# Phase transitions in Interacting Systems

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## RESEARCH ARTICLES AS PART OF THE HABILITATION


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[H2] J. G. Conlon and A. Schlichting. A non-local problem for the Fokker-Planck equation related to the Becker-Döring model. *Discret. Contin. Dyn. Syst.* 39.4 (Apr. 2019), pp. 1821–1889.

[H3] M. Erbar, M. Fathi, and A. Schlichting. Entropic curvature and convergence to equilibrium for mean-field dynamics on discrete spaces. *accepted at Lat. Am. J. Probab. Math. Stat.* (Aug. 2020), p. 26.

[H4] R. S. Gvalani and A. Schlichting. Barriers of the McKean–Vlasov energy via a mountain pass theorem in the space of probability measures. *under minor revision at J. Funct. Anal.* (May 2020), p. 26.

[H5] A. Schlichting. Macroscopic limit of the Becker-Döring equation via gradient flows. *ESAIM Control. Optim. Calc. Var.* 25.22 (July 2019), p. 36.

[H6] A. Schlichting. The exchange-driven growth model: basic properties and longtime behavior. *J Nonlinear Sci* 30.3 (Nov. 2019), pp. 793–830.

[H7] A. Schlichting and M. Slowik. Poincaré and logarithmic Sobolev constants for metastable Markov chains via capacitary inequalities. *Ann. Appl. Probab.* 29.6 (Dec. 2019), pp. 3438–3488.

CONTENTS

# 1. Introduction and overview

This thesis analyzes evolutionary models possessing nonlinearities emerging from interactions. The analysis considers dynamical aspects and, in particular, the behavior of these systems in the presence of phase transitions. Here, a phase transition is understood as a sudden change of the equilibrium states, if one of the system parameters crosses a critical threshold. This phenomenon is studied from several different aspects to highlight that this topic touches many different fields of mathematics.

1.1. **Models of interacting agents.** In Section 2, so-called mean-field limits originating from models of interacting agents are considered. These models are described by the McKean–Vlasov partial differential equations, also called diffusion-aggregation equations. The interactions are modeled through a potential function, which encodes repulsive and attractive forces between agents. Moreover, each agent undergoes a Brownian stochastic forcing, which acts as an additional repulsive force.

For this reason, there are two situations: The two forces on the agents could act proportional or reciprocal. If the interaction potential is repulsive, the agents avoid each other and dissolved states are preferred. A striking phenomenon occurs for attractive potentials where, depending on the ratio between the self-diffusion and interaction force, the system prefers a uniform state or a clustered state as equilibrium. The emergence of a clustered state is called consensus formation in application to opinion dynamic.

The project [H1] described in Section 2.1 establishes a method to verify the occurrence of such consensus formation and to obtain the critical parameters for those. Moreover, in statistical mechanics [Rue99], two kinds of phase transitions are considered: First order phase transitions, also called discontinuous ones, are those where an order parameter shows a jump, whereas second-order phase transitions, also called continuous ones, show a continuous change of the order parameter. The work [H1] provides criteria on the interaction potential identifying the type of the phase transition. Mathematically, the continuous phase transitions are accessible by local bifurcation analysis. The investigation of the discontinuous phase transition is more subtle and relies on the fact that the McKean–Vlasov model possesses a free energy. Each critical point of the free energy corresponds to a stationary state, and local minima are also locally stable equilibria for the dynamic. Hence, discontinuous phase transitions can be observed from the free energy landscape by finding and constructing suitable competitor states.

The observation of discontinuous phase transitions for the McKean–Vlasov dynamic is the starting point of the project [H4] described in Section 2.2. Here, several observations and results from the literature are connected and extended to prove the metastable behavior of the stochastic many agent dynamic. First, due to the works [LS95; JKO98; Ott01], it is well-known that the free energy for the McKean–Vlasov equation is not only a Lyapunov function for the dynamic but also the driving energy function for a gradient flow formulation with respect to the Wasserstein distance. This interpretation justifies that many properties of the McKean–Vlasov dynamic can be read off the free energy landscape.

The gradient flow interpretation formally justifies also the observation that the *stochastic* dynamic with finitely many agents in the parameter regime of a discontinuous phase transition shows metastable behavior, see also Section 1.2 below. That is, the stochastic dynamic of the agents has a unique equilibrium Gibbs state, but the ergodicity is lost in the limit of infinite agents. This manifests itself in a very slow convergence to equilibrium of the system.

The question is whether the slow time-scale of the metastable dynamic can be read of the energy landscape in terms of an energy barrier similar to the Arrhenius law for chemical reactions. That this is the case can be proven thanks to the seminal work of Dawson and Gärtner [DG87], which connects the free energy with the large deviation rate function for the stochastic dynamic. Hence, the remaining step for making this observation rigorous is a mountain pass theorem in the space of probability measures for the driving free energy functional, which is the main result presented in Section 2.2.

Another indicator of the presence of a phase transition is the *breakdown of convexity* of the free energy. The reasoning is that if the free energy of a model from statistical mechanics is convex, then the system cannot have a phase transition. Hence, if the statement is considered the other way round, then a loss of convexity indicates the existence of a phase transition. Moreover, the critical parameter for the phase transition should be related to the breakdown of convexity.

In Section 2.3 a class of mean-field interacting agent systems on graphs is considered for which the notion of convexity is refined, since the free energy is a functional of probability measures on the graph. The notion of displacement convexity pioneered by [McC97] is used with respect to a discrete transportation metric for which the dynamic becomes a gradient flow for the free energy [Maa11; 10]. The seminal works of Sturm [Stu06] and Lott-Villani [LV09] connect for Riemannian manifolds displacement convexity of the entropy to the lower Ricci curvature bounds, which justifies the name entropic curvature bound.

1.2. **Metastability.** Metastability is related to the dynamics of a first-order phase transition from the statistical mechanics' point of view: a quick change of a system parameter across the line of the phase transition reveals the existence of multiple time scales. On the short time scale, subsets of the state space emerge which effectively trap the system and form quasi-equilibrium states within the subset. These states are called metastable states. On longer time scales, a transition between these metastable states can be observed.

In many applications of metastability, especially in statistical mechanics [Geo11], one deals with discrete state spaces with very few structural assumptions. The work [H7] described in Section 3 provides a mathematical definition of metastability for Markov chains being able to *quantify* the time scale separation and, equally important, being *verifiable* for non-trivial concrete systems. This definition of metastability extends the one from the potential theoretic approach introduced by Bovier and coauthors in [Bov+01; Bov+02; BH15].

The proposed definition of metastability permits to express the time-scale separation in terms of capacities, which are *computable* thanks to various variational principles for relevant models of statistical mechanics [BBI09; BBI12]. Moreover,

under suitable size and regularity properties on the metastable states, sharp asymptotic estimates on the Poincaré and logarithmic Sobolev constant are established, which provide asymptotic sharp convergence estimates in variance and relative entropy.

The main ingredient is a capacitary inequality, a generalization of the co-area formula, along the lines of V. Maz'ya [Maz72; Maz11] relating regularity properties of harmonic functions and capacities. These notions and assumptions are well adapted to models from statistical mechanics, which is illustrated with an application to the random field Curie Weiss model.

1.3. **Longtime behavior of models for nucleation.** One of the fundamental phase transitions, the vapor-liquid transition, is investigated in section 4. The basic modeling assumptions go back to the work of Becker and Döring [BD35] which describe a mean-field theory for the initial era of condensation in which droplets form out of oversaturated vapor, called *homogeneous nucleation*. It describes the emergence of a new liquid phase out of an oversaturated vapor phase and to differentiate it from the phase transition discussed before, it is called *phase separation*.

The underlying modeling assumption is that the vapor phase consists of monomers, and the droplets are clusters consisting of at least two monomers. It is assumed that only the monomers can freely move on a faster time scale and that the clusters are fixed in space. This allows modeling the system under the mean-field assumption and neglect any spatial information. Hence, the state of the system is solely described by the population of monomers and clusters. In particular, the only possible coagulation events are those of single monomers with other monomers or clusters and the fragmentation of a single monomer from a cluster. This rules out coagulation and fragmentation of clusters as in the Smoluchowski equation [Smo16].

Becker and Döring [BD35] used further thermodynamic consideration to determine the rates of attachment and detachment of monomers and derived a model for the evolution of the population of clusters. They assumed that the monomer concentration stays constant, which makes the system a countable family of linear ordinary differential equations and accessible to their analysis. Later, Penrose and Lebowitz [PL79] revised this and proposed that the whole system should be thermodynamically closed, which in particular prohibits the exchange of mass with the environment. Hence, the total mass density consisting of the total number of monomers, also taking the ones in the clusters into account, stays constant. This model is a coupled countable system of ordinary differential equations, where the coupling in the equation happens through the monomer density.

The importance of the (thermodynamically closed) Becker–Döring equations for the kinetic description of solutes—just as the Boltzmann equation for the rarefied gas dynamics—cannot be overestimated. A first mathematically rigorous treatment was done by Ball, Carr, and Penrose [BCP86] proving well-posedness and the trend toward equilibrium. The equilibrium of the Becker–Döring system shows a phase separation phenomenon depending on the total mass density $\varrho$. For a range of physical relevant rates exists a critical mass density $\varrho_c$ below and above the equilibria take a different form. If $\varrho \leq \varrho_c$, then there exists an equilibrium state with

the same mass density, whereas for $\varrho > \varrho_c$ there does not exist a matching equilibrium state. In the first case, convergence can be shown, whereas in the second case, the system convergences actually to the equilibrium state with mass density $\varrho_c$ and hence the excess mass $\varrho - \varrho_c$ vanishes. This vanishing is interpreted as the formation of larger and larger clusters.

After this observation, it was formally argued by Penrose [Pen97] that the evolution of the excess mass satisfies a transport equation known from the theory of coarsening developed independently by Lifshitz–Slyozov [LS61] and Wagner [Wag61], for short LSW in the following. The rigorous connection was obtained by Niethammer [Nie03] based on exploiting the free energy–dissipation relation satisfied by both equations.

In Section 4.1 based on [H5], an alternative proof of the connection between the Becker–Döring system and the LSW model is presented. It is based on the observation that the (thermodynamically closed) Becker–Döring system is the gradient flow of its free energy with respect to a discrete transportation metric similar to the one introduced in [Cho+12; Maa11; Mie11; 10] and explained in Section 2.3. The gradient flow formulation comes with a variational characterization of the solution, which provides a robust way of passing to the limit in a family of evolutionary systems based on the stability of gradient flows initiated by Sandier and Serfaty [SS04; Ser11].

In Section 4.2 based on [H2], a nonlinear and nonlocal Fokker–Planck description of the Becker–Döring equation is introduced. The model is based on the assumption that the monomers are very small in comparison to the nucleated droplets, which makes it reasonable to use a positive real number for their cluster sizes and track the monomer concentration in a separate variable.

A Fokker–Planck description is very appealing from the mathematical side since it opens new toolboxes from the theory of partial differential equations as well as stochastic processes. In this way, it is possible to show that the Fokker–Planck model possesses a phase separation phenomenon of the same type as the Becker–Döring model, and the convergence to equilibrium is obtained. Additionally, it is also possible to obtain quantitative convergence rates to equilibrium for initially subcritical mass densities.

Ben-Naim and Krakivsky introduced in [BK03] the *exchange-driven growth* model, which describes a process in which pairs of clusters consisting of an integer number of monomers can grow or shrink only by the exchange of single monomers. The very close relationship to the classical Becker–Döring system was so far not observed in the literature and is discussed in Section 4.3 based on [H6]. It is then shown that the exchange-driven growth system shares many of the qualitative properties of the Becker–Döring equations. In particular, the model shows for exchange rate kernels satisfying a detailed balance condition the same type of phase separation in terms of some critical mass density $\varrho_c$, where depending on the initial mass density $\varrho$ the system convergences to an equilibrium with the same mass or in the case $\varrho > \varrho_c$ to the one having mass $\varrho_c$.

