Coarse-graining for gradient systems and Markov processes

DISSERTATION

zur Erlangung des akademischen Grades

doctor rerum naturalium
(Dr. rer. nat.)

im Fach Mathematik

eingereicht an der
Mathematisch-Naturwissenschaftlichen Fakultät
der
Humboldt-Universität zu Berlin

von

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eingereicht am: 11. Januar 2021
Tag der mündlichen Prüfung: 11. Mai 2021

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Abstract

This thesis deals with coarse-graining for gradient systems and Markov processes. Coarse-graining is a well-established tool in mathematical and natural sciences for reducing the complexity of a physical system and for deriving effective models. The mathematical problems in this work originate from interacting particle systems. The aim is twofold: first, providing mathematically rigorous results for physical coarse-graining, and secondly, formulating mathematically equivalent descriptions for the effective models in order to obtain complement information that provides new mathematical and modeling insights.

The first three parts of the thesis deal with fast-reaction limits for reaction systems and reaction-diffusion systems. Instead of deriving effective models by solely investigating the associated reaction-rate equation, we derive effective models using the underlying gradient structure of the evolution equation. The starting point is that reaction systems and reaction-diffusion systems that satisfy detailed balance can be understood as a gradient flow equation. For gradient systems a structural convergence, the so-called *EDP-convergence*, has been derived in recent years. In this thesis, this coarse-graining procedure has been applied to the following systems with slow and fast reactions: linear reaction systems (or Markov process on finite state space), nonlinear reaction systems of mass-action type, and linear reaction-diffusion systems. For the fast-reaction limit, we perform rigorous and structural coarse-graining on the level of the gradient system by proving EDP-convergence. In all cases, the effective dual dissipation potential of the limit gradient system incorporates the slow reactions and a restriction of the chemical potentials to a linear submanifold. Moreover, it induces a slow reaction system or reaction-diffusion system on a slow manifold with Lagrange multipliers. Equivalently, the effective gradient systems can be described in coarse-grained slow variables, which provides a coarse-grained gradient system as well as a coarse-grained gradient flow equation. In the case of nonlinear reactions, the main assumption is the so-called *Unique Fast Equilibrium Condition*, which provides a parametrization of the slow manifold in terms of slow variables. The reaction-diffusion system is interpreted as a gradient flow of the free energy in the space of probability measures. The dissipation potential extends the well-established Otto gradient structure for diffusion, also incorporating the linear reactions.

In the fourth part, the connection between memory equations and Markov processes is investigated. Considering linear memory equations, which can be motivated from spatial homogenization, we explicitly construct a larger Markov process that includes the memory equation as a subsystem. The Markov process is defined by introducing hidden states or quasi particles, which capture the loss of mass in the evolution. In particular, analytical tools from the theory of Markov processes can now be used to investigate these types of memory equations.

The last part deals with numerical discretizations for the Fokker–Planck operator. These finite volume discretizations can also be understood as a physical coarse-graining procedure since they reduce an infinite dimensional problem to a finite dimensional approximation preserving the physics of the model. Different finite volume schemes, including the well-established Scharfetter-Gummel as well as the recently developed SQRA discretization, are numerically and analytically investigated.

Zusammenfassung

Diese Arbeit beschäftigt sich mit Coarse-Graining (dt. *Vergröberung*, *Zusammenfassung von Zuständen*) für Gradientensysteme und Markov-Prozesse. Coarse-Graining ist ein etabliertes Verfahren in der Mathematik und in den Naturwissenschaften und hat das Ziel, die Komplexität eines physikalischen Systems zu reduzieren und effektive Modelle herzuleiten. Die mathematischen Probleme in dieser Arbeit stammen aus der Theorie der Systeme interagierender Teilchen. Hierbei werden zwei Ziele verfolgt: Erstens, Coarse-Graining mathematisch rigoros zu beweisen, zweitens, mathematisch äquivalente Beschreibungen für die effektiven Modelle zu formulieren, welche ergänzende Informationen enthalten und somit neue Erkenntnisse zur Mathematik und Modellierung beisteuern.

Die ersten drei Teile der Arbeit befassen sich mit dem Grenzwert schneller Reaktionen für Reaktionssysteme und Reaktions-Diffusions-Systeme. Um effektive Modelle herzuleiten, werden nicht nur die zugehörigen Reaktionsratengleichungen betrachtet, sondern auch die zugrunde liegende Gradientenstruktur. Der Ausgangspunkt dabei ist, dass Reaktionssysteme und Reaktions-Diffusions-Systeme unter der Voraussetzung von detaillierter Balance als Gradientenfluss verstanden werden können. Für Gradientensysteme wurde in den letzten Jahren eine strukturelle Konvergenz, die sogenannte *EDP-Konvergenz*, entwickelt. Dieses Coarse-Graining-Verfahren wird in der vorliegenden Arbeit auf folgende Systeme mit langsamen und schnellen Reaktionen angewandt: lineare Reaktionssysteme (bzw. Markov-Prozesse auf endlichem Zustandsraum), nichtlineare Reaktionssysteme, die das Massenwirkungsgesetz erfüllen, und lineare Reaktions-Diffusions-Systeme. Für den Grenzwert schneller Reaktionen wird eine mathematisch rigorose und strukturerhaltende Vergröberung auf dem Level des Gradientensystems bewiesen, indem EDP-Konvergenz gezeigt wird. In allen drei Fällen beinhaltet das effektive duale Dissipationspotential des Limes-Gradientensystems die langsamen Reaktionen und eine Einschränkung der chemischen Potentiale auf einen linearen Unterraum. Außerdem induziert es ein langsames Reaktionssystem oder Reaktions-Diffusions-System auf einer langsamen Mannigfaltigkeit mit Lagrange-Multiplikatoren. Dazu mathematisch äquivalent können die effektiven Gradientensysteme in groben langsamen Variablen beschrieben werden, was sowohl ein grobes Gradientensystem als auch eine grobe Gradientenflussgleichung liefert. Im Falle nichtlinearer Reaktionen ist die wesentliche Annahme die sogenannte *Unique Fast Equilibrium Condition*, die eine Parametrisierung der langsamen Mannigfaltigkeit durch langsame Variablen liefert. Das Reaktions-Diffusions-System wird als Gradientenfluss der freien Energie im Raum der Wahrscheinlichkeitsmaße interpretiert. Das Dissipationspotential erweitert die etablierte Otto-Gradientenstruktur für die Diffusion und bezieht auch Reaktionen mit ein.

Im vierten Teil wird der Zusammenhang zwischen Gleichungen mit Gedächtnis und Markov-Prozessen untersucht. Dabei werden Gedächtnisintegrale betrachtet, die durch einen räumlichen Homogenisierungprozess motiviert werden können. Für solche Gleichungen wird explizit ein größer Markov-Prozess konstruiert, der die Gleichung mit Gedächtnis als Teilsystem enthält. Der Markov-Prozess wird durch die Einführung verborgener Zustände bzw. Quasiteilchen definiert, die den Massenverlust in der Evolution erfassen. Insbesondere können nun analytische Hilfsmittel aus der Theorie der Markov-Prozesse verwendet werden, um diese Arten von Gleichungen mit Gedächtnis zu untersuchen.

Der letzte Teil beschäftigt sich mit numerischen Diskretisierungen für den Fokker-Planck-Operator. Die hier betrachteten Finite-Volumen-Diskretisierungen können auch als ein physikalisches Coarse-graining verstanden werden, da sie, unter Erhaltung der Physik des Systems, ein unendlichdimensionales Problem auf eine endlichdimensionale Approximation reduzieren. Verschiedene Finite-Volumen-Verfahren, darunter das etablierte Scharfetter-Gummel- sowie das neu entwickelte SQRA-Diskretisierungsverfahren, werden numerisch und analytisch untersucht.

Acknowledgment

At this stage, I would like to thank all people who supported me during my studies and while writing my thesis.

Special thanks go to my teacher, supervisor and mentor Alexander Mielke. I am thankful that he took the time to enthusiastically discuss mathematical research, and for letting me learn from his rich mathematical knowledge. He introduced me to wonderful scientific topics, and his asking questions at the right time undoubtedly enriched my research. His support and advice regarding scientific and organizational questions have helped me to complete my PhD.

I also thank all my coauthors, namely Martin Heida, Markus Kantner, Alexander Mielke, Mark A. Peletier, and Holger Stephan, with whom I had the chance to collaborate. The results of my thesis have obtained due to their contribution. Doing collaborative science has been a really great experience.

I would like to thank Mark A. Peletier for his invitation to visit Eindhoven. I enjoyed my research stay at CASA very much. From Mark, I learned a lot about mathematics and human integrity.

I am grateful to the Weierstrass Institute for Applied Analysis and Stochastics, and, especially, to the members of research group 1 for the fantastic working atmosphere. I thank Thomas Eiter, Thomas Frenzel, Annegret Glitzky, Markus Kantner, Matthias Liero, Markus Mittnenzweig, Robert Patterson, Dirk Peschka, Joachim Rehberg, and Michiel Renger, who where interested in my research and with whom I had great scientific discussions. Here, I would also like to thank my friend and colleague Hagen Neidhardt, who passed away very unexpectedly. His enthusiasm provided a good basis for my scientific career. There are a lot of things I would have liked to discuss with him about science and life.

Moreover, I thank the defense committee and the co-examiners of my PhD thesis for agreeing to evaluate my dissertation.

The research would not have been possible without funding. I would like to thank the Berlin Mathematical School for the scholarship and for travel money so I could participate in workshops and conferences, where I got introduced into the scientific community. Since October 2018, my research has been funded by Deutsche Forschungsgemeinschaft (DFG) through the Collaborative Research Center SFB 1114 "Scaling Cascades in Complex Systems" (Project no. 235221301), Subproject C05 "Effective models for materials and interfaces with multiple scales". In general, the CRC 1114 with its broad and interdisciplinary framework provided a very good opportunity to dig into applied mathematics.

In addition, I would also like to thank the German educational system I entered more than 20 years ago, where all the knowledge I have acquired did not cost me much money.

Undoubtedly, I would not have been here without my family. All of them, with their support and love, have played their part in my development and education. My father Holger and my brother Anton have supported me from the beginning of my mathematical education. The long and fruitful discussions with my father helped me not to lose sight of the broader picture in science. Finally, I would like to thank my beloved wife Elisa and my sons Friedrich and Nikolai. They have shown me that the most important thing in life is love.

Für meine Familie

Content

Introduction

Coarse-graining

The mathematical description of complex processes in physics involves many challenging difficulties. It results from the fact that mathematical models are governed by the trade-off between accuracy and simplicity. A more accurate description, involving more physical states, provides richer information about the physical problem, which is desirable for a detailed understanding of the physical process. In contrast, a precise description involves many challenges affecting all branches of applied mathematics, namely modeling, analysis and simulation: First, the validation of an applicable model requires precise measurements that become practically impossible if the state space is too large. Secondly, the analytic difficulties grow when increasing the complexity of the problem. Thirdly, good numerical algorithms may become too costly if the number of parameters and dimensions increase.

A procedure that reduces the complexity of a system is often called *coarse-graining*. It is a prominent research component in all areas of natural sciences. These reductions or approximations are often physically motivated by scale separations of the problem. On different temporal or spatial scales, different processes may govern the physical system, resulting in different levels of description. The derivation of effective systems by reducing a system involving different scales to a smaller system with less scales, for example only one distinguished scale, is one of the main focuses of this work.

Having derived an effective system, the scientific tasks are usually not finished, because effective systems can often be formulated in mathematically different but equivalent ways. These mathematically equivalent descriptions are relevant for applications, as they provide new valuable insights, extending mathematical models with complementary information. As we will see, a mathematically equivalent description can be obtained by introducing new additional variables and enlarging the state space, or, conversely, by reducing the system to less variables and shrinking the state space. A prominent example for that are models for semiconductor physics, where, in addition to the electrons, also electron holes as their physical counterpart may be included in the model for capturing, for example, charge conservation. Although mathematically equivalent, different models may provide additional information about the physical process.

Mathematically, the two aspects of reduction and equivalent description are the main focus of my thesis. They are motivated by the two questions:

1. How can the coarse-graining procedure be mathematically justified?

2. Are there mathematically equivalent descriptions of the effective system that provide new mathematical and modeling insights?

Of course, the two terms "justification" and "insights" need a philosophical clarification, because they depend on the proposed question. These two different but closely related problems are explained in detail in the next sections. Although coarse-graining is often already a part of the modeling process, in this thesis, we are interested in a mathematically rigorous justification of the coarse-graining procedure. In particular, we are interested in a reduction procedure respecting the underlying physical structure, which is the gradient structure of the evolution system. Additionally, we will derive mathematically equivalent descriptions on both levels, namely the evolution equation as well as its gradient structure (whenever it exists). The physical examples in all five parts of the thesis originate from stochastic particle systems and chemical reaction systems. For these problems, the models are either Markov processes that describe the evolution of the number of particles of the chemical species, or the corresponding master equation for the distribution. After introducing gradient systems and the reduction machinery, the mathematical results for the five parts of the thesis are explained in detail. The results can be found in [MiS20, MPS21, Ste21, StS19, HKS20], which either refer to the published article or to the WIAS preprint of the submitted publication.

EDP-convergence and deriving the effective gradient system

The first three parts of the thesis investigate reaction systems and reaction-diffusion systems. In many applications the number of chemical species can be huge and the reaction coefficients for the chemical reactions may vary in a large range. In such cases not only the measurement of all necessary physical quantities, but also analytical or numerical treatment is out of reach. A natural simplification is made by the assumption that reactions can happen with different and distinguished magnitudes of speed. We will consider the case that slow and fast reactions are distinguished, namely the slow ones of order 1 and the fast ones of order $1/\varepsilon$ for a small parameter $\varepsilon > 0$. There are many instances for this kind of assumption in chemical literature, see e.g. [HaR02]. As an example we refer to [KaK13, Ex. 6.1], where an mRNA-DNA system for 6 species with 8 slow reactions and 2 fast reactions is considered.

The first three parts deal with the fast-reaction limit if $\varepsilon \to 0$. Mathematically, fast-reaction limits for linear and nonlinear reaction systems have attracted attention for decades starting from the pioneering work by Tikhonov [Tik52] and Fenichel [Fen79]. We refer to [Bot03, KaK13, DLZ18] for modern approaches. Traditionally, ODE or PDE results provide effective reaction systems or reaction-diffusion systems that are defined on the slow manifold described by either a projection or an algebraic relation together with the corresponding Lagrange multipliers. In contrast, here, the motivation and starting point was different. The fundamental idea is that these systems have an underlying variational structure because they can be understood as a gradient flow. Gradient flows are inevitable in modeling physical problems in mechanics and thermodynamics, starting from the pioneering work of Onsager [Ons31, OnM53]. They describe an evolution of the steepest descent of a driving functional, where the steepness is defined in terms of the dissipation mechanism. Mathematically, gradient flows are evolution equations that are induced by a so-called *gradient system* $(Q, \mathcal{E}, \mathcal{R}^*)$ [Mie11, Pel14, Mie16], consisting of a state space Q (a subspace of a Banach space X), a driving (or energy) functional $\mathcal{E}$, and a geometric or dissipative structure in the form of a dissipation potential $\mathcal{R}$ that describes

the geometry of the underlying state space Q. Here, $\mathcal{R}$ is called a *dissipation potential* if $\mathcal{R}(q,\cdot) : X \to [0,\infty]$ is lower semicontinuous, convex and satisfies $\mathcal{R}(q,0) = 0$. Then, $\mathcal{R}^*$ is the (partial) Legendre-Fenchel transform given by

$$\mathcal{R}^*(q,\xi) := \sup_{v\in X} \{\langle \xi, v\rangle - \mathcal{R}(q,v)\}.$$

The induced gradient flow equation is then defined by

$$\dot q = \partial \mathcal{R}^*(q, -\mathrm{D}\mathcal{E}(q)) \quad \text{ or equivalently } \quad 0 = \mathrm{D}_{\dot q}\mathcal{R}(q,\dot q) + \mathrm{D}\mathcal{E}(q). \tag{0.1}$$

The first equation is a rate equation in the state space $Q \subset X$. The second equation is a force balance, where the viscous force $\mathrm{D}_{\dot q}\mathcal{R}(q,\dot q)$ is balanced by the potential restoring force $-\mathrm{D}\mathcal{E}(q)$.

Adding thermodynamic information to the evolution equation, gradient structures are of great importance from the modeling perspective. In general, an evolution equation may have many different gradient structures. However, a gradient system uniquely defines the gradient flow evolution. A great challenge in modeling is to determine the gradient structure of a physical system. It provides mathematical features for analytical and numerical investigation.

Another equivalent formulation of the gradient flow equation (0.1) plays an important role. Introducing the total dissipation functional

$$\mathfrak{D}(q) = \int_0^T \mathcal{R}(q,\dot q) + \mathcal{R}^*(q, -\mathrm{D}\mathcal{E}(q))\,\mathrm{d}t, \tag{0.2}$$

the gradient flow evolution can equivalently be described by the so-called *energy-dissipation balance*

$$\mathcal{E}(q(T)) + \mathfrak{D}(q) = \mathcal{E}(q(0)).$$

This energy-dissipation balance compares the energy at initial time $t = 0$ with the energy at final time $t = T$. The difference is given by the dissipation functional $\mathfrak{D}(q)$, which has a particular form, consisting of two terms $\mathcal{R}$ and $\mathcal{R}^*$. This formulation has many interesting properties. First, the energy-dissipation principle states that the energy-dissipation balance is an equivalent formulation of the gradient flow equation (0.1). Secondly, it rewrites the former evolution equation defined on an (in general) infinite dimensional space to a relation involving real-valued functionals. The gradient flow evolution equation is given by the trajectory that provides the optimal relation between energy and dissipation. Both features together allow for investigating families of gradient systems $(Q, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon)$ depending on a small parameter $\varepsilon > 0$.

For families of gradient systems $(Q, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon)$, where $\varepsilon > 0$ is a small parameter coming from a microstructure, a structural convergence, the so-called *EDP-convergence* has been established in recent years [LM*17, DFM19, MMP21]. The aim is to identify the effective gradient system $(Q, \mathcal{E}_{\mathrm{eff}}, \mathcal{R}^*_{\mathrm{eff}})$ in the limit as $\varepsilon \to 0$. This convergence relies on the energy-dissipation principle, which allows for the use of methods from calculus of variations. Roughly speaking, EDP-convergence is defined by two Γ-convergences: for the energy functionals $\mathcal{E}_\varepsilon$, defined on the state space Q, and the dissipation functionals $\mathfrak{D}_\varepsilon$ given by

$$\mathfrak{D}_\varepsilon(q) = \int_0^T \mathcal{R}_\varepsilon(q,\dot q) + \mathcal{R}^*_\varepsilon(q, -\mathrm{D}\mathcal{E}_\varepsilon(q))\,\mathrm{d}t,$$

defined on the dynamic space of trajectories (in a suitable topology). The limit is again given by

$$\mathfrak{D}_0(q) = \int_0^T \mathcal{R}_{\text{eff}}(q, \dot{q}) + \mathcal{R}^*_{\text{eff}}(q, -\mathrm{D}\mathcal{E}(q)) \, \mathrm{d}t.$$

The effective gradient system is, then, given by $(Q, \mathcal{E}_{\text{eff}}, \mathcal{R}^*_{\text{eff}})$. The dissipation functionals $\mathfrak{D}_\varepsilon$ are defined not only for the solution of the gradient flow equation (0.1), but on general trajectories around solutions. These trajectories can be understood as fluctuations, which is in accordance with the deep connection between gradient systems and the stochastic description via large-deviation principles [MPR14]. These fluctuations provide a more detailed description of the physical problem, since thermodynamical randomness is also taken into account. In general, these fluctuations have less time regularity than the solution of the gradient flow equation, which yields several technical problems.

An almost trivial consequence of EDP-convergence is that solutions of the gradient flow of $(Q, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon)$ converge to the solution of the gradient flow of the effective gradient system $(Q, \mathcal{E}_{\text{eff}}, \mathcal{R}^*_{\text{eff}})$. The great advantage of EDP-convergence is that the limit gradient system is uniquely determined, and hence, the previously hidden physical principles of the effective evolution equation become evident (see Figure 1).

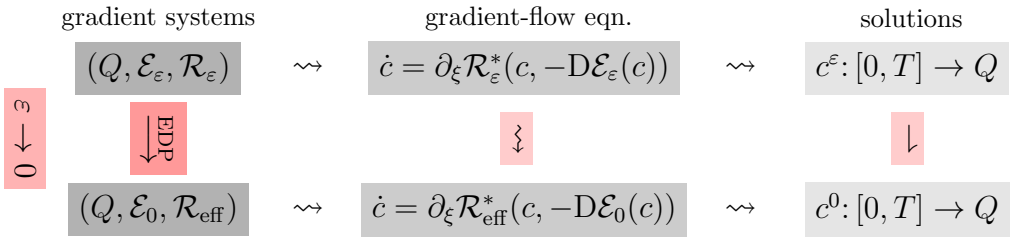


Figure 1: EDP-convergence leads to a commuting diagram. In particular, EDP-convergence generates the correct limit equation $\dot{c} = \mathcal{R}^*_{\text{eff}}(c, -\mathrm{D}\mathcal{E}_0(c))$ and the solutions c^ε converge to solutions c^0 of the limit equation. However, $\mathcal{R}_{\text{eff}}$, which is uniquely determined by EDP-convergence, provides information not contained in the limit equation.

Recently, it has become evident that the dissipation functional $\mathfrak{D}(q)$ given by (0.2) does not contain all desired information, because only specific forces of the form $-\mathrm{D}\mathcal{E}(q)$ are present in the dissipation functional. To overcome these limitations, so-called *tilts* in the form of linear shifts of the energy $\mathcal{E}^\eta(q) = \mathcal{E}(q) + \langle \eta, q \rangle$ have been used. In particular, a stronger notion, namely *EDP-convergence with tilting*, has been introduced in [DFM19, MMP21]. Tilt-EDP-convergence then means that the effective dissipation potential $\mathcal{R}^*_{\text{eff}}$ in the limit of $\mathfrak{D}^\eta_\varepsilon$ is completely independent of the tilts η. Deriving an effective dissipation potential $\mathcal{R}^*_{\text{eff}}$ that is independent of external energy shifts provides a physically reasonable distinction between dissipation and energy in the evolution.

In fact, in the first three parts, we derive EDP-convergence with tilting for different kinds of fast-slow reaction systems and reaction-diffusion systems. The physically underlying gradient structure provides the mathematical framework for performing coarse-graining. Mathematical coarse-graining is intrinsically related to numerical methods, where complex problems are approximated finite dimensionally respecting the physics of the problem. The last part of the thesis compares different numerical schemes for discretizations of the Fokker-Planck operator. There, the finite volume discretization provides transition rates for the underlying Markov process that is connected to the gra-

dient structures used in the first three parts of the thesis for reaction systems. Instead of proving EDP-convergence here, we aim at deriving convergence rate estimates.

Equivalent model descriptions for the evolution equation and the gradient systems

So far, we have seen the mathematical framework for deriving effective models. The effective systems, either gradient systems or solely the evolution equation, can often be described in various but mathematically equivalent ways. This is also the case for slow-fast reaction systems and reaction-diffusion systems. As it turns out, the limit system can either be described on a larger space with an algebraic constraint and corresponding Lagrange multipliers, or in smaller space consisting of coarse-grained variables. Both equivalent formulations are present on the level of the evolution equation and the gradient system and have different mathematical and modeling properties. An evolution equation with an algebraic constraint and Lagrange multipliers is defined on a large space, the evolution equation in coarse-grained variables needs an explicit resolution or parametrization of the slow manifold.

The same reasoning is the motivation for the fourth part of the thesis. There, the connection between memory equations and (memoryless) Markov processes is explored. The memory equation under investigation can be motivated from a space-dependent homogenization problem [Tar90], where memory effects, as the result of a spatial microstructure have been derived. Here, we consider the simplest linear space-independent situation. It is shown that this memory equation with its rich and complex dynamics can be understood as a reduced subsystem of a Markov process defined on a larger space, but having easier analytical properties. The construction is done by introducing hidden states, or quasi particles, which, a priori, do not have any physical meaning. A posteriori they provide valuable insights in the dynamics of the original problem.

In the following, we describe the results of all five parts of the thesis in more detail.

Part 1: Coarse-graining via EDP-convergence for linear fast-slow reaction systems

In the first part of the thesis, we perform the fast-reaction limit for a fast-slow linear reaction system (i.e. a Markov process on a finite state space). The aim is to show EDP-convergence for the gradient systems under the assumption of detailed balance. On the state space

$$Q := \mathrm{Prob}(\{1,\dots,I\}) = \left\{ c \in [0,1]^I : \sum\nolimits_{i=1}^{I} c_i = 1 \right\} \subset \mathbb{R}^I =: X,$$

where we interpret c as a mass distribution, the ε-dependent evolution equation reads

$$\dot{c}^\varepsilon = A^\varepsilon c^\varepsilon = \left(A^{\mathrm{slow}} + \frac{1}{\varepsilon} A^{\mathrm{fast}} \right) c^\varepsilon . \tag{0.3}$$

Here, A^ε is a Markov generator preserving positivity and mass of the evolution. It consists of a part of slow reactions A^{slow} and a part of fast reactions A^{fast}. The basic assumption is that the *detailed-balance condition* holds, which means that there exists a positive equilibrium state $w^\varepsilon = (w_i^\varepsilon)_i \in Q$ such that

$$\forall\, i,k \in \{1,\dots,I\} : \quad A_{ik}^\varepsilon w_k^\varepsilon = A_{ki}^\varepsilon w_i^\varepsilon . \tag{0.4}$$

For reaction systems of mass-action type (which include all linear systems) satisfying detailed balance, it was shown in [Mie11] that an entropic gradient structure exists, i.e. $\mathcal{E}_\varepsilon$ is free energy of Boltzmann type

$$\mathcal{E}^\varepsilon_{\mathrm{Bz}}(c) = \sum_{i=1}^{I} w_i^\varepsilon E_{\mathrm{Bz}}(c_i/w_i^\varepsilon),$$

where the Boltzmann function E_{Bz} is given by $E_{\mathrm{Bz}}(r) = r\log r - r + 1$. Let us mention that this fact was implicitly used in earlier works, see e.g. [ÖtG97, Yon08]. For linear reaction systems, which are master equations for Markov processes, a more general theory was developed in [Maa11, CH*12] leading to a large class of possible gradient structures [MaM20].

Here, we use the physically most natural gradient structure that has its origin in the theory of large deviation, see [MPR14, MP*17]. The dual dissipation potentials $\mathcal{R}^*_\varepsilon(c,\cdot) : X \to \mathbb{R}$ are not quadratic but include exponential terms, namely

$$\mathcal{R}^*_\varepsilon(c,\xi) = \frac{1}{2}\sum_{i<k} \kappa^\varepsilon_{ik}\,\sqrt{c_i c_k}\;\mathsf{C}^*(\xi_i - \xi_k) \quad \text{with } \mathsf{C}^*(\zeta) = 4\cosh(\zeta/2) - 4 \tag{0.5}$$

and $\kappa^\varepsilon_{ik} = A^\varepsilon_{ik}\sqrt{w^\varepsilon_k/w^\varepsilon_i}$. The gradient system $(Q, \mathcal{E}^\varepsilon_{\mathrm{Bz}}, \mathcal{R}^*_\varepsilon)$ exactly generates the gradient-flow evolution (0.3), i.e.

$$\dot c = \partial_\xi \mathcal{R}^*_\varepsilon(c, -\mathrm{D}\mathcal{E}_\varepsilon(c)).$$

The main technical assumption is that the stationary measure is not degenerate for $\varepsilon \to 0$, i.e. $w^\varepsilon \to w^0$ and $w^0 > 0$, which means that mass is present in all states in the limit $\varepsilon \to 0$. This assumption immediately implies that $\mathcal{E}^\varepsilon_{\mathrm{Bz}} \xrightarrow{\mathrm{M}} \mathcal{E}^0_{\mathrm{Bz}}$. To prove tilt-EDP-convergence, we show that $\mathfrak{D}^\eta_\varepsilon \xrightarrow{\mathrm{M}} \mathfrak{D}^\eta_0$, where

$$\mathfrak{D}^\eta_0(q) = \int_0^T \mathcal{R}_{\mathrm{eff}}(q,\dot q) + \mathcal{R}^*_{\mathrm{eff}}(q, -\eta - \mathrm{D}\mathcal{E}(q))\mathrm{d}t.$$

To obtain an explicit form of the dissipation potential $\mathcal{R}^*_{\mathrm{eff}}$, we introduce the following notation. By the non-degeneracy assumption $w^0 > 0$, the fast part A^{fast} of the reactions defines an equivalent relation on the set of states $\{1,\dots,I\}$. This equivalence relation separates the states that are connected via fast reactions into different $J < I$ clusters. This defines a coarse-graining map

$$M : \mathrm{Prob}(\{1,\dots,I\}) \to \mathrm{Prob}(\{1,\dots,J\}),$$

which is a Markov operator. The crucial idea is that, respecting the microscopic equilibrium w^0, we may uniquely define a linear reconstruction operator

$$N : \mathrm{Prob}(\{1,\dots,J\}) \to \mathrm{Prob}(\{1,\dots,I\}),$$

which inverts the coarse-graining operator M in a physically reasonable sense. The effective dissipation potential $\mathcal{R}^*_{\mathrm{eff}}$ of the limit gradient structure $(Q, \mathcal{E}^0_{\mathrm{Bz}}, \mathcal{R}^*_{\mathrm{eff}})$ is then given by

$$\mathcal{R}^*_{\mathrm{eff}}(c,\xi) = \mathcal{R}^*_{\mathrm{slow}}(c,\xi) + \chi_{\mathrm{Range}(M^*)}(\xi).$$

The effective gradient structure defines an effective evolution equation of the form

$$\dot c \in A^{\mathrm{slow}}c + \ker M, \quad A^{\mathrm{fast}}c = 0\,,$$

which describes the slow evolution on the linear slow manifold with Lagrange multipliers.

Equivalently, the effective gradient system can be understood as a gradient system in coarse-grained slow variables. On the coarse-grained state space

$$\hat{Q} := M\left(\mathrm{Prob}(\{1,\dots,I\})\right) = \mathrm{Prob}(\{1,\dots,J\}),$$

we define the coarse-grained energy functional and dissipation potential via

$$\hat{\mathcal{E}}(\hat{c}) = \mathcal{E}^0_{\mathrm{Bz}}(N\hat{c}), \quad \hat{\mathcal{R}}^*(\hat{c},\hat{\xi}) = \mathcal{R}^*_{\mathrm{eff}}(N\hat{c}, M^*\hat{\xi}).$$

As it turns out, both gradient systems, $(Q,\mathcal{E}^0_{\mathrm{Bz}},\mathcal{R}^*_{\mathrm{eff}})$ or the coarse-grained gradient systems $(\hat{Q},\hat{\mathcal{E}},\hat{\mathcal{R}}^*)$, contain the same information, because there is a one-to-one correspondence between concentrations c on the slow manifold and coarse-grained concentrations $\hat{c}$. The coarse-grained evolution equation is then given by

$$\dot{\hat{c}} = \hat{A}\hat{c}\,,$$

where the coarse-grained Markov generator is simply $\hat{A} = MA^{\mathrm{slow}}N$.

Part 2: EDP-convergence for nonlinear fast-slow reaction systems with detailed balance

The second part of the thesis deals with the study of nonlinear reaction systems with different time scales. We assume that the species X_i, $i \in I := \{1,\dots,i_*\}$ undergo r_* forward-backward chemical reactions of mass-action type

$$\alpha^r_1 X_1 + \cdots + \alpha^r_{i_*} X_{i_*} \quad \rightleftharpoons \quad \beta^r_1 X_1 + \cdots + \beta^r_{i_*} X_{i_*},$$

where $\alpha^r = (\alpha^r_i)_{i\in I}$ and $\beta^r = (\beta^r_i)_{i\in I}$ are the stoichiometric vectors in $\mathbb{N}_0^{i_*}$. The reaction-rate equation has the form

$$\dot{c} = -\sum_{r=1}^{r_*} \left(k^{\mathrm{fw}}_r c^{\alpha^r} - k^{\mathrm{bw}}_r c^{\beta^r}\right)\left(\alpha^r - \beta^r\right), \quad \text{where } c^\alpha = c_1^{\alpha_1}\cdots c_{i_*}^{\alpha_{i_*}}.$$

The main assumption is that the reaction-rate equation satisfies the *detailed-balance condition*, which requires the existence of a positive concentration vector $c_* = (c^*_i)_{i\in I} \in \mathbf{C}_+ :=]0,\infty[^{i_*}$ such that all r_* reactions are in equilibrium:

$$\exists\, c_* = (c^*_i)_{i\in I} \in \mathbf{C}_+ \;\forall\, r \in R := \{1,\dots,r_*\}: \quad k^{\mathrm{fw}}_r c_*^{\alpha^r} = k^{\mathrm{bw}}_r c_*^{\beta^r}\,.$$

For notational convenience, we introduce the ratios

$$\widetilde{\kappa}_r = k^{\mathrm{fw}}_r \left(c_*^{\alpha^r}/c_*^{\beta^r}\right)^{1/2} = k^{\mathrm{bw}}_r \left(c_*^{\beta^r}/c_*^{\alpha^r}\right)^{1/2}.$$

For studying systems with different time scales, we introduce a small parameter $\varepsilon > 0$ measuring the ratio between the slow and the fast time scale. We decompose the set of reaction pairs into slow and fast reactions (i.e. $R = R_{\mathrm{slow}} \cup R_{\mathrm{fast}}$) and we assume that $\widetilde{\kappa}_r = \kappa_r$ for the slow reactions and $\widetilde{\kappa}_r = \kappa_r/\varepsilon$ for the fast reactions (where $\kappa_r > 0$ are fixed numbers). Then the fast-slow reaction-rate equation is given by

$$\dot{c} = \boldsymbol{R}_{\mathrm{slow}}(c) + \frac{1}{\varepsilon}\boldsymbol{R}_{\mathrm{fast}}(c) \quad \text{with} \quad \boldsymbol{R}_{\mathrm{xy}}(c) := -\sum_{r\in R_{\mathrm{xy}}} \kappa_r \left(c_*^{\alpha^r} c_*^{\beta^r}\right)^{1/2} \left(\frac{c^{\alpha^r}}{c_*^{\alpha_r}} - \frac{c^{\beta^r}}{c_*^{\beta_r}}\right)(\alpha^r - \beta^r). \tag{0.6}$$

Following [Mie11, MPR14], the fast-slow reaction-rate equation can be understood as a gradient flow of the cosh-type gradient structure $(\mathbf{C}, \mathcal{E}, \mathcal{R}^*)$, where the energy functional is the free energy of Boltzmann type

$$\mathcal{E}(c) = \sum_{i=1}^{i^*} c_i^* E_{\mathrm{Bz}}(c_i/c_i^*), \quad E_{\mathrm{Bz}}(r) = r\log r - r + 1\,.$$

The dual dissipation potential consists of a slow part and a fast part and is given by

$$\mathcal{R}_\varepsilon^*(c,\xi) = \mathcal{R}_{\mathrm{slow}}^*(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}_{\mathrm{fast}}^*(c,\xi)$$

with

$$\mathcal{R}_{\mathrm{xy}}^*(c,\xi) = \sum_{r\in R_{\mathrm{xy}}} \kappa_r \big(c^{\alpha^r} c^{\beta^r}\big)^{1/2}\, \mathsf{C}^*\big((\alpha^r - \beta^r)\cdot\xi\big),$$

where the cosh-function C^* is defined exactly like for linear reactions (0.5). It follows that the reaction-rate equation (0.6) is indeed given by the gradient flow equation

$$\dot c = \partial_\xi \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c)).$$

The aim of the second part of the thesis is to derive the effective gradient structure $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ by proving EDP-convergence for the fast-reaction limit $\varepsilon \to 0$. Since the energy functional $\mathcal{E}$ is ε-independent, the major challenge lies in proving Γ-convergence for the tilted dissipation functional

$$\mathfrak{D}_\varepsilon^\eta(c) = \int_0^T \mathcal{R}_\varepsilon(c,\dot c) + \mathcal{R}_\varepsilon^*(c, \eta - \mathrm{D}\mathcal{E}(c))\,\mathrm{d}t.$$

As in the linear situation, the evolution gets constrained to a submanifold, which is nonlinear in general. To capture this, we introduce the subspace of fast stoichiometric vectors

$$\Gamma_{\mathrm{fast}} = \mathrm{span}\,\{\alpha^r - \beta^r : r \text{ is fast}\}\,, \quad \Gamma_{\mathrm{fast}}^\perp = \big\{\xi \in \mathbb{R}^{i_*} : \forall\,\gamma\in\Gamma_{\mathrm{fast}} :\ \gamma\cdot\xi = 0\big\}\ .$$

Moreover, we define the matrix $Q_{\mathrm{fast}} \in \mathbb{R}^{m_{\mathrm{fast}}\times i_*}$ that captures the conserved quantities of the fast reactions, i.e. $\ker Q_{\mathrm{fast}} = \Gamma_{\mathrm{fast}}$ and Q_{fast} is surjective. The matrix Q_{fast} defines the coarse-grained slow variables in a linear way and plays the same role as the matrix M in the linear situation of the first part of the thesis. Then it turns out that $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ converges in the sense of EDP with tilting to $(\mathbf{C}, \mathcal{E}_{\mathrm{eff}}, \mathcal{R}_{\mathrm{eff}}^*)$, where the effective gradient system is given by

$$\mathcal{E}_{\mathrm{eff}} = \mathcal{E}, \quad \mathcal{R}_{\mathrm{eff}}^* = \mathcal{R}_{\mathrm{slow}}^* + \chi_{\Gamma_{\mathrm{fast}}^\perp}.$$

The dissipation potential again consists of two parts: one part that captures the slow reactions and one part that restricts the evolution to the set of fast equilibria

$$\mathscr{E}_{\mathrm{fast}} = \{c\in\mathbf{C} : \boldsymbol{R}_{\mathrm{fast}}(c) = 0\}\,.$$

The main assumption is that these equilibria are uniquely determined in each invariant subspace $\mathbf{C}_q^{\mathrm{fast}} = \{c\in\mathbf{C} : Q_{\mathrm{fast}}c = q\}$. This *Unique Fast Equilibrium Condition* (UFEC) ensures the definition of a non-linear reconstruction map Ψ, which "inverts" the linear coarse-graining map Q_{fast}. The slow manifold can then be parametrized by Ψ, i.e.

$$\mathscr{M}_{\mathrm{slow}} = \{\Psi(q) : q\in Q_{\mathrm{fast}}\mathbf{C}\} = \{c\in\mathbf{C} : \boldsymbol{R}_{\mathrm{fast}}(c) = 0\}\,.$$

Considering only positive concentrations, the UFEC is no restriction. In particular, the UFEC is not needed when considering non-trivial solutions of the reaction-rate equation. In contrast, the concept of EDP-convergence is more general and considers fluctuations around solutions that are not necessarily positive.

