Macroscopic limit of the Becker-Döring equation via gradient flows

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State space $u \in \mathcal{M} \subseteq \{\mathbb{R}^n, \text{functions}, \text{measures}\}$ 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 $\mathcal{F} : \mathcal{M} \to \mathbb{R}$

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

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

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

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

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

Then, each $(u,\psi) \in \mathrm{CE}_T$ 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 $(\blacklozenge)$.

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Gradient flow formalism – technical ingredients

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 $\mathcal{F}(u_T) + \int_0^T \mathcal{D}(u_t)\,\mathrm{d}t = \mathcal{F}(u_0)$

Technical ingredients:

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

$$|\mathcal{F}(u_t) - \mathcal{F}(u_s)| \le \int_s^t \sqrt{\mathcal{A}(u_\tau,\psi_\tau)}\sqrt{\mathcal{D}(u_\tau)}\,\mathrm{d}\tau.$$

- Compactness and lower semicontinuity of $\mathcal{J}$:
  Let $(u^n,\psi^n) \in \mathrm{CE}_T$ starting from u_0 such that $\mathcal{J}(u^n) \le C < \infty$, then there exists a limit $(u,\psi) \in \mathrm{CE}_T$ such that

$$\liminf_{n\to\infty} \mathcal{J}(u^n) \ge \mathcal{J}(u).$$

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

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Gradient flow formalism – limit

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 $\Pi^\varepsilon : \mathcal{M}^\varepsilon \times \mathcal{T}^*\mathcal{M}^\varepsilon \to \mathcal{M} \times \mathcal{T}^*\mathcal{M}$ such that for all $(u^\varepsilon, \psi^\varepsilon) \in \mathrm{CE}_T^\varepsilon$ with $J^\varepsilon(u^\varepsilon) \leq C$, there exists a subsequence with $\Pi^\varepsilon(u^\varepsilon, \psi^\varepsilon) \to (u, \psi) \in \mathrm{CE}_T$ satisfying the following $\liminf$-estimates

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

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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 $\mathcal{F}^\varepsilon(u_0^\varepsilon) \to \mathcal{F}(u_0)$, then the sequence of gradient flow solutions converge to a gradient flow solution.

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Becker-Döring equation – derivation

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

$$X_1 + X_{l-1} \underset{b_l}{\overset{a_{l-1}}{\rightleftharpoons}} X_l, \qquad l = 2, 3, \ldots$$

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

$$\dot{n}_l(t) = J_{l-1}(t) - J_l(t) \qquad l = 2, 3 \ldots.$$

Mass conversation implies

$$\dot{n}_1(t) = -\sum_{l=1}^{\infty} J_l(t) - J_1(t) =: J_0(t) - J_1(t).$$

The flux is determined from mass-action-kinetics

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Stationary states are characterized by the detailed balance condition

$$J_l = 0 \quad \Rightarrow \quad a_l \omega_1 \omega_l = b_{l+1} \omega_{l+1} \quad \Rightarrow \quad \omega_l(z) = z^l Q_l \quad \text{with } Q_l := \frac{a_{l-1} \cdots a_1}{b_l \cdots b_2}.$$

Has $\omega(z)$ finite mass?

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

Concrete physical relevant rates: Defined for $\alpha \in [0,1)$, $\gamma \in (0,1)$ and $z_s, q > 0$ by

$$a_l := l^\alpha \qquad \text{and} \qquad b_l := l^\alpha \left(z_s + q l^{-\gamma} \right).$$

Then

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

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Becker-Döring equation – stationary states and rates

Stationary states are characterized by the detailed balance condition

$$J_l = 0 \quad \Rightarrow \quad a_l \omega_1 \omega_l = b_{l+1} \omega_{l+1} \quad \Rightarrow \quad \omega_l(z) = z^l Q_l \quad \text{with } Q_l := \frac{a_{l-1} \cdots a_1}{b_l \cdots b_2}.$$

Has $\omega(z)$ finite mass?

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Becker-Döring equation – free energy and long-time behavior

Consider free energy

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

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

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

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Becker-Döring – Gradient flow formulation

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

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

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

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

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

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

Then $\dot{n} = -\mathcal{K}(n) D\mathcal{F}(n)$ follows from

$$\Lambda\left(\frac{n^{\alpha^l}}{\omega^{\alpha^l}}, \frac{n^{\beta^l}}{\omega^{\beta^l}}\right) D\mathcal{F}(n) \cdot (\alpha^l - \beta^l) = \frac{n^{\alpha^l}}{\omega^{\alpha^l}} - \frac{n^{\beta^l}}{\omega^{\beta^l}}$$

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Becker-Döring – formal expansion [Penrose '97]

Assumption: $\rho_0 > \rho_s$ and $\omega = \omega(z_s)$.

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

$$\nu^\varepsilon(\mathrm{d}\lambda) := (\Pi^\varepsilon_{\mathrm{mac}} n)(\mathrm{d}\lambda) := \varepsilon \sum_{l \geq l_0} \delta_{\varepsilon l}(\lambda) \frac{n_l}{\varepsilon^2} \qquad \Rightarrow \qquad \int \lambda \, \nu^\varepsilon(\mathrm{d}\lambda) = \sum_{l \geq l_0} l n_l .$$

Expansion of free energy $\psi(x) = x \log x - x + 1$

$$\mathcal{F}(n) \geq \sum_{l \geq l_0} \omega_l \, \psi\left(\frac{n_l}{\omega_l x}\right) = \varepsilon^\gamma \frac{q}{z_s(1-\gamma)} \int \lambda^{1-\gamma} \, \nu^\varepsilon(\mathrm{d}\lambda)(1 + o(1)).$$

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Becker-Döring – rescaled gradient structure

Onsager matrix $\mathcal{K}^\varepsilon(n)w^\varepsilon := \frac{1}{\varepsilon^{1-\alpha+\gamma}}\mathcal{K}(n)\psi$ with $w^\varepsilon(\varepsilon l) = \varepsilon^{-\gamma}(\psi_1 + \psi_l - \psi_{l+1})$.