## 2. Phase transitions for models of interacting agents

2.1. **The McKean–Vlasov dynamic on the torus.** In [H1], an evolution of a collection of $N$ agents with position $\mathbf{X}_t^N = \left(X_t^{i,N} \in \mathbb{T}^d\right)_{i=1}^N$ at time $t \geq 0$ on the $d$-dimensional torus $\mathbb{T}^d$ of length $L > 0$ is considered. The agents evolve according to the following system of stochastic differential equations

$$\begin{cases} dX_t^{i,N} = -\dfrac{\kappa}{N} \displaystyle\sum_{i \neq j, j=1}^{N} \nabla W(X_t^{i,N} - X_t^{j,N})\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,dB_t^{i,N} \\ \mathrm{Law}(\mathbf{X}_0^N) = \rho_0^{\otimes N}(\mathrm{d}x) \end{cases}$$

where $B_t^{i,N}$ are independent $\mathbb{T}^d$-valued Brownian motions, $W$ is a sufficiently smooth even potential which describes the pairwise interaction between agents, and the constants $\kappa, \beta > 0$ represent the strength of interaction and inverse temperature respectively. One of the two parameters is redundant and $\beta$ is from now one fixed and $\kappa$ treated as the only parameter of the system.

If $\rho_N(x,t)$ denotes the law at time $t$ of $\mathbf{X}_t^N$, then by passing to the limit as $N \to \infty$, commonly referred to as the mean-field limit, one obtains (cf. [Gra+96]) that $\rho_N(x,t)$ converges to $\rho^{\otimes N}$. Here, the density $\rho(x,t)$ of the agents at position $x$ and time $t$ is a solution of the McKean–Vlasov equation

$$\begin{cases} \partial_t \rho = \beta^{-1}\Delta\rho + \kappa\nabla\cdot(\rho\nabla W \star \rho) & (x,t) \in \mathbb{T}^d \times (0,\infty) \\ \rho(x,0) = \rho_0(x) & x \in \mathbb{T}^d \end{cases}. \tag{2.1}$$

The nonlocal parabolic partial differential equation (2.1) describes the mean behavior of the probability density of agents in the large $N$-limit. The equation (2.1) is characterized by a natural competition between aggregation and diffusion depending on the value of the parameter $\beta$. This arises from the fact that, if $W$ is chosen to be attractive, the second term on the right hand side causes the agents to aggregate while the Laplacian causes them to diffuse. It is well-known since the seminal work in [JKO98] that (2.1) is a gradient flow of a free energy $\mathscr{F} : \mathscr{P}(\mathbb{T}^d) \to \mathbb{R} \cup \{+\infty\}$,

$$\mathscr{F}(\rho) := \beta^{-1} \int_{\mathbb{T}^d} \rho \log \rho \; \mathrm{d}x + \frac{\kappa}{2} \iint_{\mathbb{T}^d \times \mathbb{T}^d} W(x-y)\rho(x)\rho(y)\,\mathrm{d}x\,\mathrm{d}y\,, \tag{2.2}$$

with respect to the 2-Wasserstein metric on the space of probability measures. For this reason, $\mathscr{F}$ is a (strict) Lyapunov function for the dynamics of (2.1) and it holds

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{F}(\rho) = -\int_{\mathbb{T}^d} \left|\beta^{-1}\nabla \log\frac{\rho}{\mu} + \kappa\nabla W * \rho\right|^2 \mathrm{d}\rho.$$

The gradient flow formulation implies that critical points of $\mathscr{F}$ correspond exactly to steady states of (2.1) and satisfy the self-consistency condition

$$\rho_\infty = \frac{\exp(-\beta\kappa W * \rho_\infty)}{\int_{\mathbb{T}^d} \exp(-\beta\kappa W * \rho_\infty)}.$$

One can notice immediately that $\rho_\infty := L^{-d}$ is a steady state of (2.1) for all $\kappa > 0$. The question addressed in [H1] is whether non-constant steady states exist and if they do exist, how to characterize and classify them. By the variational characterization, this question is closely related to the existence and uniqueness of minimizers of $\mathscr{F}$. The absence of uniqueness is exactly the case for which phase

transitions in the system will occur and the critical value of the parameter $\kappa_c$ is the one for which there is a change in the set of minimizers of $\mathscr{F}$.

In the presence of a phase transition, the work [H1] also answers the question, which kind of phase transition occurs. Second order phase transitions are characterized that a new minimizer bifurcates from an existing one in a continuous manner while $\kappa$ crosses $\kappa_c$, hence those are called *continuous phase transition*. Complementary for first order transition, a new minimizer emerges after the transition beyond $\kappa_c$, which is not close in the chosen topology and those are called *discontinuous*. This definition is robust for a range of topologies and in the present case the total variation is used.

Before considering phase transitions, the global stability of (2.1) is investigated. The main results of [H1] are stated here only in one dimension and the additional notation needed to state them is the cosine transform of $W$ denoted by

$$\widetilde{W}(k) := \left(\frac{2}{L}\right)^{1/2} \int W(x) \cos\left(\frac{2\pi k}{L} x\right) \mathrm{d}x \quad \text{for} \quad k \in \mathbb{Z}.$$

The global stability result uses the compactness of the torus implying that the Laplacian has a spectral gap and also satisfies a logarithmic Sobolev inequality. By treating the first order part of (2.1) as a perturbation, it is possible to show the following result.

**Theorem.** *(Convergence to equilibrium) Let $\varrho$ be a classical solution of the McKean–Vlasov equation* (2.1) *with smooth initial data and smooth, even, interaction potential $W$. Then we have:*

*(i) If $0 < \kappa < \frac{2\pi}{3\beta L \|\nabla W\|_\infty}$, then $\left\| \varrho(\cdot,t) - \frac{1}{L} \right\|_2 \to 0$, exponentially, as $t \to \infty$,*

*(ii) If $\widetilde{W}(k) \geq 0$ for all $k \in \mathbb{Z}, k > 0$, or $0 < \kappa < \frac{2\pi^2}{\beta L^2 \|\Delta W\|_\infty}$, then $\mathscr{H}\left(\varrho(\cdot,t) | \frac{1}{L}\right) \to 0$, exponentially, as $t \to \infty$ ,*

*where $\mathscr{H}\left(\varrho(\cdot,t) | \frac{1}{L}\right) := \int \varrho(\cdot,t) \log\left(\frac{\varrho(\cdot,t)}{\varrho_\infty}\right) \mathrm{d}x$ denotes the relative entropy.*

The previous theorem implies that the uniform state can fail to be the unique stationary solution only if the interaction potential has at least one negative Fourier mode. The reason is that in the derivative of the $L^2$-norm or entropy convolution integrals occur, which relate to the Fourier modes by the identity

$$\int\!\!\int_{\mathbb{T}\times\mathbb{T}} W(x-y) g(x) g(y) \,\mathrm{d}x \,\mathrm{d}y = \sum_{k \in \mathbb{N}} \widetilde{W}(k) \frac{1}{N_k} \sum_{\sigma \in \{-1,1\}} |\widetilde{g}(\sigma(k))|^2. \tag{2.3}$$

Here, the symmetry of $W$ is used and $N_k$ is a suitable normalizing factor. The identity (2.3) shows that potentials with nonnegative Fourier modes are $H$-stable as introduced by Ruelle [Rue99]. From this observation, it is expected that phase transition can only occur for interaction potentials $W$, which are not $H$-stable as noticed in [CP10].

The first main result of [H1] on phase transitions provides conditions on $W$ in terms of its Fourier modes that guarantee the existence of non-constant steady states which bifurcate from the constant branch $(1/L, \kappa)$. This allows to construct interaction potentials $W$ with a prescribed bifurcation diagram, for instance $W$ with infinitely many such bifurcation points.

**Theorem.** *(Local bifurcations) Let $W$ be smooth and even and let $(1/L, \kappa)$ represent the trivial branch of solutions. Then every $k^* \in \mathbb{Z}, k^* > 0$ such that*

*(i)* $\operatorname{card}\{k \in \mathbb{Z}, k > 0 : \widetilde{W}(k) = \widetilde{W}(k^*)\} = 1$ ,

*(ii)* $\widetilde{W}(k^*) < 0$,

*leads to the bifurcation point $(1/L, \kappa_*)$ of the stationary McKean–Vlasov equation through the formula*

$$\kappa_* = -\frac{(2L)^{1/2}}{\beta \widetilde{W}(k^*)}.$$

The results for the classification of the type of phase transition are based on the analysis of the free energy $\mathscr{F}$. For $\kappa$ sufficiently small the contribution of the entropy in (2.2) dominates and minimizers of $\mathscr{F}$ are unique and given by $\rho_\infty$. However, for a large class of $W$ and large values of $\kappa$, uniqueness is lost and there exists a value $\kappa_c > 0$, the point of phase transition, at which a new non-constant minimizer of $\mathscr{F}$ arises. The results in [H1] provide verifiable conditions on $W$ in terms of its Fourier coefficients for which this transition is continuous or discontinuous, extending considerably the results in [CP10].

**Theorem.** *(Discontinuous and continuous phase transitions) Let $W$ be smooth, even and not H-stable. Then the free energy $\mathscr{F}$ defined in* (2.2) *exhibits a transition point, $\kappa_c < \infty$. The transition point can be classified in the following two scenarios:*

*(i) If there exist strictly positive $k^a, k^b, k^c \in \mathbb{Z}$ with $\widetilde{W}(k^a) \approx \widetilde{W}(k^b) \approx \widetilde{W}(k^c) \approx \min_k \widetilde{W}(k) < 0$ such that $k^a = k^b + k^c$, then $\kappa_c$ is a discontinuous transition point.*

*(ii) Let $k^\sharp = \arg\min_k \widetilde{W}(k)$ be well-defined with $\widetilde{W}(k^\sharp) < 0$. Let $W_\alpha$ denote the potential obtained by multiplying all the negative Fourier modes $\widetilde{W}(k)$ except $\widetilde{W}(k^\sharp)$ by some $\alpha \in (0, 1]$. If $\alpha$ is made small enough, then the transition point $\kappa_c$ is continuous.*

The condition in (i) can be understood as a near-resonance condition on the Fourier modes, which is crucial for the construction of competitor states for $1/L$ having lower free energy. Although this condition seems to be quite specific, it is possible to verify it for sufficiently short-range attractive interaction potentials $W$, which is explained in the next Section 2.2.

The condition (ii) describes the situation in which one mode dominates all other modes in a quantitative way. Here, the occurring constant $\alpha$ is in principle explicit, however hard to compute for two reasons: Firstly, it depends on the error in the local bifurcation analysis, which involves at least second derivatives of the fixed point map and hence estimates on its eigenvalues. Secondly, is also depends on a defect inequality between the relative entropy and any Fourier mode of the density

$$\mathscr{H}(\rho|\rho_\infty) - \tfrac{L}{2}|\widetilde{\rho}(k)| \geq \mathscr{G}(|\widetilde{\rho}(k)|),$$

where $\mathscr{G} : \mathbb{R}^+ \to \mathbb{R}^+$ with $\mathscr{G}(0) = 0$ is given only through a power series representation. Nevertheless, the condition (i) and (ii) provide a general characterization of continuous and discontinuous phase transition for the McKean–Vlasov dynamic in this perturbative regime

2.2. **A mountain pass theorem in the space of probability measures and application to the McKean–Vlasov free energy.** The setting of this section is the same as in Section 2.1, where $W$ is chosen such that $\mathscr{F}$ possesses a discontinuous transition point at some $\kappa = \kappa_c$. This implies that $\mathscr{F}$ has at least two distinct global minimizers $\rho_\infty$ and $\rho^*$ at $\kappa = \kappa_c$. That this is a generic situation for localized interaction energies is shown in [H4].