Similar to [MiS20], the effective system can equivalently be described in coarse-grained slow variables with the nonlinear reconstruction function Ψ. On the state space $\hat{\mathbf{C}} = Q_{\mathrm{fast}}\mathbf{C}$, we define

$$\hat{\mathcal{E}}(q) = \mathcal{E}(\Psi(q)), \quad \hat{\mathcal{R}}^*(q,\hat{\xi}) = \mathcal{R}^*_{\mathrm{slow}}(\Psi(q), Q^{\mathrm{T}}_{\mathrm{fast}}\hat{\xi}).$$

The coarse-grained driving functional is no longer of Boltzmann type, since it takes into account the curved nonlinear submanifold given by the dissipation. The coarse-grained evolution equation for the slow variables is given by

$$\dot{q} = \partial_{\hat{\xi}}\hat{\mathcal{R}}^*(q, -\mathrm{D}\hat{\mathcal{E}}(q)) = Q_{\mathrm{fast}}\boldsymbol{R}_{\mathrm{slow}}(\Psi(q))\,.$$

As an application, a reduction from two bimolecular chemical reactions to one trimolecular reaction can be performed. Considering two reactions

$$\text{fast}: \ X_1 + X_2 \rightleftharpoons X_3 \quad \text{and} \quad \text{slow}: \ X_3 + X_4 \rightleftharpoons X_5\,,$$

the coarse-grained gradient structure corresponds to a chemical reaction of the form

$$X_1 + X_2 + X_4 \rightleftharpoons X_5,$$

if, in addition, the limit $c_3^* \to 0$ is performed.

Part 3: EDP-convergence for a linear reaction-diffusion system with fast reversible reaction

The third part of the thesis considers a linear reaction-diffusion system with a fast reversible reaction. On a given bounded domain $\Omega \subset \mathbb{R}^d$, the corresponding evolution equation is given by

$$\begin{aligned} \dot{c}_1 &= \delta_1\Delta c_1 - \frac{1}{\varepsilon}\left(\sqrt{\tfrac{\alpha}{\beta}}c_1 - \sqrt{\tfrac{\beta}{\alpha}}c_2\right) \\ \dot{c}_2 &= \delta_2\Delta c_2 + \frac{1}{\varepsilon}\left(\sqrt{\tfrac{\alpha}{\beta}}c_1 - \sqrt{\tfrac{\beta}{\alpha}}c_2\right)\,, \end{aligned} \tag{0.7}$$

where $\delta_1, \delta_2 > 0$ are diffusion coefficients and $\alpha, \beta > 0$ are reaction rates (complemented by no-flux boundary conditions and initial conditions). The aim is to perform the fast-reaction limit if $\varepsilon \to 0$. As in the space-independent situation of the first and the second part, we are not primarily interested in the convergence of solutions of the linear reaction-diffusion system (0.7), which was shown in [BoH02]. Our starting point is that reaction-diffusion systems such as (0.7) can be written as a gradient-flow equation induced by a gradient system $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$, where the state space Q is the space of probability measures $Q = \mathrm{Prob}(\Omega \times \{1,2\})$ and the driving functional is the free energy

$$\mathcal{E}(\mu) = \int_\Omega \sum_{j=1}^{2} E_{\mathrm{Bz}}\left(\frac{c_j}{w_j}\right) w_j \,\mathrm{d}x$$

for measures $\mu = c\,\mathrm{d}x$, with the Boltzmann function $E_{\mathrm{Bz}}(r) = r\log r - r + 1$ and the (in general space-dependent) stationary measure $w = (w_1, w_2)^{\mathrm{T}} \in Q$. Here, the dissipation potential $\mathcal{R}^*_\varepsilon$ is given by two parts

$$\mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\mathrm{diff}} + \mathcal{R}^*_{\mathrm{react},\varepsilon},$$

separately describing diffusion and reaction. Since the pioneering work of Otto and coauthors [JKO98, Ott01], it is known that many diffusion type problems can be understood as a gradient flow driven by the free energy in the space of probability measures equipped with the Wasserstein distance. The corresponding dissipation potential $\mathcal{R}^*_{\mathrm{diff}}$ is quadratic and given by

$$\mathcal{R}^*_{\mathrm{diff}}(\mu,\xi) = \frac{1}{2}\int_\Omega \sum_{i=1}^{2} \delta_i\,|\nabla\xi_i|^2 \;\mathrm{d}\mu_i.$$

Later, Mielke [Mie11] also proposed a quadratic gradient structure for reaction-diffusion systems with the same driving functional, combining diffusion and reaction. Following [MPR14] and the first two parts of the thesis, we use the *cosh-type gradient structure* for the reaction part. In the space-dependent situation, the ε-dependent dissipation for reaction is given by

$$\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu,\xi) = \frac{1}{\varepsilon}\int_\Omega \mathsf{C}^*(\xi_1(x) - \xi_2(x))\;\sqrt{\mathrm{d}\mu_1\mathrm{d}\mu_2}.$$

Setting $\mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\mathrm{diff}} + \mathcal{R}^*_{\mathrm{react},\varepsilon}$, the reaction-diffusion system (0.7) can now formally be written as a gradient flow equation

$$\dot\mu = \partial_\xi \mathcal{R}^*_\varepsilon(\mu, -\mathrm{D}\mathcal{E}(\mu)).$$

For proving EDP-convergence with tilting, the main challenge is in deriving the Γ-convergence for the dissipation functional $\mathfrak{D}_\varepsilon$ as the energy functional $\mathcal{E}$ is ε-independent. The tilts η are given by an external potential and correspond to a linear shift of the energy, which has now the form

$$\mathcal{E}^V(\mu) = \mathcal{E}(\mu) + \sum_{i=1}^{2}\int_\Omega V_i\;\mathrm{d}\mu_i.$$

The total dissipation functional is given by

$$\mathfrak{D}^\eta_\varepsilon(\mu) = \int_0^T \mathcal{R}_\varepsilon(\mu,\dot\mu) + \mathcal{R}^*_\varepsilon(\mu, \eta - \mathrm{D}\mathcal{E}(\mu))\;\mathrm{d}t,$$

where the primal dissipation potential $\mathcal{R}_\varepsilon$ is an inf-convolution of the primal dissipation potentials $\mathcal{R}_{\mathrm{diff}}$ and $\mathcal{R}_{\mathrm{react},\varepsilon}$, and is given by

$$\mathcal{R}_\varepsilon(\mu,v) = \inf_{J,b}\left\{\left(\sum_{j=1}^{2}\int_\Omega \widetilde{\mathsf{Q}}\,(\delta_j c_j, J_j)\mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\tfrac{\sqrt{c_1c_2}}{\varepsilon}, b_2(x)\right)\mathrm{d}x\right) : (c,J,b)\in(\mathrm{gCE})\right\}.$$

Here, the infimum is taken over all diffusion fluxes J_j and reaction fluxes b_j, which are coupled through a linear generalized continuity equation. For $v = \dot\mu$ we have that

$$(c,J,b)\in(\mathrm{gCE}) \quad\Leftrightarrow\quad \left\{b_1 + b_2 = 0 \text{ and } \left\{\begin{array}{l}\dot c_1 = -\mathrm{div}J_1 + b_1\\ \dot c_2 = -\mathrm{div}J_2 + b_2\end{array}\right\}\right\}.$$

Without the reaction part, this correspond to the Benamou-Brenier formulation of the Wasserstein distance on Q. Here, the dissipation potential $\mathcal{R}_\varepsilon$ is extended and the corresponding cost function takes the reaction flux into account as well. Since the reaction part is not quadratic, the velocity part $\int_0^T \mathcal{R}_\varepsilon \,\mathrm{d}t$ of the dissipation functional does not define a metric on the space of probability measures. The induced gradient flow equation is then a reaction-drift-diffusion system with space-dependent reaction rates

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \operatorname{div}\left(\begin{pmatrix} \delta_1 \nabla c_1 \\ \delta_2 \nabla c_2 \end{pmatrix} + \begin{pmatrix} \delta_1 c_1 \nabla V_1 \\ \delta_2 c_2 \nabla V_2 \end{pmatrix}\right) + \frac{1}{\varepsilon}\begin{pmatrix} -\sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & \sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \\ \sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & -\sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}.$$

In the potential free situation (i.e. $V = \text{const}$), we recover the original reaction-diffusion system (0.7).

The main result is the proof of EDP-convergence with tilting. Again, the effective gradient system consists of two terms and is given by

$$\mathcal{R}^*_{\text{eff}} = \mathcal{R}^*_{\text{diff}} + \chi_{\{\xi_1=\xi_2\}},$$

where the first term describes the diffusion of the species and the second term provides a coupling together with the restriction onto the linear slow manifold respecting the stationary measure

$$w^V = (w_1^V, w_2^V)^{\mathrm{T}}, \quad w_i^V = \frac{1}{Z} w_i \mathrm{e}^{-V_i}, \quad Z = \sum_{i=1}^{2} w_i \mathrm{e}^{-V_i}.$$

The effective gradient system defines a system of drift-diffusion equations on the slow manifold with Lagrange multipliers of the form

$$\begin{aligned} \dot{c_1} &= \operatorname{div}\left(\delta_1 \nabla c_1 + \delta_1 c_1 \nabla V_1\right) - \lambda \\ \dot{c_2} &= \operatorname{div}\left(\delta_2 \nabla c_2 + \delta_2 c_2 \nabla V_2\right) + \lambda \end{aligned} \quad , \quad \frac{c_1}{w_1^V} = \frac{c_2}{w_2^V}.$$

Like in the first two parts of the thesis the gradient systems can equivalently be described using coarse-grained slow variables $\hat{c} = c_1 + c_2$. The coarse-grained state space is given by $\hat{Q} = \mathrm{Prob}(\Omega)$. The coarse-grained energy functional and dissipation potential are defined by

$$\begin{aligned} \hat{\mathcal{R}}^*(\hat{\mu}, \hat{\xi}) &:= \mathcal{R}^*_{\text{eff}}\left(\left(\frac{w_1^V}{w_1^V + w_2^V}\hat{\mu}, \frac{w_2^V}{w_1^V + w_2^V}\hat{\mu}\right), (\hat{\xi}, \hat{\xi})\right) = \frac{1}{2}\int_\Omega \hat{\delta}^V |\nabla \hat{\xi}|^2 \,\mathrm{d}\hat{\mu}\,, \\ \hat{\mathcal{E}}(\hat{\mu}) &:= \mathcal{E}^V\left(\frac{w_1^V}{w_1^V + w_2^V}\hat{\mu}, \frac{w_2^V}{w_1^V + w_2^V}\hat{\mu}\right) = \int_\Omega \left(\log \hat{\mu} + \hat{V}\right) \mathrm{d}\hat{\mu}, \end{aligned} \tag{0.8}$$

where the mixed space-dependent diffusion coefficient and the mixed potential are given by

$$\hat{\delta}^V = \frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}, \quad \hat{V} = -\log\left(w_1 \mathrm{e}^{-V_1} + w_2 \mathrm{e}^{-V_2}\right),$$

respectively. The coarse-grained evolution equation is, a scalar drift-diffusion equation of the form

$$\dot{\hat{c}} = -\operatorname{div}\left(\hat{\delta}^V \hat{c}\, \nabla\left(-\mathrm{D}\hat{\mathcal{E}}(\hat{\mu})\right)\right) = \operatorname{div}\left(\hat{\delta}^V \nabla \hat{c} + \hat{\delta}^V \hat{c} \nabla \hat{V}\right).$$

In particular, for the potential free case $V = \text{const}$, the PDE-result of Bothe and Hilhorst [BoH02] is recovered.

Part 4: Memory equations as reduced Markov processes

In the fourth part of the thesis we investigate the connection between memory equations and Markov processes. Memory equations are evolution equations that may explicitly depend on the whole history of the evolution. In contrast, Markov processes are evolution equations, where solely the current state and rate determines the future evolution. It seems that memory equations describe much more physical problems than Markov processes. The aim of that part is to show that a large and important class of Memory equations can be understood as a reduction of a larger Markov process by introducing hidden states, which may be interpreted as quasi-particles. The memory equation here can be understood as an evolution equation that loses mass in time. Since Markov processes describe physical problems that conserve the total probability in time, we aim at introducing hidden state variables that captures the loss of mass. This procedure shows the already mentioned trade-off between analytical simplicity and large geometry. Moreover, it continues reasoning of the first three parts of the thesis, which show the advantage of two different but equivalent descriptions. It is well-known that non-autonomous evolution equations can also be understood as autonomous equations in the space of trajectories (see e.g. [HaV93] for general functional-differential equations or [NSZ18, NSZ20], where this reformulation is used for linear abstract Cauchy problems). There the underlying state space is the space of trajectories and becomes immediately infinite dimensional. This procedure is not meant here, where a large but still finite state space is constructed.

In this part, we focus on the linear Memory equation of the form

$$\dot{u}(t) = -au(t) + \int_0^t K(t-s)u(s)\,\mathrm{d}s,\ t \geq 0, \quad u(0) = u_0 > 0, \tag{0.9}$$

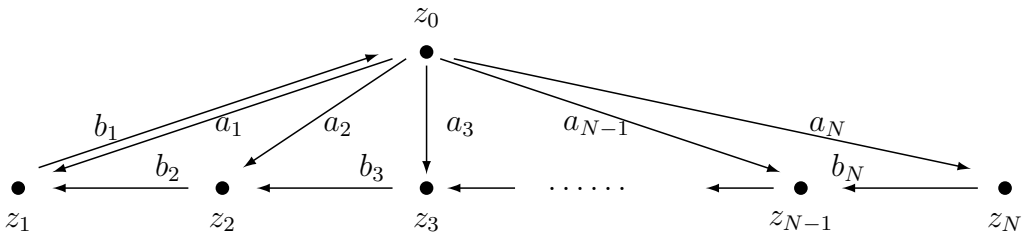
where $a > 0$ is a constant and $K : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is a positive kernel satisfying $\int_0^\infty K(t)\mathrm{d}t = a$. We interpret $u \in \mathbb{R}_{\geq 0}$ as a mass of a species. These kinds of evolution equations appear, for example, as effective limits of homogenization of space-dependent evolution equations [Tar90]. In general, memory equations as (0.9) encounter various analytical and modeling difficulties. For example, dynamical properties as stationary solutions and asymptotic behavior are not obvious. Moreover, modeling aspects of deriving a proper memory kernel K for a given physical system are not trivial.

Without memory (i.e. putting $K = 0$), the evolution is governed by usual damping, which equilibrates in zero. With the memory term (i.e. $K \gneq 0$), we heuristically expect that the damping is slower due to the presence of former mass and u equilibrates at $u_\infty > 0$.

Here, the aim is to construct a Markov process, which captures the loss of the mass, and hence, can be interpreted as a full description of the underlying physical process. The Markov process $\dot{p} = A^*p$ is explicitly constructed via an approximation of the memory kernel K. Since we are aiming at a Markov process that provides a physically reasonable interpretation, not all general memory kernels K can be approximated in that way. Instead, we focus on kernels K that are a linear combination of exponentials, where each addend is a first moment approximation of the corresponding discrete model

$$K(t) = \sum_{j=1}^{N} \alpha_j K_j(t), \quad K_j(t) \approx \delta(t - t_j),$$

where $0 = t_0 < t_1 < \cdots < t_N$ are given fixed time values and $a_j \geq 0$ satisfy $\sum_{j=1}^{N} a_j = a$. Here, the approximation respects the mean value, i.e. we have that $\int_0^\infty K_j \, \mathrm{d}t = 1$ and $\int_0^T t K_j \, \mathrm{d}t = t_j$. Defining the rates $b_j = \frac{1}{t_j - t_{j-1}}$ for $j = 1, \ldots, N$, the corresponding Markov generator A^* on $\mathbb{R}^{N+1}$ is given via the following network



showing the mass transfer between the original state z_0 and the different quasi-particles z_i, $i \in \{1, \ldots, N\}$. As it turns out, the first component of $\dot{p} = A^* p$ with concentrated initial value $p_0 = (u_0, 0 \ldots, 0)^{\mathrm{T}} \in \mathbb{R}^{N+1}$ is the solution of the memory equation (0.9). The Markov generator A^* is defined in such a way that mass is distributed from state z_0 to the N states, which then returns on a loop determined by the rates b_j providing the memory effect. Apart from trivial cases, the generator A^* does not satisfy the detailed balance condition. This construction provides interesting modeling and analytical insights. For example, the stationary solution, which had previously not been obvious, can be computed easily and is given by

$$u_\infty = \frac{1}{Z} u_0, \quad Z = 1 + \sum_{i=1}^{N} \left((t_j - t_{j-1}) \sum_{j=i}^{N} a_j \right).$$

Moreover, it allows for a procedure to model memory kernels in a comprehensible way, describing the memory effects as an interaction with given former states.

Finally, we apply the above construction to the degenerate situation of a delay-differential equation of the form

$$\begin{aligned} \dot{u}(t) &= -a u(t), \ t \in [0, T], \quad u(0) = u_0 > 0, \\ \dot{u}(t) &= -a u(t) + a u(t - T), \ t \geq T, \end{aligned}$$

which can be approximated by a reaction network of infinite size.

Part 5: Consistency and convergence for a family of finite volume discretizations of the Fokker–Planck operator

The last part compares different finite volume discretization schemes and proves their convergence for the Fokker–Planck operator. The Fokker-Planck equation is one of the most important equations in applied mathematics. It describes the time-evolution of the probability density of a particle, which is exposed to a potential force field. The stationary Fokker-Planck equation is given by

$$-\nabla \cdot (\kappa \nabla u) - \nabla \cdot (\kappa u \nabla V) = \operatorname{div} \mathbf{J}(u, V) = f,$$

where $\mathbf{J}(u, V) = -\kappa (\nabla u + u \nabla V)$ is the flux, $\kappa > 0$ is a diffusion coefficient and $V : \Omega \to \mathbb{R}$ is a given potential. The finite volume discretization is defined on a decomposition of

the domain $\Omega = \bigcup_j \Omega_j$ and is given by

$$-\sum_{j:\, j\sim i} \frac{m_{ij}}{h_{ij}}\, \kappa_{ij}\, S_{ij} \left(\frac{u_j}{\pi_j} - \frac{u_i}{\pi_i}\right) = f_i,$$

where for two neighboring cells Ω_i and Ω_j, m_{ij} denotes the mass of the common interface and h_{ij} denotes the distance between their cell centers. Moreover, κ_{ij} denotes a suitable approximation of the diffusion coefficient κ, f_i approximates the right-hand side f, $\pi = \mathrm{e}^{-V(x_i)}$ is an average of the Boltzmann distribution $\pi = \mathrm{e}^{-V}$. The finite volume discretization provides a Markov generator that captures the transitions between neighboring cells. This approximation scheme respects the underlying physical model and can be understood as a coarse-graining procedure from an infinite dimensional system to a finite dimensional reduction.

The function $S_{ij} = S(\pi_i, \pi_j)$ denotes a mean value of the Boltzmann distributions and is the starting point for our research. The choice of the mean function determines the weight in the flux between two neighboring cells. In the past, different choices of the mean value function S were derived. The well-established Scharfetter-Gummel discretization, which considers a particular choice of S, has been derived for drift-diffusion models for charge carrier transport in semiconductor devices [ScG69]. It provides a robust flux discretization since it interpolates well between the drift and the diffusion dominated regime. Recently and motivated from high-dimensional molecular dynamics simulations, the so-called *square-root approximation* (SQRA) scheme has been derived. The SQRA scheme results from the choice of a different mean function S and, mathematically, has been investigated only sparsely. Understanding the different cells as species and the diffusion as a mass exchange in the form of a linear reaction, the SQRA scheme corresponds to the gradient structure of the linear reaction system (0.5).

Our starting point was to compare both discretization schemes from the analytical as well as the numerical perspective. In fact, both schemes are special choices of a general class of Stolarsky means, which are defined by

$$S_{\alpha,\beta}(x,y) = \left(\frac{\beta(x^\alpha - y^\alpha)}{\alpha(x^\beta - y^\beta)}\right)^{\frac{1}{\alpha-\beta}}, \quad x, y > 0,\ \alpha, \beta \in \mathbb{R}.$$

As it turns out, the mean for the Scharfetter-Gummel discretization is given by $(\alpha, \beta) = (0, -1)$ and the mean for the SQRA scheme is given by $(\alpha, \beta) = (1, -1)$.

In order to compare different discretization schemes, we rewrite the Fokker–Planck operator to a purely diffusive second order operator, by introducing relative densities

$$U = \frac{u}{\pi}, \quad U_i = \frac{u_i}{\pi_i},$$

which results in

$$-\nabla \cdot (\kappa \pi \nabla U) = f, \quad \text{and} \quad -\sum_{j:\, j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \,(U_j - U_i) = f_i.$$

This reformulation allows for deriving convergence rates independent of the chosen mean if the mesh-discretization is appropriate for the pure Laplace operator. To capture the mesh-discretization, the notion of *consistency* is introduced, which basically ensures a proper finite volume discretization for $-\Delta u = f$ [DiD18]. We show that the convergence rate mainly depends on the mesh-discretization and only secondarily on the chosen

weights. In general, the convergence is of order $O(h)$ and can be improved for cubic grids to $O(h^2)$, where h is given by the mesh size of the discretization. For a comparison between different weights S, we investigate the convergence rate constants. As it turns out, the actual convergence constant depends non-trivially on the chosen Stolarsky mean S. In geometrically simple situations, the multifaceted behavior is indicated in numerical examples.

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Part 1

Coarse-graining via EDP-convergence for linear fast-slow reaction systems

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Electronic version of an article published as: Mathematical Models and Methods in Applied Sciences, Vol. 30, No. 09 (2020), 1765-1807, DOI:10.1142/S0218202520500360

However, the present version contains a corrected version of Lemma 3.4, since in the published version a part of the assumption was mistakenly stated as assertion. The author is grateful to Mark Peletier for spotting this error.

Coarse-graining via EDP-convergence for linear fast-slow reaction systems*

Alexander Mielke† and Artur Stephan‡

Abstract

We consider linear reaction systems with slow and fast reactions, which can be interpreted as master equations or Kolmogorov forward equations for Markov processes on a finite state space. We investigate their limit behavior if the fast reaction rates tend to infinity, which leads to a coarse-grained model where the fast reactions create microscopically equilibrated clusters, while the exchange mass between the clusters occurs on the slow time scale.

Assuming detailed balance the reaction system can be written as a gradient flow with respect to the relative entropy. Focusing on the physically relevant cosh-type gradient structure we show how an effective limit gradient structure can be rigorously derived and that the coarse-grained equation again has a cosh-type gradient structure. We obtain the strongest version of convergence in the sense of the Energy-Dissipation Principle (EDP), namely EDP-convergence with tilting.

1 Introduction

Considering $I \in \mathbb{N}$ particles that interact linearly with each other with given rates A_{ik}, the evolution of the probability or concentration $c_i \in [0,1]$ of a species $i \in \{1,\dots,I\} =: \mathcal{I}$ can be described by the master equation

$$\dot{c} = Ac, \tag{1.1}$$

where A is the adjoint of the Markov generator $\mathcal{L} : \mathbb{R}^I \to \mathbb{R}^I$ of the underlying Markov process, i.e. $A = \mathcal{L}^*$, see e.g. [Dyn65, Bob05, Dur10] for more information. In particular, this means $A_{ki} \geq 0$ for $i \neq k$ and $\sum_{k=1}^I A_{ki} = 0$ for all $i \in \mathcal{I}$. We interpret the master equation as a *rate equation* defined on the state space

$$\mathsf{Q} = \mathrm{Prob}(\mathcal{I}) := \Big\{ c \in [0,1]^I \,\Big|\, \sum\nolimits_{i=1}^I c_i = 1 \Big\} \subset \mathbb{R}^I.$$

*This research has been funded by Deutsche Forschungsgemeinschaft (DFG) through SFB 1114 "*Scaling Cascades in Complex Systems*", Project C05 "Effective Models for Materials and Interfaces with Multiple Scales".

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In many applications the number I of particles can be huge and the reaction coefficients A_{ik} may vary in a huge range. In such cases the analysis or the numerical treatment of system (1.1) is out of reach, and hence suitable simplifications are necessary. One natural assumption is that reactions can happen with different speeds. We will consider the case the slow and fast reactions are distinguished, the slow ones of order 1 and the fast ones of order $1/\varepsilon$ for a small parameter $\varepsilon \to 0$. Hence, we decompose $A = A^\varepsilon$ into $A^\varepsilon = A^S + \frac{1}{\varepsilon}A^F$, "$S$" for slow and "$F$" for fast reactions. Our equation then is ε-dependent and reads

$$\dot{c}^\varepsilon = A^\varepsilon c^\varepsilon = \big(A^S + \frac{1}{\varepsilon}A^F\big)\, c^\varepsilon. \tag{1.2}$$

The limit passage for $\varepsilon \to 0$ in linear and nonlinear slow-fast reaction systems is a well-established field starting from pioneering work by Tikhonov [Tik52] and Fenichel [Fen79]. We refer to [Bot03, DLZ18, Ste19b] for modern approaches and to [KaK13] for nonlinear fast-slow reaction systems under the influence of stochastic fluctuations, see e.g. Example 6.1 there for a mRNA-DNA system for $I = 6$ species with 8 slow reactions and 2 fast reactions.

While we repeat some of these arguments in Section 2, the main goal of this paper is the study of the associated *gradient structures* for (1.2), which exist under the additional assumption that the *detailed-balance condition* holds. The latter condition means that there exists a positive equilibrium state $w^\varepsilon = (w_i^\varepsilon)_{i\in\mathcal{I}} \in \mathsf{Q}$ such that

$$\text{detailed-balance condition (DBC):} \qquad \forall\, i,k \in \mathcal{I}: \quad A_{ik}^\varepsilon w_k^\varepsilon = A_{ki}^\varepsilon w_i^\varepsilon. \tag{1.3}$$

Following [Mie11, Pel14, Mie16], a gradient structure for a rate equation $\dot{c} = V_\varepsilon(c)$ on the state space Q means that there exist a differentiable energy functional $\mathcal{E}_\varepsilon$ and a dissipation potential $\mathcal{R}_\varepsilon$ such that the rate equation can be generated as the associated gradient-flow equation, namely

$$\dot{c} = V_\varepsilon(c) = \mathrm{D}_\xi \mathcal{R}_\varepsilon^*(c, -\mathrm{D}\mathcal{E}_\varepsilon(c)) \quad \text{ or equivalently } \quad 0 = \mathrm{D}_{\dot{c}}\mathcal{R}_\varepsilon(c,\dot{c}) + \mathrm{D}\mathcal{E}_\varepsilon(c). \tag{1.4}$$

Here $\mathcal{R}_\varepsilon$ is called a dissipation potential if $\mathcal{R}_\varepsilon(c,\cdot) : \mathrm{T}_c\mathsf{Q} \to [0,\infty]$ is lower semicontinuous and convex and satisfies $\mathcal{R}_\varepsilon(c,0) = 0$. Then, $\mathcal{R}_\varepsilon^*$ is the (partial) Legendre-Fenchel transform

$$\mathcal{R}_\varepsilon^*(c,\xi) := \sup\big\{\, \langle \xi, v\rangle - \mathcal{R}_\varepsilon(c,v) \,\big|\, v \in \mathrm{T}_c\mathsf{Q} \,\big\}.$$

For reaction systems of mass-action type (which includes all linear systems) satisfying detailed balance, it was shown in [Mie11] that an entropic gradient structure exists, i.e. $\mathcal{E}_\varepsilon$ is the relative Boltzmann entropy $\mathcal{E}_{\mathrm{Bz}}^\varepsilon(c) := \mathcal{H}(c|w^\varepsilon)$ of c with respect to w^ε, see Section 4.3.2. However, this fact was used implicitly in earlier works, see e.g. [ÖtG97, Eqn. (113)] and [Yon08, Sec. VII]. For linear reaction systems, which are master equations for Markov processes, a more general theory was developed in [Maa11, CH*12] leading to a large class of possible gradient structures, see Section 3 and [MaM20, Sec. 2.5].

Here, we use the physically most natural gradient structure that has its origin in the theory of large deviation, see [MPR14, MP*17]. The dual dissipation potentials $\mathcal{R}_\varepsilon^*(c,\cdot) : \mathrm{T}_c\mathsf{Q} \to \mathbb{R}$ are not quadratic but rather exponential due to cosh terms, namely

$$\mathcal{R}_\varepsilon^*(c,\xi) = \frac{1}{2}\sum_{i<k} \kappa_{ik}^\varepsilon \sqrt{c_i c_k}\, \mathsf{C}^*(\xi_i - \xi_k) \quad \text{with } \mathsf{C}^*(\zeta) = 4\cosh(\zeta/2) - 4 \tag{1.5}$$

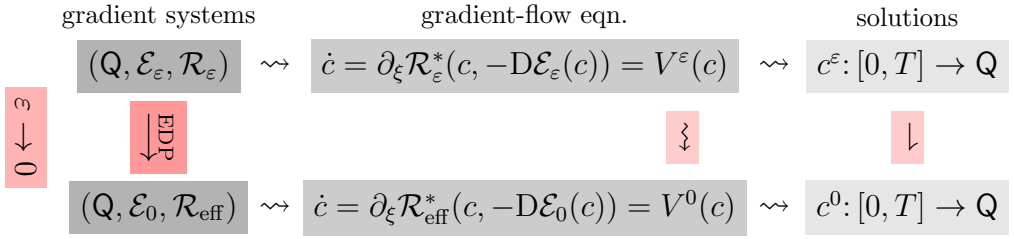


Figure 1: EDP-convergence leads to a commuting diagram, in particular EDP-convergence generates the correct limit equation $\dot c = V^0(c)$ and (subsequences of) the solutions c^ε converge to solutions c^0 of the limit equation. However, $\mathcal{R}_{\mathrm{eff}}$ provides information not contained in the limit equation.

and $\kappa_{ik}^\varepsilon = A_{ik}^\varepsilon\sqrt{w_k^\varepsilon/w_i^\varepsilon}$. The gradient structure $(\mathsf{Q},\mathcal{E}_{\mathrm{Bz}}^\varepsilon,\mathcal{R}_\varepsilon^*)$ exactly generates the gradient-flow evolution (1.2), and we call it simply the *cosh gradient structure*. Note that the dissipation potential $v\mapsto\mathcal{R}_\varepsilon(c,\cdot)$ is still superlinear, but grows only like $|v|\log(1+|v|)$. In particular, $\mathcal{R}_\varepsilon$ does not induce a metric on Q.

This gradient structure is also in line with the first derivation of exponential kinetic relations by Marcellin in 1915, see [Mar15]. Moreover, it arises as effective gradient structure in EDP converging systems, see [LM*17, FrL19]. In [FrM20] it is shown that the exponential function "cosh" arises due to the Boltzmann entropy as inverse of the logarithm. For L^p-type entropies $\mathcal{R}^*$ will have a growth like $|\xi|^{c_0/(p-1)}$.

Instead of passing to the limit $\varepsilon\to 0$ in the equation (1.2), our goal is to perform the limit passage in the gradient system $(\mathsf{Q},\mathcal{E}_{\mathrm{Bz}}^\varepsilon,\mathcal{R}_\varepsilon^*)$ to obtain directly an effective gradient system $(\mathsf{Q},\mathcal{E}_0,\mathcal{R}_{\mathrm{eff}}^*)$ via the notion of EDP-convergence as introduced in [LM*17, DFM19, MMP19]. Roughly spoken this convergence asked for the Γ-convergence of the energies, namely $\mathcal{E}_{\mathrm{Bz}}^\varepsilon\xrightarrow{\Gamma}\mathcal{E}_0$ on Q, and for the dissipation functionals $\mathfrak{D}_\varepsilon\xrightarrow{\Gamma}\mathfrak{D}_0$ on $\mathrm{L}^2([0,T];\mathsf{Q})$ with

$$\mathfrak{D}_\varepsilon(c)=\int_0^T\Big(\mathcal{R}_\varepsilon(c,\dot c)+\mathcal{R}_\varepsilon^*(c,-\mathrm{D}\mathcal{E}_\varepsilon(c))\Big)\,\mathrm{d}t \quad\text{and}$$
$$\mathfrak{D}_0(c)=\int_0^T\Big(\mathcal{R}_{\mathrm{eff}}(c,\dot c)+\mathcal{R}_{\mathrm{eff}}^*(c,-\mathrm{D}\mathcal{E}_0(c))\Big)\,\mathrm{d}t.$$

The notion of EDP-convergence produces a *unique limit gradient system*, and we may have $\mathcal{R}_\varepsilon\xrightarrow{\Gamma}\mathcal{R}_0$ while $\mathcal{R}_{\mathrm{eff}}\neq\mathcal{R}_0$, see [LM*17, DFM19]. As a trivial consequence of EDP-convergence we then find that $0=\mathrm{D}\mathcal{R}_{\mathrm{eff}}(c,\dot c)+\mathrm{D}\mathcal{E}_0(c)$ is the limit equation, cf. Lemma 3.4. In general the limit equation may have many gradient structures. However, we emphasize that constructing $\mathcal{R}_{\mathrm{eff}}$ adds thermodynamical information to the limit equation, since the gradient structure reflects the underlying microscopic properties of the model, see [MPR14, MP*17]. Thus, we turn around the usual limit analysis where one first works on the gradient-flow equations (1.4) and the solutions $c^\varepsilon:[0,T]\to\mathsf{Q}$, and then studies gradient structures for the limit equations. As shown in Figure 1, EDP-convergence works solely on the gradient systems and produces $\mathcal{R}_{\mathrm{eff}}$ as a nontrivial result, which then gives the limit equation and the accumulation points $c^0:[0,T]\to\mathsf{Q}$ of the solutions $c^\varepsilon:[0,T]\to\mathsf{Q}$.

In [LM*17, Sec. 3.3] an example of a simple linear reaction systems (with $I=3$) is considered, where it is shown that the cosh structure is distinguished by the fact that it is the only one that is stable under EDP-convergence. It is one of our major results that

in our situation the same stability is true, i.e. EDP-convergence yields a limit gradient structure of cosh-type again.

We now describe our results more precisely. We mainly work under the assumption that our system (1.2) satisfies the DBC (1.3) for w^ε and assume that $w^\varepsilon \to w^0 \in]0,1[^I$, i.e. all components w_i^0 are positive. Then, clearly A^F satisfies the DBC for w^0. As is shown in Section 2, the fast reactions encoded in A^F separate $\mathcal{I} = \{1,\dots,I\}$ into $J < I$ clusters, and we define a coarse graining operator $M \in \mathbb{R}^{J\times I}$ and a reconstruction operator $N \in \mathbb{R}^{I\times J}$ satisfying

$$MA^F = 0 \in \mathbb{R}^{J\times I}, \quad A^F N = 0 \in \mathbb{R}^{I\times J}, \quad \text{and} \quad MN = \mathrm{id}_{\mathbb{R}^J}.$$

The coarse graining operator M satisfies $M_{ji} \in \{0,1\}$ indicating whether the species i belongs to the cluster j. The limit equation, which is derived in Theorem 2.9 independently of any EDP-convergence for clarity, then reads

$$M\dot c(t) = MA^S c(t) \qquad \text{and} \qquad A^F c(t) = 0. \tag{1.6}$$

Although convergence of solutions of (1.2) is indeed well-known, we added a short proof, as it shows similarities to the proof of EDP-convergence in using complementary information to derive compactness. Using the coarse-grained states $\hat c(t) = Mc(t) \in \hat{\mathsf{Q}} \subset \mathbb{R}^J$ with probabilities $\hat c_j(t)$ for the cluster $j \in \mathcal{J}$ one obtains the coarse-grained linear reaction systems

$$\dot{\hat c}(t) = \hat A\, \hat c(t) \qquad \text{with} \quad \hat A = MA^S N \in \mathbb{R}^{J\times J}. \tag{1.7}$$

See Section 2.4 for a detailed description and an interpretation of the coarse-grained equation.