Action $\mathcal{A}^\varepsilon(n, w^\varepsilon) := \frac{1}{\varepsilon^{1-\alpha+2\gamma}}\langle\psi, \mathcal{K}(n)\psi\rangle$

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 $\dot{n}^\varepsilon(t) = \mathcal{K}^\varepsilon\big(n^\varepsilon(t)w^\varepsilon(t)\big)$, denoted by $(n^\varepsilon, w^\varepsilon) \in \mathcal{CE}_T^\varepsilon$, is called a rescaled curve of finite action if

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

Moreover, for such a curve the functional

$$\mathcal{J}^\varepsilon(n^\varepsilon) := \mathcal{F}^\varepsilon(n^\varepsilon(T)) - \mathcal{F}^\varepsilon(n^\varepsilon(0)) + \frac{1}{2}\int_0^T \mathcal{D}^\varepsilon(n^\varepsilon(t))\,\mathrm{d}t + \frac{1}{2}\int_0^T \mathcal{A}^\varepsilon(n^\varepsilon(t), w^\varepsilon(t))\,\mathrm{d}t.$$

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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LSW equation – formal gradient structure

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

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

Formal gradient structure [Niethammer '04]

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

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

Onsager operator (compare formal expansion) and action

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

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

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

$$DE(\nu) \cdot s = \frac{q}{1-\gamma} \int \lambda^{1-\gamma} s\, \mathrm{d}\lambda = -\int \Bigl(\lambda u - \frac{q}{1-\gamma}\lambda^{1-\gamma}\Bigr) s\, \mathrm{d}\lambda = -\int \lambda^\alpha \bigl(u - q\lambda^{-\gamma}\bigr) w\, \mathrm{d}\nu.$$

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

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Proposition (Dissipation is strong upper gradient of the energy)

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

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

Then, it holds the moment estimate $\int_0^T \int \lambda^\alpha \, \mathrm{d}\nu_t \, \mathrm{d}t < \infty$.
Moreover, the minimization problem has a unique solution $u \in L^2([0,T])$ such that

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

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

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

is a strong upper gradient for the energy E

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

Proposition (Compactness)

Assume $\alpha \geq 1 - 3\gamma$ and let $(\nu^n, w^n) \in \mathrm{CE}_T$ 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 $(\nu, w) \in \mathrm{CE}_T$, such that

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

In addition, the action and dissipation satisfy the $\liminf$ estimates

$$\liminf_{n\to\infty} \int_0^T A(\nu_t^n, w_t^n)\,\mathrm{d}t \geq \int_0^T A(\nu_t, w_t)\,\mathrm{d}t$$
$$\liminf_{n\to\infty} \int_0^T D(\nu_t^n)\,\mathrm{d}t \geq \int_0^T D(\nu_t)\,\mathrm{d}t$$

Proposition (LSW as curves of maximal slope)

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

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

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

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Moreover, equality holds if and only if ν_t is a weak 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 $\nu_0^\varepsilon := \Pi_{\mathrm{mac}}^\varepsilon n^\varepsilon(0)$ is tight, then there exists a limiting curve $t \mapsto (\nu_t, w_t) \in \mathrm{CE}_T$

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

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

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

The energy, the action and the dissipation satisfy the following $\liminf$ estimates

$$\forall t \in [0,T] : \qquad \lim_{\varepsilon \to 0} \mathcal{F}_{\mathrm{mac}}^\varepsilon(\nu_t^\varepsilon) \geq \frac{1}{z_s} E(\nu_t),$$

$$\liminf_{\varepsilon \to 0} \int_0^T \mathcal{A}_{\mathrm{mac}}^\varepsilon(\nu_t^\varepsilon, w_t^\varepsilon)\,\mathrm{d}t \geq \frac{1}{z_s}\int_0^T A(\nu_t, w_t)\,\mathrm{d}t,$$

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Macroscopic Limit of the Becker-Döring gradient structure

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

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

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

then there exists a limiting $(\nu, w) \in \mathrm{CE}_T$ such that $\liminf_{\varepsilon\to 0} \mathcal{J}^\varepsilon(n^\varepsilon) \geq J(\nu) \geq 0$.
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

$$\lim_{\varepsilon\to 0} E\left(\Pi^\varepsilon_{\mathrm{mac}} n^\varepsilon(0)\right) = E(\nu_0).$$

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 $\lim_{\varepsilon\to 0} E(\nu_0^\varepsilon) = E(\nu_0)$.
Then there exists a solution $\nu \in C_c^\infty([0,T]\times\mathbb{R}_+)^*$ to the LSW equation such that $\nu_t^\varepsilon \stackrel{*}{\rightharpoonup} \nu_t$ 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 $\mathcal{J}^\varepsilon(n^\varepsilon) \le C$ and $\Pi^\varepsilon_{\mathrm{mac}} n^\varepsilon(0)$ tight. Then, it holds

$$\int_0^T \mathcal{H}_{\mathrm{mic}}\big(n^\varepsilon(t) \mid \omega(n_1^\varepsilon(t))\big)\,\mathrm{d}t \le C\varepsilon^{\gamma+(1-x)(1-\alpha+\gamma)} \int_0^T \mathcal{D}^\varepsilon_{\mathrm{mic}}(n_t^\varepsilon)\,\mathrm{d}t,$$

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

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

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!