**Lemma.** *Let $W \in C^2(\mathbb{T}^d)$ be a compactly supported interaction potential with support. If for some $C > 0$ and all $\varepsilon > 0$ it holds*

$$\int_{\mathbb{T}^d} W(x) e^{i\frac{2\pi\epsilon k\cdot x}{L}}\,\mathrm{d}x \geq \int_{\mathbb{T}^d} W := -C \quad \text{for all } k \in \mathbb{Z}^d,$$

*Then, the associated free energy $\mathscr{F}^\epsilon$ to the rescaled potential $W_\epsilon(x) = \varepsilon^{-d} W(x/\varepsilon)$ possesses for some $\epsilon$ small enough a discontinuous transition point.*

The result raises the question if $\mathscr{F}$ has in this situation also a saddle point $\rho^{**}$ at $\kappa = \kappa_c$ which admits a minimax characterization in the spirit of the well-known Ambrosetti–Rabinowitz mountain pass theorem [AR73]. The mountain pass theorem is a classical result in nonlinear analysis which is extensively used to prove the existence of solutions to nonlinear elliptic partial differential equations. If such a point exists it captures exactly the energy barrier between $\rho_\infty$ and $\rho^*$, i.e., $\Delta = \mathscr{F}(\rho^{**}) - \mathscr{F}(\rho_\infty) = \mathscr{F}(\rho^{**}) - \mathscr{F}(\rho^*)$, where $\Delta$ is defined as

$$\Delta := \inf_{\gamma\in\Gamma} \max_{t\in[0,1]} \mathscr{F}(\gamma(t)), \tag{2.4}$$

with $\Gamma$ the set of all continuous curves that start at $\rho_\infty$ and end at $\rho^*$.

The main issue with applying a mountain pass type argument is that the functional $\mathscr{F}$ is not continuous, it is only lower semicontinuous on $\mathscr{P}(\mathbb{T}^d)$ equipped with the Wasserstein metric. Hence, the classical mountain pass theorem or even generalizations to continuous functions on metric spaces like [Kat94] do not apply.

The first main result of [H4] overcomes this difficulties and is a general mountain pass theorem for lower semicontinuous functionals $I$ on $\mathscr{P}(M)$, where $M$ is some compact Riemannian manifold, and $\mathscr{P}(M)$ is equipped with the 2-Wasserstein topology. The compactness is used in this section for convenience to avoid the introduction of some Palais–Smale condition [PS64].

Moreover, the additional regularity making the mount pass theorem achievable in this situation is $\lambda$-convexity of $I$ in the sense of McCann [McC97]: There exists $\lambda \in \mathbb{R}$ such that for all $W_2$-geodesics $(\mu_t)_{t\in[0,1]}$ holds

$$I(\mu_t) \leq (1-t)I(\mu_0) + tI(\mu_1) - \lambda\frac{t(1-t)}{2} W_2(\mu_0,\mu_1)^2\,.$$

Since $(\mathscr{P}(M), W_2)$ is a metric space, one would expect to formulate critical points in terms of the metric slope of $I$ defined as

$$|\partial I|(\mu) = \begin{cases} \limsup\limits_{\nu\to\mu} \frac{(I(\mu)-I(\nu))_+}{W_2(\mu,\nu)} & \mu \in \mathrm{Dom}(I) \\ +\infty & \text{otherwise}\,. \end{cases}$$

However, due to missing regularity a detour through the weak metric slope $|dI|$ is needed. The notion goes back to Ioffe and Schwartzman [IS96] who provided the definition in the Banach space setting. For this introduction the definition is

omitted (see [H4, Definition 2.1]) because it is shown in [H4, Proposition 4.8] that for $\lambda$-convex $I$ it holds $|\partial I| = |dI|$ for all $\mu \in \mathrm{Dom}(I)$.

**Theorem.** *Let $I : \mathscr{P}(M) \to \mathbb{R} \cup \{+\infty\}$ be a proper, lower semicontinuous, and $\lambda$-geodesically convex functional and assume that if $\mu \in \mathrm{Dom}(I)$, then $\mu \ll \mathrm{vol}$. Suppose $\mu, \nu \in \mathscr{P}(M) \cap \mathrm{Dom}(I)$, $\Gamma$ is the set of all continuous curves $\gamma : [0,1] \to \mathscr{P}(M)$ with $\gamma(0) = \mu$ and $\gamma(1) = \nu$, and the function $\Upsilon : \Gamma \to \mathbb{R}$ is defined by:*

$$\Upsilon(\gamma) = \max_{t \in [0,1]} I(\gamma(t)) .$$

*Let $c = \inf_{\gamma \in \Gamma} \Upsilon(\gamma)$ and $c_1 = \max\{I(\mu), I(\nu)\}$. If $c > c_1$ then there exists a $c' \geq c$ such that $c'$ is a critical value of $I$, i.e., there exists a $\eta \in \mathscr{P}(M)$ with $I(\eta) = c'$ such that $|\partial I|(\eta) = |dI|(\eta) = 0$.*

The strategy to cope with the lower semicontinuity of $I$ is based on an idea introduced by Di Giorgi et al. in [DMT80]: Extend the energy functional $I$ to its epigraph by setting

$$\mathscr{G}_I(\rho, \xi) := \xi, \quad (\rho, \xi) \in \mathrm{epi}(I) := \{(u, \xi) \in \mathscr{P}(M) \times \mathbb{R} : I(u) \leq \xi\} .$$

By also extending the metric to the epigraph, the functional $\mathscr{G}_I$ is continuous, which is enough extra regularity to prove a mountain pass theorem for the extended functional. The other crucial ingredient comes from the $\lambda$-convexity, which ensures that this saddle point lies on the boundary of the epigraph and is thus a saddle point of $I$ in the classical sense. This is the first result of its kind which shows a mountain pass theorem in a nonsmooth setting. Even though the result is proved in the 2-Wasserstein setting, it easily generalizes to the $p$-Wasserstein case and might be also applicable to similar transportation distances.

In the second part of [H4], the mount pass theorem is illustrated and applied to the functional $\mathscr{F}$ from (2.2) and it is shown that at $\kappa = \kappa_c$ in the presence of a discontinuous phase transition, there exists mountain pass point $\rho^{**}$ which realizes the energy barrier $\Delta$ in (2.4). This result along with the classical Dawson–Gärtner large deviations principle [DG87] allows to compute upper bounds on the escape probabilities of the $N$-particle system $\mathbf{X}_t^N$ at the very beginning of Section 2.1. For this let $\rho^{(N)}$ be the empirical measure associated to $\mathbf{X}_t^N$, i.e., $\rho^{(N)}(t) = N^{-1} \sum_i \delta_{X_t^{i,N}}$ and let $\rho^N(0)$ be close to $\rho_\infty$. Then, the probability that $\rho^{(N)}(t)$ reaches close to $\rho^*$ in time $T > 0$ is bounded by $\exp(-N\Delta)$, which confirms the Arrhenius law in this situation.

2.3. **Convexity breakdown for entropic curvature.** The work [10] considers, similarly to the derivation of (2.1) described in Section 2.1, the scaling limit of particle system with mean-field interaction on discrete state spaces. Let $\mathscr{X}$ be finite set and $\mathscr{P}(\mathscr{X})$ the set of probability measures on $\mathscr{X}$. It is assumed that the equilibrium distribution of a $N$-particle system is given by a Gibbs measure $\pi^N \in \mathscr{P}(\mathscr{X}^N)$ of the form

$$\pi^n(\boldsymbol{x}) = \frac{1}{Z_N} \exp\big(-U^N(\boldsymbol{x})\big) ,$$

where the Hamiltonian $U^N : \mathscr{X}^N \to \mathbb{R}$ is of mean-field type, that is the state $\boldsymbol{x} = (x_1, \ldots, x_N)$ enters solely via its empirical distribution $L^N(\boldsymbol{x}) = \frac{1}{N} \sum_i \delta_{x_i}$. Hence, it is assumed that $U^N(\boldsymbol{x}) = U\big(L^N(\boldsymbol{x})\big)$ for some suitable function $U : \mathscr{P}(\mathscr{X}) \to \mathbb{R}$. A

typical example mimicking the situation of Section 2.1 is the choice

$$U^N(\boldsymbol{x}) = \sum_i V(x_i) + \frac{1}{N}\sum_{i,j} W(x_i, x_j)\,,$$

where $V$ is an external potential and $W$ is an interaction potential with similar interpretation as introduced in Section 2.1. Note that $U\big(L^N(\boldsymbol{x})\big) = U^N(\boldsymbol{x})$ in this case is of the form

$$U(\mu) = \sum_{x\in\mathscr{X}} \mu_x K_x(\mu) \quad \text{with} \quad K_x(\mu) = V(x) + \sum_y W(x,y)\mu_y\,. \tag{2.5}$$

This motivates the general assumption that $U$ takes precisely the form (2.5) for an arbitrary$< C^2$ function $K : \mathscr{P}(\mathscr{X}) \to \mathbb{R}^{\mathscr{X}}$. Based on this preliminary assumption, it is straightforward to construct a reversible Markov chain with respect to the Gibbs measure $\pi^N$. The jump of the $i$-th single particle from $x_i$ to $y$ is denoted by $\boldsymbol{x} \to \boldsymbol{x}^{i,y} = (x_1, \dots, x_{i-1}, y, x_{i+1}, \dots, x_N)$. With this notation the jump rates are given by

$$Q^N(\boldsymbol{x}, \boldsymbol{x}^{i,y}) = \sqrt{\frac{\pi^N_{\boldsymbol{x}^{i,y}}}{\pi^N_{\boldsymbol{x}}}} A_{x_i,y}\big(L^N(\boldsymbol{x})\big)\,. \tag{2.6}$$

This is a generalized Glauber dynamic for the Gibbs measure $\pi^N$, where the symmetric irreducible family of matrices $\big(A(\mu)\big)_{\mu\in\mathscr{P}(\mathscr{X})}$ describes and weights the admissible jumps. The construction so far ensures that $Q^n(\boldsymbol{x}, \boldsymbol{x}^{i,y}) = Q_{x_i,y}\big(L^N(\boldsymbol{x})\big)$ for explicit family of rate matrices $Q : \mathscr{P}(\mathscr{X}) \times \mathscr{X} \times \mathscr{X} \to \mathbb{R}_+$.

Thanks to the results of [Maa11; Mie11], the Markov chain $(\mathscr{X}^N, Q^N, \pi^N)$ possesses a gradient flow structure with respect to the relative entropy

$$\mathscr{F}^N(\mu^N) = \sum_{\boldsymbol{x}^N} \mu^N(\boldsymbol{x}) \log \frac{\mu^N(\boldsymbol{x})}{\pi^N(\boldsymbol{x})}\,.$$

In addition the jump rates $Q^N$ give rise to a discrete transportation metric $\mathscr{W}^N$.