From the solutions $\hat c$ we obtain all solutions of the limit equation (1.6) via $c(t) = N\hat c(t)$. In fact, setting $\hat w := Mw^0 \in]0,1[^J$ and defining the diagonal mappings $\mathbb{D}_{w^0} = \mathrm{diag}(w_i^0)_{i\in\mathcal{I}}$ and $\mathbb{D}_{\hat w} = \mathrm{diag}(\hat w_j)_{j\in\mathcal{J}}$ the reconstruction operator N is given via $N = \mathbb{D}_{w^0} M^* \mathbb{D}_{\hat w}^{-1}$. The intrinsic definition of N becomes clear from duality theory as $\mathbb{D}_{w^0}$ can be seen as a duality mapping from relative densities $\varrho \in (\mathbb{R}^I)^*$ to concentrations $c \in \mathbb{R}^I$.

$$\begin{array}{ccc} c \in \mathbb{R}^I & \xrightarrow{\mathbb{D}_{w^0}^{-1}} & \varrho \in (\mathbb{R}^I)^* \supset M^*(\mathbb{R}^J)^* \\ M \downarrow \quad \uparrow N & & \uparrow M^* \\ \hat c \in \mathbb{R}^J & \xrightarrow{\mathbb{D}_{\hat w}^{-1}} & \hat\varrho \in (\mathbb{R}^J)^* \end{array}$$

In Section 3 we discuss general gradient systems and define different notions of EDP-convergence as in [DFM19, MMP19], while Section 4 recalls the different possible gradient structures for linear reaction systems satisfying the DBC (1.3). In Section 4.4 we address the important notion of tilting of Markov processes which means the change of the equilibrium measure w into $w^\eta = \frac{1}{Z}\big(\mathrm{e}^{-\eta_i} w_i\big)_{i\in\mathcal{I}}$. It is another remarkable feature of the cosh gradient structure that it is invariant under tilting (see Proposition 4.1).

In Section 5 we present our main result on the EDP-convergence with tilting of the cosh-gradient systems $(\mathsf{Q}, \mathcal{E}_{\mathrm{Bz}}^\varepsilon, \mathcal{R}_\varepsilon^*)$ defined via (1.5). While the Γ-convergence $\mathcal{E}_{\mathrm{Bz}}^\varepsilon \xrightarrow{\Gamma} \mathcal{E}_{\mathrm{Bz}}^0$ follows trivially from $w^\varepsilon \to w^0$, the Γ-convergence $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma} \mathfrak{D}_0$ in $\mathrm{L}^2([0,T],\mathsf{Q})$ is much more delicate. In fact, Theorem 5.3 even provides the Mosco-convergence of $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}} \mathfrak{D}_0$, i.e. (i)

the liminf estimate $\liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) \geq \mathfrak{D}_0(c^0)$ holds even under the weak convergence $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^2([0,T];\mathsf{Q})$ and (ii) for each $c^0 \in \mathrm{L}^2([0,T];\mathsf{Q})$ there exists a recovery sequence $c^\varepsilon \to c^0$ strongly(!) in $\mathrm{L}^2([0,T];\mathsf{Q})$ such that $\limsup_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) \leq \mathfrak{D}_0(c^0)$.

The main point of the result is the exact characterization of $\mathcal{R}_{\mathrm{eff}}$. Indeed, we have

$$\mathfrak{D}_0(c) = \begin{cases} \displaystyle\int_0^T \Big(\mathcal{R}_{\mathrm{eff}}(c,\dot c) + \mathcal{R}^*_{\mathrm{eff}}(c, -\mathrm{D}\mathcal{E}^0_{\mathrm{Bz}}(c)) \Big)\,\mathrm{d}t & \text{for } c \in \mathrm{W}^{1,1}([0,1];P\mathsf{Q}), \\ \infty & \text{otherwise in } \mathrm{L}^2([0,1];\mathsf{Q}), \end{cases}$$

where, for $c \in P\mathsf{Q}$ the effective dissipation potential $\mathcal{R}_{\mathrm{eff}}$ is given by

$$\mathcal{R}^*_{\mathrm{eff}}(c,\xi) = \mathcal{R}^*_S(c,\xi) + \chi_{M^*(\mathbb{R}^J)^*}(\xi) \quad \text{or equivalently} \quad \mathcal{R}_{\mathrm{eff}}(c,v) = \inf_{z\in\mathbb{R}^I : Mz = Mv} \mathcal{R}_S(c,z).$$

Here $P = NM$ is the projection mapping general $c \in \mathsf{Q}$ into microscopically equilibrated reactions $c = N\hat c$ with $\hat c = Mc$, and $\mathcal{R}^*_S$ is the dual dissipation potential defined as in (1.5) but using only the slow reactions. Finally, the characteristic function χ_Ξ is 0 for $\xi \in \Xi$ and ∞ else. The condition $\chi_\Xi(-\mathrm{D}\mathcal{E}^0_{\mathrm{Bz}}(c)) < \infty$ is in fact equivalent to $c \in P\mathsf{Q}$ (see Section 5.2).

It is easy to see that the degenerate gradient system $(\mathsf{Q}, \mathcal{E}^0_{\mathrm{Bz}}, \mathcal{R}^*_{\mathrm{eff}})$ generates exactly the limit equation (1.6). Moreover, using the bijective linear mapping $M : P\mathsf{Q} \to \hat{\mathsf{Q}} := \big\{ \hat c \in [0,1]^J \,\big|\, \hat c_1 + \cdots + \hat c_J = 1 \big\} \subset \mathbb{R}^J$ with inverse $N : \hat{\mathsf{Q}} \to P\mathsf{Q} \subset \mathbb{R}^I$ we can define the coarse-grained gradient system $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ for the coarse-grained states $\hat c = Mc$ via

$$\hat{\mathcal{E}}(\hat c) = \mathcal{E}^0_{\mathrm{Bz}}(N\hat c), \quad \hat{\mathcal{R}}(\hat c, \hat v) = \mathcal{R}_{\mathrm{eff}}(N\hat c, N\hat v), \quad \hat{\mathcal{R}}^*(\hat c, \hat\xi) = \mathcal{R}^*_{\mathrm{eff}}(N\hat c, M^*\hat\xi).$$

The construction and the explicit formula for $\mathcal{R}^*_{\mathrm{eff}}$ yield that $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ is again a cosh gradient structure and the associated gradient-flow equation is the coarse-grained equation (1.7), see Proposition 5.7.

This is indeed a rigorous coarse-graining in the sense of [MaM20, Sec. 6.1]. This paper is intended to be an easy-to-understand first result for more general results for EDP-convergence that will finally cover nonlinear reaction systems [MPS20] (where the coarse-graining procedure based on Markov operators does not work) and reaction-diffusion systems as in [FrL19, FrM20] and [Ste20] (where also the reaction fluxes are coarse-grained and reconstructed). We expect that the cosh gradient structure will also be stable in these more general situations.

2 Fast-slow reaction network

On $\mathsf{Q} := \mathrm{Prob}(\mathcal{I}) := \big\{ c \in [0,1]^I \,\big|\, \sum_{i\in\mathcal{I}} c_i = 1 \big\} \subset X := \mathbb{R}^I$ we consider the Kolmogorov forward equation or master equation

$$\dot c = Ac \quad \text{with} \quad A \in \mathbb{R}^{I\times I},$$

where A is the adjoint of a Markov generator, i.e.

$$A_{ik} \geq 0 \quad \text{for all } i \neq k \quad \text{and} \quad \forall\, k \in \mathcal{I} : \quad 0 = \sum\nolimits_{i=1}^I A_{ik}.$$

Some comments on the notation are in order. Usually, in the theory of Markov operators and stochastic processes the state space is the set of probability measures which is a

subset of the dual space of continuous functions. So it would be more convenient to denote the space of interest by X^* and not X. Certainly, since we are dealing with finite dimensional spaces, both are isomorphic and the notation is just a question of manner. In that paper, the master equation is understood as a *rate equation* of a gradient system in the sense of Section 3 which is an equation in X. Strictly speaking, the operator A is the adjoint of a Markov generator $\mathcal{L}$ which generates a semigroup of Markov operators $\mathrm{e}^{t\mathcal{L}} : X^* \to X^*$. By definition, a Markov operator $M^* : X^* \to Y^*$ on a finite dimensional state space maps positive vectors on positive vectors and the constant one vector $\mathbb{1}_{X^*}$ to a constant one vector $\mathbb{1}_{Y^*}$. Its adjoint maps the set of probability vectors onto the set of probability vectors.

The linear reactions given by A, naturally define a graph or reaction network, where edges e_{ik} from node x_i to node x_k correspond to the entries $A_{ik} > 0$. The graph is directed, i.e. edges e_{ik} and e_{ki} are different and have an orientation. We assume that A is irreducible, which means that the corresponding graph is irreducible, or in other words, that any two nodes are connected via a directed path. This implies that there is a unique steady state $w \in \mathrm{Prob}(\mathcal{I})$ which is positive, i.e. $w_j > 0$ for all $j \in \mathcal{I}$, see e.g. [Dur10].

The crucial assumption for our systems is the following symmetry condition. The Markov process satisfies is called to satisfy the *detailed-balance condition* (DBC) with respect to its stationary measure $w > 0$, if $A_{ik}w_k = A_{ki}w_i$ for all $i, k \in \mathcal{I}$. Assuming detailed balance, the evolution equation $\dot{c} = Ac$, which is an equation on X, can also be written in another form. Let us introduce the duality operator

$$\mathbb{D}_w = \mathrm{diag}(w) : \left\{ \begin{array}{ccc} X^* & \to & X, \\ \varrho & \mapsto & c = \mathbb{D}_w \varrho \end{array} \right. \qquad \text{and} \qquad X \ni c \xrightarrow{\mathbb{D}_w^{-1}} \varrho \in X^*.$$

Hence, $\mathbb{D}_w$ maps the relative densities ϱ to the concentrations c, i.e. $c_i = \varrho_i w_i$. The linear master equation can now be written as

$$\dot{c} = B\varrho \quad \text{with } B = A\mathbb{D}_w \,.$$

Because of the DBC, $B = A\mathbb{D}_w : X^* \to X$ is a symmetric operator on X, i.e. $B^* = B$.

For our slow-fast systems, we introduce a scaling parameter $1/\varepsilon$ for $\varepsilon > 0$ and the rates A_{ik} on the right-hand side decompose into $A = A^\varepsilon = A^S + \frac{1}{\varepsilon}A^F$, where "$S$" stands for slow and "$F$" for fast reactions. Our equation is ε-dependent and reads

$$\dot{c}^\varepsilon = A^\varepsilon c^\varepsilon = (A^S + \frac{1}{\varepsilon}A^F)c^\varepsilon. \tag{2.1}$$

The aim of the paper is to investigate the system in the limit $\varepsilon \to 0$. To do this, some assumptions on the ε-dependent reaction network are needed.

2.1 Assumptions on the ε-dependency of the network

Our paper will be restricted to the case where the stationary measure $w^\varepsilon \in \mathsf{Q}$ converges to a positive limit measure $w^\varepsilon \to w^0 \in]0,1[^I$:

For all $\varepsilon > 0$, the reaction graph defined by A^ε is connected. Moreover, if there is a transition from state i to k (i.e. $A_{ki} > 0$), then there is also a transition backwards from k to i. (2.Aa)

For all $\varepsilon > 0$ there is a unique and positive stationary measure $w^\varepsilon \in \mathsf{Q}$, and the stationary measure converges $w^\varepsilon \to w^0$, where w^0 is positive. (2.Ab)

(DBC): For all $\varepsilon > 0$ the detailed-balance condition with respect to w^ε holds, i.e. $A^\varepsilon_{ik} w^\varepsilon_k = A^\varepsilon_{ki} w^\varepsilon_i$ for all $i,k \in \mathcal{I}$. (2.Ac)

These three conditions are not independent of each other, but it is practical to state them as above. In particular, if (2.Aa) and the DBC (2.Ac) hold, then (2.Ab) follow, which is the content of the following results. See [Ste19a] and the references therein for generalizations.

Proposition 2.1. *Let the reaction network satisfy* (2.Aa) *and* (2.Ac) *and define, for transitions according* (2.Aa)*, the transition quotients*

$$q^\varepsilon_{ik} = \frac{A^\varepsilon_{ik}}{A^\varepsilon_{ki}} = \frac{A^S_{ik} + \frac{1}{\varepsilon} A^F_{ik}}{A^S_{ki} + \frac{1}{\varepsilon} A^F_{ki}} \,.$$

If there is a (universal) bound $q^* < \infty$ such that for all transitions from i to k and for all $\varepsilon \ge 0$ the transition quotients q^ε_{ik} satisfy $1/q^* \le q^\varepsilon_{ik} \le q^*$, then w^ε converges and its limit w^0 is positive, i.e. (2.Ab) *holds.*

Proof. Using the DBC (2.Ac), the stationary measure w^ε only depends on the transition quotient q^ε_{ik}. Hence, each $\varepsilon \mapsto w^\varepsilon_i \in [0,1]$ is a rational polynomial in ε and thus converges to w^0_i with $w^0 \in \mathsf{Q} = \mathrm{Prob}(\mathcal{I})$ with polynomial dependency on $\varepsilon > 0$. Moreover, $q^\varepsilon_{ik} = 1/q^\varepsilon_{ki}$ converges to $q^0_{ik} \in [1/q^*, q^*]$. Since the limit w^0 again depends only q^0_{ik}, we conclude that it is positive. □

We now comment on the relevance of the above assumptions and give two nontrivial examples.

Remark 2.2.

(a) In the chemical literature, our assumption (2.Aa) is often called (weak) *reversibility*. It implies already that the stationary measure w^ε for A^ε is unique and positive.

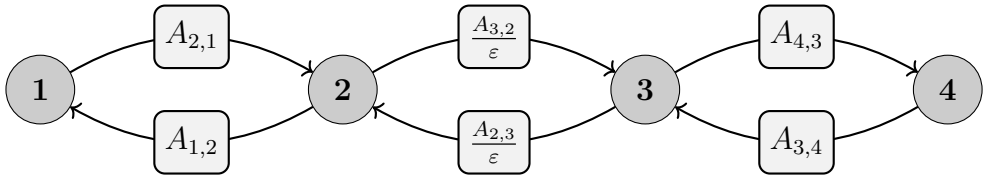
(b) The assumptions in Proposition 2.1 say that the quotients q^ε_{ij} are bounded even for $\varepsilon \to 0$ and hence, they converge. In particular, this means that if there is a fast reaction $A^F_{ik} \ne 0$ then necessarily also the backward reaction is fast, i.e. $A^F_{ki} \ne 0$. So, the graph does not change its topology in the limit process $\varepsilon \to 0$. Without this assumption the mass w^ε_i may vanish for some species i, see Example 2.3(b). This case is more delicate and will be considered in subsequent work.

(c) It was observed in [Yon08, Mie11] that reaction systems of mass-action type have an entropic gradient structure, if the DBC holds. For linear reaction systems this was independently found in [Maa11, CH*12]. However, our work will not use the quadratic gradient structure derived in the latter works, but will rely on the cosh-type generalized gradient structure derived in [MPR14, MP*17], see Section 4.

(d) Assuming (2.Aa), (2.Ac), and additionally that the reaction quotients q_{ik}^{ε} scale either with 1 or with $1/\varepsilon$, i.e. $A_{ik}^F \neq 0 \Rightarrow A_{ik}^S = 0$, then the transition quotients q_{ik}^{ε} are ε-independent. In particular, the stationary measure w_ε as well as the energy $\mathcal{E}_\varepsilon$ (see Section 4.2) are independent of ε.

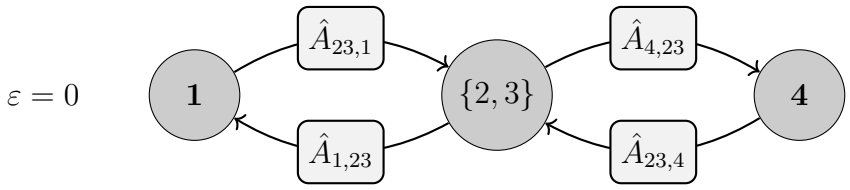
Example 2.3. We discuss two cases highlighting the relevance of our assumptions.

(a) A prototype example is the following, where four states are involved:

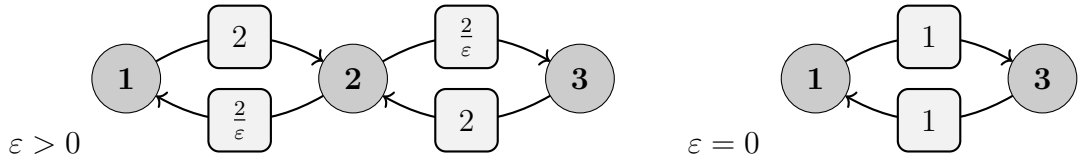


As in all reaction chains, this example satisfies the DBC (2.Ac).

We observe that the reaction rates A_{ik}^{ε} scale either with 1 or with $1/\varepsilon$ and hence, the reaction ratios as well as the stationary measure do not depend on ε, see Remark 2.2(d). Hence, the assumptions (2.A) are satisfied. We expect that in the limit $\varepsilon \to 0$ a local equilibrium between the states 2 and 3 occur, which means that the system can be described by only three states.



(b) In [LM*17], the authors considered the following reaction chain:



The DBC (2.Ac) is again satisfied. The stationary measure is $w_\varepsilon = \frac{1}{2+\varepsilon}(1, \varepsilon, 1)$. The transition quotients are $q_{12}^{\varepsilon} = \varepsilon$ and $q_{23}^{\varepsilon} = \frac{1}{\varepsilon}$, which converge to 0 or ∞, respectively. Hence assumption (2.Ab) is violated. In fact the limit stationary measure is $w^0 = (\frac{1}{2}, 0, \frac{1}{2})$, which is no longer strictly positive. In [LM*17, Sec. 3.3] the EDP-convergence is performed for different gradient structures and only the cosh-gradient structure as defined in Section 4.3.3 turned out to be stable.

2.2 Capturing the states connected by fast reactions

In the limit species which are connected by fast reactions have to be treated like one large particle. Let $i_1 \sim_F i_2$ denote the relation if states i_1 and i_2 are connected via fast reactions. Assumptions (2.Aa),(2.Ab),(2.Ac) guarantees that $\sim_F$ defines an equivalence relation on $\mathcal{I}$ and decomposes $\mathcal{I}$ into different equivalence classes $\mathcal{J} := \{\alpha_1, \dots, \alpha_J\}$, where the index of $\sim_F$, i.e. the number of (different) equivalence classes, is denoted by

J. By definition all α_j are non-empty. Obviously, we have $1 \le J \le I$. In particular, $J = I$ means that there are no fast reactions; $J = 1$ means that each two species are connected via at least one reaction path consisting only of fast reactions. Let $\phi : \{1, \dots, I\} \to \{\alpha_1, \dots, \alpha_J\}$ be the function, which maps a state i to its equivalence class α_j, i.e. $i \mapsto \phi(i) = [i]_{\sim_F} = \alpha_j$. To make notation simpler, we denote the set of equivalence classes by $\mathcal{J} = \{1, \dots, J\}$ and further use $j \in \mathcal{J}$ and $i \in \mathcal{I}$.

The function $\phi : \mathcal{I} \to \mathcal{J}$ defines a deterministic Markov operator $M^* : Y^* \to X^*$, where Y^* is a J-dimensional real vector space, by

$$(M^*\hat{\varrho})_i := \hat{\varrho}_{\phi(i)}, \qquad \hat{\varrho} \in Y^*,\ i \in \mathcal{I}.$$

Deterministic Markov operator means that its dual $M : X \to Y$ maps pure concentrations, i.e. unit vectors e_i, to pure concentrations.

Some facts on deterministic Markov operators are in order. Clearly for a deterministic Markov operator it holds $M^*(\hat{\varrho} \cdot \hat{\psi}) = M^*\hat{\varrho} \cdot M^*\hat{\psi}$ where the multiplication is meant pointwise. (This, by the way, characterizes all deterministic Markov operator.) We want to write the multiplicative relation in form of operators. To do this let us define the multiplication by $\hat{\varrho}$ as $\Pi_{\hat{\varrho}} : Y^* \to Y^*$, with $(\Pi_{\hat{\varrho}}\hat{\psi})_j = \hat{\varrho}_j \cdot \hat{\psi}_j$. Hence, we conclude for a deterministic Markov operator that $M^*\Pi_{\hat{\varrho}} = \Pi_{M^*\hat{\varrho}}M^*$. Dualizing this equation, we get $\Pi^*_{\hat{\varrho}}M = M\Pi^*_{M^*\hat{\varrho}}$. Note, that the adjoint operator has a simple form: $\Pi^*_{\hat{\varrho}} : Y \to Y$, $\Pi^*_{\hat{\varrho}}\hat{c} = \mathbb{D}_{\hat{c}}\hat{\varrho}$. So summarizing

$$\Pi^*_{\hat{\varrho}}M = M\Pi^*_{M^*\hat{\varrho}} \qquad \text{and} \qquad \Pi^*_{\hat{\varrho}}\hat{c} = \mathbb{D}_{\hat{c}}\hat{\varrho}. \tag{2.3}$$

In the limit process the species connected by fast reactions are identified. This is done by a linear *coarse-graining-operator*, which is the adjoint of M^*, $M : X \to Y$. In matrix representation induced by the canonical basis, we have

$$M : X \approx \mathbb{R}^I \to Y \approx \mathbb{R}^J, \quad M_{ji} := \begin{cases} 1, & \text{for } \ i \in \alpha_j, \\ 0, & \text{otherwise .} \end{cases}$$

Note that the construction is such that M maps $X \supset \mathrm{Prob}(\mathcal{I})$ onto $Y \supset \mathrm{Prob}(\mathcal{J})$. Since for α_j there is at least one i with $i \in \alpha_j$, the matrix of M has full rank and each column is a unit vector. Moreover, we point out that M and M^* only depend on the reaction network topology and the locations of the fast reactions, the specific reaction rates A_{ij} do not matter (see Example 2.6 below).

2.3 Properties of the coarse-graining operator M and the reconstruction operator N

Recall the duality map $\mathbb{D}_{w^0}$, which is a represented by a diagonal matrix with entries $w^0 > 0$, connects the concentrations and the relative densities, i.e.

$$\varrho \in X^* \xrightarrow{\mathbb{D}_{w^0}} c \in X.$$

The subset of X^* which consists of the equilibrated densities ϱ_i is denoted by X^*_{eq}, i.e.

$$X^*_{\mathrm{eq}} := \big\{\, \varrho \in X^* \,\big|\, \forall\, i_1 \sim_F i_2 :\ \varrho_{i_1} = \varrho_{i_2} \,\big\}.$$

For the limit system, we define the stationary measure (denoted by $\hat{w}$) by $\hat{w} = Mw^0$. Since M^* is a deterministic Markov operator, we have the following characterization of the multiplication operator induced by $\hat{w}$.

Lemma 2.4. *Let $M^* : Y^* \to X^*$ be a deterministic Markov operator induced by a function $\phi : \{1,\dots,I\} \to \{1,\dots,J\}$ and let $w \in X$. Then $Mw = \hat{w}$ if and only if $\mathbb{D}_{\hat{w}} = M\mathbb{D}_w M^*$.*

Proof. Assume that $\mathbb{D}_{\hat{w}} = M\mathbb{D}_w M^*$ holds. Evaluating both sides at the constant vector $\mathbb{1}_{Y^*}$, we get $\mathbb{D}_{\hat{w}}\mathbb{1}_{Y^*} = \hat{w}$ and $M\mathbb{D}_w M^*\mathbb{1}_{Y^*} = M\mathbb{D}_w\mathbb{1}_{X^*} = Mw$, since M^* is a Markov operator which maps $\mathbb{1}_{Y^*} \mapsto \mathbb{1}_{X^*}$. This proves the claim in one direction.

Assume $\hat{w} = Mw$ we have to show that $\mathbb{D}_{Mw} = M\mathbb{D}_w M^*$. We use statement (2.3) for deterministic Markov operators and find $\mathbb{D}_{Mw}\hat{\varrho} = \Pi^*_{\hat{\varrho}} Mw = M\Pi^*_{M^*\hat{\varrho}} w = M\mathbb{D}_w M^*\hat{\varrho}$. □

If M^* is not a deterministic Markov operator but a general one, then the above relation will not hold.

We assumed that all equivalence classes α_j are non-empty and hence, each row of M has at least one entry "1". In particular, this implies that $\hat{w}$ is strictly positive and hence, $\mathbb{D}_{\hat{w}}$ is invertible. In particular, we proved that the following diagram commutes:

$$\begin{array}{ccc} c \in X & \xrightarrow{\mathbb{D}_{w^0}^{-1}} & \varrho \in X^* \supset X^*_{\mathrm{eq}} = \left\{ \varrho \in X^* \,\middle|\, \forall\, i_1 \sim_F i_2 :\ \varrho_{i_1} = \varrho_{i_2} \right\} \\ {\scriptstyle M}\downarrow & & \uparrow{\scriptstyle M^*} \\ \hat{c} \in Y & \xrightarrow{\qquad\qquad \mathbb{D}_{\hat{w}}^{-1} \qquad\qquad} & Y^* \end{array}$$

The crucial object is the following operator $N : Y \to X$, which "inverts" the coarse-graining operator $M : X \to Y$, by mapping coarse-grained concentrations $\hat{c} \in Y$ to concentrations $c \in X$ (see also [Ste13], where the operator is introduced for its connection to the direction of time). We call N a *reconstruction operator* as it reconstructs the full information on the density $c \in X$ from the coarse-grained vector $\hat{c} \in Y$ assuming, of course, microscopic equilibrium. More precisely, N is defined via

$$N := \mathbb{D}_{w^0} M^* \mathbb{D}_{\hat{w}}^{-1} : Y \to X \quad \text{such that} \quad N^* = \mathbb{D}_{\hat{w}}^{-1} M \mathbb{D}_{w^0} : X^* \to Y^*. \tag{2.4}$$

The operator N and its adjoint N^* have several important properties which are summarized in the next proposition, which is independent of the generators $A^\varepsilon = A^S + \frac{1}{\varepsilon}A^F$.

Proposition 2.5. *Let $M^* : Y^* \to X^*$ be a deterministic Markov operator as in Lemma 2.4 with adjoint $M : X \to Y$ and let $\hat{w} := Mw^0$ for some $w^0 \in]0,1[^I \subset \mathsf{Q}$. Moreover, N and N^* be defined as in (2.4), then the following holds:*

1. *N^* is a Markov operator.*
2. *$MN = \mathrm{id}_Y$ or $N^*M^* = \mathrm{id}_{Y^*}$, i.e. N^* is a left-inverse of the Markov operator M^*.*
3. *NM is a projection on X, which leaves the range of $\mathbb{D}_{w^0}M^* : Y^* \to X$ invariant. The adjoint M^*N^* is a projection as well, which leaves the range of M^* invariant.*
4. *$N\hat{w} = w^0$, i.e. N inverts w.r.t. the stationary measure.*
5. *The operator $P^* := M^*N^*$ is a Markov operator on X^* and its adjoint $P = NM$ has the stationary measure w^0. Moreover, P^* satisfies detailed balance w.r.t. w^0.*

Proof. Clearly, N^* is non-negative and $N^*\mathbb{1}_{X^*} = \mathbb{D}_{\hat{w}}^{-1} M \mathbb{D}_{w^0} \mathbb{1}_{X^*} = \mathbb{D}_{\hat{w}}^{-1} M w^0 = \mathbb{1}_{Y^*}$ holds. This proves the first statement.

Lemma 2.4 implies that $MN = \mathrm{id}_Y$ and that NM is a projection on X, which leaves the range of $\mathbb{D}_{w^0} M^* : Y^* \to X$ invariant. The fourth claim is also trivial. It is also not hard to see that P^* is a Markov operator and that its adjoint has the stationary measure w^0. Moreover, detailed balance holds:

$$\mathbb{D}_{w^0} P^* = \mathbb{D}_{w^0} M^* N^* = \mathbb{D}_{w^0} M^* \mathbb{D}_{\hat{w}}^{-1} M \mathbb{D}_{w^0} = NM \mathbb{D}_{w^0} = P \mathbb{D}_{w^0}.$$

This proves the result. □

The following example shows how the operators look like in a specific case.

Example 2.6. For the reaction network in Example 2.3(a) we have $I = 4$ with only one fast reaction $2 \sim_F 3$, hence $J = 3$. Using the numbering $\alpha_1 = \{1\}$, $\alpha_2 = \{2, 3\}$, and $\alpha_3 = \{4\}$ and the stationary measures $w = (w_1, w_2, w_3, w_4)^\top \in X$ and $\hat{w} = (w_1, w_2{+}w_3, w_4)^\top \in Y$, respectively, we find

$$M = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \; N = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{w_2}{w_2+w_3} & 0 \\ 0 & \frac{w_3}{w_2+w_3} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \text{ and } P = NM = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{w_2}{w_2+w_3} & \frac{w_2}{w_2+w_3} & 0 \\ 0 & \frac{w_3}{w_2+w_3} & \frac{w_3}{w_2+w_3} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

2.4 The limit equation and the coarse-grained equation

As a direct consequence of Proposition 2.5 we obtain a decomposition of the state space $X \approx \mathbb{R}^I$ into the microscopically equilibrated states

$$c = Pc \in \mathsf{Q}_{\mathrm{eq}} := P\mathsf{Q} \subset X_{\mathrm{eq}} := PX = \big\{ c \in X \,\big|\, A^F c = 0 \big\},$$

which are measures having constant density with respect to w^0, and a component $(I{-}P)c \in X_{\mathrm{fast}} := (I{-}P)X$ that disappears exponentially on the time scale of the fast reactions. We emphasize that the following result does not use the DBC (2.Ac).

Proposition 2.7. *Under the assumptions* (2.Aa)–(2.Ab) *we have*

$$PA^F = A^F P = 0 \in \mathbb{R}^{I\times I}, \quad MA^F = 0 \in \mathbb{R}^{J\times I}, \quad A^F N = 0 \in \mathbb{R}^{I\times J}, \tag{2.5a}$$

$$X = X_{\mathrm{eq}} \oplus X_{\mathrm{fast}} \quad \textit{with} \tag{2.5b}$$

$$X_{\mathrm{eq}} = \mathrm{kernel}(A^F) = \mathrm{range}(P) = \mathrm{range}(N) \textit{ and} \tag{2.5c}$$

$$X_{\mathrm{fast}} = \mathrm{range}(A^F) = \mathrm{kernel}(P) = \mathrm{kernel}(M). \tag{2.5d}$$

Here, X_{fast} depends on M only, i.e. only on the reaction graph of A^F, whereas X_{eq} depends on A^S and A^F through w^0.

Proof. By construction of M from the reaction network induced by A^F we immediately obtain $\mathrm{range}(A^F) = \mathrm{kernel}(M)$. Indeed, the entries of M are all 0 or 1, where the jth row contains only the entry 1 exactly for $i \in \alpha(j)$. Thus, these 1s correspond to the mass conservation in the corresponding equivalence class $\alpha(j) \subset \{1, \dots, I\}$, and $MA^F = 0$ follows, which implies $\mathrm{range}(A^F) \subset \mathrm{kernel}(M)$. Dimension counting gives the desired equality.

Using the injectivity of N and $P = NM$ we have shown (2.5d).

To establish the relation for $X_{\rm eq}$ it suffices to show kernel$(A^F) =$ range(N), since the surjectivity of M and $P = NM$ gives range$(N) =$ range(P).

Using the dimension counting it is even sufficient to show $A^F N = 0$. Firstly, we use $0 = A^\varepsilon w^\varepsilon = (A^S + \frac{1}{\varepsilon} A^F) w^\varepsilon$, which gives $A^F w^\varepsilon \to 0$. Hence, $A^F w^0 = 0$. Moreover, we observe that the jth column of $N = \mathbb{D}_{w^0} M^* \mathbb{D}_{\hat w}$ contains the unique equilibrium measure associated with the equivalence class $\alpha(j) \subset \{1, \dots, I\}$, which implies that $A^F N = 0$. □

Based on the above result we can formally pass to the limit in our linear reaction system $\dot c^\varepsilon = (A^S + \frac{1}{\varepsilon} A^F) c^\varepsilon$. Multiplying the equation from the left by M we can use $MA^F = 0$ and see that the term of order $\frac{1}{\varepsilon}$ disappears. Moreover, it is expected that the fast reactions equilibrate, so in the limit $\varepsilon \to 0$ we expect the microscopic equilibrium condition $A^F c^\varepsilon \to 0$. Hence, we expect that $c^\varepsilon : [0,T] \to \mathsf{Q}$ converges to a function $c^0 : [0,T] \to \mathsf{Q}$ which solves the limit equation

$$M\dot c(t) = MA^S c(t) \quad \text{and} \quad A^F c(t) = 0. \tag{2.6}$$

Before giving a proof for the convergence $c^\varepsilon \to c$ we want state that this system has a unique solution for each initial condition $c(0)$ that is compatible, i.e. $A^F c(0) = 0$ and that this solution is characterized by solving the so-called *coarse-grained equation*.

Theorem 2.8 (Coarse-grained equation)**.** *For each $c_0 \in \mathsf{Q}$ with $A^F c_0 = 0$ there is a unique continuous solution $c : [0,T] \to \mathsf{Q}$ of (2.6) with $c(0) = c_0$. This solution is obtained by solving the coarse-grained ODE*

$$\dot{\hat c} = MA^S N\, \hat c, \quad \hat c(0) = Mc_0 \tag{2.7}$$

and setting $c(t) = N\hat c(t)$. Moreover, the stationary solution is $\hat w = Mw^0$.

Proof. On the one hand, by (2.5c) we know that $A^F c = 0$ is equivalent to $c = Pc = NMc$. Thus, for any solution c of (2.6) the coarse-grained state $\hat c = Mc$ satisfies the coarse-grained equation (2.7).

On the other hand, (2.7) is a linear ODE in $\hat{\mathsf{Q}} \subset Y$ which has a unique solution satisfying $\hat c(t) \in \hat{\mathsf{Q}}$. This proves the first result.

To see that $\hat w = Mw^0$ is a stationary measure, we use $A^F w^0 = 0$ and (2.5b) implies $Pw^0 = w^0$. On the other hand using $MA^F = 0$ we can pass to the limit in $0 = M0 = MA^\varepsilon w^\varepsilon = MA^S w^\varepsilon$ to obtain $MA^S w^0 = 0$. Combing the two results we find

$$\hat A \hat w = MA^S N(Mw^0) = MA^S\, Pw^0 = MA^S w^0 = 0,$$

which is the desired result. □

We emphasize that the coarse-grained equation (2.7) is again a linear reaction system, describing the master equation for a Markov process on $\mathcal{J} = \{1, \dots, J\}$. The effective operator $\hat A := MA^S N$ can be interpreted in the following way: N divides the coarse-grained states into microscopically equilibrated states, A^S is the part of the slow reactions, and M collects the states according to their equivalence classes $\alpha(j)$.

Using $M_{ji} = \delta_{j\phi(i)}$ and $N_{ij} = \frac{w_i^0}{\hat w_j} \delta_{j\phi(i)}$ the coefficients of the generator $\hat A = MA^S N$ are easily obtained by a suitable average, namely

$$\hat A_{j_1 j_2} = \sum_{i_1 \in \alpha_{j_1}} \sum_{i_2 \in \alpha_{j_2}} A^S_{i_1 i_2} \frac{w^0_{i_2}}{\hat w_{j_2}}. \tag{2.8}$$

2.5 Convergence of solutions on the level of the ODE

Finally, for mathematical completeness, we provide a simple and short convergence proof. It can also be obtained as a special case of the result in [Bot03]. Of course, the convergence of solutions is also a byproduct of the EDP-convergence given below, see Lemma 3.4. The latter result, which is the main goal of this work, provides convergence of the gradient structures, which is a significantly stronger concept, because the coarse-grained equation (2.7) has many different gradient structures, while the EDP-limit is unique.

Theorem 2.9 (Convergence of c^ε to c^0)**.** *Assume* (2.A) *and consider solutions* $c^\varepsilon : [0,T] \to \mathsf{Q}$ *of* (1.2) *such that* $Mc^\varepsilon(0) \to \hat{c}_0$*. Then, we have the convergences*

$$Mc^\varepsilon \to Mc^0 \text{ in } \mathrm{C}^0([0,T];X) \qquad \text{and} \qquad c^\varepsilon \to c^0 \text{ in } \mathrm{L}^2([0,T];X),$$

where c^0 *is the unique solution of* (2.6) *with* $c^0(0) = N\hat{c}_0$*.*

Proof. Step 1: Weak compactness. We first observe that $c^\varepsilon : [0,T] \to \mathsf{Q} \subset [0,1]^I$ provides a trivial a priori bound for c^ε in $\mathrm{L}^\infty([0,T];\mathbb{R}^I)$. Hence, we may choose a subsequence (not relabeled) such that $c^\varepsilon \to c^0$ weakly in $\mathrm{L}^2([0,T];\mathbb{R}^I)$.

Step 2: Compactness of coarse-grained concentrations. With Step 1 we see that $\hat{a}^\varepsilon := Mc^\varepsilon$ is bounded in $\mathrm{C}^{\mathrm{Lip}}([0,T];\mathbb{R}^I)$, because of $\dot{\hat{a}}^\varepsilon = M\dot{c}^\varepsilon = MA^S c^\varepsilon$. Thus, there is a subsequence (not relabeled) such that $\hat{a}^\varepsilon \to \hat{a}^0$ in $\mathrm{C}^0([0,T];\mathbb{R}^J)$ and $\hat{a}^0(0) = \hat{c}_0$. Moreover, with Step 1 we have $\hat{a}^0 = Mc^0$.

