho_s =: \bar{\rho}\}$

Tangent space $T_\nu M := \{s \in C_c^0(\mathbb{R}_+)^* \mid \int \lambda s(d\lambda) = 0\}$.

Onsager operator (compare formal expansion) and action

$$K(\nu)w := -\partial_\lambda (\lambda^\alpha w \nu) \quad \text{and} \quad A(\nu, w) := \langle w, Kw \rangle := \int \lambda^\alpha |w|^2 d\nu.$$

Cotangent space $T_\nu^* M := \{w \mid \int \lambda^\alpha w \nu(d\lambda) = 0\}$.

Energy $E(\nu) = \frac{q}{1-\gamma} \int \lambda^{1-\gamma} \nu(d\lambda)$, in general $DE(\nu) \notin T_\nu^* M$! For $s \in T_\nu M$ holds

$$DE(\nu) \cdot s = \frac{q}{1-\gamma} \int \lambda^{1-\gamma} s d\lambda = - \int \left(\lambda u - \frac{q}{1-\gamma} \lambda^{1-\gamma} \right) s d\lambda = - \int \lambda^\alpha (u - q\lambda^{-\gamma}) w d\nu.$$

where $u = u(\nu)$ is chosen such that $\lambda \mapsto u - q\lambda^{-\gamma} \in T_\nu^* M$.

The [Lifshitz–Slyozov, Wagner '61] (LSW) equation models the coarsening of large clusters and solves the **nonlocal conservation law**

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Formal gradient structure [Niethammer '04]

State space $M := \{\nu \in C_c^0(\mathbb{R}_+)^* \mid \int \lambda \nu(d\lambda) = \rho_0 - \rho_s =: \bar{\rho}\}$

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Proposition (Dissipation is strong upper gradient of the energy)

Assume $\alpha \geq 1 - 3\gamma$. Let $(\nu, w) \in CE_T$ be a curve of finite action in M such that

$$\inf_{u \in L^2([0, T])} \int_0^T \int \lambda^\alpha (u(t) - q\lambda^{-\gamma})^2 d\nu_t dt < \infty.$$

Then, it holds the **moment estimate** $\int_0^T \int \lambda^\alpha d\nu_t dt < \infty$.

Moreover, the minimization problem has a **unique solution** $u \in L^2([0, T])$ such that

$$\lambda \mapsto u(t) - q\lambda^{-\gamma} \in T_{\nu_t}^* M \quad \text{for a.e. } t \in [0, T]$$

and the **dissipation** defined for a.e. $t \in [0, T]$ by

$$D(\nu_t) := \int \lambda^\alpha (u(t) - q\lambda^{-\gamma})^2 d\nu_t \quad \text{with} \quad u(t) := \frac{q \int \lambda^{\alpha-\gamma} d\nu_t}{\int \lambda^\alpha d\nu_t},$$

is a **strong upper gradient** for the energy E

$$|E(\nu_t) - E(\nu_s)| \leq \int_s^t \sqrt{D(\nu_r)} \sqrt{A(\nu_r, w_r)} dr, \quad \forall 0 \leq s < t \leq T.$$

Proposition (Compactness)

Assume $\alpha \geq 1 - 3\gamma$ and let $(\nu^n, w^n) \in \text{CE}_T$ for $n \in \mathbb{N}$ be a family of curves of uniformly **bounded action and dissipation** such that $\{\nu_0^n\}_{n \in \mathbb{N}}$ is **tight**. Then, there exists a subsequence and a couple $(\nu, w) \in \text{CE}_T$, such that

$$\forall t \in [0, T] : \nu_t^n \xrightarrow{*} \nu_t \quad \text{and} \quad w^n \nu^n \xrightarrow{*} w \nu.$$

In addition, the action and dissipation satisfy the **lim inf estimates**

$$\begin{aligned} \liminf_{n \rightarrow \infty} \int_0^T A(\nu_t^n, w_t^n) dt &\geq \int_0^T A(\nu_t, w_t) dt \\ \liminf_{n \rightarrow \infty} \int_0^T D(\nu_t^n) dt &\geq \int_0^T D(\nu_t) dt \end{aligned}$$

Proposition (LSW as curves of maximal slope)

Let $\alpha \geq 1 - 3\gamma$. For $(\nu, w) \in \text{CE}_T$ with finite action holds

$$J(\nu) := E(\nu_T) - E(\nu_0) + \frac{1}{2} \int_0^T D(\nu_t) dt + \frac{1}{2} \int_0^T A(\nu_t, w_t) dt \geq 0.$$

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Moreover, equality holds if and only if ν_t is a solution to the LSW equation.