In [10], the evolution $c^N(t) = L^N_{\#}\mu^N(t) \in \mathscr{P}(\mathscr{P}(\mathscr{X}))$ of the empirical measure obtained from the $N$-particle Markov dynamic $\mu^N(t)$ is considered. In the scaling limit $N \to \infty$, $c^N(t)$ converges towards a deterministic measure $c^N(t) \rightharpoonup \delta_{\mu(t)}$ with $\mu$ the solution to a suitable discrete McKean–Vlasov equation

$$\dot\mu_x(t) = \sum_{y\in\mathscr{X}} \mu_y(t) Q_{y,x}\big(\mu(t)\big)\,. \tag{2.7}$$

The equation (2.7) looks like the master equation for a linear Markov chain, but it is indeed nonlinear through the dependence of the transition matrix $Q$ on $\mu$. The construction $Q$ in (2.6) ensures that there exists a local Gibbs measure

$$\pi(\mu)_x = \frac{1}{Z}\exp\big(-H(\mu)_x\big) \quad \text{with} \quad H(\mu)_x = \partial_{\mu_x} U(\mu)\,, \tag{2.8}$$

satisfying the local detailed balance condition

$$\pi(\mu)_x Q_{x,y}(\mu) = \pi(\mu)_y Q_{y,x}(\mu) \qquad \text{for all} \qquad \mu \in \mathscr{P}(\mathscr{X})\,. \tag{2.9}$$

Hence, any stationary point $\pi^*$ for the dynamic (2.7) is a fixed point of the mapping $\mu \mapsto \pi(\mu)$, that is $\pi(\pi^*) = \pi^*$. This situation resembles very much the one of

Section 2.1. In particular the non-uniqueness is possible and the loss of a unique stationary point implies a phase transition for this particular system parameter.

Systems of the type (2.7) appeared in the work [Bud+15], where it is shown that the free energy

$$\mathscr{F}(\mu) = \sum_x \mu_x(\log \mu_x - 1) + U(\mu) \tag{2.10}$$

is a Lyapunov function for the dynamic. In [10] a gradient structure implying the monotonicity of the free energy is introduced, which allows to write (2.7) as

$$\dot{\mu}_x(t) = \sum_{y\in\mathscr{X}} \mu_y(t) Q_{y,x}\big(\mu(t)\big) = -\mathscr{K}_{\mu(t)} D\mathscr{F}\big(\mu(t)\big)\,,$$

where the operator $\mathscr{K}_\mu$ is given by

$$(\mathscr{K}_\mu \psi)(x) = -\sum_y \Lambda\big(\mu_x Q_{x,y}(\mu), \mu_y Q_{y,x}(\mu)\big)\nabla\psi(x,y)\,, \tag{2.11}$$

and $D\mathscr{F}$ identified with the vector $D\mathscr{F}(\mu)_x = \partial_{\mu_x}\mathscr{F}(\mu) = \left(\log \frac{\mu_x}{\pi(\mu)_x}\right)$. The through $\mathscr{K}$ induced Riemannian geometry on $\mathscr{P}(\mathscr{X})$ is the natural nonlinear counterpart of the results from [Maa11; Mie13] for linear Markov chains.

Furthermore, the work [10] also studies the associated discrete transportation distance, which based on the minimizer action formalism introduced in [BB00] is obtained from

$$\mathscr{A}(\mu,\psi) = \frac{1}{2}\sum_{x,y\in\mathscr{X}} |\nabla\psi(x,y)|^2 \Lambda\big(\mu_x Q_{x,y}(\mu), \mu_y Q_{y,x}\big)\,,$$

through the minimization problem

$$\mathscr{W}^2(\mu_0,\mu_1) = \inf_{\mu,\psi}\left\{\int_0^1 \mathscr{A}(\mu_t,\psi_t)\,\mathrm{d}t\right\}\,, \tag{2.12}$$

over all pairs $\mu : [0,1] \to \mathscr{P}(\mathscr{X})$ and $\psi : [0,1] \to \mathbb{R}^{\mathscr{X}}$, such that $\mu(0) = \mu_0$, $\mu(1) = \mu_1$, satisfying the continuity equation

$$\dot{\mu}(t) + \mathscr{K}_{\mu(t)}\psi = 0\,.$$

The main theorem regarding the metric of [10] is the following.

**Theorem.** *$\mathscr{W}$ defines a complete, separable and geodesic metric on $\mathscr{P}(\mathscr{X})$. The discrete McKean–Vlasov equation* (2.7) *is the gradient flow of $\mathscr{F}$ with respect to $\mathscr{W}$.*

The above Theorem is the starting point for the project [H3] in which displacement convexity properties of $\mathscr{F}$ from (2.10) are studied with respect to the metric (2.12). The definition of the notion of convexity in this situation is motivated from [LV09; Stu06].

**Definition.** A nonlinear Markov triple $(\mathscr{X}, Q, \pi)$, that is $\pi$ is given by (2.8) and satisfies (2.9) with respect to $Q$, has *Ricci curvature bounded below by* $\kappa \in \mathbb{R}$ (for short $\mathrm{Ric}(\mathscr{X}, Q) \geq \kappa$) if for any $\mathscr{W}$-geodesic $(\mu_t)_{t\in[0,1]}$:

$$\mathscr{F}(\mu_t) \leq (1-t)\mathscr{F}(\mu_0) + t\mathscr{F}(\mu_1) - \frac{\kappa}{2}t(1-t)\mathscr{W}(\mu_0,\mu_1)^2\,.$$

It show that Ricci curvature lower bounds can be characterized in terms of a discrete Bochner-type inequality by deriving the Hessian of $\mathscr{F}$ in the Riemannian

structure $\mathscr{W}$, as well as in terms of the Evolution Variational inequality $\mathrm{EVI}_\kappa$ for the solutions to (2.7)

$$\frac{1}{2}\frac{\mathrm{d}^+}{\mathrm{d}t}\mathscr{W}(\mu_t,\nu)^2+\frac{\kappa}{2}\mathscr{W}(\mu_t,\nu)^2\le\mathscr{F}(\nu)-\mathscr{F}(\mu_t)\,.$$

Further, it is shown that a positive lower bound on the Ricci curvature entails a number of functional inequalities that control the convergence to equilibrium of the mean-field systems. These involve a discrete Fisher information functional $\mathscr{I}:\mathscr{P}(\mathscr{X})\to[0,\infty]$ given by

$$\mathscr{I}(\mu)=\frac{1}{2}\sum_{x,y}\Theta\big(\mu_xQ_{xy}(\mu),\mu_yQ_{yx}(\mu)\big)\,,\qquad\Theta(a,b)=(a-b)(\log a-\log b)\,,$$

which arises from the dissipation of $\mathscr{F}$ along solutions to (2.7) as $\frac{d}{dt}\mathscr{F}(\mu_t)=-\mathscr{I}(\mu_t)$. One of our main results is the following theorem which can be seen as a discrete analog of [CMV03, Thm. 2.1].

**Theorem.** *Assume that* $\mathrm{Ric}(\mathscr{X},Q,\pi)\ge\lambda$ *for some* $\lambda>0$*. Then the following hold:*

*(i) there exists a unique stationary point* $\pi^*$ *for the evolution* (2.7)*, it is the unique minimizer of* $\mathscr{F}$*. Let* $\mathscr{F}_*(\cdot):=\mathscr{F}(\cdot)-\mathscr{F}(\pi^*)$*;*

*(ii) the* modified logarithmic Sobolev inequality *with constant* $\lambda>0$ *holds, i.e. for all* $\mu\in\mathscr{P}(\mathscr{X})$*,*

$$\mathscr{F}_*(\mu)\le\frac{1}{2\lambda}\mathscr{I}(\mu)\,;\qquad\qquad\mathrm{MLSI}(\lambda)$$

*(iii) for any solution* $(\mu_t)_{t\ge0}$ *to* (2.7) *the free energy decays exponentially*

$$\mathscr{F}_*(\mu_t)\le e^{-2\lambda t}\mathscr{F}_*(\mu_0)\,;$$

*(iv) the* entropy-transport inequality *with constant* $\lambda>0$ *holds, i.e. for all* $\mu\in\mathscr{P}(\mathscr{X})$*,*

$$\mathscr{W}(\mu,\pi_*)\le\sqrt{\frac{2}{\lambda}\mathscr{F}_*(\mu)}\,.\qquad\qquad\mathrm{ET}(\lambda)$$

The above theorem characterizes the situation where strict convexity is present in the system implying good contraction properties for the dynamic. This type of results is then established for several examples of mean-field interacting dynamics.

The Curie–Weiss model is obtained by setting $\mathscr{X}=\{0,1\}$ and defining $K$ as in (2.5) with $V\equiv0$, $W(0,0)=0=W(1,1)$, and $W(0,1)=\beta=W(1,0)$ for some $\beta>0$. In particular, it holds

$$U(\mu)=2\beta\mu_0\mu_1\,.$$

The free energy (2.10) becomes

$$\mathscr{F}(\mu)=\mu_0\log\mu_0+\mu_1\log\mu_1+2\beta\mu_0\mu_1\,.$$

Since $\mu\in\mathscr{P}(\mathscr{X})$, it holds $\mu_0+\mu_1=1$ and $\mathscr{F}$ can be portrayed as a one-dimensional function and it is easily checked that this function is convex as a one-dimensional real function if and only if $\beta\in[0,1]$. Indeed, $\beta_c=1$ is the critical temperature in the statistical mechanics sense [Kac69].

To prove this observation on the level of entropic curvature, a dynamic needs to be imposed. A canonical choice in this case is the Glauber dynamic, which reads

$$Q(\mu;0,1)=\sqrt{\frac{\pi_1(\mu)}{\pi_0(\mu)}}=\exp\big(-\beta(\mu(0)-\mu(1))\big)=\frac{1}{Q(\mu;1,0)}\ .$$

Therewith it holds that $\mathrm{Ric}(\mathscr{X},Q,\pi)\geq\kappa_{\text{Curie–Weiss}}=2(1-\beta)$ and hence the *breakdown of convexity* in the sense of entropic curvature happens exactly also for $\beta_c=1$.

The other class of models are mean-field zero range and misanthrope processes, which are given with rates of the type

$$Q(\mu;x,y)=p(x,y)c(\mu_x,\mu_y)\,.$$

These systems generalize usual linear Markov chains encoded in $p(x,y)$ by an additional dependency of the jump rate on the population density of the departure and arrival site of the jump given by the function $c:[0,1]\times[0,1]\to\mathbb{R}_+$. This model, first introduced in [Coc85], incorporates many examples, such as for instance the zero range process [Spi70], for which $c(\mu_x,\mu_y)=b(\mu_x)$, but also interacting agent/voter models [Vil19], for which $c(\mu_x,\mu_y)=a(\mu_y)$. To ensure the detailed balance condition (2.9) more structural assumptions on $c$ are needed and separability is a sufficient condition, which seems to be very related to the observation for a similar model discussed in Section 4.3. The result for the entropic Ricci lower bound is perturbative and based on the comparison with the complete graph.

**Theorem** (Curvature for separable kernels)**.** *Assume the rates are separable, given by*

$$Q(\mu;x,y)=b(\mu_x)a(\mu_y)\,. \tag{2.13}$$

*Suppose that*

$$0<\underline{a}\leq a(\cdot)\qquad\text{and}\qquad 0<\underline{b}\leq b(\cdot)\,.$$

*Moreover, assume that* $\frac{\max\{\mathrm{Lip}\,a,\mathrm{Lip}\,b\}}{\min\{\underline{a},\underline{b}\}}=:\eta\ll 1$*, then it holds that*

$$\mathrm{Ric}(\mathscr{X},Q,\pi)\geq\kappa=d\,\underline{a}\,\underline{b}\big(1+O(\eta)\big)\,.$$

For the full result making $O(\eta)$ explicit see [H3, Theorem 5.3].