Step 3: Generation of microscopic equilibrium. We take the dot product of the ODE with the vector of relative densities $c^\varepsilon/w^\varepsilon := (c_i^\varepsilon/w_i^\varepsilon)_{i=1,..,I}$. Defining the quadratic form $\mathcal{B}_\varepsilon(c) = \sum_{i=1}^I \frac{c_i^2}{2w_i^\varepsilon}$ we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{B}_\varepsilon(c^\varepsilon) = \dot{c}^\varepsilon \cdot \frac{c^\varepsilon}{w^\varepsilon} = \big(A^\varepsilon c^\varepsilon\big) \cdot \frac{c^\varepsilon}{w^\varepsilon} = \frac{1}{\varepsilon}\big(B^\varepsilon c^\varepsilon\big) \cdot c^\varepsilon \quad \text{with } \varepsilon \mathbb{D}_{w^\varepsilon}^{-1} A^\varepsilon =: B^\varepsilon = (B^\varepsilon)^* \geq 0. \tag{2.9}$$

The latter relations follow from the DBC (2.Ac). Defining the quadratic functional $\mathfrak{Q}_\varepsilon(c) := \int_0^T B^\varepsilon c(t) \cdot c(t) \mathrm{d}t$ and integrating (2.9) over $[0,T]$ gives

$$\mathfrak{Q}_\varepsilon(c^\varepsilon) = \varepsilon \mathcal{B}(c^\varepsilon(0)) - \varepsilon \mathcal{B}(c^\varepsilon(T)) \leq C_1 \varepsilon.$$

Moreover, using $|w^\varepsilon - w^0| \leq C_2\varepsilon$ we find $|\mathfrak{Q}_\varepsilon(c) - \mathfrak{Q}_0(c)| \leq C_3\varepsilon$. Hence $\mathfrak{Q}_0(c^\varepsilon) \leq \mathfrak{Q}_\varepsilon(c^\varepsilon) + C_3\varepsilon \leq C_1\varepsilon + C_3\varepsilon$. Using the convexity of $\mathfrak{Q}_0$ the weak limit c^0 of c^ε satisfies

$$0 \leq \mathfrak{Q}_0(c^0) \leq \liminf_{\varepsilon \to 0} \mathfrak{Q}_0(c^\varepsilon) \leq \liminf_{\varepsilon \to 0} (C_1 + C_3)\varepsilon = 0.$$

Since $B^0 = \mathbb{D}_{w^0}^{-1} A^F$ is symmetric and positive semidefinite we conclude $A^F c^0(t) = 0$ a.e. in $[0,T]$. More precisely, by (2.5d) $c \mapsto \big(B^0 c \cdot c\big)^{1/2}$ defines a norm on X_{fast} that is equivalent to $c \mapsto |(I-P)c|$. Thus, we conclude $(I-P)c^\varepsilon \to (I-P)c^0$. Moreover, Step 2 gives $Pc^\varepsilon = NMc^\varepsilon = N\hat{a}^\varepsilon \to NMc^0 = Pc^0$ such that $c^\varepsilon \to c^0$ in $\mathrm{L}^2([0,T;\mathbb{R}^I)$ follows.

Step 4. Limit passage in the ODE. To see that c^0 satisfies the limit equation (2.6) we pass to the limit in

$$Mc^\varepsilon(t) = Mc^\varepsilon(0) + \int_0^t MA^S c^\varepsilon(s) \mathrm{d}s,$$

where the left-hand side converges by Step 2 and the right-hand side by the assumption on the initial condition and by Step 3 and Lebesgue's' dominated convergence theorem. Thus, $Mc^0(t) = Mc^0(0) + \int_0^t MA^S c^0(s)\mathrm{d}\,s$, and with $A^F c^0 = 0$ from Step 3 the desired limit equation (2.6) is established.

As we already know that the solution of (2.6) is unique, we conclude convergence of the whole family $(c^\varepsilon)_{\varepsilon>0}$, instead of a subsequence only. □

In the above proof the DBC (2.Ac) is not really necessary, but it simplified our proof considerably.

3 Generalized gradient structures

This small section provides the general notions of gradient systems, gradient-flow equations, the energy-dissipation principle (EDP), and the three notions of EDP convergence. We follow the survey article [Mie16] and the more recent works [DFM19, MMP19].

3.1 Gradient systems and the Energy-Dissipation Principle

A triple $(\mathsf{Q}, \mathcal{E}, \mathcal{R})$ is called a *gradient system* if

- Q is a closed convex subset of a Banach space X,
- $\mathcal{E} : \mathsf{Q} \to \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ is a differentiable functional (e.g. free energy, negative entropy)
- $\mathcal{R} : \mathsf{Q} \times X \to \mathbb{R}_\infty$ is a dissipation potential, i.e. for all $u \in \mathsf{Q}$ the functional $\mathcal{R}(u, \cdot) : X \to \mathbb{R}_\infty$ is lower semicontinuous (lsc), nonnegative, convex and satisfies $\mathcal{R}(u, 0) = 0$.

(More general, Q can be a manifold, then $\mathcal{R}$ is defined on the tangent bundle $\mathrm{T}\mathsf{Q}$, but this generalization is not needed in this work.) A gradient system $(\mathsf{Q}, \mathcal{E}, \mathcal{R})$ is called *classical* if $\mathcal{R}(u, \cdot)$ is quadratic, i.e. if there are symmetric and positive definite operators $\mathbb{G}(u) : X \to X^*$ such that $\mathcal{R}(u, v) = \frac{1}{2}\langle \mathbb{G}(u)v, v\rangle$. But often $\mathcal{R}(u, \cdot)$ is not quadratic (e.g. for rate-independent processes such as elastoplasticity), see [Mie16] and reference therein. We define the dual dissipation potential $\mathcal{R}^*$ using the Legendre transform via

$$\mathcal{R}^*(u, \xi) = (\mathcal{R}(u, \cdot))^*(\xi) := \sup\big\{\, \langle \xi, v\rangle - \mathcal{R}(u, v) \,\big|\, v \in X \,\big\}.$$

The gradient system is uniquely described by $(Q, \mathcal{E}, \mathcal{R})$ or, equivalently by $(Q, \mathcal{E}, \mathcal{R}^*)$ and, in particular, in this paper we use the second representation.

The evolution of the states $u(t)$ in a gradient system are given in terms of the so-called *gradient-flow equation* that is given in terms of $\mathcal{E}$ and $\mathcal{R}$ and can be formulated in three equivalent ways:

$$\begin{aligned}
&\text{(I) } \textit{force balance in } X^*. && 0 \in \partial_{\dot u}\mathcal{R}(u, \dot u) + \mathrm{D}\mathcal{E}(u) \in X^*,\\
&\text{(II) } \textit{power balance in } \mathbb{R}. && \mathcal{R}(u, \dot u) + \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u)) = -\langle \mathrm{D}\mathcal{E}(u), \dot u\rangle,\\
&\text{(III) } \textit{rate equation in } X. && \dot u \in \partial_\xi \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u)) \in X,
\end{aligned} \tag{3.1}$$

where ∂ is the set-valued partial subdifferential with respect to the second variable.

In general, we cannot expect that the solution of the gradient-flow equation fill the whole state space. Clearly, along solutions we want to have $\mathcal{E}(u(t)) < \infty$ for $t > 0$. Moreover, relation (III) asks that $-\mathrm{D}\mathcal{E}(u(t))$ lies in the domain of $\partial_\xi \mathcal{R}^*(u(t), \cdot)$ for a.a. $t \in [0,T]$. Thus, we set

$$\mathrm{Dom}(\mathsf{Q}, \mathcal{E}, \mathcal{R}) := \big\{ u \in \mathsf{Q} \,\big|\, \mathrm{D}\mathcal{E}(u) \text{ exists, } \partial_\xi \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u)) \text{ is nonempty } \big\}. \tag{3.2}$$

Typically, one expects that solutions exist for all initial conditions in the closure of $\mathrm{Dom}(\mathsf{Q}, \mathcal{E}, \mathcal{R})$.

These three formulations are the same due to the so-called *Fenchel equivalences* (cf. [Fen49]): Let Z be a reflexive Banach space and $\Psi : Z \to \mathbb{R}_\infty$ be a proper, convex and lsc, then for every all pairs $(v, \xi) \in Z \times Z^*$ the following holds:

$$\text{(i) } \xi \in \partial\Psi(v) \quad \Longleftrightarrow \quad \text{(ii) } \Psi(v) + \Psi^*(\xi) = \langle \xi, v \rangle \quad \Longleftrightarrow \quad \text{(iii) } v \in \partial\Psi^*(\xi).$$

We emphasize that (ii) and (II) should be seen as scalar optimality conditions, because the definition of the Legendre transform easily gives the Young-Fenchel inequality, namely $\Psi(v) + \Psi^*(\xi) \geq \langle \xi, v \rangle$ for all $(v, \xi) \in Z \times Z^*$.

Integrating the power balance (II) in (3.1) over $[0,T]$ along a solution $u : [0,T] \to \mathsf{Q}$ and using the chain rule $\langle \mathrm{D}\mathcal{E}(u(t)), \dot{u}(t) \rangle = \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}(u(t))$ we find the *Energy-Dissipation Balance* (EDB):

$$\mathcal{E}(u(T)) + \int_0^T \Big(\mathcal{R}(u(t), \dot{u}(t)) + \mathcal{R}^*(u(t), -\mathrm{D}\mathcal{E}(u(t))) \Big) \,\mathrm{d}\, t = \mathcal{E}(u(0)). \tag{3.3}$$

The following *Energy-Dissipation Principle* (EDP) states that solving (3.3) is equivalent to solving the gradient-flow equation (3.1).

Theorem 3.1 (Energy-dissipation principle, see e.g. [Mie16, Th. 3.2])**.** *Assume that* Q *is a closed convex subset of* $X = \mathbb{R}^I$*, that* $\mathcal{E} \in \mathrm{C}^1(\mathsf{Q}, \mathbb{R})$*, and that the dissipation potential* $\mathcal{R}(u, \cdot)$ *is superlinear uniformly in* $u \in \mathsf{Q}$*. Then, a function* $u \in \mathrm{W}^{1,1}([0,T]; \mathsf{Q})$ *is a solution of the gradient-flow equation* (3.1) *if and only if* u *solves the energy-dissipation balance* (3.3)*.*

Again, the EDB is an optimality condition, because integrating the Young-Fenchel inequality for arbitrary $\widetilde{u} \in \mathrm{W}^{1,1}([0,T]; \mathsf{Q})$ and using the chain rule we obtain the estimate

$$\mathcal{E}(\widetilde{u}(T)) + \int_0^T \Big(\mathcal{R}(\widetilde{u}(t), \dot{\widetilde{u}}(t)) + \mathcal{R}^*(\widetilde{u}(t), -\mathrm{D}\mathcal{E}(\widetilde{u}(t))) \Big) \,\mathrm{d}\, t \geq \mathcal{E}(\widetilde{u}(0)). \tag{3.4}$$

The above considerations show that an important quantity associated with a gradient system $(\mathsf{Q}, \mathcal{E}, \mathcal{R})$ is given by the *dissipation functional*

$$\mathfrak{D}(u) := \int_0^T \Big(\mathcal{R}(u(t), \dot{u}(t)) + \mathcal{R}^*\big(u(t), -\mathrm{D}\mathcal{E}(u(t))\big) \Big) \,\mathrm{d}\, t,$$

which is defined for all curves $u \in \mathrm{W}^{1,1}([0,T]; \mathsf{Q})$.

3.2 General gradient systems and EDP-convergence

In the following, we consider a family of gradient systems $(X, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ and define a notion of convergence on the level of gradient systems which uniquely defines the limit or effective system $(\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$. Our notion relies on the the energy-dissipation principle from above and the so-called sequential Γ-convergence for functionals, which is defined as follows.

Definition 3.2 (Γ-convergence, see e.g. [Att84])**.** For functionals $(I_\varepsilon)_{\varepsilon>0}$ on a Banach space Z we say I_ε *(strongly)* Γ*-converges to* I, and write $I_\varepsilon \xrightarrow{\Gamma} I$, if the following two conditions hold:

1. *Liminf estimate.*
   if $u_\varepsilon \to u$ in Z, then $\quad I(u) \ \le \ \liminf_{\varepsilon\to 0} I_\varepsilon(u_\varepsilon)$,
2. *Existence of recovery sequences.*
   for all $\tilde u \in Z$ there exists $(\tilde u_\varepsilon)_{\varepsilon>0}$ such that $\quad \tilde u_\varepsilon \to \tilde u$ and $\lim_{\varepsilon\to 0} I_\varepsilon(\tilde u_\varepsilon) = I(\tilde u)$.

If the same conditions hold when the strong convergences "$\to$" are replaced by weak convergences "$\rightharpoonup$", we say that I_ε *weakly* Γ*-converges to* I and write $I_\varepsilon \xrightarrow{\Gamma} I$. If $I_\varepsilon \xrightarrow{\Gamma} I$ and $I_\varepsilon \xrightarrow{\Gamma} I$ holds, we say that I_ε *Mosco converges to* I and write $I_\varepsilon \xrightarrow{\text{M}} I$.

Clearly, for finite-dimensional Banach spaces Z the convergences $\xrightarrow{\Gamma}$, $\xrightarrow{\Gamma}$, and $\xrightarrow{\text{M}}$ coincide.

The energy dissipation principle allows us to formulate the gradient-flow equation in terms of the two functionals $\mathcal{E}_\varepsilon$ and $\mathfrak{D}_\varepsilon$. However, to explore the full structure of gradient systems it is useful to embed the given gradient system into a family of tilted gradient systems $(\mathsf{Q}, \mathcal{E}^\eta, \mathcal{R})$, where the *tilted energies* $\mathcal{E}^\eta$ are given by

$$\mathcal{E}^\eta(u) = \mathcal{E}(u) - \ell^\eta(u) \quad \text{with } \ell^\eta(u) := \langle \eta, u\rangle \tag{3.5}$$

with an arbitrary tilt $\eta \in X^*$. Moreover, introducing the *tilted dissipation functional*

$$\mathfrak{D}^\eta_\varepsilon(u) := \int_0^T \Big(\mathcal{R}_\varepsilon(u,\dot u) + \mathcal{R}^*_\varepsilon(u, \eta - \mathrm{D}\mathcal{E}_\varepsilon(u))\Big)\,\mathrm{d}t, \tag{3.6}$$

we can now define three versions of EDP-convergence for a family $\big((\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)\big)_{\varepsilon>0}$ as follows.

Definition 3.3 (EDP-convergence [DFM19, MMP19])**.** Let Q be a closed convex subset of a Banach space X and let $\mathcal{E}_\varepsilon$ be Gateaux differentiable.

(A) We say that the gradient systems $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)_{\varepsilon>0}$ *converges in the simple EDP sense to* $(\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$, and write $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon) \xrightarrow{\text{EDP}} (\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$, if the following conditions hold:

(i) $\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_0$ on $\mathsf{Q} \subset X$, and

(ii) $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma} \mathfrak{D}_0$ on $\mathrm{L}^2([0,T];\mathsf{Q})$ with $\mathfrak{D}_0(u) = \int_0^T \big(\mathcal{R}_{\text{eff}}(u,\dot u) + \mathcal{R}^*_{\text{eff}}(u, -\mathrm{D}\mathcal{E}_0(u))\big)\,\mathrm{d}t$.

(B) We say that $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ *EDP-converges with tilting to* $(\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$, if for all $\eta \in X^*$ we have $(\mathsf{Q}, \mathcal{E}_\varepsilon - \ell_\eta, \mathcal{R}_\varepsilon) \xrightarrow{\text{EDP}} (\mathsf{Q}, \mathcal{E}_0 - \ell_\eta, \mathcal{R}_{\text{eff}})$.

(C) We say that $(\mathsf{Q},\mathcal{E}_\varepsilon,\mathcal{R}_\varepsilon)$ *contact EDP-converges with tilting to* $(\mathsf{Q},\mathcal{E}_0,\mathcal{R}_{\text{eff}})$, if (i) holds and for all $\eta\in X^*$ we have $\mathfrak{D}_\varepsilon^\eta \overset{\Gamma}{\rightharpoonup} \mathfrak{D}_0^\eta$ with $\mathfrak{D}_0^\eta(u)=\int_0^T \mathcal{M}(u(t),\dot u(t),\eta-\mathrm{D}\mathcal{E}_0(u(t))\big)\,\mathrm{d}\,t$, where $\mathcal{M}$ satisfies the contact conditions

$$\begin{aligned}&\text{(c1)}\quad \mathcal{M}(u,v,\xi)\ge\langle\xi,v\rangle \text{ for all } (v,\xi)\in X\times X^*,\\ &\text{(c2)}\quad \mathcal{M}(u,v,\xi)=\langle\xi,v\rangle \iff \mathcal{R}_{\text{eff}}(u,v)+\mathcal{R}_{\text{eff}}^*(u,\xi)=\langle\xi,v\rangle.\end{aligned}$$

Clearly, 'tilted EDP-convergence' is a stronger notion than 'contact EDP-convergence' since the contact potential $\mathcal{M}$ is explicitly given in $\mathcal{R}+\mathcal{R}^*$ form. We refer to [DFM19, MMP19] for a general discussions of EDP-convergence and remark that 'contact EDP-convergence with tilting' was called 'relaxed EDP-convergence' in [DFM19]. We emphasize that there are cases where we have the Γ (or even Mosco) convergence $\mathcal{R}_\varepsilon\to\mathcal{R}_0$, but EDP-convergence yields $\mathcal{R}_{\text{eff}}\neq\mathcal{R}_0$. In general, EDP-convergence allows for effective dissipation potentials $\mathcal{R}_{\text{eff}}$ that inherit properties of the family $(\mathcal{E}_\varepsilon)_{\varepsilon>0}$.

A first important feature of the different notions of EDP-convergence is that the effective gradient system is uniquely determined. This is a much stronger statement than determining the effective or limit gradient-flow equation, since a given equation can have several gradient structures, as we will see below for linear reaction systems.

A further interesting observation is that the notion of EDP-convergence does not involve the solutions of the associated gradient-flow equation. This may look like an advantage, since solutions need not be characterized, however typically showing EDP-convergence is at least as difficult.

Another important feature is that, under suitable technical assumptions, EDP-convergence automatically implies the convergence of the corresponding solutions u^ε of the gradient-flow equations to the solutions u of the effective equation

$$0\in\partial_v\mathcal{R}_{\text{eff}}(u(t),\dot u(t))+\mathrm{D}\mathcal{E}_0(u(t))\quad\text{for a.a. } t\in[0,T]. \tag{3.7}$$

The following result gives one possible variant of such a result, see [MMP19, Lem. 2.8] for another. We do not enforce the condition $u^\varepsilon(0)\to u(0)$ but only $\mathcal{E}_\varepsilon(u^\varepsilon(0))\to\mathcal{E}_0(u(0))$ as well as the continuity of the limit encoded in the assumption $u\in\mathrm{W}^{1,1}([0,T];X)$. Thus, the result still applies to fast-slow reaction systems, where jumps at initial time $t=0$ may develop for $\varepsilon\to0$, see e.g. the example treated in [MPS20, Sec. 2.5]. Then, it is important to take into account that $\lim_{\varepsilon\to0}u^\varepsilon(0)$ may be different from $u(0)=\lim_{t\to0^+}u(t)$.

Lemma 3.4. *Let the assumption of Theorem 3.1 be satisfied for all $\varepsilon\ge0$. Assume that the gradient systems $(\mathsf{Q};\mathcal{E}_\varepsilon,\mathcal{R}_\varepsilon)$ EDP-converge to $(\mathsf{Q},\mathcal{E}_0,\mathcal{R}_{\text{eff}})$ in one of the three senses of Definition 3.3, then the following holds. If $u^\varepsilon:[0,T]\to\mathsf{Q}$ are solutions for* (3.1) *and $u:[0,T]\to\mathsf{Q}$ is such that $u\in\mathrm{W}^{1,1}([0,T];X)$,*

$$\mathcal{E}_\varepsilon(u^\varepsilon(0))\to\mathcal{E}_0(u(0)),\quad u^\varepsilon\rightharpoonup u \text{ in } \mathrm{L}^2([0,T];\mathsf{Q}),\quad \text{and } u^\varepsilon(t)\to u(t) \text{ for all } t\in]0,T],$$

then u is a solution of the effective gradient-flow equation (3.7).

Proof. By Theorem 3.1 we know that the EDB (3.3) holds for u^ε as solutions for the gradient system $(\mathsf{Q},\mathcal{E}_\varepsilon,\mathcal{R}_\varepsilon)$, namely $\mathcal{E}_\varepsilon(u^\varepsilon(T))+\mathfrak{D}_\varepsilon(u^\varepsilon)=\mathcal{E}_\varepsilon(u^\varepsilon(0))$.

Using $u^\varepsilon(T)\to u(T)$ and $u^\varepsilon\rightharpoonup u$ in L^2 we have the liminf estimates

$$\mathcal{E}_0(u(T))\le\liminf_{\varepsilon\to0}\mathcal{E}_\varepsilon(u^\varepsilon(T))\quad\text{and}\quad\mathfrak{D}_0(u)\le\liminf_{\varepsilon\to0}\mathfrak{D}_\varepsilon(u^\varepsilon).$$

Together with the assumed convergence of the energies at $t = 0$ and the representation of $\mathfrak{D}_0$ via $\mathcal{R}_{\text{eff}}$, we obtain

$$\mathcal{E}_0(u(T)) + \int_0^T \Big(\mathcal{R}_{\text{eff}}(u(t), \dot{u}(t)) + \mathcal{R}^*_{\text{eff}}(u(t), -\mathrm{D}\mathcal{E}_0(u(t))) \Big) \,\mathrm{d}t \le \mathcal{E}_0(u(0)). \tag{3.8}$$

Together with (3.4) and the EDP in Theorem 3.1 we see that u solves (3.7). □

4 Gradient structures for linear reaction systems

In this section we discuss several gradient structures for linear reaction systems satisfying the detailed balance condition. Moreover, following the theory of Markov processes we define a natural way of tilting such systems in such a way that a new global equilibrium state w arises. This will show that the entropic gradient structure with cosh-type dual dissipation plays a distinguished role.

4.1 A special representation for generators

We start from a general linear reaction system with the finite index space $\mathcal{I} := \{1, \dots, I\}$. On the state space $\mathsf{Q} = \mathrm{Prob}(\mathcal{I})$ we consider the general linear reaction system

$$\dot{c} = Ac \qquad \text{where } A_{in} \ge 0 \text{ for } i \ne n \quad \text{and} \quad \sum_{i=1}^{I} A_{in} = 0 \text{ for all } n \in \mathcal{I}. \tag{4.1}$$

Throughout we assume that there exists a positive equilibrium state $w \in \mathsf{Q}$, i.e. $Aw = 0$ and $w_i > 0$ for all $i \in \mathcal{I}$. At this stage we don't need the detailed-balance condition.

As we later want to change the equilibrium state w (and hence also the generator A) we write A in a specific form, namely

$$\begin{aligned} &A = \mathbb{D}_w^{1/2} K \mathbb{D}_w^{-1/2} - \mathbb{D}_b \qquad \text{with } K = (\kappa_{in}) \in \mathbb{R}^{I\times I} \text{ and } b \in \mathbb{R}^I \text{ given by} \\ &\kappa_{in} = A_{in} \big(\frac{w_n}{w_i}\big)^{1/2} > 0 \text{ for } i \ne n, \qquad \kappa_{ii} = 0, \quad \text{and} \\ &b_i = -A_{ii} = \sum_{n=1}^{I} \kappa_{ni} \big(\frac{w_n}{w_i}\big)^{1/2} > 0. \end{aligned} \tag{4.2}$$

This representation is useful, because we can keep K fixed, while varying w to obtain Markov generators $A = A^{w,K}$ such that $A^{w,K} w = 0$. The evolution equation (4.1) can be written in the symmetric form

$$\dot{c}_n = \sum_{i:\, i\ne n} \kappa_{ni} \Big(\big(\frac{w_n}{w_i}\big)^{1/2} c_i - \big(\frac{w_i}{w_n}\big)^{1/2} c_n \Big) \qquad \text{for } n \in \mathcal{I}. \tag{4.3}$$

Moreover, we see that A and w satisfies the DBC $A_{in} w_n = A_{ni} w_i$ if and only if K is symmetric. Thus, fixing a symmetric K and changing w does automatically generate the DBC for $A^{K,w}$ and w.

4.2 A general class of gradient structures

We now assume the DBC $A\mathbb{D}_w = (A\mathbb{D}_w)^*$ or equivalently $K = K^*$ in (4.2) and discuss a general class of gradient structures for (4.1) following the general approach in [MaM20, Sec. 2.5].

Let $\Phi : [0,\infty[\to [0,\infty[$ and $\Psi_{in} : \mathbb{R} \to [0,\infty[$ for $1 \le i < n \le I$ be lower semicontinuous and strictly convex C^2 functions such that $\Psi_{in}(0) = 0$ and $\Psi''_{in}(0) > 0$. We search for a gradient system $(\mathsf{Q}, \mathcal{E}, \mathcal{R}^*)$ with an energy functional $\mathcal{E}$ and a dual dissipation potential in the form

$$\mathcal{E}(c) = \sum_{i=1}^{I} w_i\, \Phi\big(\frac{c_i}{w_i}\big) \qquad \text{and} \qquad \mathcal{R}^*(c,\xi) = \sum_{i=1}^{I-1} \sum_{n=i+1}^{I} a_{in}(c)\, \Psi_{in}(\xi_i - \xi_n),$$

where the coefficient functions a_{in} must be chosen appropriately, but need to be nonnegative to guarantee that $\mathcal{R}^*(c,\cdot)$ is a dissipation potential.

With $\partial_{\xi_n}\mathcal{R}^*(c,\xi) = \sum_{k=n+1}^{I} a_{nk}(c)\Psi'_{nk}(\xi_n - \xi_k) - \sum_{i=1}^{n-1} a_{in}(c)\Psi'_{in}(\xi_i - \xi_n)$ and $\mathrm{D}\mathcal{E}(c) = \big(\Phi'(\frac{c_k}{w_k})\big)_k$ we find the relation

$$\partial_{\xi_n}\mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c)) = \sum_{i=n+1}^{I} a_{ni}(c)\Psi'_{ni}\Big(\Phi'\big(\frac{c_i}{w_i}\big) - \Phi'\big(\frac{c_n}{w_n}\big)\Big) - \sum_{i=1}^{n-1} a_{in}(c)\Psi'_{in}\Big(\Phi'\big(\frac{c_n}{w_n}\big) - \Phi'\big(\frac{c_i}{w_i}\big)\Big).$$

Thus, the equations $\dot c_n = \partial_{\xi_n}\mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c))$ are the same as in (4.3), provided we choose the coefficient functions a_{in} as

$$a_{ni}(c) := \frac{\kappa_{ni}\sqrt{w_n w_i}\,\big(\frac{c_i}{w_i} - \frac{c_n}{w_n}\big)}{\Psi'_{ni}\big(\Phi'(\frac{c_i}{w_i}) - \Phi'(\frac{c_n}{w_n})\big)} \text{ for } \tfrac{c_i}{w_i} \neq \tfrac{c_n}{w_n} \quad \text{and} \quad a_{ni}(c) := \frac{\kappa_{ni}\sqrt{w_n w_i}}{\Psi''_{ni}(0)\Phi''(\frac{c_i}{w_i})} \text{ for } \tfrac{c_i}{w_i} = \tfrac{c_n}{w_n} \tag{4.4}$$

and exploit the DBC $\kappa_{in} = \kappa_{ni}$. We also emphasize that Φ' is strictly increasing such that $\frac{c_i}{w_i} - \frac{c_n}{w_n}$ and $\Phi'(\frac{c_i}{w_i}) - \Phi'(\frac{c_n}{w_n})$ always have the same sign. Since $\Psi'(\zeta)$ and ζ also always have the same sign, we conclude that $a_{in}(c) \ge 0$ as desired for dissipation potentials.

As the choice of entropy functional density Φ and of the dual dissipation potentials Ψ_{in} is general quite arbitrary we see that we can generate a whole zoo of different gradient structures for (4.1) or (4.3). The following choices relate to situation where all Ψ_{in} are given by one function Ψ, but more general cases are possible.

From the construction it is clear that $\mathcal{R}^*$ is linear in the generator A, i.e. if $A = A^1 + A^2$ and the equilibrium w is fixed, then $\mathcal{R}^* = \mathcal{R}^*_{A^1} + \mathcal{R}^*_{A^2}$ where $\mathcal{R}^*_{A^m}$ is constructed as above.

4.3 Some specific gradient structures for linear reaction systems

We now realize special choices for the general gradient structures in the previous subsection. These choices are singled out because they lead to natural entropy functionals and relatively simple coefficient functions a_{in} in (4.4).

4.3.1 Quadratic energy and dissipation

The quadratic gradient structure is given by quadratic energy and dissipation, i.e.

$$\Phi_{\mathrm{quad}}(\varrho) = \frac{1}{2}\varrho^2 \quad \text{and} \quad \Psi_{\mathrm{quad}}(\zeta) = \frac{1}{2}\zeta^2.$$

The coefficient functions are constant and read $a_{in}(c) = \kappa_{in}\sqrt{w_i w_n}$. Thus, we find

$$\mathcal{E}_{\rm quad}(c) = \frac{1}{2}\sum_{i=1}^{I}\frac{c_i^2}{w_i} \quad \text{and } \mathcal{R}^*_{\rm quad}(c,\xi) = \frac{1}{2}\sum_{i=1}^{I-1}\sum_{n=i+1}^{I}\kappa_{in}\sqrt{w_i w_n}(\xi_i-\xi_n)^2 = \frac{1}{2}\langle \xi, \mathbb{K}_{\rm quad}\xi\rangle.$$

In this case the dual dissipation functional does not depend on the concentration $c \in \mathsf{Q}$, which means that the equation $\dot c = Ac = -\mathbb{K}\mathrm{D}\mathcal{E}(c)$ can be treated as self-adjoint linear evolution problem in the Hilbert space with the norm induced by $\mathcal{R}$. This leads to the classical Hilbert space approach for reversible Markov operators.

4.3.2 Boltzmann entropy and quadratic dissipation

The *quadratic-entropic* gradient structure is defined by the choices

$$\Phi_{\rm Boltzmann}(\varrho) = \lambda_{\rm Bz}(\varrho) := \varrho\log\varrho - \varrho + 1 \quad \text{and} \quad \Psi_{\rm quad}(\zeta) = \frac{1}{2}\zeta^2.$$

This gradient structure for was first introduced in [Mie11, Maa11, ErM12, CH*12, Mie13] as a possible generalization of Otto's gradient structure for the Fokker-Planck and more general diffusion equations equation, cf. [JKO98, Ott01]. However, similar structures also appear earlier in the physics literature, see e.g. [ÖtG97, Eqn. (113)]

The associated entropy is Boltzmann's relative entropy and, using the logarithmic mean $\Lambda(a,b) = \int_0^1 a^s b^{1-s}\,\mathrm{d}s = \frac{a-b}{\log a - \log b}$, the dual dissipation potential $\mathcal{R}^*$ reads

$$\mathcal{E}_{\rm Bz}(c) := \sum_{i=1}^{I} w_i\,\lambda_{\rm Bz}\big(\frac{c_i}{w_i}\big) \quad \text{and} \quad \mathcal{R}^*(c,\xi) = \frac{1}{2}\sum_{i=1}^{I-1}\sum_{n=i+1}^{I}\kappa_{in}\,\sqrt{w_i w_n}\,\Lambda\big(\frac{c_i}{w_i},\frac{c_n}{w_n}\big)\,(\xi_i-\xi_n)^2.$$

Again $\mathcal{R}^*$ is quadratic in ξ but now also depends nontrivially on $c \in \mathsf{Q}$, viz. $\mathcal{R}^*(c,\xi) = \frac{1}{2}\langle \xi, \mathbb{K}_{\rm Bz}(c)\xi\rangle$. This means that Q can be equipped with the Riemannian metric induced by $\mathcal{R}$, see [Maa11].

Note that $\mathbb{K}_{\rm Bz}(w) = \mathbb{K}_{\rm quad}$ and $\mathcal{E}_{\rm quad}(c) = \frac{1}{2}\mathrm{D}^2\mathcal{E}_{\rm Bz}(w)[c,c]$, which is the desired compatibility under linearization at $c = w$.

4.3.3 Boltzmann entropy and cosh-type dissipation

The following, so-called *entropic cosh-type gradient structure*, was derived via a large-deviation principle from an interacting particle system in [MPR14, MP*17]. We refer to Marcellin's PhD thesis [Mar15] from 1915 for a historical, first physical derivation of exponential kinetic relations in the context of Boltzmann statistics. Only little of this important result penetrated into the main stream thermomechanical modeling of reaction systems, see [Grm10, Item iii on p. 77 and eqn. (69)] for a discussion.

For this gradient structure the choices are

$$\Phi_{\rm Boltzmann}(\varrho) = \lambda_{\rm Bz}(\varrho) := \varrho\log\varrho - \varrho + 1 \quad \text{and} \quad \Psi_{\cosh}(\zeta) = \mathsf{C}^*(\zeta) := 4\cosh\big(\frac{\zeta}{2}\big) - 4,$$

giving Boltzmann's relative entropy $\mathcal{E}_{\rm Bz}$ and the cosh-type dual dissipation potential:

$$\mathcal{E}_{\rm Bz}(c) := \sum_{i=1}^{I} w_i\,\lambda_{\rm Bz}\big(\frac{c_i}{w_i}\big) \quad \text{and} \quad \mathcal{R}^*_{\cosh}(c,\xi) = \sum_{i=1}^{I-1}\sum_{n=i+1}^{I}\kappa_{in}\,\sqrt{c_i c_n}\,\mathsf{C}^*(\xi_i-\xi_n). \tag{4.5}$$

The especially simple form of the coefficient functions arises from the interaction of the cosh function with the the Boltzmann function λ_{Bz}, namely

$$\mathsf{C}^{*\prime}\big(\lambda'_{\mathrm{Bz}}(p)-\lambda'_{\mathrm{Bz}}(q)\big)=2\sinh\big(\log\sqrt{p/q}\,\big)=\sqrt{p/q}-\sqrt{q/p}=\frac{p-q}{\sqrt{pq}}.$$

With this we easily find the simple formula $a_{in}(c)=\kappa_{in}\sqrt{c_ic_n}$.

Because of the close connection between the cosh-type function C^* and the Boltzmann function λ_{Bz}, it is obvious that using C^* means that we also use the Boltzmann entropy. Hence, it will not lead to confusion if we simply call $(\mathsf{Q},\mathcal{E}_{\mathrm{Bz}},\mathcal{R}_{\cosh})$ the *cosh gradient structure*.

Again, the quadratic gradient structure in Section 4.3.1 is obtained by linearization:

$$\mathcal{E}_{\mathrm{quad}}(c)=\frac{1}{2}\mathrm{D}^2\mathcal{E}_{\mathrm{Bz}}(w)[c,c]\quad\text{and}\quad\mathbb{K}_{\mathrm{quad}}=\mathrm{D}^2_\xi\mathcal{R}^*_{\cosh}(w,0).$$

4.4 Tilting of Markov processes

Tilting, also called exponential tilting, is a standard procedure in stochastics (in particular in the theory of large deviations) to change the dynamics of a Markov process in a controlled way. In particular, the equilibrium measure w is changed into another one, let us say $\widetilde{w}$. For more motivation and theory we refer to [MMP19] and the references therein.

Defining two entropy functionals, namely the Boltzmann entropies for w and $\widetilde{w}$,

$$\mathcal{E}_{\mathrm{Bz}}(c)=\sum_{i=1}^I w_i\,\lambda_{\mathrm{Bz}}\big(\frac{c_i}{w_i}\big)\quad\text{and}\quad\widetilde{\mathcal{E}}_{\mathrm{Bz}}(c)=\sum_{i=1}^I \widetilde{w}_i\,\lambda_{\mathrm{Bz}}\big(\frac{c_i}{\widetilde{w}_i}\big)$$

the special structure of λ_{Bz} leads to the relation

$$\widetilde{\mathcal{E}}_{\mathrm{Bz}}(c)=\mathcal{E}_{\mathrm{Bz}}(c)-\langle\eta,c\rangle\quad\text{with }\eta=\big(\log(w_i/\widetilde{w}_i)\big)_{i\in\mathcal{I}}.$$

Thus, we see that a change of the equilibrium measure leads to a tilt in the sense of (3.5) for the entropy. Moreover, for every tilt $\eta\in X^*$ there is a unique new equilibrium state w^η, namely the minimizer of $c\mapsto\mathcal{E}^\eta(c)=\mathcal{E}_{\mathrm{Bz}}(c)-\langle\eta,c\rangle$. We easily find

$$w_i^\eta=\frac{1}{Z}\mathrm{e}^{-\eta_i}w_i\quad\text{with }Z=\sum_{n=1}^I\mathrm{e}^{-\eta_n}w_n.$$

This explains the name 'exponential tilting'.

For a time-dependent linear reaction systems the tilting is defined in a consistent way, namely using the representation (4.2). Given $\dot c=Ac$ with positive equilibrium w and a tilt η we first construct the equilibrium w^η and then, using $K=(\kappa_{in})$ from (4.2), we define the evolution

$$\dot c=A^\eta c\quad\text{with }A^\eta:=\mathbb{D}_{w^\eta}^{1/2}K\mathbb{D}_{w^\eta}^{-1/2}-\mathbb{D}_{b^\eta}.\tag{4.6}$$

One of the important observations in [MMP19] is that the cosh gradient structure is invariant under tilting, i.e. the dissipation potential does not change if the Boltzmann entropy is tilted. This can now be formulated as follows:

$$A^\eta c=\mathrm{D}_\xi\mathcal{R}^*_{\cosh}\big(c,-\mathrm{D}\mathcal{E}^\eta(c)\big).\tag{4.7}$$

This relation can easily checked by noting that (4.6) has the form (4.3), where now w is replaced by w^η. But $\mathcal{E}^\eta$ is exactly the relative entropy with respect to w^η such that the results in Section 4.3.3 yield identity (4.7).

Using the formula (4.4) for $a_{in}(c)$ we can find all possible gradient structures in terms of Φ and Ψ_{in} such that the $a_{in}(c)$ is independent for w. The result shows that, up to a trivial scaling, the only tilt-invariant gradient structures in the form of Section 4.2 are given by the cosh gradient structure. Indeed, in [MPR14] the case $\gamma = 1/2$ is obtained from the theory of large deviations.