Theorem (Convergence of curves of finite action)

Suppose that $\alpha \geq 1 - 3\gamma$. Let $(n^\varepsilon, w^\varepsilon) \in \mathcal{CE}_T^\varepsilon$ be such that $\mathcal{J}^\varepsilon(n^\varepsilon) \leq C$ and $\nu_0^\varepsilon := \Pi_{\text{mac}}^\varepsilon n^\varepsilon(0)$ is tight, then there exists a limiting curve $t \mapsto (\nu_t, w_t) \in \text{CE}_T$

$$\forall t \in [0, T] : \nu_t^\varepsilon := \Pi_{\text{mac}}^\varepsilon n^\varepsilon(t) \xrightarrow{*} \nu_t \quad \text{and} \quad w_t^\varepsilon(\lambda) \nu_t^\varepsilon(d\lambda) dt \xrightarrow{*} w_t(\lambda) d\nu_t(d\lambda) dt.$$

There exists $u \in L^2((0, T))$ such that

$$\frac{n_1(\cdot) - z_s}{\varepsilon^\gamma} \xrightarrow{L^2} u(\cdot) \quad \text{with} \quad u(\nu_t) := \frac{\int \lambda^{\alpha-\gamma} \nu_t(d\lambda)}{\int \lambda^\alpha \nu_t(d\lambda)}.$$

The energy, the action and the dissipation satisfy the following lim inf estimates

$$\begin{aligned} \forall t \in [0, T] : \quad & \lim_{\varepsilon \rightarrow 0} \mathcal{F}_{\text{mac}}^\varepsilon(\nu_t^\varepsilon) \geq \frac{1}{z_s} E(\nu_t), \\ \liminf_{\varepsilon \rightarrow 0} \int_0^T \mathcal{A}_{\text{mac}}^\varepsilon(\nu_t^\varepsilon, w_t^\varepsilon) dt & \geq \frac{1}{z_s} \int_0^T A(\nu_t, w_t) dt, \\ \liminf_{\varepsilon \rightarrow 0} \int_0^T \mathcal{D}_{\text{mac}}^\varepsilon(\nu_t^\varepsilon) dt & \geq \frac{1}{z_s} \int_0^T D(\nu_t) dt. \end{aligned}$$

Corollary (Convergence of solutions) [cp. Niethammer '03]

In addition, assume $n^\varepsilon(0)$ to be **well-prepared** in the sense that

$$\lim_{\varepsilon \rightarrow 0} \mathcal{F}^\varepsilon(n^\varepsilon(0)) = E(\nu_0)$$

then there exists a limiting $(\nu, w) \in CE_T$ such that $\liminf_{\varepsilon \rightarrow 0} \mathcal{J}^\varepsilon(n^\varepsilon) \geq J(\nu) \geq 0$.
Especially, solutions converge: $\mathcal{J}^\varepsilon(n^\varepsilon) = 0 \Rightarrow J(\nu) = 0$.

Conjecture

The statement holds by assuming only **macroscopic well-prepared** initial data

$$\lim_{\varepsilon \rightarrow 0} E(\Pi_{\text{mac}}^\varepsilon n^\varepsilon(0)) = E(\nu_0).$$

Continuous dependence on the initial data of the LSW-equation

Let $\{\nu_0^\varepsilon\}_{\varepsilon > 0}$ be a tight sequence of initial data such that $\lim_{\varepsilon \rightarrow 0} E(\nu_0^\varepsilon) = E(\nu_0)$.
Then there exists a solution $\nu \in C_c^\infty([0, T] \times \mathbb{R}_+)^*$ to the LSW equation such that $\nu_t^\varepsilon \xrightarrow{*} \nu_t$ in $C_c^0(\mathbb{R}_+)$ for all $t \in [0, T]$.

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Theorem (Quasistationary distribution)

Let $(n^\varepsilon, w^\varepsilon) \in \mathcal{CE}_T^\varepsilon$ be such that $\mathcal{J}^\varepsilon(n^\varepsilon) \leq C$ and $(\Pi_{\text{mac}}^\varepsilon n^\varepsilon)(0)$ tight. Then, it holds

$$\int_0^T \mathcal{H}_{\text{mic}}(n^\varepsilon(t) \mid \omega(n_1^\varepsilon(t))) dt \leq C\varepsilon^{\gamma+(1-x)(1-\alpha+\gamma)} \int_0^T \mathcal{D}_{\text{mic}}^\varepsilon(n_t^\varepsilon) dt,$$

where $\omega_l(z) = z^l Q_l$ and \mathcal{H}_{mic} is the relative entropy defined by

$$\mathcal{H}_{\text{mic}}(n \mid \omega(z)) := \sum_{l=1}^{l_0-1} \omega_l(z) \eta\left(\frac{n_l}{\omega_l(z)}\right) \quad \text{with} \quad \eta(x) = x \log x - x + 1.$$

In particular, for a.e. $t \in [0, T]$ it holds

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 A. Schlichting, *Macroscopic limit of the Becker-Döring equation via gradient flows*, arXiv:1607.08735

Thank you for your attention!