2.4. **Open questions.** There are various other equations related to (2.1) for which phase transitions of similar type are expected. First, it would be desirable to add an external potential $V : \mathbb{R}^d \to \mathbb{R}$ and consider the equation on $\mathbb{R}^d$:

$$\partial_t \rho = \beta^{-1}\Delta\rho + \nabla \cdot (\kappa_1 \rho \nabla V + \kappa_2 \rho \nabla W \star \rho) \qquad (x,t) \in \mathbb{R}^d \times (0,\infty). \tag{2.14}$$

One difficulty in this case is that the ground state $\rho_\infty$ itself will in general depend on the bifurcation parameters $\beta, \kappa_1$ and $\kappa_2$. The choice of an suitable orthonormal basis, which was before the Fourier basis on $\mathbb{T}^d$, is not obvious. However, there are generalizations of the results in preparation which consider variants of (2.1) still defined on the torus, where there exists a fixed ground state $\rho_\infty$ independent of the relevant order parameter. This is for instance the case by considering fast or slow diffusion of porous medium type, that is replacing $\Delta\rho$ by $\Delta\rho^m$ for some $m > 0$ in (2.1).

The mountain pass theorem in Section 2.2 gives a general description of the dynamic around a discontinuous phase transition. However, it does not provide much information for specific applications in opinion formation, like for the shape of the critical state constituting the saddle point. In contrast, for the classical Ginzburg–Landau energy, there exists a detailed description of the droplet [GW15; GWW17]. Also, in microscopic models of crystals, the Wulff shape is studied in great detail in [DKS92; BCK02]. Since the interaction potential in consensus formation is not derived from physical means, there is some freedom in its choice, and one could investigate some treatable examples. One choice is the Gaussian interaction, for which preliminary analysis leads to explicit expressions for some of the relevant quantities, like $\Delta$ in (2.4).

The work [CMV03] gives a full characterization of the displacement convexity of the equation (2.14) in terms of convexity of the potentials $V$ and $W$. A translation of this type of result to the discrete McKean–Vlasov system considered in Section 2.3 is an interesting question. Significant difficulties pose the identification of the discrete counterparts of the convexity conditions on $V, W$. The so-called Bochner approach pioneered in the works [CDP09] and translated to the entropic Ricci curvature in [FM16] is likely generalizable to the mean-field setting, which might be able to improve the bounds for mean-field interacting birth-death chains similar to (2.13).

It is also worth mentioning that nonlinear systems could have more than one conserved quantity. At the moment, the setup for the definition of the entropic curvature in Section 2.3 neglects further conserved quantities besides the total mass, which has the consequence that positive curvature cannot be proven in such models. Therefore, a general setup covering models like the one considered in Section 4.3 is desirable. Lastly, any relationship between entropic curvature bounds of the $N$-particle process and the mean-field gradient structure is except for very specific cases mainly open.

## 3. Metastability close to phase transitions in discrete systems

The setting of the project [H7] is given in terms of the generator of a Markov chain on a countable state space $\mathscr{S}$ in the form

$$(Lf)(x) := \sum_{y\in\mathscr{S}} p(x,y)(f(y)-f(x)).$$

The process is assumed to be positively recurrent and reversible with respect to a probability measure $\mu$. The notion of metastability for a Markov chain with generator $L$ is based on a qualitative comparison of hitting probabilities encoding the time-scale separation of metastable dynamics.

**Definition 3.1** (Metastable sets)**.** For fixed $\varrho > 0$ and $K \in \mathbb{N}$ let $\mathscr{M} = \{M_1, \dots, M_K\}$ be a set of subsets of $\mathscr{S}$ such that $M_i \cap M_j = \emptyset$ for all $i \neq j$. A Markov chain $(X(t) : t \geq 0)$ is called $\varrho$-metastable with respect to a *set of metastable sets* $\mathscr{M}$, if

$$|\mathscr{M}| \, \frac{\max_{M\in\mathscr{M}} \mathbb{P}_{\mu_M}\big[\tau_{\bigcup_{i=1}^K M_i\setminus M} < \tau_M\big]}{\min_{A\subset\mathscr{S}\setminus\bigcup_{i=1}^K M_i} \mathbb{P}_{\mu_A}\big[\tau_{\bigcup_{i=1}^K M_i} < \tau_A\big]} \leq \varrho \ll 1,$$

where $\mu_A[x] = \mu[x \mid A]$, $x \in A \neq \emptyset$ denotes the conditional probability on the set $A$ and $|\mathscr{M}|$ denotes the cardinality $K$ of $\mathscr{M}$. Moreover, for $A \subset \mathscr{S}$ denotes $\tau_A$ the first hitting time of the set $A$ for the Markov chain with generator $L$.

The main novelty of Definition 3.1 is the modification of the denominator compared to [BH15, equation (8.1.5)]. The main advantage of this particular form is the fact that sharp estimates on the mean exit time to "deeper" metastable sets are proven without using additional regularity and renewal estimates, which was the state of the art so far.

The crucial role of capacities in the potential theoretic approach to metastability comes from the fact that the hitting probabilities occurring in Definition 3.1 are related to capacities by the identity

$$\mathbb{P}_{\mu_A}[\tau_B < \tau_A] = \frac{\operatorname{cap}(A,B)}{\mu[A]}, \tag{3.1}$$

Hereby, the capacity between two disjoint sets $A, B \subset \mathscr{S}$ is given by

$$\operatorname{cap}(A,B) := \langle -Lh_{A,B}, h_{A,B}\rangle = \mathscr{E}(h_{A,B}),$$

where $\mathscr{E}$ is the Dirichlet form associated with the generator $L$ and the equilibrium potential $h_{A,B}$ is defined for any two disjoint subsets $A, B \subset \mathscr{S}$ as the solution of

$$\begin{cases} Lh_{A,B} = 0, & \text{on } (A\cup B)^c \\ h_{A,B} = \mathbf{1}_A, & \text{on } A\cup B, \end{cases}$$

with $\mathbf{1}_A$ the indicator function on $A$.

This connection shows that the assumption of metastability in Definition 3.1 is essentially a quantified comparison of capacities and measures. Hence, the verifiability of Definition 3.1 relies crucially on the fact that upper and lower bounds on capacities can easily be deduced from their variational characterization. To make use of this comparison the crucial new theoretical ingredient in the discrete case is a capacitary inequality in the spirit of V. Maz'ya [Maz11].

**Theorem** (Capacitary inequality)**.** *For $f : \mathbb{R} \to \mathscr{S}$ define by $A_t \subset \mathscr{S}$ its super-level sets $A_t := \{|f| > t\}$. Moreover, assume that $f|_B \equiv 0$, then it holds*

$$\int_0^\infty 2t \, \operatorname{cap}(A_t, B) \, \mathrm{d}t \;\leq\; 4\mathscr{E}(f).$$

The capacitary inequality gives a new bridge from capacities to spectral gap and log-Sobolev constants for Markov chains. It implies that the quantitative comparison of certain measures and capacities provide upper and lower bounds on the Poincaré and logarithmic Sobolev constant. These measure-capacity inequalities are the generalization of the isoperimetric inequality for structured graphs, like $\mathbb{Z}^d$.

**Proposition** (Poincaré inequality)**.** *Let $\nu \in \mathscr{S}$ and $b \in \mathscr{S}$. Then, there exist $C_{\mathrm{var}}, C_{\mathrm{PI}} > 0$ satisfying*

$$\nu[b]\, C_{\mathrm{var}} \;\leq\; C_{\mathrm{PI}} \;\leq\; 4\, C_{\mathrm{var}}$$

*such that the following statements are equivalent:*

*a) For all $A \subset \mathscr{S} \setminus \{b\}$ it holds the inequality*

$$\nu[A] \;\leq\; C_{\mathrm{var}} \operatorname{cap}(A, b).$$

*b) It holds the mixed Poincaré inequality*

$$\operatorname{var}_\nu[f] \;\leq\; C_{\mathrm{PI}}\, \mathscr{E}(f).$$

A similar statement holds for the logarithmic Sobolev inequality.

**Proposition** (Logarithmic Sobolev inequality)**.** *Let $\nu \in \mathscr{P}(\mathscr{S})$ and $b \in \mathscr{S}$. Then, there exist $C_{\mathrm{Ent}}, C_{\mathrm{LSI}} > 0$ satisfying*

$$\frac{\nu[b]}{\ln(1+e^2)}\, C_{\mathrm{Ent}} \;\leq\; C_{\mathrm{LSI}} \;\leq\; 4\, C_{\mathrm{Ent}}$$

*such that the following statements are equivalent:*

*a) For all $A \subset \mathscr{S} \setminus \{b\}$ it holds the inequality*

$$\nu[A] \ln\left(1 + \frac{e^2}{\nu[A]}\right) \;\leq\; C_{\mathrm{Ent}} \operatorname{cap}(A, b).$$

*b) It holds the logarithmic Sobolev inequality*

$$\operatorname{Ent}_\nu[f^2] \;\leq\; C_{\mathrm{LSI}}\, \mathscr{E}(f).$$

The above results can be seen as a generalization of the Muckenhoupt criterion which is used to characterize the Poincaré and logarithmic Sobolev constant in the one dimensional case [Muc72; BG99; Mic99; BGL14].

This result is well suited to be applied to metastability, because the constants $C_{\mathrm{var}}$ and $C_{\mathrm{Ent}}$ in the inequalities a) can be connected to the metastable parameter $\varrho$ thanks to (3.1). This allows to compare local Poincaré and logarithmic Sobolev constants, providing the relaxation timescale to the metastable states, with the contribution to the full Poincaré and logarithmic Sobolev constant, describing the timescale of the full system. In the case, where the metastable sets $M \in \mathscr{M}$ consist of more than one point, suitable regularity assumptions on $M$ are needed. Therewith, the final result, stated in this section for simplicity in the case $|\mathscr{M}| = 2$, reads

**Theorem** (Poincaré and logarithmic Sobolev constant)**.** *Under additional mixing and regularity assumptions on the $\varrho$-metastable set $\mathscr{M} = \{M_1, M_2\}$ is the Poincaré constant $C_{\mathrm{PI}}$ given by*

$$C_{\mathrm{PI}} = \frac{\mu[\mathscr{S}_1]\mu[\mathscr{S}_2]}{\mathrm{cap}(M_1, M_2)} \left(1 + O\big(\sqrt{\varrho}\big)\right).$$

*Moreover, the logarithmic Sobolev constant $C_{\mathrm{LSI}}$ satisfies*

$$C_{\mathrm{LSI}} = \frac{\mu[\mathscr{S}_1]\mu[\mathscr{S}_2]}{\Lambda\left(\mu[\mathscr{S}_1], \mu[\mathscr{S}_2]\right)\, \mathrm{cap}(M_1, M_2)} \left(1 + O\big(\sqrt{\varrho}\big)\right),$$

*where $\Lambda(a, b) = \frac{a-b}{\log a - \log b}$ is the logarithmic mean for $a, b \geq 0$.*

The approach is applied to the random field Curie Weiss model, where the assumption of $\varrho$-metastability, and the further mixing and regularity assumption on the metastable sets $M$ can be verified. Moreover, this shows that the potentially theoretic approach can also produce the sharp asymptotic of the Poincaré and logarithmic Sobolev constant for this model, which was so far open (cf. [BBI09; BBI12; BH15]).

**Open questions.** There are many more reversible models, like for instance the zero-range process [AGL17; Seo19] or Kawasaki dynamic in large boxes [BHN05; GL15] for which the above technique is partially applicable and may give new results and insights for estimating the Poincaré and logarithmic Sobolev constant.

In addition, the presented capacitary inequality seems to be quite universal and robust making a generalization of the framework to the non-reversible setting achievable. For non-reversible Markov chains the theory is far from being complete, see [Lan14; GL14; LS18; Seo19] for various first results into this direction. In this way, it would be possible to obtain quantitative estimates allowing to investigate the convergence rates to equilibrium for non-reversible dynamics.