Proposition 4.1 (Characterization of tilt-invariant gradient structures)**.** *If Φ and Ψ_{in} are such that a_{in} in* (4.4) *is independent of w, then there exists $\varphi_0, \varphi_1 \in \mathbb{R}$ and $\psi_{in}, \gamma > 0$ such that*

$$\Phi(c) = \gamma\lambda_{\mathrm{Bz}}(c) + \varphi_0 + \varphi_1 c \quad \textit{and} \quad \Psi_{in}(\zeta) = \gamma\,\psi_{in}\,\mathsf{C}^*\big(\frac{\zeta}{\gamma}\big).$$

In particular, we always obtain $a_{in}(c) = \frac{\kappa_{in}}{\psi_{in}}\sqrt{c_i c_n}$. Since ψ_{in} can be integrated into κ_{in}, all tilt-invariant gradient structures are given by scaled cosh gradient structures

$$\mathcal{E}(c) = \gamma\,\mathcal{E}_{Bz}(c) + \varphi_0 I + \varphi_1 \quad \textit{and} \quad \mathcal{R}^*(c,\xi) = \gamma\,\mathcal{R}^*_{\cosh}(c, \frac{1}{\gamma}\xi).$$

Proof. We rewrite a_{in} in the form

$$a_{in}(c) = \kappa_{in}\sqrt{c_i c_n}\,\frac{\varrho_i - \varrho_n}{\sqrt{\varrho_i\varrho_n}\,\Psi'_{ni}\big(\Phi'(\varrho_i) - \Phi'(\varrho_n)\big)}, \quad \text{where } \varrho_k = \frac{c_k}{w_k}$$

Because the expression has to be independent of w_i and w_n for all $c, w \in \mathsf{Q}$, the fraction involving ϱ_i and ϱ_n has to be a constant, which we set $1/\psi_{in}$, i.e.

$$\text{(i)}\;\; \Phi'(\varrho_i) - \Phi'(\varrho_n) = G\big(\frac{\varrho_i}{\varrho_n}\big), \qquad \text{(ii)}\;\; G(\sigma) = \big(\Psi'_{in}\big)^{-1}\Big(\psi_{in}\big(\sqrt{\sigma} - \frac{1}{\sqrt{\sigma}}\big)\Big).$$

Setting $r_k = \log\varrho_k$, $f(r) = \Phi'(\mathrm{e}^r)$, and $g(s) = G(\mathrm{e}^s)$ in (i), we arrive at the relation

$$f(r_i) - f(r_n) = g(r_i - r_n) \quad \text{for all } r_i, r_n \in \mathbb{R}.$$

As f and g are continuous the only solutions of this functional relation are $f(r) = \varphi_1 + \gamma r$ and $g(s) = \gamma s$ with $\varphi_1, \gamma \in \mathbb{R}$. This implies $\Phi'(\varrho) = \varphi_1 + \gamma\log\varrho$ and, hence, $\Phi(\varrho) = \varphi_0 + \varphi_1\varrho + \gamma\lambda_{\mathrm{Bz}}(\varrho)$. Strict convexity of Φ leads to the restriction $\gamma > 0$.

Solving (ii) with $G(\sigma) = \gamma\log\sigma =: \zeta$ yields

$$\Psi'_{in}(\zeta) = \psi_{in}\big(\mathrm{e}^{\zeta/(2\gamma)} - \mathrm{e}^{-\zeta/(2\gamma)}\big) = \psi_{in}\,2\sinh\big(\frac{\zeta}{2\gamma}\big) = \psi_{in}\,\mathsf{C}^{*\prime}\big(\frac{\zeta}{\gamma}\big).$$

Because of $\Psi_{in}(0) = 0$ this determines Ψ_{in} uniquely, and the result is established. □

We also refer to [HKS20] for the connections of the cosh gradient structure to the SQRA-discretization scheme for drift-diffusion systems.

5 EDP-convergence and the effective gradient structure

In this section we fully concentrate on the cosh gradient structure, because only this gradient structure allows to prove EDP convergence with tilting.

Our energy functionals $\mathcal{E}_\varepsilon$ are the relative Boltzmann entropies, while the dual dissipation potentials $\mathcal{R}^*_\varepsilon$ is the sum of a slow and a fast part:

$$\mathcal{E}_\varepsilon(c) = \sum_{i=1}^I w_i^\varepsilon \, \lambda_{\mathrm{Bz}}\big(\frac{c_i}{w_i^\varepsilon}\big) \quad \text{and} \quad \mathcal{R}^*_\varepsilon(c,\xi) = \mathcal{R}^*_{S,\varepsilon}(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}^*_{F,\varepsilon}(c,\xi), \text{ where}$$

$$\mathcal{R}^*_{Z,\varepsilon}(c,\xi) := \sum_{i=1}^{I-1}\sum_{n=i+1}^{I} \kappa_{in}^{Z,\varepsilon}\sqrt{c_i c_n}\,\mathsf{C}^*(\xi_i - \xi_n) \quad \text{with } \kappa_{in}^{Z,\varepsilon} = A_{in}^Z\sqrt{w_n^\varepsilon / w_i^\varepsilon} \quad \text{and } Z \in \{S,F\}.$$

Here, the ε-dependencies of the coefficients $\kappa_{in}^{S,\varepsilon}$ and $\kappa_{in}^{F,\varepsilon}$ is trivial in the sense that the limits for $\varepsilon \to 0$ exist. The really important term is the factor $1/\varepsilon$ in front of $\mathcal{R}^*_{F,\varepsilon}$.

The structure of this section is as follows. In Section 5.1 we present the main results concerning the Γ-convergence of $\mathcal{E}_\varepsilon$ and $\mathfrak{D}_\varepsilon$ which then imply the EDP-convergence with tilting of $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ to the limit system $(\mathsf{Q}, \mathcal{E}, \mathcal{R}_{\mathrm{eff}})$. In Section 5.2 we show that this provides a gradient structure for the limit equation (2.6), and moreover that we obtain the natural cosh gradient structure $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ for the coarse-grained equation (2.7).

The remaining part of this section then provides the proof of the convergence $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}} \mathfrak{D}_0$, namely the a priori estimates in Section 5.3, the liminf estimate in Section 5.4, and the construction of recovery sequences in Section 5.5.

5.1 Main theorem on EDP-convergence

We now study the limit for $\varepsilon \to 0$ of the family of gradient systems $\big((\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon)\big)_{\varepsilon>0}$ by showing EDP-convergence with tilting for a suitable limit.

As a first, and trivial result we state the Mosco convergence of the energies, which follows immediately from our assumption (2.Ab), i.e. $w^\varepsilon \to w^0$.

Proposition 5.1. *On $\mathsf{Q} = \mathrm{Prob}(\mathcal{I})$, we have the uniform convergence $\mathcal{E}_\varepsilon \to \mathcal{E}_0$, where $\mathcal{E}_0(c) = \sum_{i=1}^I w_i^0 \, \lambda_{\mathrm{Bz}}(c_i/w_i^0)$. In particular, we have $\mathcal{E}_\varepsilon \xrightarrow{\mathrm{M}} \mathcal{E}_0$ on X.*

To have a proper functional analytic setting we let

$$\mathrm{L}^2([0,T];\mathsf{Q}) = \big\{\, c \in \mathrm{L}^2([0,T];\mathbb{R}^I) \,\big|\, c(t) \in \mathsf{Q} \text{ a.e. in } [0,T] \,\big\}$$

and use the weak and strong topology induced by $\mathrm{L}^2([0,T];\mathbb{R}^I)$. The dissipation functional $\mathfrak{D}_\varepsilon$ is now defined via

$$\mathfrak{D}_\varepsilon(c) := \begin{cases} \int_0^T \big(\mathcal{R}_\varepsilon(c,\dot c) + \mathcal{R}^*_\varepsilon(c, -\mathrm{D}\mathcal{E}_\varepsilon(c))\big)\,\mathrm{d}t & \text{for } c \in \mathrm{W}^{1,1}([0,T];\mathsf{Q}), \\ \infty & \text{otherwise on } \mathrm{L}^2([0,T];\mathsf{Q}), \end{cases}$$

where $\mathcal{R}_\varepsilon(c,\cdot)$ is defined implicitly as Legendre transform of $\mathcal{R}^*_\varepsilon(c,\cdot)$. To see that $\mathfrak{D}_\varepsilon$ is well defined, we derive suitable properties for $\mathcal{R}_\varepsilon$.

Proposition 5.2 (Properties of $\mathcal{R}_\varepsilon$)**.** *Let $\mathcal{R}_\varepsilon : \mathsf{Q}\times X \to [0,\infty]$ be defined by $\mathcal{R}_\varepsilon(c,\cdot) = \big(\mathcal{R}^*_\varepsilon(c,\cdot)\big)^*$. Then, $\mathcal{R}_\varepsilon : \mathsf{Q}\times X \to [0,\infty]$ is lower semicontinuous and jointly convex.*

Proof. Since $(c_i, c_n) \mapsto \sqrt{c_i c_n}$ is concave and $\xi \mapsto \mathsf{C}(\xi_i - \xi_n)$ is convex, the mapping $\mathcal{R}^* : \mathsf{Q} \times X^* \to [0, \infty]$ is concave-convex and thus its partial conjugate is convex in (c, v).

For the lower semicontinuity consider $(c_k, v_k) \to (c, v)$. Then, for all $\delta > 0$ there exist ξ_δ with $\mathcal{R}_\varepsilon(c, v) \le \langle \xi_\delta, v\rangle - \mathcal{R}^*_\varepsilon(c_k, \xi_\delta) + \delta$. The definition of the Legendre transform yields

$$\mathcal{R}_\varepsilon(c_k, v_k) \ge \langle \xi_\delta, v_k\rangle - \mathcal{R}^*_\varepsilon(c_k, \xi_\delta) \overset{k\to\infty}{\to} \langle \xi_\delta, v\rangle - \mathcal{R}^*_\varepsilon(c, \xi_\delta) \ge \mathcal{R}_\varepsilon(c, v) - \delta,$$

where we used the continuity of $c \mapsto \mathcal{R}^*_\varepsilon(c, \xi)$. Since $\delta > 0$ was arbitrary, we find $\liminf_{k\to\infty} \mathcal{R}_\varepsilon(c_k, v_k) \ge \mathcal{R}_\varepsilon(c, v)$ as desired. □

To formulate the main Γ-convergence result for $\mathfrak{D}_\varepsilon$ we define the effective dissipation $\mathcal{R}^*_{\text{eff}}$ beforehand. It can be understood as the formal limit of $\mathcal{R}^*_\varepsilon$ when taking $\varepsilon \to 0$. The slow part $\mathcal{R}^*_{S,\varepsilon}$ simply converges to its limit

$$\mathcal{R}^*_S(c, \xi) := \sum_{i=1}^{I-1} \sum_{n=i+1}^{I} \kappa^{S,0}_{in} \sqrt{c_i c_n}\, \mathsf{C}^*(\xi_i - \xi_j) \quad \text{with } \kappa^{S,0}_{in} = A^S_{in} \sqrt{w^0_n / w^0_i} = \lim_{\varepsilon\to 0} \kappa^{S,\varepsilon}_{in}.$$

For the fast part $\frac{1}{\varepsilon}\mathcal{R}^*_{F,\varepsilon}$ we obtain blow up, except for those ξ that lie in the subspace that is not affected by fast reactions. For this we set

$$\Xi = M^*Y^* = \text{range}(M^*) = \text{kernel}(M)^\perp := \big\{\, \xi \in X^* \,\big|\, \langle \xi, v\rangle = 0 \text{ for all } v \in \text{kernel}(M) \,\big\}.$$

and observe that by construction for all $\varepsilon > 0$ we have

$$\mathcal{R}^*_{F,\varepsilon}(c, \xi) = 0 \quad \text{for all } \xi \in \Xi. \tag{5.1}$$

Indeed, $\mathcal{R}^*_{F,\varepsilon}(c, \xi)$ contains $\mathsf{C}^*(\xi_i - \xi_n)$ with a positive prefactor only if $i \sim_F n$, while $\xi \in \Xi$ implies $\xi_i = \xi_n$ in that case. Together we set

$$\mathcal{R}^*_{\text{eff}}(c, \xi) := \mathcal{R}^*_S(c, \xi) + \chi_\Xi(\xi), \quad \text{where } \chi_A(a) = \begin{cases} 0 & \text{for } a \in A, \\ \infty & \text{for } a \notin A. \end{cases} \tag{5.2}$$

The dual dissipation potential $\mathcal{R}^*_{\text{eff}}$ consists of two terms: The first term $\mathcal{R}^*_S$ contains the information of the slow reactions in the limit $\varepsilon \to 0$. The second term χ_Ξ restricts the vector of chemical potentials $\xi = \mathrm{D}\mathcal{E}_0(c)$ exactly in such a way that the microscopic equilibria of the fast reactions holds, i.e. $A^F c = 0$ or equivalently $Pc = c$, see below.

Because of this constraint, it is actually irrelevant how $\mathcal{R}^*_{\text{eff}}(c, \cdot) : \Xi \to [0, \infty]$ is defined for $c \notin \mathsf{Q}_{\text{eq}} = \mathsf{Q} \cap PX$.

We note that $\mathcal{R}^*_\varepsilon(c, \cdot)$ has a Mosco limit $\mathcal{R}^*_0(c, \cdot)$ that is not necessarily equal to $\mathcal{R}^*_{\text{eff}}(c, \cdot)$. For c on the boundary of Q, where some of the c_i are 0, we may have $\mathcal{R}^*_{F,\varepsilon}(c, \xi) = 0$ for all ξ, which implies $\mathcal{R}^*_0(c, \xi) = \mathcal{R}^*_S(c, \xi)$ for these c and all $\xi \in \mathbb{R}^I$. However, the Γ-limit of $\mathfrak{D}_\varepsilon$ yields $\mathcal{R}^*_{\text{eff}} \ge \mathcal{R}^*_0$.

Theorem 5.3 (Mosco convergence of $\mathfrak{D}_\varepsilon$)**.** *On* $\mathrm{L}^2([0,T];\mathsf{Q})$ *we have* $\mathfrak{D}_\varepsilon \overset{\text{M}}{\to} \mathfrak{D}_0$ *with*

$$\mathfrak{D}_0(c) := \begin{cases} \int_0^T \big(\mathcal{R}_{\text{eff}}(c, \dot c) + \mathcal{R}^*_{\text{eff}}(c, -\mathrm{D}\mathcal{E}_0(c))\big)\,\mathrm{d}t & \text{for } c \in \mathrm{W}^{1,1}([0,T];\mathsf{Q}), \\ \infty & \text{otherwise in } \mathrm{L}^2([0,T];\mathsf{Q}), \end{cases} \tag{5.3}$$

where $\mathcal{R}^*_{\text{eff}}$ *is given in* (5.2) *and leads to the primal dissipation potential*

$$\mathcal{R}_{\text{eff}}(c, v) = \inf\big\{\, \mathcal{R}_S(c, z) \,\big|\, z \in \mathbb{R}^I \text{ with } Mz = Mv \,\big\} \quad \text{for all } c \in \mathsf{Q}_{\text{eq}} = P\mathsf{Q}.$$

The proof of this theorem is the main part of this section and will be given in Sections 5.3 to 5.5. Now, we want to use the above result to conclude the EDP-convergence with tilting. For this result, it is essential to study the dependence of the limit $\mathfrak{D}_0$ on the limit equilibrium measure w^0. One the one hand, $\mathcal{E}_0(c)$ is the relative Boltzmann entropy of c with respect to w^0, which provides a simple and well-behaved dependence on w^0. On the other hand, $\mathcal{R}^*_{\text{eff}}$ is given through $\mathcal{R}^*_S$ and χ_Ξ. The former only depends on $(\kappa^{S,0}_{in})_{i,n\in\mathcal{I}}$ and the latter depends only on $M \in \{0,1\}^{J\times I}$. Thus, there is no dependence on w^0 at all. The proof relies on the fact that the two processes of (i) tilting with driving forces η and of (ii) taking the limit $\varepsilon \to 0$ commute.

Theorem 5.4 (EDP-convergence with tilting)**.** *The gradient systems* $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ *EDP-converge with tilting to the limit gradient structure* $(\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$.

The closure of the domain of the limit gradient system in the sense of (3.2) *is* Q_{eq}.

Proof. Proposition 5.1 and Theorem 5.3 already provide the simple EDP convergence $(\mathsf{Q}, \mathcal{E}_\varepsilon, \mathcal{R}^*_\varepsilon) \xrightarrow{\text{EDP}} (\mathsf{Q}, \mathcal{E}_0, \mathcal{R}^*_{\text{eff}})$. The domain is restricted by the conditions (i) that $\mathrm{D}\mathcal{E}_0(c)$ exists, which means that $c_i > 0$ for all i, and (ii) that $\mathrm{D}\mathcal{E}_0(c)$ lies in the domain of $\partial_\xi \mathcal{R}^*_{\text{eff}}(c, \cdot\,)$. The latter condition is equivalent to $\mathrm{D}\mathcal{E}_0(c) \in \Xi$ or equivalently $c \in X_{\text{eq}}$.

For the tilted energies $\mathcal{E}^\eta_\varepsilon = \mathcal{E}_\varepsilon - \langle \eta, \cdot \rangle$ we obviously have $\mathcal{E}^\eta_\varepsilon \xrightarrow{\text{M}} \mathcal{E}^\eta_0$. We can now apply Theorem 5.3 once again for $\mathfrak{D}^\eta_\varepsilon$. Using the fact that $\mathcal{E}^\eta$ is again a relative Boltzmann entropy with respect to the exponentially tilted equilibrium state $w^{\eta,\varepsilon}$ that satisfies $w^{\eta,\varepsilon} \to w^{\eta,0}$. Thus, the Mosco limit $\mathfrak{D}^\eta_0$ of $\mathfrak{D}^\eta_\varepsilon$ again exists and has the same form as $\mathfrak{D}_0$ in (5.3), but with $\mathrm{D}\mathcal{E}_0(c)$ replaced by $\mathrm{D}\mathcal{E}(c) - \eta$. In particular, $\mathcal{R}_{\text{eff}}$ remains unchanged and EDP-convergence with tilting is established. □

5.2 The limit and the coarse-grained gradient structure

Before going into the proof of Theorem 5.3 we connect the limit gradient systems with the limit equation (2.6). The gradient-flow equation for the limit gradient systems reads

$$\dot c \in \partial_\xi \mathcal{R}^*_{\text{eff}}(c, -\mathrm{D}\mathcal{E}_0(c)) \quad \text{a.e. on } [0,T]. \tag{5.4}$$

Since $\mathcal{R}^*_{\text{eff}}$ is no longer smooth, we use the set-valued convex subdifferential ∂_ξ that satisfies, because of the continuity of $\mathcal{R}^*_S$, the sum rule

$$\partial_\xi \mathcal{R}^*_{\text{eff}}(c,\xi) = \mathrm{D}_\xi \mathcal{R}^*_S(c,\xi) + \partial\chi_\Xi(\xi) \quad \text{with } \partial\chi_\Xi(\xi) = \begin{cases} \text{kernel}(M) & \text{for } \xi \in \Xi, \\ \emptyset & \text{for } \xi \notin \Xi, \end{cases}$$

where we used the relation $\Xi = \text{range}(M^*) = \text{kernel}(M)^\perp$.

On the one hand, (5.4) implies that $\mathrm{D}\mathcal{E}_0(c) \in \Xi$ for a.a. $t \in [0,T]$. Recalling that the rows of $M \in \{0,1\}^{J\times I}$ consists of vectors having the entry 1 in exactly one equivalent class $\alpha(j) \subset \mathcal{I}$ for $\sim_F$ and 0 else, we have

$$\Xi = \text{range}(M^*) = \big\{ \xi \in \mathbb{R}^I \,\big|\, \forall\, j \in \mathcal{J}\ \forall\, i_1, i_2 \in \alpha(j) :\ \xi_{i_1} = \xi_{i_2} \big\}$$

we conclude

$$\mathrm{D}\mathcal{E}_0(c) \in \Xi \iff \forall\, j \in \mathcal{J}\ \forall\, i_1, i_2 \in \alpha(j) :\ \frac{c_{i_1}}{w^0_{i_1}} = \frac{c_{i_2}}{w^0_{i_2}} \iff c \in X_{\text{eq}} \iff A^F c = 0.$$

One the other hand, by construction of the gradient structure the term $\mathrm{D}_\xi \mathcal{R}_S^*(c, -\mathrm{D}\mathcal{E}_0(c))$ generates exactly the term $A^S c$. Thus, (5.4) is equivalent to

$$\dot{c}(t) \in A^S c(t) + \mathrm{kernel}(M), \quad A^F c(t) = 0 \qquad \text{a.e. on } [0,T]. \tag{5.5}$$

Applying M to the first equation gives the limit equation (2.6) and the following result.

Proposition 5.5 (Gradient structure for limit equation)**.** *The limit equation* (2.6) *is the gradient-flow equation generated by the limit gradient system* $(\mathsf{Q}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}}^*)$.

As a last step, we show that the gradient structure for the limit equation also provides a gradient structure for the coarse gradient equation (2.7) $\dot{\hat{c}} = MA^S N\hat{c}$ for the coarse-grained states $\hat{c} = Mc \in \hat{\mathsf{Q}}$. For this we exploit the special relations derived for coarse graining via $M : X \to Y$ and reconstruction via $N : Y \to X$.

Theorem 5.6 (Gradient structure for coarse-grained equation)**.** *The coarse-grained equation* (2.7) *(viz.* $\dot{\hat{c}} = MA^S N\hat{c}$*) is the gradient-flow equation generated by the coarse-grained gradient system* $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ *given by*

$$\hat{\mathcal{E}}(\hat{c}) = \mathcal{E}_0(N\hat{c}) = \mathcal{H}_J(\hat{c}|\hat{w}) \quad \textit{and} \quad \hat{\mathcal{R}}(\hat{c}, \hat{v}) = \mathcal{R}_{\mathrm{eff}}(N\hat{c}, N\hat{v}).$$

Moreover, we have $\hat{\mathcal{R}}^*(\hat{c}, \hat{\xi}) = \mathcal{R}_{\mathrm{eff}}^*(N\hat{c}, M^*\hat{\xi}) = \mathcal{R}_S^*(N\hat{c}, M^*\hat{\xi})$.

This result can be seen as an exact coarse graining in the sense of the formal approach developed in [MaM20, Sec. 6.1].

Before giving the proof of this result we want to highlight its relevance. First, we emphasize that the coarse-grained equation is again a linear reaction system, now in $\mathbb{R}^J$, i.e. the master equation for a Markov process on $\mathcal{J} = \{1, \dots, J\}$. Second, the coarse-grained energy functional is again the relative Boltzmann entropy, now with respect to the coarse-grained equilibrium $\hat{w} = Mw^0$. Third, the coarse-grained dual dissipation potential is again given in terms of the function C^*, i.e. the coarse-grained gradient system is again of cosh-type. In summary, the coarse-grained gradient structure $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ is again a cosh gradient structure, see Proposition 5.7 below.

We refer to [LM*17, Sec. 3.3] for an example that shows that other gradient structures may not be stable under EDP-convergence. All these results rely on the special properties of M and N developed in Section 2.3. In particular, we use that the projection $P = NM : X \to X$ is a Markov operator, i.e. it maps Q onto itself.

Proof of Theorem 5.6.

Step 1: $\hat{\mathcal{E}}$ is a relative entropy. We use the special form $N = \mathbb{D}_{w^0} M^* \mathbb{D}_{\hat{w}}$, which gives $(N\hat{c})_i = w_i^0 \hat{c}_j / \hat{w}_j$, where $i \in \alpha(j)$. With this and $\hat{w}_j = \sum_{i \in \alpha(j)} w_i^0$ we obtain

$$\begin{aligned}
\hat{\mathcal{E}}(\hat{c}) = \mathcal{E}_0(N\hat{c}) = \mathcal{H}_I(Nc|w^0) &= \sum_i w_i^0 \, \lambda_{\mathrm{Bz}}\big(\frac{(N\hat{c})_i}{w_i^0}\big) \\
&= \sum_{j=1}^J \sum_{i \in \alpha(j)} w_i^0 \lambda_{\mathrm{Bz}}\big(\frac{\hat{c}_j}{\hat{w}_j}\big) = \sum_{j=1}^J \hat{w}_j \lambda_{\mathrm{Bz}}\big(\frac{\hat{c}_j}{\hat{w}_j}\big) = \mathcal{H}_J(\hat{c}|\hat{w}).
\end{aligned}$$

Step 2: Legendre-conjugate pair $\hat{\mathcal{R}}$ and $\hat{\mathcal{R}}^*$. We start from the formula for $\hat{\mathcal{R}}^*$ and calculate $\hat{\mathcal{R}}$ as follows. Using $MN = \mathrm{id}_Y$ and $\Xi = M^* Y^*$, we obtain

$$\begin{aligned}
&\hat{\mathcal{R}}(\hat{c}, \hat{v}) = \sup\big\{ \langle \hat{\xi}, MN\hat{v}\rangle_J - \hat{\mathcal{R}}^*(\hat{c}, \hat{\xi}) \,\big|\, \hat{\xi} \in Y^* \big\} \\
&= \sup\big\{ \langle M^*\hat{\xi}, N\hat{v}\rangle_I - \hat{\mathcal{R}}^*(\hat{c}, \hat{\xi}) \,\big|\, \hat{\xi} \in Y^* \big\} = \sup\big\{ \langle \xi, N\hat{v}\rangle_I - \mathcal{R}_S^*(N\hat{c}, \xi) \,\big|\, \xi \in M^*Y^* \big\} \\
&= \sup\big\{ \langle \xi, N\hat{v}\rangle_I - \mathcal{R}_S^*(N\hat{c}, \xi) - \chi_\Xi(\xi) \,\big|\, \xi \in X^* \big\} = \mathcal{R}_{\mathrm{eff}}(N\hat{c}, N\hat{v}),
\end{aligned}$$

where we use the definition of $\mathcal{R}^*_{\mathrm{eff}}$ in (5.2).

Step 3: The gradient-flow equation for $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$. We first observe

$$M^*N^*\mathrm{D}\mathcal{E}_0(N\hat{c}) = \mathrm{D}\mathcal{E}_0(N\hat{c}). \tag{5.6}$$

Indeed, let us define the component-wise log-function on $\mathbb{R}^I$, $\log : x \mapsto (\log(x_i))_{i=1,\dots,I}$. We have $\mathrm{D}\mathcal{E}_0(c) = \log(\mathbb{D}_{w^0}^{-1}c)$. Hence, for $c = N\hat{c} = \mathbb{D}_{w^0}M^*\mathbb{D}_{\hat{w}}^{-1}\hat{c}$, we conclude

$$\mathrm{D}\mathcal{E}_0(N\hat{c}) = \log(\mathbb{D}_{w^0}^{-1}N\hat{c}) = \log(M^*\mathbb{D}_{\hat{w}}^{-1}\hat{c}) = M^*\log(\mathbb{D}_{\hat{w}}^{-1}\hat{c}) = M^*\mathrm{D}\hat{\mathcal{E}}(\hat{c}) = M^*N^*\mathrm{D}\mathcal{E}_0(N\hat{c}),$$

where we used that $\mathrm{D}\hat{\mathcal{E}}(\hat{c}) = N^*\mathrm{D}\mathcal{E}_0(N\hat{c})$.

With $\mathrm{D}\hat{\mathcal{E}}(\hat{c}) = N^*\mathrm{D}\mathcal{E}_0(N\hat{c})$ and (5.6) the gradient-flow equation for $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ reads

$$\begin{aligned}\dot{\hat{c}} &= \partial_\xi\hat{\mathcal{R}}^*(\hat{c}, -\mathrm{D}\hat{\mathcal{E}}_0(\hat{c})) = M\partial_\xi\mathcal{R}^*_S\big(N\hat{c}, -M^*\mathrm{D}\hat{\mathcal{E}}(\hat{c})\big)\\ &= M\partial_\xi\mathcal{R}^*_S\big(N\hat{c}, -M^*N^*\mathrm{D}\mathcal{E}_0(N\hat{c})\big) = M\partial_\xi\mathcal{R}^*_S(N\hat{c}, -\mathrm{D}\mathcal{E}_0(N\hat{c})) = MA^SN\hat{c},\end{aligned}$$

where we used the identity $\mathrm{D}_\xi\mathcal{R}^*_S(c, -\mathrm{D}\mathcal{E}_0(c)) = A^Sc$, which holds for all c by the construction of our gradient structure. □

In analogy to formula (2.8) providing the coefficients $\hat{A}_{j_1j_2}$ of the coarse-grained generator $\hat{A} = MA^SN$ we can also give a formula for the tilting-invariant reaction intensities $\kappa^{S,0}_{i_1i_2}$ to obtain the corresponding intensities $\hat{\kappa}_{j_1,j_2}$ for the coarse-grained equation (2.7) by a suitable averaging. In particular, the gradient systems $(\hat{\mathsf{Q}}, \hat{\mathcal{E}}, \hat{\mathcal{R}})$ provides again a cosh gradient structure in the sense of Section 4.3.3.

Proposition 5.7 (Cosh structure of $\hat{\mathcal{R}}^*$)**.** *The coarse-grained dual dissipation potential $\hat{\mathcal{R}}^*$ reads*

$$\hat{\mathcal{R}}^*(\hat{c}, \hat{\xi}) = \sum_{1\le j_1<j_2\le J} \hat{\kappa}_{j_1,j_2}\sqrt{\hat{c}_{j_1}\hat{c}_{j_2}}\,\mathsf{C}^*(\hat{\xi}_{j_1}-\hat{\xi}_{j_2}) \text{ with } \hat{\kappa}_{j_1,j_2} = \sum_{i_1\in\alpha(j_1)}\sum_{i_2\in\alpha(j_2)}\kappa^{S,0}_{i_1i_2}\big(\tfrac{w^0_{i_1}w^0_{i_2}}{\hat{w}_{j_1}\hat{w}_{j_2}}\big)^{1/2}.$$

Proof. Theorem 5.6 provides an explicit formula for $\hat{\mathcal{R}}^*$. Inserting the definitions of M and N and grouping according to equivalence classes will provide the result. Recalling the function $\phi : \mathcal{I} \to \mathcal{J}$ giving for each i the associated equivalence class $\alpha(\phi(i)) \subset \mathcal{I}$ we have $(N\hat{c})_i = w^0_i\hat{c}_{\phi(i)}/\hat{w}_{\phi(i)}$ and $(M^*\hat{\xi})_i = \hat{\xi}_{\phi(i)}$ and find

$$\begin{aligned}\hat{\mathcal{R}}^*(\hat{c}, \hat{\xi}) = \mathcal{R}^*_S(N\hat{c}, M^*\hat{\xi}) &= \frac{1}{2}\sum_{i_1\in\mathcal{I}}\sum_{i_2\in\mathcal{I}}\kappa^{S,0}_{i_1i_2}\Big(\frac{w^0_{i_1}c_{\phi(i_1)}}{\hat{w}_{\phi(i_1)}}\,\frac{w^0_{i_2}c_{\phi(i_2)}}{\hat{w}_{\phi(i_2)}}\Big)^{1/2}\,\mathsf{C}^*\big(\hat{\xi}_{\phi(i_1)}-\hat{\xi}_{\phi(i_2)}\big)\\ &= \frac{1}{2}\sum_{j_1\in\mathcal{J}}\sum_{j_2\in\mathcal{J}}\sum_{i_1\in\alpha(i_1)}\sum_{i_2\in\alpha(j_2)}\kappa^{S,0}_{i_1i_2}\Big(\frac{w^0_{i_1}c_{j_1}}{\hat{w}_{j_1}}\,\frac{w^0_{i_2}c_{j_2}}{\hat{w}_{j_2}}\Big)^{1/2}\,\mathsf{C}^*\big(\hat{\xi}_{j_1}-\hat{\xi}_{j_2}\big).\end{aligned}$$

This shows the desired result. □

5.3 A priori bounds and compactness

We start the proof of the Γ-convergence for the dissipation functional $\mathfrak{D}_\varepsilon$ on $\mathrm{L}^2([0,T],\mathsf{Q})$ by deriving the necessary a priori bounds for proving the compactness for a family $(c^\varepsilon)_{\varepsilon>0}$ of functions satisfying $\mathfrak{D}_\varepsilon(c^\varepsilon) \le C < \infty$.

Clearly since for all $t \in [0,T]$ we have $c^\varepsilon(t) \in \mathsf{Q}$ we get immediately uniform L^∞-bounds on c^ε. Hence, we have (after extracting a suitable subsequence, which is not relabeled) a weak limit $c^0 \in \mathrm{L}^2([0,T],\mathsf{Q})$. We want to improve the convergence to strong convergence. Already in the proof of the convergence of the solutions c^ε in Section 2.5 it became clear that there are two different controls, namely (i) the tendency to go to microscopic equilibrium and (ii) the dissipation through the slow reactions. From (i) we will obtain control of the distance of c^ε from $X_{\mathrm{eq}} = PX$ by estimating $(I-P)c^\varepsilon$, but we are not able to control $(I-P)\dot{c}^\varepsilon$. From (ii) we obtain an a priori bound for $P\dot{c}^\varepsilon$, and the major task is to show that these two complementary pieces of information are enough to obtain compactness.

Subsequently, we will drop ε in the notations for w^ε, $\kappa_{in}^{\alpha,\varepsilon}$, and $\mathcal{R}_{S,\varepsilon}$, and so on. Of course, we will keep the important factor $1/\varepsilon$ in $\mathcal{R}_\varepsilon^* = \mathcal{R}_S^* + \frac{1}{\varepsilon}\mathcal{R}_F^*$.

The following result shows the convergence of sequences to the subspace $X_{\mathrm{eq}} = PX$ of microscopic equilibria. Recall the decomposition $X = X_{\mathrm{eq}} \oplus X_{\mathrm{fast}}$ from (2.5) and the projection $P = NM$ such that $X_{\mathrm{eq}} = PX$ and $X_{\mathrm{fast}} = (I-P)X$. In particular, the semi-norm $c \mapsto |(I-P)c|$ is equivalent to $c \mapsto \mathrm{dist}(c, X_{\mathrm{eq}})$.

Lemma 5.8 (Convergence in the direction of fast reactions)**.** *Consider a sequence (c^ε) in $\mathrm{L}^2([0,T],\mathsf{Q})$ with $\mathfrak{D}_\varepsilon(c^\varepsilon) \le C_{\mathfrak{D}} < \infty$ and $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^2([0,T],\mathbb{R}^I)$. Then, there is a constant $C > 0$ such that*

$$\int_0^T |(I-P)c^\varepsilon(t)|^2 \mathrm{d}t \le C\varepsilon.$$

In particular, we have $c^0(t) \in \mathsf{Q}_{\mathrm{eq}} = P\mathsf{Q}$ for a.a. $t \in [0,T]$.

Proof. The bound on the dissipation functional $\mathfrak{D}_\varepsilon$, $\mathcal{R}_\varepsilon \ge 0$, $\mathcal{R}_S^* \ge 0$ and the relation $\mathsf{C}^*(\log p - \log q) = 2\big(\sqrt{p/q} + \sqrt{q/p} - 2\big)$ imply

$$C_{\mathfrak{D}} \ge \mathfrak{D}_\varepsilon(c^\varepsilon) \ge \frac{1}{\varepsilon}\int_0^T \sum_{(i,n)\in\mathbb{F}} \frac{4\kappa_{in}^F}{\sqrt{w_i w_n}} \left(\sqrt{\frac{c_i^\varepsilon}{w_i}} - \sqrt{\frac{c_n^\varepsilon}{w_n}}\right)^2 \mathrm{d}t,$$

where the set $\mathbb{F}$ is given in term of the equivalence relation $\sim_F$, viz.

$$\mathbb{F} := \big\{\, (i,n) \in \mathcal{I}\times\mathcal{I} \,\big|\, i \sim_F n \text{ and } i < n \,\big\}.$$

Using the decomposition $X = X_{\mathrm{eq}} \oplus X_{\mathrm{fast}}$ from (2.5), we see that the semi-norm

$$\|c\|_{\mathbb{F}} := \Big(\sum\nolimits_{(i,n)\in\mathbb{F}} \big(\frac{c_i}{w_i} - \frac{c_n}{w_n}\big)^2\Big)^{1/2}$$

defines a norm on X_{fast} and there exists $C_2 > 0$ such that $|(I-P)c| \le C_2\|c\|_{\mathbb{F}}$ on Q.

Denoting by $\underline{w} > 0$ and $\underline{\kappa} > 0$ lower bounds for all w_i^ε and all κ_{in}^F with $i \sim_F n$, respectively, we obtain the estimate

$$\begin{aligned}
&\int_0^T |(I-P)c^\varepsilon(t)|^2 \mathrm{d}t \le C_2^2 \int_0^T \|c^\varepsilon(t)\|_{\mathbb{F}}^2 \mathrm{d}t \\
&\le C_2^2 \int_0^T \sum_{(i,n)\in\mathbb{F}} \Big(\sqrt{\frac{c_i^\varepsilon}{w_i}} - \sqrt{\frac{c_n^\varepsilon}{w_n}}\Big)^2 \Big(\sqrt{\frac{c_i^\varepsilon}{w_i}} + \sqrt{\frac{c_n^\varepsilon}{w_n}}\Big)^2 \mathrm{d}t \\
&\le \frac{C_2^2}{\underline{w}^2\underline{\kappa}} \int_0^T \sum_{(i,n)\in\mathbb{F}} \frac{4\kappa_{in}^F}{\sqrt{w_i w_n}} \Big(\sqrt{\frac{c_i^\varepsilon}{w_i}} - \sqrt{\frac{c_n^\varepsilon}{w_n}}\Big)^2 \mathrm{d}t \le \frac{C_2^2}{\underline{w}^2\underline{\kappa}}\, C_{\mathfrak{D}}\, \varepsilon.
\end{aligned}$$

By weak lower semicontinuity of semi-norms we find $\int_0^T |(I-P)c^0(t)|^2 \mathrm{d}\, t = 0$ and conclude $c^0(t) = Pc^0(t)$ a.e. on $[0,T]$. This proves the result. □

The next result shows that we are able to control the time derivative of Pc^ε. Using $\mathrm{range}(P) = \mathrm{range}(N)$ and $NM = \mathrm{id}_Y$ it suffices to control $M\dot{c}^\varepsilon$. For this, we show that $\mathcal{R}_\varepsilon(c,\cdot)$ restricted to PX has a uniform lower superlinear bound in terms of the superlinear function C, see (A.2).