## 4. Dynamics in the presence of phase separation for nucleation models

4.1. **Macroscopic limit of the Becker–Döring system.** The Becker–Döring model [BD35] describes the evolution of the number density $c_l$ of clusters consisting of an integer number $l \in \mathbb{N}$ of monomers. Although the attachment and detachment of monomers to and from cluster is not necessarily mitigated by a chemical reaction, it is helpful to think of the system as the following reaction network

$$X_1 + X_l \underset{b_{l+1})}{\overset{a_l}{\rightleftharpoons}} X_{l+1}\,, \qquad \text{for} \quad l \geq 1\,. \tag{4.1}$$

Hereby, $\{a_l\}_{l=1}^{\infty}$ and $\{b_l\}_{l=2}^{\infty}$ denote the kinetic rates of attachment and detachment of a monomer to or from an $l$-cluster. It is reasonable to model the dynamics for (4.1) by mass-action and one arrives at a countable number of ordinary differential equations describing the evolution of the cluster number densities

$$\frac{\mathrm{d}c_l}{\mathrm{d}t} = J_{l-1}(t) - J_l(t), \quad \text{with} \quad J_l = a_l c_1(t) c_l(t) - b_{l+1} c_{l+1}(t) \quad \text{for } l = 1, 2, \ldots \tag{4.2}$$

The system becomes closed by fixing the flux $J_0$ in such a way that the total number of monomers

$$\varrho = \sum_{i=1}^{\infty} l c_l(t) \tag{4.3}$$

is conserved which leads to $J_0(t) = -\sum_{l=1}^{\infty} J_l(t)$ and closes the system (4.2). In this case, the evolution of the clusters is coupled through the monomer concentration $c_1(t)$. The system has a one-parameter family of equilibrium states $\{\omega_l(z)\}_{l=1}^{\infty}$ satisfying the detailed balance condition $a_l \omega_1(z) \omega_l(z) = b_{l+1} \omega_{l+1}(z)$

$$\omega_l(z) = z^l Q_l \qquad \text{with} \qquad Q_l = \frac{a_1 \cdots a_{l-1}}{b_2 \cdots b_l}. \tag{4.4}$$

The relative entropy with respect to this states is a Lyapunov function for the dynamic and is given by $\mathscr{F}_z(c) = \mathscr{H}(c \mid \omega(z))$ with

$$\mathscr{H}(c \mid \omega) := \sum_{l=1}^{\infty} \omega_l \psi\left(\frac{c_l}{\omega_l}\right) \quad \text{where} \quad \psi(a) := a \log a - a + 1, \text{ for } a > 0.$$

For physical relevant rates, the convergence radius $z_s$ of the series $z \mapsto \sum_l l z^l Q_l$ is finite and $\varrho_c = \sum_l l z_s^l Q_r$ is finite, too. The following rates with these properties are used from now on: $a_l = l^{\alpha}$ and $b_l = l^{\alpha}(z_s + q l^{-\gamma})$, where $\alpha \in [0, 1)$, $\gamma \in (0, 1)$ and $z_s, q > 0$. For these rates, the stationary states satisfy for $l \ll 1$

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

The chemical potential inside of the exponent consists of two parts: The first is the bulk energy scaling with $l$ which corresponds to volume in physical units. The second term is a change of the surface energy (usually $\gamma = 1/2$ or $1/3$) due to the Gibbs–Thomson effect [BCK02; Bis+04].

In [BCP86] the effect is shown that if the initial mass $\varrho(0) = \sum_{l=1}^{\infty} l c_l(0)$ is larger than $\varrho_c$, the system is no longer mass conservative for $t \to \infty$, and the solution converges only coordinate-wise to the equilibrium distribution $\omega(z_s)$. These two cases can already be observed from a static investigation of the minimizers of $\mathscr{F}_z$

which are candidates for equilibria since $\mathscr{F}$ is a Lyapunov function:

$$\inf_{c,z>0}\left\{\mathscr{F}_z(c):\sum_{l=1}^{\infty} l c_l=\varrho_0\right\}=\begin{cases}\mathscr{F}_z(\omega(z)), & \varrho_0\le\varrho_c;\\ \mathscr{F}_{z_s}(\omega(z_s)), & \varrho_0>\varrho_c.\end{cases}$$

Hence, the overcritical mass density $\varrho_0-\varrho_c$ vanishes during the minimization. This process is interpreted as the formation of macroscopic droplets and raises the question about a possible equation for the excess mass density.

By formal asymptotic it is shown in [Pen97] that the dynamic of the excess mass $\varrho_0-\varrho_c$ relates to the Lifshitz–Slyozov–Wagner (LSW) theory of coarsening [LS61; Wag61]. The work [Nie03] makes this connection rigorous and shows that suitable rescaled solutions of the Becker–Döring system with initial relative entropy of order $\varepsilon$ converge as $\varepsilon\to 0$ to the LSW-equations

$$\partial\, \nu_t+\partial_\lambda\Big(\lambda^\alpha\Big(u-\frac{q}{\lambda^\gamma}\Big)\nu_t\Big)=0\qquad\text{with}\qquad u(t)=\frac{q\int\lambda^{\alpha-\gamma}\,\nu\,\mathrm{d}\lambda}{\int\lambda^\alpha\,\nu\,\mathrm{d}\lambda}. \tag{4.5}$$

In [Nie04], it was heuristically observed that the LSW-equations can be understood as the gradient-flow of the surface energy $E(\nu)=\int\lambda^{1-\gamma}\nu\ \mathrm{d}\lambda$ with respect to a weighted Wasserstein distance. The distance is induced by the action functional following the construction of [BB00]: For a pair $(\nu,w)$ solving the continuity equation $\partial_t\nu_t+\partial_\lambda(\lambda^\alpha w_t\nu_t)=0$ in distributions the action is defined by

$$A(\nu_t,w_t):=\int\lambda^\alpha|w_t|^2\,\mathrm{d}\nu_t.$$

The gradient structure of the Becker–Döring system was not known so far, but thanks to the interpretation (4.1) as an infinite set of ordinary differential equations with equilibria (4.4) satisfying a detailed balance condition, it is possible to apply the framework developed in [Mie11; 10]. The Becker–Döring model fits into the structure as discussed in Section 2.3 by treating $c_1$ as a mean-field variable thanks to the conservation law $c_1=\varrho-\sum_{l\ge2}lc_l$.

This raises the question whether the result of [Nie03] also holds true in the context of a passage from gradient-flows to gradient-flows. The work [H5] gives a positive answer to this question implying that not only solutions do converge, but also their gradient flow structure. The idea to show convergence is first based the variational characterization of gradient flows as curves of maximal slope introduced in [DMT80] (see also [AGS08]). In addition, suitable notions of convergence of the resulting variational principle are used as pioneered in [SS04] with many generalizations discussed in [Ser11; Arn+12; Mie16].

Solutions to the Becker–Döring equation (4.2) denoted by $[0,T]\ni t\mapsto c(t)$ are described variationally with the help of a functional in the form

$$\mathscr{J}(c)=\mathscr{F}(c(T))-\mathscr{F}(c(0))+\frac12\int_0^T|D\mathscr{F}(c(t))|^2_{\mathscr{K}(c(t))}\,\mathrm{d}t+\frac12\int_0^T|c'(t)|^2_{\mathscr{K}(c(t))^{-1}}\,\mathrm{d}t,$$

where the inner product is defined in terms of some suitable positive-definite linear operator $\mathscr{K}$ similar to the one defined in (2.11) in Section 2.3. The functional $\mathscr{J}$ is non-negative for a general mass-conserving curve. Moreover, $\mathscr{J}(c)=0$ if and only if $c$ is a solution of the Becker–Döring system on $[0,T]$. A similar functional $J(\nu)$,

non-negative and vanishing only on solution to (4.5), can be defined for the gradient flow structure of the LSW-equation. Therewith, the convergence of gradient structures is a $\Gamma$-lim inf statement on suitable rescaled versions of the functional $\mathscr{J}$ converging toward $J$.

In the mathematical analysis, the notion of local equilibrium is crucial and as a side product further estimates on the dynamics of the small clusters are obtained. It is shown that the distribution of the small clusters follow a quasi-stationary distribution dictated by the monomer-concentration. This result was so far only established by formal asymptotic.

4.2. **A Fokker–Planck equation related to the Becker–Döring model.** The starting point of this project is the observation due to [Vel98] that the Becker–Döring system (4.2) considered in Section 4.1 can be rewritten as a discrete Fokker–Planck equation. To do so, the notation $c(\ell,t)=c_\ell(t)$ is used for the density of $\ell$-clusters. It is convenient to introduce the excess monomer concentration $\theta(t)$ as

$$c(1,t) \;=\; z_s+\theta(t),$$

which in this formulation acts as the boundary condition. By doing so, the system (4.2) takes the form of a discretized parabolic diffusion advection equation

$$\frac{\partial c(\ell,t)}{\partial t} \;=\; -D^*D[b_\ell c(\ell,t)]+D^*[\{(a_\ell z_s-b_\ell)+\theta(t)a_\ell\}c(\ell,t)]\,,\quad \ell\geq 2\,, \tag{4.6}$$

where $D$ and $D^*$ are the forward and backward difference operators, respectively. The global conservation law (4.3) is still assumed to hold along the solution and gives an equation for $\theta$.

In view of (4.6), it is natural to consider a family of discrete models with scale parameter $\varepsilon>0$, for which $\varepsilon=1$ corresponds to the Becker–Döring model and the limit $\varepsilon\to 0$ will become a non-linear non-local Fokker–Planck equation on the half line $[0,\infty)$

$$\frac{\partial c(x,t)}{\partial t}+\frac{\partial}{\partial x}\left[b(x,t)c(x,t)\right]=\frac{\partial^2}{\partial x^2}\left[a(x)c(x,t)\right]\,,\quad 0<x<\infty,\ t>0 \tag{4.7}$$

$$b(x,t)=a(x)\{\theta(t)W'(x)-V'(x)\}\,, \tag{4.8}$$

where $a(\cdot)$ is continuous and strictly positive and $V(\cdot),W(\cdot)$ are $C^1$ functions. In particular, if the function $\theta(\cdot)$ in (4.8) is constant $\theta(\cdot)\equiv\theta$, then $c(x,t)=c^{\mathrm{eq}}_\theta(x)$, where

$$c^{\mathrm{eq}}_\theta(x) \;=\; a(x)^{-1}\exp\big(-V(x)+\theta W(x)\big)\,,2$$

is a steady state solution of (4.7), (4.8). Now, the Dirichlet boundary condition is chosen to be compatible with the equilibria for fixed $\theta$ and therefore given by

$$c(0,t) \;=\; c^{\mathrm{eq}}_{\theta(t)}(0) \;=\; a(0)^{-1}\exp[-V(0)+\theta(t)W(0)]\,,\quad t>0\,. \tag{4.9}$$

The system (4.7), (4.8), and (4.9) is complemented by an equation for $\theta(\cdot)$ determined by the conservation law in analogy to (4.3) from the Becker–Döring theory

$$\theta(t)+\int_0^\infty dx\; W(x)c(x,t) \;=\; \varrho\,,\quad \text{with } \varrho>0 \text{ is constant.} \tag{4.10}$$

A concrete admissible choice for $a, V, W$ reflecting the physical rates for the Becker–Döring model introduced in Section 4.1 are in terms of power laws

$$W(x) = 1 + x \qquad a(x) = (1+x)^{\alpha} \qquad \text{and} \qquad V(x) = (1+x)^{1-\gamma}. \tag{4.11}$$

In analogy to the results on the Becker–Döring model, the primary interest is the large time behavior of solutions to (4.7) and the occurrence of a phase separation.