Proposition 5.9 (Convergence in the direction of slow reactions)**.** *Consider a sequence (c^ε) in $\mathrm{L}^2([0,T],\mathsf{Q})$ with $\mathfrak{D}_\varepsilon(c^\varepsilon) \le C_\mathfrak{D} < \infty$ and $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^2([0,T];X)$. Then, there is a constant $C_\mathrm{W} > 0$ such that*

$$\int_0^T \mathsf{C}\big(\frac{1}{C_\mathrm{W}}\,|P\dot{c}^\varepsilon(t)|\big)\,\mathrm{d}\, t \le C_\mathrm{W}. \tag{5.7}$$

Moreover, $Pc^\varepsilon \rightharpoonup Pc^0 \in \mathrm{W}^{1,1}([0,T];\mathsf{Q})$ and $Pc^\varepsilon \to Pc^0$ in $\mathrm{C}^0([0,T];P\mathsf{Q})$. With Lemma 5.8 we have $c^\varepsilon \to c^0$ strongly in $\mathrm{L}^2([0,T],\mathsf{Q})$ and $c^0 = Pc^0 \in \mathrm{W}^{1,1}([0,T];\mathsf{Q})$.

Proof. To show a lower bound for $\mathcal{R}_\varepsilon(c,Pv)$ we first derive an upper bound for $\mathcal{R}^*_\varepsilon(c,\tilde{\xi})$ for $\tilde{\xi} \in P^*X^*$. Use $\mathcal{R}^*_{F,\varepsilon}(c,\tilde{\xi}) = 0$ and set $\overline{\kappa} := \sup\big\{\, \kappa_{in}^{S,\varepsilon} \,\big|\, 1 \le i < n \le I, \varepsilon \in]0,1[\,\big\}$ to obtain

$$\mathcal{R}^*_\varepsilon(c,\tilde{\xi}) = \sum_{i<j} \kappa_{in}^{S,\varepsilon}\sqrt{c_i c_j}\,\mathsf{C}^*\big((\tilde{\xi}_i - \tilde{\xi}_j\big) \le \sum_{i<j} \overline{\kappa}\,\tfrac{1}{2}\,\mathsf{C}^*(\sqrt{2}\,|\tilde{\xi}|) \le a\,\mathsf{C}^*(\sqrt{2}\,|\tilde{\xi}|)$$

with $a = I^2\overline{\kappa}/4$. Next, Legendre transform, $\mathcal{R}^*_{F,\varepsilon}(c,\tilde{\xi}) = 0$ by (5.1) and the bound $|P^*\xi| \le C_P/\sqrt{2}|\xi|$ yield the lower bound

$$\begin{aligned}
\mathcal{R}_\varepsilon(c,v) &\ge \sup\big\{\, \langle\tilde{\xi},v\rangle - \mathcal{R}^*_\varepsilon(c,\tilde{\xi}) \,\big|\, \tilde{\xi} \in P^*X^* \,\big\} = \sup\big\{\, \langle P^*\xi, v\rangle - \mathcal{R}^*_{S,\varepsilon}(c,P^*\xi) \,\big|\, \xi \in X^* \,\big\} \\
&\ge \sup\big\{\, \langle \xi, Pv\rangle - a\mathsf{C}^*(\sqrt{2}|P^*\xi|) \,\big|\, \xi \in X^* \,\big\} \ge \sup\big\{\, \langle \xi, Pv\rangle - a\mathsf{C}^*(C_P|\xi|) \,\big|\, \xi \in X^* \,\big\} \\
&= a\,\mathsf{C}\big(\frac{|Pv|}{aC_P}\big).
\end{aligned}$$

Applying this to $v = \dot{c}^\varepsilon$ we find

$$\int_0^T a\mathsf{C}\big(\frac{|P\dot{c}^\varepsilon(t)|}{aC_P}\big)\,\mathrm{d}\, t \le \int_0^T \mathcal{R}_\varepsilon(c^\varepsilon(t),\dot{c}^\varepsilon(t))\mathrm{d}\, t \le \mathfrak{D}_\varepsilon(c^\varepsilon) \le C_\mathfrak{D},$$

which gives (5.7) with $C_\mathrm{W} = \max\{aC_P, C_\mathfrak{D}/a\}$.

With the superlinearity of C, we obtain $Pc^\varepsilon \rightharpoonup Pc^0$ in $\mathrm{W}^{1,1}([0,T];PX)$. Moreover, the sequence Pc^ε is also equicontinuous, which is seen as follows. By (5.7) and (A.2) we have $\int_0^T |P\dot{c}^\varepsilon(t)| \log\big(2+|P\dot{c}^\varepsilon(t)|\big)\,\mathrm{d}\, t \le C_1$. For $R > 0$ we set $\Sigma(R,\varepsilon) = \big\{\, t \in [0,T] \,\big|\, |P\dot{c}^\varepsilon(t)| \ge R \,\big\}$. Thus, for $t_1 < t_2$ we obtain the estimate

$$\begin{aligned}
&|Pc^\varepsilon(t_2) - Pc^\varepsilon(t_1)| \le \int_{t_1}^{t_2} |P\dot{c}^\varepsilon(t)|\mathrm{d}\, t \\
&\le \int_{[t_1,t_2]\setminus\Sigma(R,\varepsilon)} |P\dot{c}^\varepsilon(t)|\mathrm{d}\, t + \int_{\Sigma(R,\varepsilon)} |P\dot{c}^\varepsilon(t)|\,\tfrac{\log(2+|P\dot{c}^\varepsilon(t)|)}{\log(2+R)}\,\mathrm{d}\, t \le (t_2-t_1)R + \frac{C_1}{\log(2+R)}.
\end{aligned}$$

The last sum can be made smaller than any $\varepsilon > 0$ by choosing first $R = R(\varepsilon) := \exp(2C_1/\varepsilon)$ and then assuming $t_2 - t_1 < \delta(\varepsilon) := \varepsilon/(2R(\varepsilon))$. This shows the estimate $|Pc^\varepsilon(t_2) - Pc^\varepsilon(t_1)| < \varepsilon$ whenever $|t_2 - t_1| < \delta(\varepsilon)$, which is the desired equicontinuity. By the Arzelà-Ascoli theorem we obtain uniform convergence.

The final convergence follows from $c^\varepsilon = Pc^\varepsilon + (I-P)c^\varepsilon$ via Lemma 5.8, and the last statement from $Pc^0(t) = c^0(t)$ a.e. in $[0,T]$. □

5.4 The liminf estimate

For the limit passage $\varepsilon \to 0$ we use a technique, which was introduced formally in [LM*17] and exploited in [MaM20] for the study of the large-volume limit in chemical master equations. It relies on the idea that the velocity part $\mathfrak{D}_\varepsilon^{\mathrm{vel}} = \int \mathcal{R}_\varepsilon \,\mathrm{d}t$ of the dissipation functional $\mathfrak{D}_\varepsilon$ can be characterized by Legendre transform using a classical result of Rockafellar:

Theorem 5.10 ([Roc68, Thm. 2]). *Let $f : [0,T]\times\mathbb{R}^n \to \mathbb{R}_\infty$ be a normal, convex integrand and with conjugate f^*. Assume there exist $u_\circ \in \mathrm{L}^1([0,T];\mathbb{R}^n)$ and $\xi_\circ \in \mathrm{L}^\infty([0,T];\mathbb{R}^n)$ such that $t \mapsto f(t,u_\circ(t))$ and $t \mapsto f^*(t,\eta_\circ(t))$ are integrable, then the functionals*

$$I_f\colon \begin{cases} \mathrm{L}^1([0,T];\mathbb{R}^n) \to & \mathbb{R}_\infty, \\ u & \mapsto \int_0^T f(t,u(t))\,\mathrm{d}t \end{cases} \quad \text{and} \quad I_{f^*} : \begin{cases} \mathrm{L}^\infty([0,T];\mathbb{R}^n) \to & \mathbb{R}_\infty, \\ \eta & \mapsto \int_0^T f^*(t,\eta(t))\,\mathrm{d}t \end{cases}$$

are proper convex functionals that are conjugate to each other with respect to the dual pairing $(u,\eta) \mapsto \int_0^T \langle \xi(t), u(t)\rangle \,\mathrm{d}t$, viz. for all $u \in \mathrm{L}^1([0,T];\mathbb{R}^n)$ we have

$$\int_0^T f(t,u(t))\,\mathrm{d}t = \sup\left\{ \int_0^T \Big(\langle \eta(t),u(t)\rangle - f^*(t,\eta(t))\Big)\,\mathrm{d}t \;\middle|\; \eta \in \mathrm{L}^\infty([0,T];\mathbb{R}^n) \right\}. \tag{5.8}$$

We apply this result with $f(t,u) = \mathcal{R}_\varepsilon(c(t),u)$ and obtain, for $\varepsilon \in [0,1]$, the identity

$$\begin{aligned} &\mathfrak{D}_\varepsilon(c) = \sup\big\{\, \mathfrak{B}_\varepsilon(c,\dot c,\xi) \,\big|\, \xi \in \mathrm{L}^\infty([0,T];X^*)\,\big\} \text{ where } \mathfrak{B}_\varepsilon(c,u,\xi) := \mathfrak{B}_\varepsilon^{\mathrm{vel}}(c,u,\xi) + \mathfrak{D}_\varepsilon^{\mathrm{slope}}(c) \\ &\text{with } \mathfrak{B}_\varepsilon^{\mathrm{vel}}(c,u,\xi) := \int_0^T \Big(\langle \xi(t),u(t)\rangle - \mathcal{R}_\varepsilon^*(c(t),\xi(t))\Big)\,\mathrm{d}t \qquad (5.9) \\ &\text{and } \mathfrak{D}_\varepsilon^{\mathrm{slope}}(c) = \int_0^T \mathcal{R}_\varepsilon^*\big(c,-\mathrm{D}\mathcal{E}_\varepsilon(c(t))\big)\,\mathrm{d}t. \end{aligned}$$

The assumptions are easily satisfied as we may choose $u_\circ \equiv 0$ and $\eta_\circ \equiv 0$.

With these preparations we obtain the liminf estimate in a straightforward manner.

Theorem 5.11 (Liminf estimate). *The weak convergence $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^2([0,T];\mathsf{Q})$ implies $\liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) \ge \mathfrak{D}_0(c^0)$, where $\mathfrak{D}_0$ is defined via $\mathcal{E}_0$ and $\mathcal{R}_{\mathrm{eff}}$ in (5.3).*

Proof. We may assume that $\alpha_* := \liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) < \infty$, since otherwise the desired estimate is trivially satisfied.

Step 1. Strong convergence and limit characterization: Using Proposition 5.9 gives

$$c^\varepsilon \to c^0 \text{ strongly in } \mathrm{L}^2([0,T];Q) \quad \text{and} \quad c^0 = Pc^0 \in \mathrm{W}^{1,1}([0,T];\mathbb{R}^I).$$

Step 2. Slope part: Because of $Pc^0(t) = c^0(t)$ we know $\xi_0(t) = \mathrm{D}\mathcal{E}_0(c^0(t)) \in M^*X^*$ which implies $\chi_\Xi\big(-\mathrm{D}\mathcal{E}_0(c^0(t))\big) = 0$ on $[0,T]$. Hence, dropping the nonnegative term $\mathcal{R}_{F,\varepsilon}^*(c^\varepsilon, -\mathrm{D}\mathcal{E}_\varepsilon(c^\varepsilon(t)))$ and setting $\mathcal{S}_\varepsilon(c) := \mathcal{R}_{S,\varepsilon}^*(c,-\mathrm{D}\mathcal{E}_\varepsilon(c))$ we obtain

$$\liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon^{\mathrm{slope}}(c^\varepsilon) \ge \liminf_{\varepsilon\to 0} \int_0^T \mathcal{S}_\varepsilon(c^\varepsilon(t))\,\mathrm{d}t \overset{*}{=} \int_0^T \mathcal{S}_0(c^0(t))\,\mathrm{d}t = \mathfrak{D}_0^{\mathrm{slope}}(c^0).$$

In the passage $\overset{*}{=}$ we use the strong convergence $c^\varepsilon \to c^0$ and the continuity of

$$[0,1]\times Q \ni (\varepsilon,c) \mapsto \mathcal{S}_\varepsilon(c) = \mathcal{R}_{S,\varepsilon}^*(c,-\mathrm{D}\mathcal{E}_\varepsilon(c)) = \sum_{i<n} \frac{4\kappa_{in}^{S,\varepsilon}}{w_i^\varepsilon w_n^\varepsilon}\Big(\sqrt{\tfrac{c_i}{w_i^\varepsilon}} - \sqrt{\tfrac{c_n}{w_n^\varepsilon}}\Big)^2. \tag{5.10}$$

Step 3. Velocity part: We exploit the Rockafellar representation (5.9) together with the fact that $\dot{c}^0(t) = P\dot{c}^0(t)$ a.e. in $[0,T]$. The latter condition allows us to test only by functions $\xi = P^*\xi \in \mathrm{L}^\infty([0,T];X^*)$, which leads to the estimate

$$\begin{aligned}\liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^\varepsilon) &\geq \liminf_{\varepsilon\to 0} \mathfrak{B}_\varepsilon^{\mathrm{vel}}(c^\varepsilon,\dot{c}^\varepsilon,P^*\xi) \overset{\mathrm{a}}{=} \liminf_{\varepsilon\to 0} \int_0^T \Big(\langle \xi, P\dot{c}^\varepsilon\rangle - \mathcal{R}^*_{S,\varepsilon}(c^\varepsilon,\xi)\Big)\,\mathrm{d}t \\ &\overset{\mathrm{b}}{=} \int_0^T \Big(\langle \xi, P\dot{c}^0\rangle - \mathcal{R}^*_{S}(c^0,\xi)\Big)\,\mathrm{d}t = \mathfrak{B}_0^{\mathrm{vel}}(c^0,\dot{c}^0,\xi),\end{aligned}$$

where in $\overset{\mathrm{a}}{=}$ we used $\mathcal{R}^*_\varepsilon(c,\xi) = \mathcal{R}^*_{S,\varepsilon}(c,\xi)$ whenever $\xi = P^*\xi$, see (5.1). In $\overset{\mathrm{b}}{=}$ we exploited the weak convergence $P\dot{c}^\varepsilon \rightharpoonup P c^0$ established in Proposition 5.9 as well as the strong convergence $c^\varepsilon \to c^0$ together with the continuity of $(\varepsilon,c)\mapsto \mathcal{R}^*_{S,\varepsilon}(c,\xi)$.

Now we exploit Rockafellar's characterization (5.9) to return to $\mathfrak{D}_0^{\mathrm{vel}}(c^0)$, namely

$$\begin{aligned}\mathfrak{D}_0^{\mathrm{vel}}(c^0) &= \sup\big\{\, \mathfrak{B}_0^{\mathrm{vel}}(c^0,\dot{c}^0,\xi) \,\big|\, \xi\in \mathrm{L}^\infty([0,T];X^*)\,\big\} \\ &= \sup\Big\{ \int_0^T \Big(\langle \xi,\dot{c}^0\rangle - \mathcal{R}^*_S(c^0,\xi) - \chi_\Xi(\xi)\Big)\,\mathrm{d}t \,\Big|\, \xi\in \mathrm{L}^\infty([0,T];X^*)\,\Big\} \\ &= \sup\big\{\, \mathfrak{B}_0^{\mathrm{vel}}(c^0,\dot{c}^0,\xi) \,\big|\, \xi = P^*\xi\in \mathrm{L}^\infty([0,T];X^*)\,\big\}.\end{aligned}$$

With the above estimate we conclude $\liminf_{\varepsilon\to 0}\mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^\varepsilon) \geq \mathfrak{D}_0^{\mathrm{vel}}(c^0)$.

Adding this to the estimate in Step 2 we obtain the full liminf estimate. □

5.5 Construction of the recovery sequence

Now we construct the recovery sequence for the Mosco-convergence of the dissipation functionals $\mathfrak{D}_\varepsilon$. This provides the required limsup estimate $\limsup_{\varepsilon\to 0}\mathfrak{D}_\varepsilon(c^\varepsilon) \leq \mathfrak{D}_0(c^0)$ along at least one sequence with the strong convergence $c^\varepsilon\to c^0$ in $\mathrm{L}^2([0,T];\mathsf{Q})$. For this we use in Step 2(b) an approximation result by piecewise affine functions $\widehat{c}_N$ introduced in [LiR18, Thm. 2.6, Step 3] and adapted to state-dependent dissipation potentials in [BEM18, Cor. 3.3].

Theorem 5.12 (Recovery sequences)**.** *For every $c^0\in \mathrm{L}^2([0,T];\mathsf{Q})$ there exists a sequence $(c^\varepsilon)_{\varepsilon\in]0,1[}$ with $c^\varepsilon\to c^0$ in $\mathrm{L}^2([0,T];\mathsf{Q})$ such that $\lim_{\varepsilon\to 0}\mathfrak{D}_\varepsilon(c^\varepsilon) = \mathfrak{D}_0(c^0)$.*

Proof. Step 1. The case $\mathfrak{D}_0(c^0)=\infty$. We choose the constant sequence $c^\varepsilon = c^0$ and claim $\mathfrak{D}_\varepsilon(c^\varepsilon) = \mathfrak{D}_\varepsilon(c^0)\to\infty$. Because of $\mathfrak{D}_0(c^0)=\infty$ one of the following conditions is false:

$$\text{(i) } c^0(t)\in \mathsf{Q}_{\mathrm{eq}} \text{ a.e. in } [0,T] \quad \text{or} \quad \text{(ii) } \mathsf{C}\big(|P\dot{c}^0(\cdot)|\big)\in \mathrm{L}^1([0,T]).$$

If (i) is false, then $c^0(t)\notin \mathsf{Q}_{\mathrm{eq}}$ for $t\in\mathcal{T}\subset[0,T]$, where $|\mathcal{T}| = \int_{\mathcal{T}} 1\,\mathrm{d}t > 0$. Setting $\mathcal{F}_\varepsilon(c) := \mathcal{R}^*_{F,\varepsilon}(c,-\mathrm{D}\mathcal{E}_\varepsilon(c))$ we have

$$\mathfrak{D}_\varepsilon^{\mathrm{slope}}(c^0) = \int_0^T \Big(\mathcal{R}^*_{S,\varepsilon}\big(c^0,-\mathrm{D}\mathcal{E}_\varepsilon(c^0)\big)+\frac{1}{\varepsilon}\mathcal{R}^*_{F,\varepsilon}\big(c^0,-\mathrm{D}\mathcal{E}_\varepsilon(c^0)\big)\Big)\,\mathrm{d}t \geq \frac{1}{\varepsilon}\int_0^T \mathcal{F}_\varepsilon(c^0(t))\mathrm{d}t.$$

However, for $t\in\mathcal{T}$ we have $\mathcal{F}_\varepsilon(c^0(t))\to\mathcal{F}_0(c^0(t))>0$. Thus, $\mathfrak{D}_\varepsilon^{\mathrm{slope}}(c^0)\to\infty$ follows which implies $\mathfrak{D}_\varepsilon(c^0)\to\infty$.

If (ii) is false, then $\mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^0)=\infty$ for all $\varepsilon>0$ and we are done.

Step 2. Preliminary recovery sequences for the case $\mathfrak{D}_0(c^0)<\infty$. In the sub-steps (a) to (c) we discuss three approximations for general c^0.

Step 2(a). Positivity for the case $\varepsilon = 0$. We set $\tilde{c}_\delta(t) := \delta w^0 + (1-\delta)c^0(t)$ and claim that $\mathfrak{D}_0(\tilde{c}_\delta) \to \mathfrak{D}_0(c^0) < \infty$ for $\delta \searrow 0$. As $\mathfrak{D}_0$ is convex and lower semicontinuous (cf. see Proposition 5.2), we have $\liminf_{\delta\searrow 0} \mathfrak{D}_0(\tilde{c}_\delta) \geq \mathcal{D}_0(c^0)$.

Obviously, $\tilde{c}_\delta \geq (1-\delta)c^0$ holds componentwise, and hence the explicit form of $\mathcal{R}_0^*$ gives

$$\mathcal{R}^*_{\mathrm{eff}}(\tilde{c}_\delta, \xi) \geq (1-\delta)\mathcal{R}^*_{\mathrm{eff}}(c^0, \xi), \quad \text{and thus } \mathcal{R}_{\mathrm{eff}}(\tilde{c}_\delta, v) \leq (1-\delta)\mathcal{R}_{\mathrm{eff}}\big(c^0, \frac{1}{1-\delta}v\big).$$

Inserting $v = \dot{\tilde{c}}_\delta = (1-\delta)\dot{c}^0$ into the latter estimate gives

$$\mathfrak{D}_0^{\mathrm{vel}}(\tilde{c}_\delta) = \int_0^T \mathcal{R}_{\mathrm{eff}}(\tilde{c}_\delta, \dot{\tilde{c}}_\delta)\,\mathrm{d}t \leq \int_0^T (1-\delta)\mathcal{R}_{\mathrm{eff}}(c^0, \dot{c}^0)\,\mathrm{d}t = (1-\delta)\mathfrak{D}_0^{\mathrm{vel}}(c^0),$$

which proves the desired claim of Step 2(a), because $\mathfrak{D}_0^{\mathrm{slope}}(\tilde{c}_\delta) \to \mathfrak{D}_0^{\mathrm{slope}}(c^0)$ is trivial.

Step 2(b). We stay with $\varepsilon = 0$ and, by Step 2(a), may assume for some $c_* > 0$ that

$$c^0(t) \in \mathsf{Q}_{c_*} := \big\{\, c \in \mathsf{Q} \,\big|\, \forall\, i \in \mathcal{I}\colon\, c_i \geq c_* \,\big\} \text{ for all } t \in [0,T].$$

We now approximate c^0 by a function $\widehat{c}_N \in \mathrm{W}^{1,\infty}([0,T]; PX)$ still satisfying $\widehat{c}_N(t) \in \mathsf{Q}_{c_*}$.

For $N \in \mathbb{N}$ we define $\widehat{c}_N : [0,T] \to PX$ as the piecewise affine interpolant of the nodal points $\widehat{c}_N(kT/N) = c^0(kT/N)$ for $k = 0, 1, \dots, N$. We also define the piecewise constant interpolant $\overline{c}_N : [0,T] \to \mathsf{Q}_{c_*}$ via $\overline{c}_N(t) = c^0(kT/N)$ for $t \in \,](k-1)T/N, kT/N]$. Then, using $c^0 \in \mathrm{W}^{1,1}([0,T]; PX) \subset \mathrm{C}^0([0,T]; PX)$ we have

$$\widehat{c}_N \to c^0 \text{ in } \mathrm{W}^{1,1}([0,T]; PX) \text{ and in } \mathrm{C}^0([0,T]; PX) \quad \text{and} \quad \overline{c}_N \to c^0 \text{ in } \mathrm{L}^\infty([0,T]; PX).$$

We now set

$$\alpha_N := \|c^0 - \widehat{c}_N\|_{\mathrm{L}^\infty} + \|c^0 - \overline{c}_N\|_{\mathrm{L}^\infty}$$

and obtain $\alpha_N \to 0$.

These uniform estimates can be used in conjunction with the uniform continuity of $c \mapsto \mathcal{R}^*_{\mathrm{eff}}(c, \xi)$ when restricted to Q_{c_*}. Clearly $\mathsf{Q}_{c_*} \ni c \mapsto \sqrt{c_i c_n}$ is Lipschitz continuous, and we call the Lipschitz constant λ^*. The special form of $\mathcal{R}^*_{\mathrm{eff}}$ then implies

$$\forall\, c, \tilde{c} \in \mathsf{Q}_{c_*}\ \forall\, \xi \in X^* :\ |\mathcal{R}^*_{\mathrm{eff}}(c, \xi) - \mathcal{R}^*_{\mathrm{eff}}(\tilde{c}, \xi)| \leq \Lambda^* |c - \tilde{c}| \mathcal{R}^*_{\mathrm{eff}}(c, \xi) \ \text{ with } \Lambda^* = \lambda^* \overline{\kappa}.$$

Assuming $|c - \tilde{c}| \leq \alpha$ and $\Lambda^* \alpha < 1$ and applying the Legendre transform we find

$$(1-\Lambda^*\alpha)\mathcal{R}_{\mathrm{eff}}(c, \tfrac{1}{1-\Lambda^*\alpha}v) \geq \mathcal{R}_{\mathrm{eff}}(\tilde{c}, v) \geq (1+\Lambda^*\alpha)\mathcal{R}_{\mathrm{eff}}(c, \tfrac{1}{1+\Lambda^*\alpha}v).$$

Exploiting the scaling property (A.4) we arrive at the estimates

$$\frac{1}{1-\Lambda^*\alpha}\,\mathcal{R}_{\mathrm{eff}}(c, v) \geq \mathcal{R}_{\mathrm{eff}}(\tilde{c}, v) \geq \frac{1}{1+\Lambda^*\alpha}\,\mathcal{R}_{\mathrm{eff}}(c, v).$$

To estimate the velocity part of the dissipation functional as in [LiR18, BEM18] we introduce

$$\mathfrak{J}(c, v) := \int_0^T \mathcal{R}_{\mathrm{eff}}(c(t), v(t))\,\mathrm{d}t,$$

which allows us to use different approximations for c^0 and for $\dot{c}^0$. We obtain

$$\begin{aligned}\mathfrak{D}_0^{\mathrm{vel}}(\widehat{c}_N) &= \mathfrak{J}(\widehat{c}_N,\dot{\widehat{c}}_N) \le (1+\Lambda^*\alpha_N)\mathfrak{J}(\overline{c}_N,\dot{\widehat{c}}_N)\\ &\overset{*}{\le} (1+\Lambda^*\alpha_N)\mathfrak{J}(\overline{c}_N,\dot{c}^0) \le (1+\Lambda^*\alpha_N)^2\mathfrak{J}(c^0,\dot{c}^0) = (1+\Lambda^*\alpha_N)^2\mathfrak{D}_0^{\mathrm{vel}}(c^0).\end{aligned}$$

For the estimate $\overset{*}{\le}$ we split $[0,T]$ into the subintervals $S_k^N :=](k-1)T/N, kT/N[$, where $\overline{c}_N$ and $\dot{\widehat{c}}_N$ are equal to the constants $c^0(kT/N)$ and $\frac{T}{N}\int_{S_N}\dot{c}^0(t)\mathrm{d}\,t$, respectively. Then, Jensen's inequality for the convex function $\mathcal{R}_{\mathrm{eff}}(\overline{c}_N,\cdot)$ gives the desired estimate.

Since $\mathfrak{D}_0^{\mathrm{slope}}(\widehat{c}_N) \to \mathfrak{D}_0^{\mathrm{slope}}(c^0)$ by the continuity of the integrand $\mathcal{S}_0$ (cf. (5.10)), the lower semicontinuity of $\mathfrak{D}_0$ yields $\mathfrak{D}_0(\widehat{c}_N) \to \mathfrak{D}_0(c^0)$.

Step 2(c). Using the Step 2(a) and 2(b), we now may assume $c^0 \in \mathrm{W}^{1,\infty}([0,T],X)$ with $c^0(t) \in \mathsf{Q}_{c_*}$ on $[0,T]$ and define c^ε via the formula

$$c^\varepsilon(t) = \mathbb{D}_{w^\varepsilon}\mathbb{D}_{w^0}^{-1}c^0(t) \text{ for } t \in [0,T].$$

This definition gives $\mathrm{D}\mathcal{E}_\varepsilon(c^\varepsilon(t)) \in \Xi$ and hence $\mathcal{S}_\varepsilon^F(c^\varepsilon(t)) = 0$. Hence, the definition of $\mathcal{S}_\varepsilon$ in terms of the ratios c_i/w_i^ε (cf. (5.10)) implies $\mathfrak{D}_\varepsilon^{\mathrm{slope}}(c^\varepsilon) \to \mathfrak{D}_0^{\mathrm{slope}}(c^0)$.

For the velocity part we again use the Rockafellar characterization, namely

$$\mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^\varepsilon) = \sup\big\{\,\mathfrak{B}_\varepsilon^{\mathrm{vel}}(c^\varepsilon,\dot{c}^\varepsilon,\xi)\,\big|\,\xi \in \mathrm{L}^\infty([0,T];X^*)\,\big\}.$$

Because of the uniform bound of $\dot{c}^\varepsilon$ in $\mathrm{L}^\infty([0,T];X)$ we indeed see that the supremum over $\mathfrak{B}_\varepsilon^{\mathrm{vel}}(c^\varepsilon,\dot{c}^\varepsilon,\cdot)$ is attained by maximizers ξ^ε that are uniformly bounded in $\mathrm{L}^\infty([0,T];X^*)$. To see this, we firstly observe that for any $(c,\dot{c}) \in \mathsf{Q}\times X$ the functional $\mathfrak{B}_\varepsilon(c,\dot{c},\cdot)$ is invariant under scaling $\xi \mapsto \xi + c\mathbb{1}$, since $\langle \mathbb{1},\dot{c}\rangle = 0$ and the dissipation potential $\mathcal{R}_\varepsilon^*(c,\xi)$ only depends on differences $\xi_i - \xi_n$. Hence, it is impossible to obtain compactness for any maximizer ξ^ε in $\mathrm{L}^\infty([0,T],X^*)$. On the contrary, one gets compactness for maximizers ξ^ε with a fixed, say first, component $\xi_1^\varepsilon = 1$. Indeed, by $c^0(t) \in \mathsf{Q}_{c_*}$ and the exponential growth of $\mathcal{R}_\varepsilon^*$ we get

$$\mathcal{R}_\varepsilon^*(c^\varepsilon(t),\xi) \ge c_\circ \sum_{i<n:A_{in}^\varepsilon>0} |\xi_i - \xi_n|^2,$$

with a positive constant $c_\circ > 0$. By the assumption on connectivity (cf. (2.Aa)) of the reaction network all vertices can be reached by a reaction path from vertex 1. Hence, there is another constant $\tilde{c}_\circ$, such that the estimate

$$\mathcal{R}_\varepsilon^*(c^\varepsilon(t),\xi) \ge c_\circ \sum_{i<n:A_{in}^\varepsilon>0} |\xi_i - \xi_n|^2 \ge \tilde{c}_\circ \sum_{i>1} |\xi_1 - \xi_i|^2$$

holds. Hence, the maximizers ξ^ε with $\xi_1^\varepsilon = 1$ satisfy

$$\langle \xi^\varepsilon, \dot{c}^\varepsilon(t)\rangle - \mathcal{R}_\varepsilon^*(c^\varepsilon(t),\xi) \le |\xi^\varepsilon|C\|\dot{c}^0\|_{\mathrm{L}^\infty([0,T],X)} - \tilde{c}_\circ|\xi^\varepsilon|^2,$$

which implies the uniform bound $\|\xi^\varepsilon\|_{\mathrm{L}^\infty([0,T],X^*)} \le C\|\dot{c}^0\|_{\mathrm{L}^\infty([0,T],X)}/\tilde{c}_\circ$.

We now first choose a subsequence $(\varepsilon_k)_{k\in\mathbb{N}}$ such that $\varepsilon_k \searrow 0$ and $\mathfrak{D}_{\varepsilon_k}^{\mathrm{vel}}(c^{\varepsilon_k}) \to \beta = \limsup_{\varepsilon\to 0}\mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^\varepsilon)$. Thus, after selecting a further subsequence (not relabeled) we may assume $\xi^{\varepsilon_k} \rightharpoonup \xi^0$ in $\mathrm{L}^2([0,T];X^*)$. With the strong convergence of $\dot{c}^\varepsilon \to \dot{c}^0$ we conclude

$$\limsup_{\varepsilon\to 0}\mathfrak{D}_\varepsilon^{\mathrm{vel}}(c^\varepsilon) = \lim_{k\to\infty}\mathfrak{B}_{\varepsilon_k}^{\mathrm{vel}}(c^{\varepsilon_k},\dot{c}^{\varepsilon_k},\xi^{\varepsilon_k}) \overset{*}{\le} \mathfrak{B}_0^{\mathrm{vel}}(c^0,\dot{c}^0,\xi^0) \le \mathfrak{D}_0^{\mathrm{vel}}(c^0),$$

where in $\overset{*}{\leq}$ we used the convergence of the duality pairing $\int_0^T \langle \xi^\varepsilon, \dot{c}^\varepsilon \rangle \mathrm{d}t$ and a Ioffe-type argument based on the convexity of $\mathcal{R}^*_\varepsilon(c^\varepsilon, \cdot)$ and the lower semicontinuity of $[0,1]\times X^* \ni (\varepsilon, \xi) \mapsto \mathcal{R}^*_\varepsilon(c^\varepsilon(t), \xi) \in [0,\infty]$, cf. [FoL07, Thm. 7.5]. Adding the convergence of the slope part, and taking into account the liminf estimate from Theorem 5.11 we obtain the convergence $\lim_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) = \mathfrak{D}_0(c^0)$.

Step 3. Construction of recovery sequences for the case $\mathfrak{D}_0(c^0)$. We now apply the approximation steps discussed in Step 2 and show that it is possible to choose an suitable diagonal sequence for getting the desired recovery sequence.

For a general c^0 we apply the approximation as indicated in the sub-steps 2(a), 2(b), and 2(c) and set

$$c^{\delta,N,\varepsilon} = \mathbb{D}_{w^\varepsilon}^{-1} \mathbb{D}_{w_0}\big(\delta w^0 + (1-\delta)\widehat{c}_N^0\big).$$

We easily obtain $\|c^0 - c^{\delta,N,\varepsilon}\|_{\mathrm{L}^2([0,T];X)} \leq C(\delta + \alpha_N + \varepsilon) \to 0$ if $\delta \to 0$, $N \to \infty$, and $\varepsilon \to 0$. Moreover, the difference in the dissipation functionals $\mathfrak{D}_\varepsilon$ can be estimated via

$$\begin{aligned}
\big|\mathfrak{D}_\varepsilon(c^{\delta,N,\varepsilon}) - \mathfrak{D}_0(c^0)\big| &\leq A(\delta) + B_\delta(N) + C_{\delta,N}(\varepsilon), \quad \text{where}\\
A(\delta) &= \big|\mathfrak{D}_0(\tilde{c}^{\,\delta}) - \mathfrak{D}_0(c^0)\big| && \text{with } \tilde{c}^{\,\delta}(t) = \delta w^0 + (1-\delta)c^0(t),\\
B_\delta(N) &= \big|\mathfrak{D}_0\big(c^{\delta,N}\big) - \mathfrak{D}_0(\tilde{c}^{\,\delta})\big| && \text{with } c^{\delta,N}(t) = \delta w^0 + (1-\delta)\widehat{c}_N^0(t),\\
C_{\delta,N}(\varepsilon) &= \big|\mathfrak{D}_\varepsilon(c^{\delta,N,\varepsilon}) - \mathfrak{D}_0(c^{\delta,N})\big|.
\end{aligned}$$

Constructing a recovery sequence $(c^\varepsilon)_{\varepsilon\in]0,1]}$ inductively, one easily sees that $\mathfrak{D}_\varepsilon(c^\varepsilon) \to \mathfrak{D}_0(c^0)$ as desired.

□

A Special properties of cosh gradient structures

Here we discuss a few special properties that are characterizing for the function C and C^* and this lead to corresponding properties of $\mathcal{R}^*_{\cosh}$.

We consider the special non-quadratic dissipation functional

$$\mathsf{C}(v) := 2v\,\operatorname{arsinh}(v/2) - 2\sqrt{4+v^2} + 4 \quad \text{and its Legendre dual} \quad \mathsf{C}^*(\xi) := 4\cosh(\xi/2) - 4.$$

Then, we have $\mathsf{C}(v) = \frac{1}{2}v^2 + O(v^4)$ and $\mathsf{C}^*(\xi) = \frac{1}{2}\xi^2 + O(\xi^4)$. The function C^* has the following properties:

$$\mathsf{C}^*(\log p - \log q) = 2\Big(\sqrt{\frac{p}{q}} + \sqrt{\frac{q}{p}} - 2\Big), \quad \mathsf{C}^{*\prime}(\log p - \log q) = \frac{p-q}{\sqrt{pq}}. \tag{A.1}$$

In addition we have superlinear growth of C:

$$\frac{1}{2}|s|\log(1+|s|) \leq \mathsf{C}(s) \leq |s|\log(1+|s|) \quad \text{for all } s \in \mathbb{R}. \tag{A.2}$$

The first of the following scaling properties follows easily by considering the power series expansion of C^*, the second by Legendre transform:

$$\forall\, \lambda \geq 1\ \forall\, s, \zeta \in \mathbb{R}: \quad \mathsf{C}^*(\lambda\zeta) \geq \lambda^2 \mathsf{C}^*(\zeta) \ \text{ and } \ \mathsf{C}(\lambda s) \leq \lambda^2 \mathsf{C}(s). \tag{A.3}$$

This implies the corresponding scaling property for $\mathcal{R}_{\cosh}$, namely

$$\begin{aligned}
&\forall\, \lambda \geq 1\ \forall\, c \in \mathsf{Q}\ \forall\, v, \xi \in \mathbb{R}^I:\\
&\quad \mathcal{R}^*_{\cosh}(c, \lambda\xi) \geq \lambda^2 \mathcal{R}^*_{\cosh}(c,\xi) \text{ and } \mathcal{R}_{\cosh}(c, \lambda v) \leq \lambda^2 \mathcal{R}_{\cosh}(c, v).
\end{aligned} \tag{A.4}$$

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Part 2

EDP-convergence for nonlinear fast-slow reaction systems with detailed balance

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EDP-convergence for nonlinear fast-slow reaction systems with detailed balance*

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Abstract

We consider nonlinear reaction systems satisfying mass-action kinetics with slow and fast reactions. It is known that the fast-reaction-rate limit can be described by an ODE with Lagrange multipliers and a set of nonlinear constraints that ask the fast reactions to be in equilibrium. Our aim is to study the limiting gradient structure which is available if the reaction system satisfies the detailed-balance condition.

The gradient structure on the set of concentration vectors is given in terms of the relative Boltzmann entropy and a cosh-type dissipation potential. We show that a limiting or effective gradient structure can be rigorously derived via EDP convergence, i.e. convergence in the sense of the Energy-Dissipation Principle for gradient flows. In general, the effective entropy will no longer be of Boltzmann type and the reactions will no longer satisfy mass-action kinetics.

1 Introduction

The study of nonlinear reaction systems with different time scales has attracted much attention over the last decades, see e.g. [Bot03, KaK13, WiS17, DLZ18, MiS19, MaM20] and the references therein. In this work we consider the simplest case of fast-slow reaction systems with mass-action kinetics that have only two time scales, namely 1 and ε,

$$\dot{c} = \boldsymbol{R}_{\mathrm{sl}}(c) + \frac{1}{\varepsilon}\boldsymbol{R}_{\mathrm{fa}}(c), \tag{1.1}$$

where $c \in \mathbf{C} := [0,\infty[^{i_*}$ denotes the vector of the concentrations c_i of the i^{th} species X_i. The typical aim of the above-mentioned work is to derive the limiting equation for the

*Research partially supported by DFG via SFB 1114 (project no. 235221301, subproject C05).

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evolution of c on the slow time scale, while the fast reactions are in equilibrium. Under suitable assumptions the limiting equation can be formulated in three equivalent ways:

$$\begin{aligned}
\text{constrained dynamics:} &\quad \dot c(t) = \boldsymbol{R}_{\rm sl}(c(t)) + \lambda(t), \quad \lambda(t) \in \Gamma_{\rm fa} \subset \mathbb{R}^{i_*}, \quad \boldsymbol{R}_{\rm fa}(c(t)) = 0,\\
\text{projected dynamics:} &\quad \dot c(t) = (I - \mathbb{P}(c(t)))\boldsymbol{R}_{\rm sl}(c(t)), \quad \boldsymbol{R}_{\rm fa}(c(0)) = 0,\\
\text{reduced dynamics:} &\quad \dot{\mathsf{q}}(t) = Q_{\rm fa}\boldsymbol{R}_{\rm sl}(\Psi(\mathsf{q}(t))), \quad c(t) = \Psi(\mathsf{q}(t)).
\end{aligned}$$

We refer to Section 4 for a discussion of these formulations.

The goal of this work is to revisit the same limit process, but now from the point of view of variational evolution. Our starting point is that reaction-rate equations such as (1.1) can be written as a gradient-flow equation if the reactions occur in pairs of forward and backward reactions and that these pairs satisfy the *detailed-balance condition*. This observation was highlighted in [Mie11, Sec. 3.1] but was observed and used implicitly earlier in [ÖtG97, Eqs. (103)+(113)] and [Yon08, Sec. VII]. A different gradient structure already occurs in [Grm10, Eqn. (69)] and has its origin in the thermodynamic considerations in [Mar15] from 1915. The latter gradient structure, which we will call the *cosh-type gradient structure* following [MiS19], was mathematically derived in [MPR14, MP*17] from microscopic chemical master equations via a large-deviation principle.

To be specific, we assume that the species X_i, $i \in I := \{1, \dots, i_*\}$ undergo r_* forward-backward reactions of mass-action type

$$\alpha_1^r X_1 + \cdots + \alpha_{i_*}^r X_{i_*} \quad \rightleftharpoons \quad \beta_1^r X_1 + \cdots + \beta_{i_*}^r X_{i_*},$$

where $\alpha^r = (\alpha_i^r)_{i\in I}$ and $\beta^r = (\beta_i^r)_{i\in I}$ are the stoichiometric vectors in $\mathbb{N}_0^{i_*}$. The reaction-rate equation (1.1) takes the form

$$\dot c = -\sum_{r=1}^{r_*} \big(k_r^{\rm fw} c^{\alpha^r} - k_r^{\rm bw} c^{\beta^r}\big)\big(\alpha^r - \beta^r\big), \quad \text{where } c^\alpha = c_1^{\alpha_1}\cdots c_{i_*}^{\alpha_{i_*}}. \tag{1.2}$$

The *detailed-balance condition* asks for the existence of a positive concentration vector $c_* = (c_i^*)_{i\in I} \in \mathbf{C}_+ :=]0,\infty[^{i_*}$ such that all r_* reactions are in

$$\exists\, c_* = (c_i^*)_{i\in I} \in \mathbf{C}_+ \ \forall\, r \in R := \{1, \dots, r_*\} : \quad k_r^{\rm fw} c_*^{\alpha^r} = k_r^{\rm bw} c_*^{\beta^r}. \tag{1.3}$$

For the subsequent analysis it is advantageous to introduce the scalars $\delta_r^* = \big(c_*^{\alpha^r} c_*^{\beta^r}\big)^{1/2}$ and $\widehat\kappa_r = k_r^{\rm fw} c_*^{\alpha^r}/\delta_r^* = k_r^{\rm bw} c_*^{\beta^r}/\delta_r^*$.

Throughout this work we will assume that c_* will not depend on the small parameter ε measuring the ratio between the slow and the fast time scale. The set of reaction pairs R will be decomposed into slow and fast reactions, namely $R = R_{\rm sl} \,\dot\cup\, R_{\rm fa}$, and we assume $\widehat\kappa_r = \kappa_r$ for $r \in R_{\rm sl}$ and $\widehat\kappa_r = \kappa_r/\varepsilon$ for $r \in R_{\rm fa}$, where κ_r are fixed numbers. With this we obtain the symmetric representation of the fast-slow reaction-rate equation via

$$\dot c = \boldsymbol{R}_{\rm sl}(c) + \frac{1}{\varepsilon}\boldsymbol{R}_{\rm fa}(c) \quad \text{with } \boldsymbol{R}_{\rm xy}(c) := -\sum_{r\in R_{\rm xy}} \kappa_r\, \delta_r^* \left(\frac{c^{\alpha^r}}{c_*^{\alpha_r}} - \frac{c^{\beta^r}}{c_*^{\beta_r}}\right)(\alpha^r - \beta^r). \tag{1.4}$$

The cosh-type gradient structure is now defined in terms of a gradient system $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$, where the energy functional is given in terms of the relative Boltzmann entropy

$$\mathcal{E}(c) = \sum_{i\in I} c_i^* \lambda_{\rm B}(c_i/c_i^*), \quad \text{where } \lambda_{\rm B}(\rho) := \rho\log\rho - \rho + 1,$$

and the dual dissipation potential $\mathcal{R}_\varepsilon^*$ in the form

$$\mathcal{R}_\varepsilon^*(c,\xi) = \mathcal{R}_{\mathrm{sl}}^*(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}_{\mathrm{fa}}^*(c,\xi) \quad \text{with } \mathcal{R}_{\mathrm{xy}}^*(c,\xi) = \sum_{r\in R_{\mathrm{xy}}} \kappa_r \big(c^{\alpha^r} c^{\beta^r}\big)^{1/2}\, \mathsf{C}^*\big((\alpha^r-\beta^r)\cdot\xi\big),$$

where $\mathsf{C}^*(\zeta) = 4\cosh(\zeta/2) - 4$. The fast-slow reaction-rate equation (1.4) can now be written as the gradient flow equation

$$\dot c(t) = \partial_\xi \mathcal{R}_\varepsilon^*\big(c(t), -\mathrm{D}\mathcal{E}(c(t))\big).$$

In fact, there are many other gradient structures for (1.4), see Remark 2.6; however the cosh-type gradient structure is special in several aspects: (i) it can be derived via large-deviation principles [MPR14, MP*17], (ii) the dual dissipation potential $\mathcal{R}^*$ is independent of c_*, and (iii) it is stable under general limiting processes, see [LM*17, Sec. 3.3]. The property (ii), also called *tilt invariance* below, will be especially important for us.

The main goal of this paper is to construct the effective gradient system $(\mathbf{C}, \mathcal{E}_{\mathrm{eff}}, \mathcal{R}_{\mathrm{eff}}^*)$ for the given family $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ in the limit $\varepsilon \to 0^+$. Here we use the notion of *convergence of gradient system in the sense of the energy-dissipation principle*, shortly called *EDP-convergence*. This convergence notion was introduced in [DFM19] and further developed in [MMP19, FrL19, MiS19] and is based on the dissipation functionals

$$\mathfrak{D}_\varepsilon^\eta(c) := \int_0^T \big\{\mathcal{R}_\varepsilon(c,\dot c) + \mathcal{R}_\varepsilon^*(c, \eta - \mathrm{D}\mathcal{E}(c))\big\}\,\mathrm{d}t,$$

which are defined for all curves $c \in \mathrm{L}^1([0,T];\mathbf{C})$. The notion of *EDP-convergence with tilting* now asks that the two Γ-convergences $\mathcal{E}_\varepsilon \overset{\Gamma}{\to} \mathcal{E}_{\mathrm{eff}}$ and $\mathfrak{D}_\varepsilon^\eta \overset{\Gamma}{\to} \mathfrak{D}_0^\eta$ (in suitable topologies) and that for all η the limit $\mathfrak{D}_0^\eta$ has the form $\mathfrak{D}_0^\eta(c) = \int_0^T \big\{\mathcal{R}_{\mathrm{eff}}(c,\dot c) + \mathcal{R}_{\mathrm{eff}}^*(c,\eta - \mathrm{D}\mathcal{E}(c))\big\}\,\mathrm{d}t$; see Section 3.1 for the exact definition.

Our main result is Theorem 3.5 which asserts EDP-convergence with tilting with

$$\mathcal{E}_{\mathrm{eff}} = \mathcal{E} \qquad \text{and} \qquad \mathcal{R}_{\mathrm{eff}}^*(c,\xi) = \mathcal{R}_{\mathrm{sl}}^*(c,\xi) + \chi_{\Gamma_{\mathrm{fa}}^\perp}(\xi),$$

where $\Gamma_{\mathrm{fa}} = \operatorname{span}\big\{\, \alpha^r - \beta^r \;\big|\; r \in R_{\mathrm{fa}} \,\big\}$, $\Gamma_{\mathrm{fa}}^\perp := \big\{\, \xi \in \mathbb{R}^{i_*} \;\big|\; \forall\, \gamma \in \Gamma_{\mathrm{fa}} :\ \gamma\cdot\xi = 0 \,\big\}$ and χ_A is the characteristic function of convex analysis taking 0 on A and ∞ otherwise. The proof relies on three observations:

(1) Tilting of the relative Boltzmann entropy $\mathcal{E}$ by η is equivalent to changing the underlying equilibrium c_* to $c_*^\eta := (\mathrm{e}^{\eta_i} c_i^*)_{i\in I}$ (see (3.7)), and $\mathcal{R}_\varepsilon^*$ is independent of c_*^η.

(2) The dual dissipation potentials $\mathcal{R}_\varepsilon^*$ increase monotonically to their limit $\mathcal{R}_{\mathrm{eff}}^*$, which is singular. Hence, the primal dissipation potentials $\mathcal{R}_\varepsilon$ decrease monotonically to their limit $\mathcal{R}_{\mathrm{eff}}$, which is degenerate. Defining $Q_{\mathrm{fa}} : \mathbb{R}^{i_*} \to \mathbb{R}^{m_{\mathrm{fa}}}$ such that $\ker Q_{\mathrm{fa}} = \Gamma_{\mathrm{fa}}$ and $\operatorname{im} Q_{\mathrm{fa}}^\top = \Gamma_{\mathrm{fa}}^\perp$, the bound $\mathfrak{D}_\varepsilon^\eta(c^\varepsilon) \le M_{\mathrm{diss}} < \infty$ does not provide a uniform bound on $\dot c^\varepsilon$, but we are able to show weak compactness of $Q_{\mathrm{fa}} c^\varepsilon$ in $\mathrm{W}^{1,1}([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$.

(3) To obtain compactness for families $(c^\varepsilon)_{\varepsilon\in]0,1[}$ from the bound $\mathfrak{D}_\varepsilon(c^\varepsilon) \le M_{\mathrm{diss}} < \infty$ we can use $\int_0^T \mathcal{R}_{\mathrm{fa}}^*(c^\varepsilon, -\mathrm{D}\mathcal{E}(c^\varepsilon))\,\mathrm{d}t \le \varepsilon\, M_{\mathrm{diss}}$, which forces c^ε into the set of equilibria of the fast equation, namely $\mathscr{E}_{\mathrm{fa}} := \big\{\, c \in \mathbf{C} \;\big|\; \boldsymbol{R}_{\mathrm{fa}}(c) = 0 \,\big\}$.

An important assumption of the fast reaction system $c'(\tau) = \boldsymbol{R}_{\mathrm{fa}}(c(\tau))$ is that it has a unique equilibrium in each invariant subset $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}} := \big\{\, c \in \mathbf{C} \,\big|\, Q_{\mathrm{fa}} c = \mathsf{q} \,\big\}$. This equilibrium is obtained as minimizer of $\mathcal{E}$ and is denoted by $\Psi(\mathsf{q})$. Thus, the *unique fast equilibrium condition* reads

$$\mathscr{M}_{\mathrm{sl}} := \big\{\, \Psi(\mathsf{q}) \;\big|\; \mathsf{q} \in Q_{\mathrm{fa}}\mathbf{C} \,\big\} \overset{!!}{=} \mathscr{E}_{\mathrm{fa}} := \big\{\, c \in \mathbf{C} \;\big|\; \boldsymbol{R}_{\mathrm{fa}}(c) = 0 \,\big\}.$$

The main difficulty is to show that the information in points (2) and (3) is enough to obtain the compactness necessary for deriving liminf estimate for the Γ-convergence $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma} \mathfrak{D}_0$ for the non-convex functionals $\mathfrak{D}_\varepsilon$. On the local level, one sees that (2) provides partial control of the temporal oscillations of $\dot{c}^\varepsilon$ via the bound on $Q_{\mathrm{fa}}\dot{c}^\varepsilon$ in $\mathrm{L}^1([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$, whereas (3) provides strong convergence towards $\mathscr{M}_{\mathrm{sl}}$, which is locally defined via $\mathrm{D}\mathcal{E}(c) \in \Gamma_{\mathrm{fa}}^{\perp}$ (see Lemma 3.7). In summary, we are able to show that $\mathfrak{D}_\varepsilon(c^\varepsilon) \le M_{\mathrm{diss}} < \infty$ implies that there exists a subsequence such that $c^{\varepsilon_n} \to \widetilde{c}$ in $\mathrm{L}^1([0,T];\mathbf{C})$ and $Q_{\mathrm{fa}}c^{\varepsilon_n} \to \mathsf{q}$ uniformly in $\mathrm{C}^0([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$, where $\widetilde{c}(t) = \Psi(\mathsf{q}(t))$ with $\mathsf{q} \in \mathrm{W}^{1,1}([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$.

As a corollary we obtain that the limiting evolution lies in $\mathscr{M}_{\mathrm{sl}}$ and is governed by the reduced (or coarse grained) equation $\dot{\mathsf{q}} = Q_{\mathrm{fa}}\boldsymbol{R}_{\mathrm{sl}}(\Psi(\mathsf{q}))$ described by the slow variables $\mathsf{q} \in Q_{\mathrm{fa}}\mathbf{C}$ and a natural gradient structure $(Q_{\mathrm{fa}}\mathbf{C}, \mathsf{E}, \mathsf{R})$. Even on the level of the limiting equations our result goes beyond those in [Bot03, DLZ18], since we do not assume that solutions are strictly positive or that the stoichiometric vectors $\gamma^r = \alpha^r - \beta^r$, $r \in R_{\mathrm{fa}}$, are linearly independent.

For illustration, we close the introduction by a simple example involving $i_* = 5$ species and one fast and one slow reaction (see Section 4.3 for the details under slightly more general conditions):

$$X_1 + X_2 \overset{\text{fast}}{\rightleftharpoons} X_3 \qquad \text{and} \qquad X_3 + X_4 \overset{\text{slow}}{\rightleftharpoons} X_5,$$

which gives rise to the stoichiometric vectors $\boldsymbol{\gamma}^{\mathrm{fa}} = (1,1,-1,0,0)^\top$ and $\boldsymbol{\gamma}^{\mathrm{sl}} = (0,0,1,1,-1)^\top$. Assuming the detailed-balance condition with respect to the steady state $c_* = (1,1,1,1,1)^\top$, the reaction-rate equation takes the form

$$\dot{c} = -\frac{\kappa^{\mathrm{fa}}}{\varepsilon}\big(c_1c_2 - c_3\big)\boldsymbol{\gamma}^{\mathrm{fa}} - \kappa^{\mathrm{sl}}\big(c_3c_4 - c_5\big)\boldsymbol{\gamma}^{\mathrm{sl}}\,.$$

The limiting reaction system can be described by the slow variables $\mathsf{q} = (c_1+c_3, c_2+c_3, c_4, c_5)^\top$ and reads

$$\dot{\mathsf{q}} = Q_{\mathrm{fa}}\boldsymbol{R}_{\mathrm{sl}}(\Psi(\mathsf{q})) = -\kappa^{\mathrm{sl}}\big(a(q_1,q_2)q_3 - q_4\big)\boldsymbol{\gamma}^{\mathrm{sl}},$$

where the slow manifold takes the form $\Psi(\mathsf{q}) = \big(q_1, q_2, a(q_1,q_2), q_3, q_4\big)$ and the reduced entropy is $\mathsf{E}(\mathsf{q}) = \mathcal{E}(\Psi(\mathsf{q}))$.

2 Modeling of reaction systems

We first introduce the classical notation for reaction systems with reaction kinetics according to the mass-action law. After briefly recalling our notation for *gradient systems*, we show that based on the condition of detailed balance, the reaction-rate equation is the gradient-flow equation for a suitable gradient system. Next we introduce our class of fast-slow systems, and finally we present a small, but nontrivial example in $\mathbb{R}^3$.

2.1 Mass action law and stoichiometric subspaces

We consider $i_* \in \mathbb{N}$ species X_i reacting with each other by $r_* \in \mathbb{N}$ reactions. The set of species is denoted by $I = \{1,\dots,i_*\}$, the set of reactions by $R = \{1,\dots,r_*\}$, and the r_* chemical reactions are given by

$$\forall\, r \in R: \quad \sum_{i=1}^{i_*} \alpha_i^r X_i \quad \rightleftharpoons \quad \sum_{i=1}^{i_*} \beta_i^r X_i,$$

where the stoichiometric vectors $\alpha^r, \beta^r \in \mathbb{N}_0^{i_*}$ contain the stoichiometric coefficients. The concentration c_i of species X_i is nonnegative, the space of concentrations is denoted by

$$\mathbf{C} = [0,\infty[^{i_*} \subset \mathbb{R}^{i_*} ,$$

which is the nonnegative cone of $\mathbb{R}^{i_*}$. Moreover, we introduce $\mathbf{C}_+ := \operatorname{int} \mathbf{C} =]0,\infty[^{i_*}$, the interior of the set of concentrations.

The mass-action law for reaction kinetics assumes that the forward and backward reaction fluxes are proportional to the product of the densities of the species, i.e. $j(c)_r = -k_r^{\mathrm{fw}} c^{\alpha^r} + k_r^{\mathrm{bw}} c^{\beta^r}$, where for stoichiometric vectors $\delta \in \mathbb{N}_0^{i_+}$ the monomials c^δ are given by $\prod_{i=1}^{i_*} c_i^{\delta_i}$. The reaction-rate equation (RRE) of the concentrations $c \in \mathbf{C}$ takes the form

$$\dot c = \boldsymbol{R}(c) = -\sum_{r=1}^{r_*} \left(k_r^{\mathrm{fw}} c^{\alpha^r} - k_r^{\mathrm{bw}} c^{\beta^r}\right)(\alpha^r - \beta^r), \tag{2.1}$$

with given forward and backward reaction rates $k_r^{\mathrm{fw}}, k_r^{\mathrm{bw}} > 0$.

For each of the r reactions we introduce the stoichiometric vector $\gamma^r := \alpha^r - \beta^r \in \mathbb{Z}^{i_*}$. The span of all vectors γ^r is the *stoichiometric subspace* $\Gamma \subset \mathbb{R}^{i_*}$, i.e. $\Gamma := \operatorname{span}\left\{ \gamma^r \,\middle|\, r \in R \right\}$. We do not assume any properties of the stoichiometric vectors, in particular they are not assumed to be linearly independent.

Conservation directions are vectors $q \in \mathbb{R}^{i_*}$ such that $q \in \Gamma^\perp$ (also written $q \perp \Gamma$), where the annihilator $\Gamma^\perp$ is defined as $\Gamma^\perp = \left\{ q \in \mathbb{R}^{i_*} \,\middle|\, \forall\, \gamma \in \Gamma : \ q \cdot \gamma = 0 \right\}$. By construction we have $\boldsymbol{R}(c) \in \Gamma$, thus for all solutions $t \mapsto c(t)$ of the RRE (2.1), the value of $q \cdot c(t)$ is constant, i.e. $q \cdot c$ is a conserved quantity for (2.1). Fixing a basis $\{q_1, \dots, q_m\}$ of $\Gamma^\perp$, we introduce a matrix $Q \in \mathbb{R}^{m \times i_*}$ by defining its adjoint $Q^\top = (q_1, \dots, q_m)$. By construction, $Q^\top : \mathbb{R}^m \to \mathbb{R}^{i_*}$ is injective, $Q : \mathbb{R}^{i_*} \to \mathbb{R}^m$ is surjective, and $\ker Q = \Gamma$. The image of the nonnegative cone $\mathbf{C}$ under Q is denoted by $\mathscr{Q}$, i.e. $Q : \mathbf{C} \to \mathscr{Q} \subset \mathbb{R}^m$. Fixing a vector $q \in \mathscr{Q}$, we define the stoichiometric subsets

$$\mathbf{C}_q := \left\{ c \in \mathbf{C} \,\middle|\, Qc = q \right\}.$$

They provide a decomposition $\mathbf{C} = \cup_{q \in \mathscr{Q}} \mathbf{C}_q$ into affine sets that are invariant under the flow of the RRE (2.1).

Notation: In the whole paper we consider all vectors as column vectors. In particular $\mathrm{D}\mathcal{E}(c) \in X^*$ is also a column vector although it is an element of the dual space and might be understood as a covector.

2.2 Notations for gradient systems

Following [Mie11, Mie16], we call a triple $(\mathbf{X}, \mathcal{E}, \mathcal{R})$ a (generalized) *gradient system* (GS) if

1. the state space $\mathbf{X}$ is a closed and convex subspace of a Banach space X,
2. $\mathcal{E} : \mathbf{X} \to \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ is a sufficiently smooth functional (such as a free energy, a relative entropy, or a negative entropy, etc.),
3. $\mathcal{R} : \mathbf{X} \times X \to \mathbb{R}_\infty$ is a dissipation potential, which means that for any $u \in \mathbf{X}$ the functional $\mathcal{R}(u, \cdot) : X \to \mathbb{R}_\infty$ is lower semicontinuous, nonnegative and convex, and satisfies $\mathcal{R}(u, 0) = 0$.

The dynamics of a gradient system is given by the associated *gradient-flow equation* that can be formulated in three different, but equivalent ways: as an equation in X, in $\mathbb{R}$, or in X^* (the dual Banach space of X), respectively:

$$\text{(I)}\quad \textbf{Force balance in } X^*: \qquad 0 \in \partial_{\dot u}\mathcal{R}(u,\dot u) + \mathrm{D}\mathcal{E}(u) \quad \in X^*, \tag{2.2a}$$

$$\text{(II)}\quad \textbf{Power balance in } \mathbb{R}: \quad \mathcal{R}(u,\dot u) + \mathcal{R}^*(u,-\mathrm{D}\mathcal{E}(u)) = -\langle \mathrm{D}\mathcal{E}(u),\dot u\rangle \quad \in \mathbb{R}, \tag{2.2b}$$

$$\text{(III)}\quad \textbf{Rate equation in } X: \qquad \dot u \in \partial_{\xi}\mathcal{R}^*(u,-\mathrm{D}\mathcal{E}(u)) \quad \subset X. \tag{2.2c}$$

Here, $\mathcal{R}^*$ is the *dual dissipation potential* obtained by Legendre-Fenchel transform, $\mathcal{R}^*(u,\xi) := \sup_{v\in X}\big\{\langle \xi, v\rangle - \mathcal{R}(u,v)\big\}$. The partial derivatives $\partial_{\dot u}\mathcal{R}(u,\dot u)$ and $\partial_{\xi}\mathcal{R}^*(u,\xi)$ are the possibly set-valued convex subdifferentials.

For a given evolution equation $\dot u = \boldsymbol{V}(u)$ we say that it has a *gradient structure* if there exists a gradient system $(\mathbf{X},\mathcal{E},\mathcal{R})$ such that the evolution equation is the gradient-flow equation for this gradient system, namely $\boldsymbol{V}(u) = \partial_{\xi}\mathcal{R}^*(u,-\mathrm{D}\mathcal{E}(u))$. We emphasize that a given evolution equation may have none or many gradient structures; see Remark 2.6 for the case of our nonlinear reaction systems.

Integrating the power balance (II) in time over $[0,T]$ and using the chain rule for the time-derivative of $t\mapsto \mathcal{E}(u(t))$, we obtain another equivalent formulation of the dynamics of the gradient system, which is called *Energy-Dissipation-Balance*:

$$\text{(EDB)}\qquad \mathcal{E}(u(T)) + \int_0^T \big\{\mathcal{R}(u,\dot u) + \mathcal{R}^*(u,-\mathrm{D}\mathcal{E}(u))\big\}\,\mathrm{d}t = \mathcal{E}(u(0)). \tag{2.3}$$

This gives rise to the *dissipation functional*

$$\mathfrak{D}(u) := \int_0^T \big\{\mathcal{R}(u,\dot u) + \mathcal{R}^*(u,-\mathrm{D}\mathcal{E}(u))\big\}\,\mathrm{d}t,$$

which is now defined on trajectories $u:[0,T]\mapsto \mathbf{X}$.

The following *Energy-Dissipation Principle* (EDP) states that, under natural technical conditions, solving the EDB (2.3) is equivalent to solving any of the three versions of the gradient-flow equation (2.2).

Theorem 2.1 (Energy-dissipation principle, cf. [AGS05, Prop. 1.4.1] or [Mie16, Th. 3.2])**.** *Assume that $\mathbf{X}$ is a closed convex subset of $X=\mathbb{R}^{i_*}$, that $\mathcal{E}\in \mathrm{C}^1(\mathbf{X},\mathbb{R})$, and that the dissipation potential $\mathcal{R}(u,\cdot)$ is superlinear uniformly in $u\in\mathbf{X}$. Then, a function $u\in \mathrm{W}^{1,1}([0,T];\mathbb{R}^{i_*})$ is a solution of the gradient-flow equation (2.2) if and only if u solves the EDB (2.3).*

2.3 The detailed balance condition induces gradient structures

Already in Section 2.1, we have assumed that each reaction occurs in both forward and backward directions. Such reaction systems are called *weakly reversible*. A much stronger assumption is the so-called *detailed-balance condition* which states that there is a strictly positive state $c_*=(c_i^*)\in\mathbf{C}_+$ in which all reactions are in equilibrium, i.e. $j_r(c_*)=0$ for all r:

$$\text{(DBC)}\qquad \exists\, c_*\in\mathbf{C}_+\ \forall\, r\in\mathbb{R}: \quad k_r^{\mathrm{fw}} c_*^{\alpha^r} = k_r^{\mathrm{bw}} c_*^{\beta^r}. \tag{2.4}$$

Under this assumption, one can rewrite the RRE (2.1) in the symmetric form

$$\begin{aligned} &\dot{c} = \boldsymbol{R}(c) = -\sum_{r=1}^{r_*} \widehat{\kappa}_r\, \delta_r^* \Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}} - \frac{c^{\beta^r}}{c_*^{\beta^r}} \Big) \big(\alpha^r - \beta^r\big) \\ &\text{with } \ \delta_r^* = \big(c_*^{\alpha^r} c_*^{\beta^r}\big)^{1/2} \ \text{ and } \ \widehat{\kappa}_r := k_r^{\mathrm{fw}} c_*^{\alpha^r} / \delta_r^* = k_r^{\mathrm{bw}} c_*^{\beta^r} / \delta_r^* \,. \end{aligned} \tag{2.5}$$

Subsequently, we will use the notion of a *reaction system satisfying the detailed-balance condition*, or shortly a detailed-balance reaction system.

Definition 2.2 (Detailed-balance reaction systems (DBRS))**.** For $i_*, r_* \in \mathbb{N}$ consider the stoichiometric matrices $A = \big(\alpha_i^r\big) \in \mathbb{N}_0^{i_* \times r_*}$ and $B = \big(\beta_i^r\big) \in \mathbb{N}_0^{i_* \times r_*}$ and the vectors $c_* = (c_i^*) \in \,]0,\infty[^{i_*}$ and $\widehat{\kappa} = (\widehat{\kappa}_r) \in \,]0,\infty[^{r_*}$. Then, the quadruple $(A, B, c_*, \widehat{\kappa})$ is called a *detailed-balance reaction systems* with i_* species and r_* reactions. The associated RRE is given by (2.5).

It was observed in [Mie11] (but see also [ÖtG97, Eqn. (103)+(113)] and [Yon08, Sec. VII] for earlier, but implicit statements) that RREs in this form have a gradient structure. Here we will use the gradient structure derived in [MP*17] by a large-deviation principle from a microscopic Markov process. In Remark 2.6 we will shortly comment on other possible gradient structures.

With $\mathbf{C}$ as above we define the energy as the relative Boltzmann entropy

$$\mathcal{E} : \left\{ \begin{array}{ccc} \mathbf{C} & \to & \mathbb{R}, \\ c & \mapsto & \sum_{i=1}^{i_*} c_i^* \lambda_{\mathrm{B}}(c_i/c_i^*), \end{array} \right. \qquad \text{with } \lambda_{\mathrm{B}}(r) = \begin{cases} r\log r - r + 1 & \text{for } r > 0, \\ 1 & \text{for } r = 0, \\ \infty & \text{for } r < 0. \end{cases} \tag{2.6a}$$

The dissipation functional $\mathcal{R}$ will be defined by specifying the dual dissipation potential $\mathcal{R}^*$ of "cosh-type" as

$$\mathcal{R}^* : \left\{ \begin{array}{ccc} \mathbf{C} \times \mathbb{R}^{i_*} & \to & \mathbb{R}, \\ (c, \xi) & \mapsto & \displaystyle\sum_{r=1}^{r_*} \widehat{\kappa}_r \sqrt{c^{\alpha^r} c^{\beta^r}}\, \mathsf{C}^*\big((\alpha^r - \beta^r) \cdot \xi \big), \end{array} \right. \qquad \text{with } \mathsf{C}^*(\zeta) = 4\cosh(\zeta/2) - 4\,. \tag{2.6b}$$

We will often use the following formulas for C^*:

$$\begin{aligned} &\text{(a) } \mathsf{C}^*(\log p - \log q) = 2\frac{\big(\sqrt{p} - \sqrt{q}\big)^2}{\sqrt{pq}}, \\ &\text{(b) } \big(\mathsf{C}^*\big)'(\zeta) = \mathrm{e}^{\zeta/2} - \mathrm{e}^{-\zeta/2}, \qquad \text{(c) } \big(\mathsf{C}^*\big)'(\log p - \log q) = \frac{p-q}{\sqrt{pq}}. \end{aligned} \tag{2.7}$$

The following result is also easily checked by direct calculations using (2.7)(b) and the logarithm rules

$$\alpha^r \mathrm{D}\mathcal{E}(c) = \log(c^{\alpha^r}) - \log(c_*^{\alpha^r}) = \log\big(c^{\alpha^r}/c_*^{\alpha^r}\big). \tag{2.8}$$

This identity also follows as a special case of Remark 2.6. The primal dissipation potential $\mathcal{R}$ is given by the Legendre-Fenchel transformation:

$$\mathcal{R}(u, v) = \sup\big\{ \xi \cdot v - \mathcal{R}^*(c, \xi) \,\big|\, \xi \in \mathbb{R}^{i_*} \big\}. \tag{2.9}$$

Proposition 2.3 (Gradient structure, [MP*17, Thm. 3.6]). *The RRE* (2.5) *is the gradient-flow equation associated with the cosh-type gradient system* $(\mathbf{C}, \mathcal{E}, \mathcal{R})$ *with* $\mathcal{E}$ *and* $\mathcal{R}$ *given in* (2.6).

An important property of this gradient structure, which is not shared with the ones discussed in Remark 2.6 below, is that the dissipation potential $\mathcal{R}^*$ does not depend on the equilibrium state c_*. This might seen an artifact of our special choice of the definition of $\widehat{\kappa}_r$ in terms of c_*; however, we already see this in the example treated in Section 2.5. This property will be even more relevant when we use "tilting" in our main result Theorem 3.5, which state the "EDP-convergence with tilting". In [MiS19, Prop. 4.1] it was shown that this tilt-invariance is a special property of the cosh-gradient structure; see also Remark 2.6.

Moreover, we have identified c_* as a "static" property of the RRE (2.5), whereas the stoichiometric matrices $A, B \in \mathbb{N}_0^{i_* \times r_*}$ and the reaction coefficients $\widehat{\kappa}_r$ encode the "dissipative" properties.

Because we are going to use the energy-dissipation principle, we explicitly state the cosh-type dissipation functional given by

$$\mathfrak{D}(c) = \int_0^T \big\{ \mathcal{R}(c, \dot{c}) + \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c)) \big\} \,\mathrm{d}t \;=\; \int_0^T \big\{ \mathcal{R}(c, \dot{c}) + \mathcal{S}(c) \big\} \,\mathrm{d}t. \tag{2.10}$$

We will mostly write the dissipation functional $\mathfrak{D}$ in the first "$\mathcal{R}$+$\mathcal{R}^*$ form" to highlight its duality structure. However, for mathematical purposes it will be advantageous to use the second representation via the *slope function*

$$\mathcal{S}(c) : \mathbf{C} \to [0, \infty[;\; c \mapsto \mathcal{S}(c) := \sum_{r=1}^{r_*} 2\widehat{\kappa}_r \delta_r^* \Big(\big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}\big)^{1/2} - \big(\frac{c^{\beta^r}}{c_*^{\beta^r}}\big)^{1/2} \Big)^2, \tag{2.11}$$

which is continuous on $\mathbf{C}$ and satisfies $\mathcal{S}(c) = \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c))$ for $c \in \mathbf{C}_+$. Sometimes $\mathcal{S}$ is also called the (discrete) Fisher information as it corresponds to $\int_\Omega 4k|\nabla\sqrt{\rho}|^2 \,\mathrm{d}x = \int_\Omega k|\nabla\rho|^2/\rho \,\mathrm{d}x$ in the diffusion case.

A special feature of DBRS is that all equilibria have the property that they provide an equilibrium to each individual reaction $r \in R$, where we do not need linear independence of $(\gamma^r)_{r\in R}$, see also [MHM15, Sec. 2] or [Mie17].

Lemma 2.4 (Equilibria in DBRS). *Let* $(A, B, c_*, \widehat{\kappa})$ *be a DBRS with slope function* $\mathcal{S}$ *defined in* (2.11). *Then, the following identities hold:*

$$\begin{aligned} \mathscr{E}_{\boldsymbol{R}} &:= \big\{\, c \in \mathbf{C} \,\big|\, \boldsymbol{R}(c) = 0 \,\big\} \;=\; \big\{\, c \in \mathbf{C} \,\big|\, \mathcal{S}(c) = 0 \,\big\} \\ &= \; \big\{\, c \in \mathbf{C} \,\big|\, \forall\, r \in R :\; \tfrac{c^{\alpha^r}}{c_*^{\alpha^r}} = \tfrac{c^{\beta^r}}{c_*^{\beta^r}} \,\big\}\,. \end{aligned} \tag{2.12}$$

Moreover, if $\widetilde{c}_* \in \mathscr{E}_{\boldsymbol{R}} \cap \mathbf{C}_+$, *then the two DBRS* $(A, B, c_*, \widehat{\kappa})$ *and* $(A, B, \widetilde{c}_*, \widehat{\kappa})$ *generate the same RRE.*

Proof. Step 1. For $c \in \mathbf{C}_+$ the gradient structure $\boldsymbol{R}(c) = \partial\mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c))$ of the DBRS gives

$$\mathcal{R}(c, \boldsymbol{R}(c)) + \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c)) = -\mathrm{D}\mathcal{E}(c) \cdot \boldsymbol{R}(c). \tag{2.13}$$

Thus, $\boldsymbol{R}(c) = 0$ implies $\mathcal{S}(c) = \mathcal{R}^*(c, -\mathrm{D}\mathcal{E}(c)) = 0$, and since $\mathcal{S}(c)$ is the sum of r_* nonnegative terms (cf. (2.11)) we conclude $\frac{c^{\alpha^r}}{c_*^{\alpha^r}} = \frac{c^{\beta^r}}{c_*^{\beta^r}}$ as desired.

Step 2. If $c \in \partial\mathbf{C}$ satisfies $\boldsymbol{R}(c) = 0$, then consider $c_\delta = c + \delta c_* \in \mathbf{C}_+$ for $\delta \in]0,1[$. With $|\boldsymbol{R}(c_\delta)| \le C_0\delta$, $\mathcal{R}(c_\delta, v) \ge 0$, and $|\mathrm{D}\mathcal{E}(c_\delta)| \le i_* \log(1/\delta)$ we find

$$\mathcal{S}(c_\delta) = \mathcal{R}^*(c_\delta, -\mathrm{D}\mathcal{E}(c_\delta)) = -\mathrm{D}\mathcal{E}(c_\delta)\cdot \boldsymbol{R}(c_\delta) - \mathcal{R}(c_\delta, \boldsymbol{R}(c_\delta)) \le i_* C_0 \delta \log(1/\delta) + 0\,.$$

Using the continuity of $\mathcal{S}$ we obtain $\mathcal{S}(c) = \lim_{\delta\to 0^+} \mathcal{S}(c_\delta) = 0$ and conclude as in Step 1.