To specify the long-time limit, let $W$ be positive such that $W(\cdot)a(\cdot)^{-1}\exp[-V(\cdot)]$ is integrable on $(0,\infty)$, then $W(\cdot)c_\theta^{\mathrm{eq}}(\cdot)$ is integrable for $\theta \le 0$. Furthermore, the function $\theta \mapsto \theta + \|W(\cdot)c_\theta^{\mathrm{eq}}(\cdot)\|_1$ is strictly increasing and maps $(-\infty, 0]$ to $(-\infty, \varrho_c]$ where

$$\varrho_c = \|W(\cdot)c_0^{\mathrm{eq}}(\cdot)\|_1 = \int_0^\infty W(x)a(x)^{-1}\exp\bigl(-V(x)\bigr)\,\mathrm{d}x\ .$$

The inverse function with domain $(-\infty, \varrho_c]$ is denoted with $\theta_{\mathrm{eq}}(\cdot)$. Evidently, it holds $\theta_{\mathrm{eq}}(\varrho_c) = 0$, and so $\theta_{\mathrm{eq}}(\cdot)$ extends in a continuous way to the domain $\mathbb{R}$ by setting $\theta_{\mathrm{eq}}(\varrho) = 0$ for $\varrho > \varrho_c$. The first main result of [H2] is that $c^{\mathrm{eq}}_{(\varrho)} = c^{\mathrm{eq}}_{\theta^{\mathrm{eq}}(\varrho)}$ with $\varrho$ given as right hand side of (4.10) is the long-time limit of the evolution equation (4.7), (4.8), (4.10), (4.9), which can be seen as the analog of the one of [BCP86] for the Becker–Döring model.

**Theorem.** *Let $c(x,0),\ x > 0$, be a non-negative measurable function such that*

$$\int_0^\infty W(x)c(x,0)\,\mathrm{d}x\ <\ \infty\ . \tag{4.12}$$

*Then there exists a unique solution $c(\cdot,t),\ t > 0$, to the Cauchy problem* (4.7)*,* (4.8)*,* (4.10)*,* (4.9) *with initial condition $c(\cdot,0)$.*

*For all $t > 0$ the function $c(\cdot,t) \in C^1([0,\infty))$ and $\theta \in C^1([0,\infty))$.*

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

$$\lim_{t\to\infty}\int_0^\infty W(x)|c(x,t) - c_\theta^{\mathrm{eq}}(x)|\,\mathrm{d}x\ =\ 0\ . \tag{4.13}$$

In addition to the well-posedness result, a quantified rate of convergence to equilibrium is derived in the subcritical case $\varrho < \varrho_c$. The proof relies on the entropy method and the convergence statement is shown with respect to a free energy decreasing along the solution and adapts ideas for the proof of convergence established for the Becker–Döring model [JN03; CEL15], but also for gradient-flows with constraints from [9]. For the formal calculations with the free energy it is convenient to rewrite the set of equations (4.7), (4.8), (4.9) in the form

$$\partial_t c(x,t) = \partial_x\bigl(a(x)c(x,t)\,\partial_x \log\frac{c(x,t)}{c^{\mathrm{eq}}_{\theta(t)}(x)}\bigr) \quad \text{with b.c.} \quad \log\frac{c(0,t)}{c^{\mathrm{eq}}_{\theta(t)}(0)} = 0$$

together with the equation (4.10) for $\theta(t)$. In this form, the following energy dissipation estimate is formally deduced and rigorously established after proving enough regularity properties of the solution

$$\frac{\mathrm{d}^+}{\mathrm{d}t}\mathscr{G}\bigl(c(\cdot,t),\theta(t)\bigr) \le -\mathscr{D}\bigl(c(t),\theta(t)\bigr)$$

where $\frac{\mathrm{d}^+}{\mathrm{d}t} f(t) = \limsup_{\delta\to 0^+} \frac{f(t+\delta)-f(t)}{\delta}$ and

$$\mathscr{G}(c(\cdot,t),\theta(t)) = \int (\log c - 1)c(x)\,\mathrm{d}x + \int (V+\log a)c(x)\,\mathrm{d}x + \frac{1}{2}\theta(t)^2 \quad (4.14)$$

$$\text{with} \quad \theta(t) = \varrho - \int W(x)c(x,t)\,\mathrm{d}x$$

$$\mathscr{D}(c(\cdot),\theta) = \int a(x)\left(\partial_x \log \frac{c}{c_\theta^{\mathrm{eq}}}\right)^2 c(x)\,\mathrm{d}x.$$

The term $\frac{1}{2}\theta^2$ in (4.14) is characteristic for free energies of McKean–Vlasov equations like the one considered in Section 2:

$$\mathscr{F}_{MV}(c) = \int c\log c + \int c\tilde{V} + \frac{1}{2}\iint K(x,y)c(x)c(y)\,\mathrm{d}x\,\mathrm{d}y,$$

with some kernel function $K$. For the product kernel $K(x,y) = W(x)W(y)$, the last term becomes $\left(\int Wc\right)^2$. By choosing $\tilde{V} = V - 1 + \log a - \varrho W$, the free energy $\mathscr{F}_{MV}$ agrees with $\mathscr{G}$ from (4.14) up to a constant. The connection becomes more apparent by noting that (4.7), (4.8), (4.10), (4.9) is the formal gradient flow with respect to a Wasserstein metric including a boundary condition. Hence, the presented Fokker–Planck equation has a close connection to the class of McKean–Vlasov equations with a product kernel, however with a non-local boundary condition. Let us point out that gradient flows with boundary condition are quite delicate and are first studied in [FG10] for the heat equation with Dirichlet boundary conditions.

The function $\mathscr{G}$ is proven to be convex with a unique minimizer satisfying the constraint (4.10) given by

$$\inf_c \left\{ \mathscr{G}(c,\theta) : \theta + \int W(x)c(x)\,\mathrm{d}x = \varrho \right\} = \mathscr{G}(c^{\mathrm{eq}}_{\theta_{\mathrm{eq}}}, \theta_{\mathrm{eq}})$$

where $\theta_{\mathrm{eq}} = \theta_{\mathrm{eq}}(\varrho)$ is uniquely determined by $\varrho$ through the identity $\varrho = \theta_{\mathrm{eq}} + \int W c^{\mathrm{eq}}_{\theta_{\mathrm{eq}}}$. This allows to define the normalized free energy functional

$$\mathscr{F}_\varrho(c) = \mathscr{G}(c,\theta) - \mathscr{G}(c^{\mathrm{eq}}_{\theta_{\mathrm{eq}}}, \theta_{\mathrm{eq}}) \qquad \text{with} \qquad \theta = \varrho - \int W(x)c(x)\,\mathrm{d}x.$$

Therewith, we can state the second main result on the rate of convergence to equilibrium.

**Theorem.** *Let $\varrho < \varrho_c$. In addition, assume for some $\beta \in (0,1]$ and constants $0 < c_0 < C_0 < \infty$ holds*

$$c_0 W^{1-\beta}(x) \le a(x)W'(x)^2 \qquad \text{for } x \in \mathbb{R}^+. \quad (4.15)$$

*Let $c$ be a solution to* (4.7), (4.8), (4.10), (4.9) *with initial condition $c(\cdot,0)$ satisfying* (4.12) *and for some $C_0$ and $k > 0$ the moment condition*

$$\int W(x)^{1+k\beta}\, c(x,0)\,\mathrm{d}x \le C_0, \quad (4.16)$$

*Then there exists $\lambda$ and $C$ depending on $a, V, W, \theta_{\mathrm{eq}}, C_0, k$ such that for all $t \ge 0$*

$$\mathscr{F}_\varrho(c(t)) \le \frac{1}{(C+\lambda t)^k}\,. \quad (4.17)$$

*Moreover, if* (4.15) *holds with* $\beta = 0$*, that is* $c_0 W(x) \le a(x)W'(x)^2 \le C_0 W(x)$ *for* $x \in \mathbb{R}^+$*, then there exists* $C > 0$ *and* $\lambda > 0$ *such that*

$$\mathscr{F}_\varrho(c(t)) \le Ce^{-\lambda t}. \tag{4.18}$$

By a suitable weighted Pinsker inequality similar to [BV05], the quantified convergence statements (4.17) and (4.18) imply the quantified version of the statement (4.13) as well as a quantified convergence statement for $\theta(t)$: There exists for any $T > 0$ an explicit constant $C > 0$ such that

$$\left(\int W(x)|c(x,t) - c^{\mathrm{eq}}_{\theta^{\mathrm{eq}}}(x)|\,\mathrm{d}x\right)^2 + \left(\theta(t) - \theta^{\mathrm{eq}}\right)^2 \le C\,\mathscr{F}_\varrho(c(\cdot,t)) \qquad \text{for all } t \ge T.$$

In particular, the rates given in (4.11) satisfy the refined assumption (4.15) with $\beta = 1 - \alpha \in [0,1]$.

To explain the additional assumption (4.16), let $\omega(x) = W(x)/\big(a(x)W'(x)^2\big)$ and observe that using (4.15), it holds $\omega(x) \le c_0^{-1} W(x)^\beta$ and the moment condition (4.16) gives a bound on

$$\int \omega(x)^k\, W(x)\, c(x,0)\,\mathrm{d}x \le C_0.$$

The weight function $\omega(x)$ is essential for the derivation of suitable functional inequalities, in this case weighted logarithmic Sobolev inequalities, which use the connection between entropy and suitable Orlicz-norms from [BG99]. Together with an interpolation argument, this is the essential ingredient to obtain a suitable differential inequality for the time-derivative of $\mathscr{F}_\varrho$ leading to the algebraic decay in (4.17).

4.3. **Exchange-driven growth.** Exchange-driven growth is a process in which pairs of clusters consisting of an integer number of monomers can grow or shrink only by the exchange of single monomers [BK03]. To make the connection to the Becker–Döring model form Section 4.1 apparent, it is helpful to interpret the exchange-driven growth as a reaction network of the form

$$X_{k-1} + X_l \underset{K(k,l-1)}{\overset{K(l,k-1)}{\rightleftharpoons}} X_k + X_{l-1}\,, \qquad \text{for} \quad k,l \ge 1\,. \tag{4.19}$$

There are two main-differences to the Becker–Döring system (4.1): Firstly, monomers are able to jump directly from a $k$-cluster to an $l$-cluster with rate $K(k,l)$. Secondly, the system possesses the new variable $X_0$ accounting for empty volume. The situation, where only the rates with $l = 1$ in (4.19) are nonzero resembles closest the Becker–Döring system and (4.19) becomes $X_{k-1} + X_1 \rightleftharpoons X_k + X_0$, which can be best called a Becker–Döring system in finite volume, since a detachment of a monomer from a $k$ cluster also depends on the available empty volume $X_0$ in the system.

The governing system of ordinary differential equations for the concentrations $c_k$ of $X_k$ for $k \ge 0$ can be directly read off the reaction network (4.19) assuming mass-action kinetics. The resulting system has the form of a master equation for a nonlinear continuous-time birth-death chain on $\mathbb{N}_0$

$$\dot{c}_k = A_{k-1}[c]c_{k-1} - (A_k[c] + B_k[c])c_k + B_{k+1}[c]c_{k+1}\,, \tag{4.20}$$

with state dependent birth and death rates given by

$$A_{k-1}[c] = \sum_{l\geq 1} K(l,k-1)\, c_l \qquad \text{and} \qquad B_k[c] = \sum_{l\geq 0} K(k,l)\, c_l \qquad \text{for } k \geq 1 \,.$$

The chemical reaction representation (4.19) gives rise to two conservation laws. Firstly, on each side of the reaction, there are two clusters or a cluster and empty volume, which leads to the conservation of the total number of clusters and empty volume. Due to each reaction performing an exchange of a single monomer, no mass is generated nor destroy, which gives the conservation of the total number of monomers. On the level of the densities $(c_k)_{k\geq 0}$, these two conservation laws take the form of

$$M_0 = \sum_{k\geq 0} c_k \qquad \text{and} \qquad \varrho = \sum_{k\geq 1} k\, c_k \,. \tag{4.21}$$

By a linear time-change $M_0$ can be fixed as one, which allows to interpret $(c_k)_{k\geq 0}$ as probability density on $\mathbb{N}_0$. Nevertheless, the system has two conservation laws, which makes the occurrence of phase separation possible [GSS03].

The system (4.20) is also the mean-field limit of a microscopic stochastic interacting particle system. The system consists of $N$ particles are distributed on a lattice $\Lambda$ with $|\Lambda| = L$ sites. Let $(\eta_x)_{x\in\Lambda}$ be the occupation number of each site and define the generator of the system by

$$\mathscr{L} f(\eta) = \frac{1}{L-1} \sum_{x,y\in\Lambda} K(\eta_x, \eta_y)(f(\eta^{x,y}) - f(\eta)) \,, \tag{4.22}$$

where $\eta^{x,y}$ is the configuration obtained from $\eta$ after one particles jumps from $x$ to $y$. Because the rate kernel $K$ does not only depend on the site of departure but also on the one of arrival, the jump dynamic (4.22) is a generalization of the well-studied zero range process [Spi70]. In particular, exclusion rules can be also taken into account by this general model, which was considered under the name os misanthrope processes [Coc85].

The mean-field limit is obtained by letting $N, L \to \infty$ such that $\frac{N}{L} \to \varrho \in (0,\infty)$. Then, it is shown in [GJ19] that for a at most linear growing jump kernel

$$0 \leq K(k,l-1) \leq C_K\, k\, l \qquad \text{for } k,l \geq 1 \,. \tag{$\mathrm{K}_1$}$$

and suitable tightness on the initial datum $\eta(0)$ the empirical cluster distribution $C_k^L(\eta) = \frac{1}{L}\sum_{x\in\Lambda} \delta_{\eta_x,k}$ converges to the solution of (4.20). This makes the study of qualitative properties of the system (4.20) also appealing for applications to those particle systems.

The main results of [H6] are the well-posedness of the system (4.20) for at most linear growing kernels ($\mathrm{K}_1$) and the study of the long-time behavior proving that this system possesses the same kind of phase separation phenomenon as the Becker–Döring model from Section 4.1 and the Fokker–Planck model in Section 4.2.

In view of the two conservation laws (4.21), it is natural to study the system in the space

$$\mathscr{P}^{\varrho} = \left\{ c \in \ell^1(\mathbb{N}_0) \,:\, c_l \geq 0 \,,\, \sum_{l\geq 0} c_l = 1 \,,\, \sum_{l\geq 1} l\, c_l = \varrho \right\}$$

equipped with the weighted $\ell^1$-norm $\|c\| = \sum_{l\geq 0}(1+l)|c_l|$. The existence for the exchange-driven growth (4.20) can be shown solely under Assumption ($K_1$). However, the uniqueness demands some continuity of the rate kernel for large clusters and reads

$$|K(l,k)-K(l,k-1)| \leq C_K\, l \quad \text{and} \quad |K(l+1,k-1)-K(l,k-1)| \leq C_K\, k\,. \tag{$K_2$}$$

Under the two assumptions ($K_1$) and ($K_2$) the solutions to (4.20) constitute a semigroup on $\mathscr{P}^\varrho$ for any $\varrho > 0$.

The investigation of the longtime behavior of the system is based on a free energy, which only exists if the rate kernel satisfies a suitable detailed balance condition: The rate kernel $K : \mathbb{N}\times\mathbb{N}_0 \to [0,\infty)$ satisfies the *Becker-Döring assumption*, that is for all $k,l \geq 1$ it holds $K(k,l-1) > 0$ and

$$\frac{K(k,l-1)}{K(l,k-1)} = \frac{K(k,0)K(1,l-1)}{K(l,0)K(1,k-1)}\,. \tag{BDA}$$

The Assumption (BDA) is called the *Becker-Döring assumption* because, instead of a direct exchange of a single monomer from an $l$-cluster to a $(k-1)$-cluster, the jump is achieved through a jump to empty volume. This is visualized by the following network, where two intermediate reactions involving the monomers $X_1$ and empty volume $X_0$ with the other occurring rates in (BDA) are added

$$\begin{array}{ccc} X_{k-1}+X_l+X_0 & \underset{K(k,l-1)}{\overset{K(l,k-1)}{\rightleftharpoons}} & X_k+X_{l-1}+X_0 \\ {\scriptstyle K(l,0)}\searrow\;\nwarrow{\scriptstyle K(1,l-1)} & & {\scriptstyle K(1,k-1)}\nearrow\;\swarrow{\scriptstyle K(k,0)} \\ & X_{k-1}+X_{l-1}+X_1 & \end{array} \tag{4.23}$$

From the chemical network representation (4.23), the Assumption (BDA) rewritten in the form

$$K(k,l-1)K(1,k-1)K(l,0) = K(l,k-1)K(1,l-1)K(k,0)$$

can be viewed as a curl-free property of the rate kernel on the reaction graph.

For this reason it is not surprising that under Assumption (BDA), there exists a chemical potential $(Q_k)_{k\geq 0}$ defined by

$$Q_0 = 1 \qquad \text{and} \qquad Q_l = \prod_{k=1}^{l} \frac{K(1,k-1)}{K(k,0)}\,.$$

If the kernel $K$ satisfies

$$\lim_{k\to\infty} \frac{K(k,0)}{K(1,k-1)} = \phi_c \in (0,\infty]\,. \tag{$K_c$}$$

then it holds that

$$\lim_{k\to\infty} Q_k^{1/k} = \phi_c^{-1} \qquad \text{with the convention } \phi_c^{-1} = 0 \text{ when } \phi_c = \infty\,.$$

Thanks to (BDA), the chemical potential $(Q_k)_{k\geq 0}$ satisfies the detailed balance condition

$$K(k,l-1)Q_kQ_{l-1} = K(l,k-1)Q_lQ_{k-1} \qquad \text{for } k,l \geq 1 \tag{DBC}$$

and it is easily verified that (DBC) is actually equivalent to Assumption (BDA). The two conversation laws (4.21) are also encoded in (DBC), since $(Z^{-1}\phi^k Q_k)_{k\geq 0}$ satisfies (DBC) for any $Z, \phi > 0$.

This observation is used to search for suitable equilibrium states in $\mathscr{P}^\varrho$ with $\varrho > 0$. The Assumption ($\mathrm{K}_c$) allows to define the partition sum $Z(\phi) \in [0,\infty)$ for $\phi \in [0,\phi_c)$ by

$$Z(\phi) = \sum_{l\geq 0} \phi^l Q_l \in [0,\infty) \,.$$

For $\phi \in [0,\phi_c)$, the normalized equilibrium states $\omega(\phi)$ are given by

$$\omega_l(\phi) = Z(\phi)^{-1}\,\phi^l\, Q_l \qquad \text{for } l \geq 0 \,.$$

The critical equilibrium density $\varrho_c \in (0,\infty]$ is defined by

$$\varrho_c = \limsup_{\phi\uparrow\phi_c} Z(\phi)^{-1} \sum_{l\geq 1} l\phi^l Q_l \,.$$

For $\varrho < \infty$ with $0 \leq \varrho \leq \varrho_c$, there exists a unique $\phi = \phi(\varrho) \in [0,\phi_c]$ such that

$$\sum_{l\geq 1} l\,\omega_l(\phi) = Z(\phi)^{-1} \sum_{l\geq 1} l\phi^l Q_l = \varrho \,.$$

Hence, the set of all normalized equilibria is given by

$$\left\{\omega^\varrho = \omega(\phi(\varrho)) \,:\, \varrho < \infty, 0 \leq \varrho \leq \varrho_c\right\} \,.$$

The main tool of the proof of convergence to equilibrium is the free energy functional of the form

$$\mathscr{F}[c] = \sum_{k\geq 0} c_k \log\frac{c_k}{Q_k} \,,$$

which turns out to be a Lyapunov function for the evolution (4.20) and the main tool in proving the following theorem.

**Theorem** (Convergence to equilibrium)**.** *Suppose that $K$ satisfies* (BDA) *and* ($\mathrm{K}_c$) *with $\phi_c \in (0,\infty)$. Moreover, $K$ is assumed to have sublinear growth and certain continuity at infinity. Then for any $\varrho_0 \in [0,\infty)$ and any $\bar{c} \in \mathscr{P}^{\varrho_0}$ the unique solution $c$ of* (4.20) *with $c(0) = \bar{c}$ satisfies:*

*(i) If $\varrho \leq \varrho_c$, it holds $c(t) \to \omega^\varrho$ strongly in $\mathscr{X}$ as $t \to \infty$ and*

$$\lim_{t\to\infty} \mathscr{F}[c(t)] = \mathscr{F}[\omega^\varrho] \,.$$

*(ii) If $\varrho > \varrho_c$, it holds $c_k(t) \to \omega_k^{\varrho_c}$ for all $k \geq 0$ as $t \to \infty$ and*

$$\lim_{t\to\infty} \mathscr{F}[c(t)] = \mathscr{F}[\omega^{\varrho_c}] + (\varrho - \varrho_c)\log\phi_c \,.$$

The convergence statement in *(2)* implies in particular that the excess mass $\varrho - \varrho_c$ vanishes for long time, which is interpreted as a condensation phenomenon due to the formation of larger and larger clusters similar to LSW regime for the Becker–Döring model described in Section 4.1.

4.4. **Open questions.** The results in Section 4.1 describe the coarsening regime for the Becker–Döring equation, which starts when the free energy functional is $\varepsilon$-close to its global minimum. However, the system first needs to get very close to the global minimum of the free energy, and it is show in [Pen89] that this could take a very long time for specific initial values, which get trapped in metastable states. It is widely believed and observed in numerical simulations [CDW95] that this is the generic behavior of the system. Although the gradient flow interpretation of the Becker–Döring system does not provide any immediate insight into this issue, it strengthens the point that the observed metastability is an out of equilibrium behavior and cannot be understood by studying the free energy landscape solely without taking the dissipation mechanism into account. In this regard, a study of the metric or generalization thereof induced by the dissipation mechanism is ongoing work.

After having established the phase separation phenomenon in the Fokker–Planck model (Section 4.2) and the exchange-driven growth dynamic (Section 4.3), the next step is to deduce the macroscopic limit for the excess mass in the supercritical case. A result in this direction will most likely connect the evolutions with the Lifshitz–Slyozov–Wagner theory of coarsening [LS61; Wag61] and continue the studies along the lines of [Pen97; LM02; Nie03; H5].

In addition, the dynamic of the exchange-driven growth is even richer as the Becker–Döring dynamic, since it allows for non detailed balance dynamic if the rates not satisfy (BDA). The work [BK03] gives very strong indications of self-similar behavior for the product kernel $K(k,l) = (kl)^\lambda$ with $\lambda \in [0,2)$. Since $K(k,0) = 0$ for all $k \geq 1$ for this kernel, it is not admissible for the result on the longtime behavior in Section 4.3. However, it can be interpreted as the special case $\varrho_c = 0$, where no bulk mass remains, and all mass is moving in a self-similar way towards larger and larger clusters. Preliminary promising results are able to make this observation rigorous.

## Further research articles


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