Step 3. The equilibrium condition of Step 1 implies $\widetilde{c}_*^{\beta^r}/\widetilde{c}_*^{\alpha^r} = c_*^{\beta^r}/c_*^{\alpha^r} =: \mu_r^2$ for all $r \in R$. Because in the RRE (2.5) only the terms $\delta_*^r/c_*^{\alpha^r} = \big(c_*^{\beta^r}/c_*^{\alpha^r}\big)^{1/2} = \mu_r$ and $\delta_*^r/c_*^{\beta^r} = 1/\mu_r$ appear, the last statement follows. □

The next lemma shows that $\mathcal{R}(c,\cdot)$ forbids velocities v outside of the stoichiometric subspace Γ. Moreover, for all trajectories $c : [0,T] \to \mathbf{C}$ with $\mathfrak{D}(c) < \infty$, which are much more than the solutions of the RRE (2.1), we find that they have to lie in one stoichiometric subset $\mathbf{C}_q$, i.e. the conserved quantities are already encoded in $\mathfrak{D}$.

Below we use the characteristic function χ_A of convex analysis, which is defined via $\chi_A(v) = 0$ for $v \in A$ and $\chi_A(v) = \infty$ otherwise.

Lemma 2.5 (Conserved quantities via $\mathfrak{D}$)**.** *Let Γ, Q, $\mathbf{C}_q$, and $\mathscr{Q}$ be defined as in Section 2.1, and let $\mathcal{R}^*$ and $\mathcal{R}$ be defined as in* (2.6b) *and* (2.9)*, respectively.*

(a) For all $(c,v) \in \mathbf{C}\times\mathbb{R}^{i_*}$ we have $\mathcal{R}(c,v) \ge \chi_\Gamma(v)$.

(b) If $c \in \mathrm{W}^{1,1}([0,T];\mathbf{C})$ satisfies $\mathfrak{D}(c) < \infty$, then $Q\dot c = 0$ a.e., or equivalently there exists $q \in \mathscr{Q}$ such that $c(t) \in \mathbf{C}_q$ for all $t \in [0,T]$.

Proof. Using $\gamma^r = \alpha^r - \beta^r$ we find $\mathcal{R}^*(c,\xi) = 0$ for $\xi \perp \Gamma = \ker(Q)$ and conclude

$$\mathcal{R}(c,v) = \sup_\xi(\xi\cdot v - \mathcal{R}^*(c,\xi)) \ge \sup_{\xi\perp\Gamma}(\xi\cdot v - \mathcal{R}^*(c,\xi)) = \sup_{\xi\perp\Gamma}(\xi\cdot v) = \chi_\Gamma(v).$$

This proves part (a).

The bound $\mathfrak{D}(c) < \infty$ implies that $\int_0^T \mathcal{R}(c,\dot c)\,\mathrm{d}t < \infty$ and hence $\dot c \in \Gamma = \ker(Q)$ a.e. This proves $Q\dot c(t) = 0$ a.e. and by the absolute continuity of c, the function $t \mapsto Qc(t)$ must be constant. Hence part (b) is established as well. □

Remark 2.6 (Different gradient structures). We emphasize that the symmetric RRE (2.5), which was obtained from the DBC, indeed has many other gradient structures with the same relative entropy $\mathcal{E}$ given in (2.6a). Choosing arbitrary smooth and strictly convex functions $\Phi_r : \mathbb{R} \to [0,\infty[$ with $\Phi_r(0) = 0$ and $\Phi_r(-\zeta) = \Phi_r(\zeta)$ we may define

$$\mathcal{R}_\Phi^*(c,\xi) = \sum_{r=1}^{r_*} \widehat{\kappa}_r \delta_r^* \Lambda_r\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}, \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)\,\Phi_r\big((\alpha^r-\beta^r)\cdot\xi\big) \quad \text{with } \Lambda_r(a,b) = \frac{a-b}{\Phi_r'\big(\log a - \log b\big)}$$

and $\delta_r^* = \big(c_*^{\alpha^r} c_*^{\beta^r}\big)^{1/2}$. Note that Λ_r can be smoothly extended by $\Lambda_r(a,a) = a/\Phi_r''(0)$.

To show that the gradient system $(\mathbf{C},\mathcal{E},\mathcal{R}_\Phi)$ indeed generates (2.5) as the associated gradient-flow equation, it suffices to consider the r^{th} reaction pair, because the dual potential $\mathcal{R}_\Phi^*$ is additive in the reaction pairs. Inserting $\mathrm{D}\mathcal{E}(c) = \big(\log(c_i/c_i^*)\big)_{i=1,..,i_*}$ we obtain the relation

$$\begin{aligned}
\mathrm{D}_\xi \mathcal{R}_{\Phi_r}^*\big(c, -\mathrm{D}\mathcal{E}(c)\big) &= \widehat{\kappa}_r\delta_r^*\Lambda_r\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}, \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)\,\Phi_r'\big((\alpha^r-\beta^r)\cdot(-\mathrm{D}\mathcal{E}(c))\big)(\alpha^r-\beta^r)\\
&\overset{(2.8)}{=} -\widehat{\kappa}_r\delta_r^*\Lambda_r\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}, \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)\Phi_r'\Big(\log\big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}\big) - \log\big(\frac{c^{\beta^r}}{c_*^{\beta^r}}\big)\Big)(\alpha^r-\beta^r) = -\widehat{\kappa}_r\delta_r^*\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}} - \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)(\alpha^r-\beta^r),
\end{aligned}$$

which is the desired result.

The choice $\Phi_r(\zeta) = \zeta^2/2$ was used in [Mie11], while here we use $\Phi_r = \mathsf{C}^*$ leading to

$$\Lambda_r(a,b) = (ab)^{1/2} \quad \text{and} \quad \delta_r^* \Lambda_r\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}, \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big) = \big(c^{\alpha^r} c^{\beta^r}\big)^{1/2}.$$

This is the desired term in (2.6b) that is independent of c_*, while for other choice of Φ_r the last term will depend on c_* (see [MiS19]).

2.4 Fast-slow reaction-rate equation

We assume that some reactions are fast with reaction coefficients $\widehat{\kappa}_r^\varepsilon = \kappa_r/\varepsilon$, while the others are slow with reaction coefficients $\widehat{\kappa}_r^\varepsilon = \kappa_r$ (of order 1). Here we assume that the set or reaction indices $R = \{1, ..., r_*\}$ decomposes into $R_{\mathrm{sl}} \dot\cup R_{\mathrm{fa}}$. For simplicity we assume that the detailed-balance steady state c_* is independent of ε, but a soft dependence with a limit $c_*^\varepsilon \to c_* \in \mathbf{C}_+$ could be allowed as well.

$$\begin{aligned} \dot c = \boldsymbol{R}_\varepsilon(c) &= -\sum_{r=1}^{r_*} \widehat{\kappa}_r^\varepsilon \delta_r^*\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}} - \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)\big(\alpha^r - \beta^r\big) = \boldsymbol{R}_{\mathrm{sl}}(c) + \frac{1}{\varepsilon}\boldsymbol{R}_{\mathrm{fa}}(c) \\ \text{with } \boldsymbol{R}_{\mathrm{xy}}(c) &= \sum_{r\in R_{\mathrm{xy}}} \kappa_r \delta_r^*\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}} \frac{c^{\beta^r}}{c_*^{\beta^r}}\Big)\big(\alpha^r - \beta^r\big) \quad \text{for } \mathrm{xy} \in \{\mathrm{sl}, \mathrm{fa}\}. \end{aligned} \tag{2.14}$$

Obviously, for each $\varepsilon > 0$ we have a cosh-type gradient structure $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon)$ with

$$\mathcal{R}_\varepsilon^*(c,\xi) = \mathcal{R}_{\mathrm{sl}}^*(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}_{\mathrm{fa}}^*(c,\xi) \quad \text{with } \mathcal{R}_{\mathrm{xy}}^*(c,\xi) = \sum_{r\in R_{\mathrm{xy}}} \kappa_r \sqrt{c^{\alpha^r} c^{\beta^r}}\, \mathsf{C}^*\big((\alpha^r - \beta^r)\cdot\xi\big). \tag{2.15}$$

The aim of this paper is to investigate the behavior of the gradient structures $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon)$ in the limit $\varepsilon \to 0^+$. In particular, we study the Γ-limit of the induced dissipation functionals $\mathfrak{D}_\varepsilon$ obtained as in (2.10) but with the duality pair $\mathcal{R}_\varepsilon + \mathcal{R}_\varepsilon^*$.

At this stage we report on well-known results (see e.g. [Bot03, DLZ18]) about the limit evolution for $\varepsilon \to 0^+$. For small times of order ε the fast system $\boldsymbol{R}_{\mathrm{fa}}$ will dominate, while for $t \in [\sqrt{\varepsilon}, T]$ a slow dynamics takes place where the slow reactions drive the evolution and the fast reactions remain in equilibrium.

To be more precise we introduce the fast time scale $\tau = t/\varepsilon$ such that in terms of τ we obtain the rescaled system $c'(\tau) = \varepsilon \boldsymbol{R}_{\mathrm{sl}}(c(\tau)) + \boldsymbol{R}_{\mathrm{fa}}(c(\tau))$. For $\varepsilon \to 0^+$ we obtain the fast system

$$c'(\tau) = \boldsymbol{R}_{\mathrm{fa}}(c(\tau)), \quad c(0) = c_0. \tag{2.16}$$

This is again a RRE satisfying the detailed-balance condition and all constructions introduced in Sections 2.1 and 2.3. In particular we obtain the fast stoichiometric subspace

$$\Gamma_{\mathrm{fa}} := \operatorname{span}\big\{\, \gamma^r \in \mathbb{Z}^{i_*} \,\big|\, r \in R_{\mathrm{fa}} \,\big\} \;\subset\; \Gamma \subset \mathbb{R}^{i_*}.$$

For the annihilator $\Gamma_{\mathrm{fa}}^\perp := \big\{\, q \in \mathbb{R}^{i_*} \,\big|\, \forall\, \gamma \in \Gamma_{\mathrm{fa}} :\; q\cdot\gamma = 0 \,\big\}$ we have $\Gamma^\perp \subset \Gamma_{\mathrm{fa}}^\perp$ and $m_{\mathrm{fa}} := \dim \Gamma_{\mathrm{fa}}^\perp \ge m = \dim \Gamma^\perp$. Thus, we can extend the basis $\{q_1, \dots, q_m\}$ for $\Gamma^\perp$ to a basis $\{q_1, ..., q_m, ..., q_{m_{\mathrm{fa}}}\}$ for $\Gamma_{\mathrm{fa}}^\perp$ and define the conservation operator $Q_{\mathrm{fa}} : \mathbb{R}^{i_*} \to \mathbb{R}^{m_{\mathrm{fa}}}$ via

$$Q_{\mathrm{fa}}^\top := \big(q_1, \dots, q_{m_{\mathrm{fa}}}\big) : \mathbb{R}^{m_{\mathrm{fa}}} \to \mathbb{R}^{i_*} \quad \text{and set } \mathbf{Q} := \big\{\, Q_{\mathrm{fa}} c \in \mathbb{R}^{m_{\mathrm{fa}}} \,\big|\, c \in \mathbf{C} \,\big\}.$$

In particular, the important defining relations of $Q_{\rm fa}$ are

$$\ker Q_{\rm fa} = \Gamma_{\rm fa} \quad \text{and} \quad \operatorname{im} Q_{\rm fa}^\top = \Gamma_{\rm fa}^\perp. \tag{2.17}$$

Of course, our interest lies in the case $0 \le m \lneqq m_{\rm fa} \lneqq i_*$. In that case the mapping $c \mapsto Qc$ yields fewer conserved quantities for the full fast-slow RRE (2.14) than the mapping $c \mapsto \mathsf{q} = Q_{\rm fa}c$ supplies for the fast RRE (2.16). We call $\mathsf{q} \in \mathbf{Q}$ the slow variables, as they may still vary on the slow time scale. In particular, the decomposition of $\mathbf{C}$ into fast stoichiometric subsets

$$\mathbf{C} = \bigcup_{\mathsf{q}\in\mathbf{Q}} \mathbf{C}_{\mathsf{q}}^{\rm fa} \quad \text{where} \quad \mathbf{C}_{\mathsf{q}}^{\rm fa} := \big\{\, c \in \mathbf{C} \,\big|\, Q_{\rm fa}c = \mathsf{q} \,\big\} \tag{2.18}$$

is finer than $\mathbf{C} = \bigcup_{q\in\mathscr{Q}} \mathbf{C}_q$.

Starting from a general initial condition c_0, one can show that the solutions $c^\varepsilon : [0,T] \to \mathbf{C}$ of the fast-slow RRE (2.14) have a limit $c^0 : [0,T] \to \mathbf{C}$, but this limit may not be continuous at $t = 0$. On the short time scale $\tau = t/\varepsilon$ we may define $\widetilde{c}^\varepsilon(\tau) = c^\varepsilon(\varepsilon\tau)$ which has a limit $\widetilde{c}^{\,0} : [0,\infty[\to \mathbf{C}$ satisfying the fast RRE (2.16) and having a limit $\overline{c}_0 := \lim_{\tau\to\infty} \widetilde{c}^0(\tau)$ with $\boldsymbol{R}_{\rm fa}(\overline{c}_0) = 0$. Hence, we define the set of fast equilibria

$$\mathscr{E}_{\rm fa} := \big\{\, c \in \mathbf{C} \,\big|\, \boldsymbol{R}_{\rm fa}(c) = 0 \,\big\} = \Big\{\, c \in \mathbf{C} \,\Big|\, \forall\, r \in R_{\rm fa} : \tfrac{c^{\alpha^r}}{c_*^{\alpha^r}} = \tfrac{c^{\beta^r}}{c_*^{\beta^r}} \,\Big\} \tag{2.19}$$

such that for $\tau \in [0,\infty[$ the solution $\widetilde{c}^0(\tau)$ describes the approach to the slow manifold and $\overline{c}_0 \in \mathscr{E}_{\rm fa}$. On the time scale of order 1, the limits $c^0(t)$ of the solutions $c^\varepsilon(t)$ satisfy $c^0(t) \in \mathscr{E}_{\rm fa}$ for all $t \in]0,T]$, and one has the matching condition $\overline{c}_0 = \lim_{t\to 0^+} c^0(t)$.

The evolution of the solutions c^0 within $\mathscr{E}_{\rm fa}$ is driven by the slow reactions only; the fast reactions keep the solution on the fast-equilibrium manifold $\mathscr{E}_{\rm fa}$. In particular, it can be shown (see [Bot03, DLZ18] or [MiS19] for the linear case) that c^0 satisfies the limiting equation

$$\dot{c}(t) = \boldsymbol{R}_{\rm sl}(c(t)) + \lambda(t) \quad \text{with } c(t) \in \mathscr{E}_{\rm fa} \ \text{ and } \ \lambda(t) \in \Gamma_{\rm fa}, \quad c(0) = \overline{c}_0. \tag{2.20}$$

The result of our paper is quite different: We will pass to the limit in the gradient systems $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon)$ directly and obtain an effective gradient system $(\mathbf{C}, \mathcal{E}, \mathcal{R}_{\rm eff})$, see Theorem 3.5. As a consistency check, we will show in Section 4 that the gradient-flow equation for $(\mathbf{C}, \mathcal{E}, \mathcal{R}_{\rm eff})$ is indeed identical to the limiting equation (2.20), see Proposition 4.4.

2.5 A simple example for a fast-slow system

As a guiding example, we consider a reaction system consisting of three species X_i, $i = 1,2,3 = i_*$, which interact via $r_* = 2$ reactions, one being slow and one being fast:

$$\text{slow:} \quad X_1 \rightleftharpoons X_3 \qquad \text{fast:} \quad X_1 + X_2 \rightleftharpoons 2X_3\,.$$

Hence, the stoichiometric vector are given by

$$\begin{aligned} &\alpha^1 = (1,0,0)^\top, \quad \beta^1 = (0,0,1)^\top, \quad \gamma^1 = (1,0,-1)^\top, \\ &\alpha^2 = (1,1,0)^\top, \quad \beta^2 = (0,0,2)^\top, \quad \gamma^2 = (1,1,-2)^\top. \end{aligned}$$

Hence, one can easily check that the space of conserved quantities is span $\big((1,1,1)^\top\big) \in \mathbb{R}^3$ which defines the matrix $Q = (1,1,1) \in \mathbb{R}^{1\times 3}$.

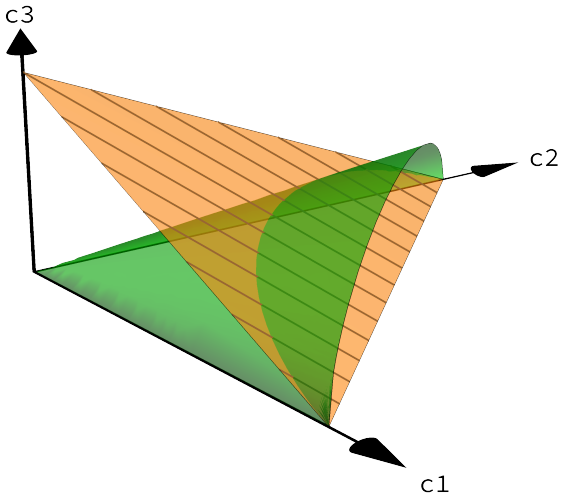

Figure 2.1: The state space $\mathbf{C} = [0,\infty[^3$ decomposes into the triangles $Qc = c_1 + c_2 + c_3 = q$ (light brown), which decompose into the straight segments $Q_{\mathrm{fa}}c = \mathsf{q}$ (brown). Each segment has exactly one intersection with the fast equilibria $\mathscr{E}_{\mathrm{fa}}$ (green).

We have $R = R_{\mathrm{fa}} \cup R_{\mathrm{sl}} = \{1\} \cup \{2\}$ and the RRE reads

$$\dot{c} = \boldsymbol{R}_\varepsilon(c) = (c_3 - 3c_1) \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + \frac{1}{\varepsilon}(c_3^2 - c_1c_2) \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}. \tag{2.21}$$

The nontrivial equilibria of this RRE are given by $c_* = (c_1^*, c_2^*, c_3^*)^\top = \sigma(1,9,3)^\top$ for $\sigma > 0$. All these c_* satisfy the detailed balance condition, and (2.21) takes the symmetric form (2.5), viz.

$$\dot{c} = -\kappa_1\delta_1^*\Big(\frac{c_1}{c_1^*} - \frac{c_3}{c_3^*}\Big) \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} - \frac{\kappa_2}{\varepsilon}\,\delta_2^*\Big(\frac{c_1c_2}{c_1^*c_2^*} - \frac{c_3^2}{(c_3^*)^2}\Big) \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}$$
$$\text{with } \delta_1^* = (c_1^*c_3^*)^{1/2} = \sigma\sqrt{3}, \quad \delta_2^* = (c_1^*c_2^*)^{1/2}c_3 = 9\sigma^2, \quad \kappa_1 = \sqrt{3}, \quad \text{and } \kappa_2 = 1.$$

Thus, we find the cosh-type gradient structure $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ of Section 2.3 with

$$\mathcal{E}(c) = \sigma\lambda_{\mathrm{B}}(c_1/\sigma) + 9\sigma\lambda_{\mathrm{B}}(c_2/(9\sigma)) + 3\sigma\lambda_{\mathrm{B}}(c_3/(3\sigma)),$$
$$\mathcal{R}_\varepsilon^*(c,\xi) = \sqrt{3c_1c_3}\,\mathsf{C}^*(\xi_1 - \xi_3) + \frac{1}{\varepsilon}\sqrt{c_1c_2c_3^2}\,\mathsf{C}^*(\xi_1 + \xi_2 - 2\xi_3).$$

As noted just after Proposition 2.3, $\mathcal{R}_\varepsilon^*$ is independent of c_*.

The associated fast system consists simply of one reaction, hence we find

$$\Gamma_{\mathrm{fa}} = \mathrm{span}(1,1,-2)^\top, \quad Q_{\mathrm{fa}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 0 \end{pmatrix}, \quad \mathbf{Q} = \big\{\, \mathsf{q} \in \mathbb{R}^2 \,\big|\, \mathsf{q}_1 \geq 0 \,\big\}.$$

The stoichiometric sets $\mathbf{C}_q$ with $Qc = q \in \mathbb{R}^1$ are triangles, which decompose into the straight segments $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}}$ given by $Q_{\mathrm{fa}}c = \mathsf{q}$, whereas the set of fast equilibria

$$\mathscr{E}_{\mathrm{fa}} = \big\{\, c \in \mathbf{C} \,\big|\, c_1c_2 = c_3^2 \,\big\}.$$

is curved. See Figure 2.5 for an illustration.

Finally, we discuss the evolution for our example starting with the initial condition $c_0 = (10,4,0)^\top$ such that $Qc^\varepsilon(t) = c_1^\varepsilon(t) + c_2^\varepsilon(t) + c_3^\varepsilon(t) = 14$ is the conserved quantity.

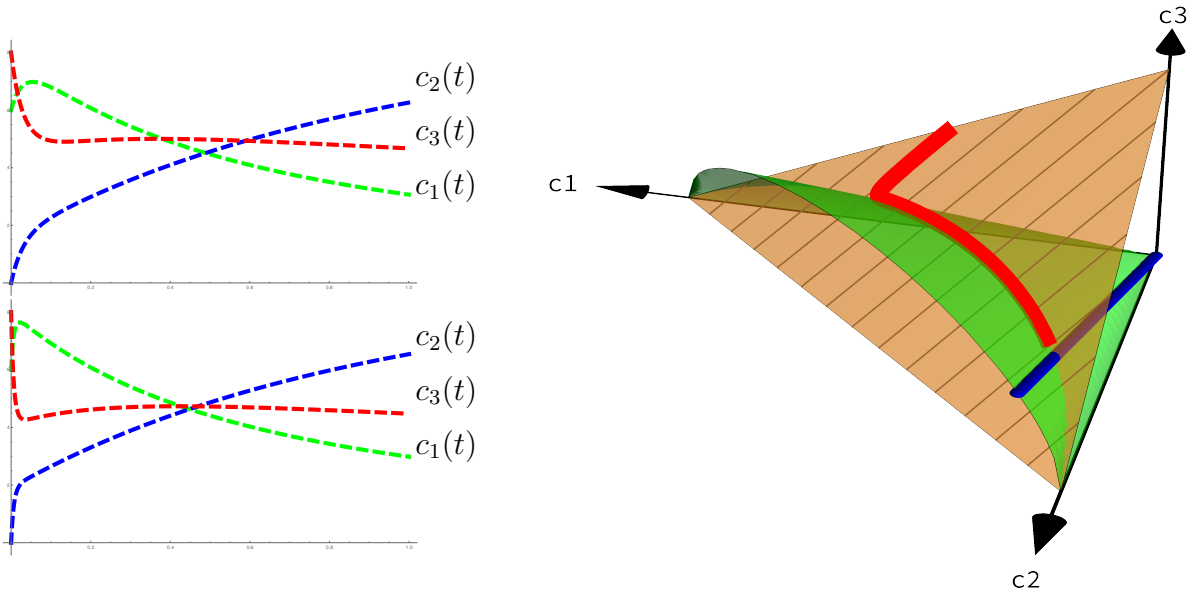

Figure 2.2: Numerical calculation of the solutions $c^\varepsilon(t)$ for the RRE (2.21) with $c^\varepsilon(0) = (4,0,10)^\top$ with $\varepsilon = 1$ (upper left) and $\varepsilon = 0.2$ (lower left). The lower left figure shows the fast convergence to $\overline{c}_0 = (8,2,4)^\top$. The right graphs displays the curve $t \mapsto c^\varepsilon(t)$ (red), which lies in the plane $Qc = 14$ (light brown). It quickly approaches $\mathscr{M}_{\rm sl}$ (green) and then moves towards the set of steady states (blue).

Since there is only one fast reaction, the second conserved quantity $c_1 - c_2 = \mathsf{q}_2 = 6$ shows that $\widetilde{c}^\varepsilon(\tau) = c^\varepsilon(\varepsilon t)$ converges to $\widetilde{c}(\tau)$ and $\widetilde{c}(\tau) \to \overline{c}_0 = (8,2,4)^\top \in \mathscr{E}_{\rm fa}$ for $\tau \to \infty$.

Thus, the limit solution c^0 satisfies the limiting equation (2.20), which reads in our case

$$\dot{c} = (c_3 - 3c_1)\begin{pmatrix}1\\0\\-1\end{pmatrix} + \lambda_0 \begin{pmatrix}1\\1\\-2\end{pmatrix}, \quad c_1(t)c_2(t) = c_3(t)^2, \quad c(0) = \overline{c}_0 = (8,2,4)^\top.$$

By eliminating the Lagrange multiplier $\lambda_0 \in \mathbb{R}$ and using the conserved quantity $Qc = 14$ this system is equivalent to the system

$$\dot{c}_1 - \dot{c}_2 = c_3 - 3c_1, \quad c_1 c_2 = c_3^2, \quad c_1 + c_2 + c_3 = 14.$$

Simulations are shown in Figure 2.5, which show the fast convergence to $\mathscr{E}_{\rm fa}$ and then the slow convergence to the final steady state $c_{\rm eq} = (1,9,4)^\top$.

3 EDP-convergence and effective gradient structure

In this section we first provide the precise definitions of EDP-convergence for gradient systems. Next we present the our main result concerning the EDP-limit of the cosh-type gradient structure for the fast-slow RRE with detailed-balance condition as introduced in Section 2.4, where the proofs are postponed to later sections. Finally, in Section 4 we discuss the obtained effective gradient system $(\mathbf{C}, \mathcal{E}, \mathcal{R}_{\rm eff})$ and show that the induced gradient-flow equation indeed is the same as the limiting equation (2.20).

3.1 Definition of different types of EDP-convergence

The definition of EDP-convergence for gradient systems relies on the notion of Γ-convergence for functionals (cf. [Dal93]). If Y is a Banach space and $I_\varepsilon : Y \to \mathbb{R}_\infty$ we write $I_\varepsilon \xrightarrow{\Gamma} I_0$ and $I_\varepsilon \xrightarrow{\Gamma\text{-}} I_0$ for Γ-convergence in the strong and weak topology, respectively. If both holds this is called Mosco convergence and written as $I_\varepsilon \xrightarrow{\mathrm{M}} I_0$.

For families of gradient systems $(X, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$, three different levels of EDP-convergence are introduced and discussed in [DFM19, MMP19], called simple EDP-convergence, EDP-convergence with tilting, and contact EDP-convergence with tilting. Here we will only use the first two notions. For all three notions the choice of weak or strong topology is still to be decided according to the specific problem. Here in the state space $X = \mathbb{R}^{i_*}$ this question is irrelevant, but it is relevant for curves $u : [0,T] \to \mathsf{X}$ lying in $Y = \mathrm{L}^1([0,T];X)$, where the state space X is a closed convex subset with non-empty interior of the Banach space X. For our paper, the strong topology will be sufficient.

Definition 3.1 (Simple EDP-convergence)**.** A family of gradient structures $(\mathsf{X}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ is said to *EDP-converge* to the gradient system $(\mathsf{X}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$ if the following conditions hold:

1. $\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_0$ on $\mathsf{X} \subset X$;
2. $\mathfrak{D}_\varepsilon$ strongly Γ-converges to $\mathfrak{D}_0$ on $\mathrm{L}^1([0,T];\mathsf{X})$ conditioned to bounded energies (we write $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma_{\mathrm{E}}} \mathfrak{D}_0$), i.e. we have
   (a) (Liminf) For all strongly converging families $u_\varepsilon \to u$ in $\mathrm{L}^1([0,T];\mathsf{X})$ which satisfy $\sup_{\varepsilon>0} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}_\varepsilon(u_\varepsilon(t)) < \infty$, we have $\liminf_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(u_\varepsilon) \geq \mathfrak{D}_0(u)$.
   (b) (Limsup) For all $\widetilde{u} \in \mathrm{L}^1([0,T];\mathsf{X})$ there exists a strongly converging family $\widetilde{u}_\varepsilon \to \widetilde{u}$ in $\mathrm{L}^1([0,T];\mathsf{X})$ with $\sup_{\varepsilon>0} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}_\varepsilon(\widetilde{u}_\varepsilon(t)) < \infty$ such that $\limsup_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(\widetilde{u}_\varepsilon) \leq \mathfrak{D}_0(\widetilde{u})$;
3. there is an effective dissipation potential $\mathcal{R}_{\mathrm{eff}} : \mathsf{X} \times X \to \mathbb{R}_\infty$ such that $\mathfrak{D}_0$ takes the form of a dual sum, namely $\mathfrak{D}_0(u) = \int_0^T \{\mathcal{R}_{\mathrm{eff}}(u,\dot{u}) + \mathcal{R}^*_{\mathrm{eff}}(u, -\mathrm{D}\mathcal{E}_{\mathrm{eff}}(u))\}\,\mathrm{d}t$.

Similarly, one can also use weak Γ or Mosco convergence conditioned to bounded energy, which we will then write as $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma\text{-}_{\mathrm{E}}} \mathfrak{D}_0$ and $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}_{\mathrm{E}}} \mathfrak{D}_0$. In fact, for our fast-slow reaction systems we are going to prove $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}_{\mathrm{E}}} \mathfrak{D}_0$.

A general feature of EDP-convergence is that under suitable conditions the gradient-flow equation $\dot{u} = \partial_\xi \mathcal{R}^*_{\mathrm{eff}}(u, -\mathrm{D}\mathcal{E}_0(u))$ of the effective gradient system $(X, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$ is indeed the limiting equation equation for the family $\dot{u} = \partial_\xi \mathcal{R}^*_\varepsilon(u, -\mathrm{D}\mathcal{E}_\varepsilon(u))$, i.e. limits u^0 of solutions u^ε of latter equations solve the former equation, see e.g. [Bra14, Thm. 11.3], [MiS19, Lem. 3.4], or [MMP19, Lem. 2.8]. For our case, such a result is given in Propositions 4.3 and 4.4.

A strengthening of simple EDP-convergence is the so-called *EDP-convergence with tilting*. This notion involves the tilted energy functionals $\mathcal{E}^\eta_\varepsilon : \mathsf{X} \ni u \mapsto \mathcal{E}_\varepsilon(u) - \langle \eta, u\rangle$, where the tilt η (also called forcing) varies through the whole dual space X^*.

Definition 3.2 (EDP-convergence with tilting (cf. [MMP19, Def. 2.14]))**.** A family of gradient structures $(\mathsf{X}, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ is said to *EDP-converge with tilting* to the gradient system $(\mathsf{X}, \mathcal{E}_0, \mathcal{R}_{\mathrm{eff}})$, if for all tilts $\eta \in X^*$ we have $(\mathsf{X}, \mathcal{E}^\eta_\varepsilon, \mathcal{R}_\varepsilon)$ EDP-converges to $(\mathsf{X}, \mathcal{E}^\eta_\varepsilon, \mathcal{R}_{\mathrm{eff}})$.

We observe that $\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_0$ implies $\mathcal{E}_\varepsilon^\eta \xrightarrow{\Gamma} \mathcal{E}_0^\eta$ for all $\eta \in X^*$ (and similarly for weak Γ-convergence), since the linear tilt $u \mapsto -\langle \eta, u\rangle$ is weakly continuous. The main and nontrivial assumption is that additionally

$$\mathfrak{D}_\varepsilon^\eta : u \mapsto \int_0^T \big\{\mathcal{R}_\varepsilon(u,\dot u) + \mathcal{R}_\varepsilon^*(u, \eta - \mathrm{D}\mathcal{E}_\varepsilon(u))\big\}\,\mathrm{d}t$$

Γ-converges in $\mathrm{L}^1([0,T];\mathbf{X})$ to $\mathfrak{D}_0^\eta$ for all $\eta \in X^*$ and that this limit $\mathfrak{D}_0^\eta$ is given in dual-sum form with $\mathcal{R}_{\mathrm{eff}}$ via

$$\mathfrak{D}_0^\eta(u) = \int_0^T \big\{\mathcal{R}_{\mathrm{eff}}(u,\dot u) + \mathcal{R}_{\mathrm{eff}}^*(u, \eta - \mathrm{D}\mathcal{E}_{\mathrm{eff}}(u))\big\}\,\mathrm{d}t.$$

The main point is that $\mathcal{R}_{\mathrm{eff}}$ remains independent of $\eta \in X^*$. We refer to [MMP19] for a discussion of this and the other two notions of EDP-convergence.

3.2 Our main EDP-convergence result

Since we have assumed that the stationary measure does not depend on $\varepsilon > 0$, also the energy $\mathcal{E}_\varepsilon = \mathcal{E}$ is ε-independent. Since $\mathcal{E}$ is also convex and lower semicontinuous, we have the trivial Mosco convergence $\mathcal{E}_\varepsilon \xrightarrow{\mathrm{M}} \mathcal{E}$.

To study the Γ-limit of the dissipation functionals $\mathfrak{D}_\varepsilon$ we first extend them to the space

$$\mathrm{L}^1([0,T];\mathbf{C}) := \big\{\, c \in \mathrm{L}^1([0,T];\mathbb{R}^{i_*}) \;\big|\; c(t) \in \mathbf{C} \text{ a.e.} \,\big\}.$$

For this we also use the slope functions (where $\mathrm{xy} \in \{\mathrm{fa}, \mathrm{sl}\}$)

$$\mathcal{S}_\varepsilon(c) = \mathcal{S}_{\mathrm{sl}}(c) + \frac{1}{\varepsilon}\mathcal{S}_{\mathrm{fa}}(c) \quad \text{with } \mathcal{S}_{\mathrm{xy}}(c) = \sum_{r \in R_{\mathrm{xy}}} 2\kappa_r \delta_r^*\Big(\big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}\big)^{1/2} - \big(\frac{c^{\beta^r}}{c_*^{\beta^r}}\big)^{1/2}\Big)^2. \tag{3.1}$$

For $\varepsilon > 0$ the dissipation functional $\mathfrak{D}_\varepsilon : \mathrm{L}^1([0,T];\mathbf{C}) \to [0,\infty]$ is now given by

$$\mathfrak{D}_\varepsilon(c) = \begin{cases} \int_0^T \big\{\mathcal{R}_\varepsilon(c,\dot c) + \mathcal{S}_\varepsilon(c)\big\}\,\mathrm{d}t & \text{for } c \in \mathrm{W}^{1,1}([0,T];\mathbf{C}), \\ \infty & \text{otherwise.} \end{cases} \tag{3.2}$$

We recall that the dual dissipation potentials are given by (with $\gamma^r = \alpha^r - \beta^r$)

$$\mathcal{R}_\varepsilon^*(c,\xi) = \mathcal{R}_{\mathrm{sl}}^*(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}_{\mathrm{fa}}^*(c,\xi) \quad \text{with } \mathcal{R}_{\mathrm{xy}}^*(c,\xi) = \sum_{r \in R_{\mathrm{xy}}} \kappa_r \sqrt{c^{\alpha^r} c^{\beta^r}}\; \mathsf{C}^*\big(\gamma^r \cdot \xi\big).$$

Because $\mathcal{S}_{\mathrm{fa}}(c) \ge 0$ and $\mathcal{R}_{\mathrm{fa}}^*(c,\xi) \ge 0$ we observe that $\mathcal{S}_\varepsilon(c)$ and $\mathcal{R}_\varepsilon^*(c,\xi)$ are monotonously increasing for $\varepsilon \downarrow 0$. Thus, their Γ-limits exist and are equal to the pointwise limits, which are denoted by $\mathcal{S}_0$ and $\mathcal{R}_0^*$ respectively (this uses [Dal93, Rem. 5.5] and the continuity of $\mathcal{S}_{\mathrm{fa}}$ and $\mathcal{R}_{\mathrm{fa}}^*$.)

Using (2.12) for the fast system we know that for $c \in \mathbf{C}$ the three conditions $\boldsymbol{R}_{\mathrm{fa}}(c) = 0$, $\mathcal{S}_{\mathrm{fa}}(c) = 0$, and $c \in \mathscr{E}_{\mathrm{fa}}$ are equivalent. Hence, we conclude

$$\lim_{\varepsilon \to 0^+} \mathcal{S}_\varepsilon(c) =: \mathcal{S}_0(c) = \mathcal{S}_{\mathrm{sl}}(c) + \chi_{\mathscr{E}_{\mathrm{fa}}}(c), \quad \text{where } \chi_A(b) = \begin{cases} 0 & \text{for } b \in A, \\ \infty & \text{for } b \notin A. \end{cases}$$

Obviously, we have $\lim_{\varepsilon\to 0^+} \mathcal{R}^*_\varepsilon(c,\xi) =: \mathcal{R}^*_0(c,\xi) = 0$ for $\xi \in \Gamma_{\rm fa}^\perp$ and for $c \in \mathbf{C}_+$ we obtain $\mathcal{R}^*_0(c,\xi) = \infty$ for $\xi \notin \Gamma_{\rm fa}^\perp$. Thus, we define the effective dual dissipation potential as

$$\mathcal{R}^*_{\rm eff}(c,\xi) = \mathcal{R}^*_{\rm sl}(c,\xi) + \chi_{\Gamma_{\rm fa}^\perp}(\xi)\,. \tag{3.3}$$

Note that $\mathcal{R}^*_{\rm eff}(c,\xi) \geq \mathcal{R}^*_0(c,\xi)$ where inequality may happen on the boundary of $\mathbf{C}$, e.g. at $c = 0$. Nevertheless, we have the important relation

$$\forall\, c \in \mathbf{C}_+ :\ \mathcal{R}^*_{\rm eff}(c, -\mathrm{D}\mathcal{E}(c)) = \mathcal{S}_0(c) := \mathcal{S}_{\rm sl}(c) + \chi_{\mathscr{E}_{\rm fa}}(c)\,. \tag{3.4a}$$

The primal effective dissipation potential $\mathcal{R}_{\rm eff}$ is given by the Legendre–Fenchel transformation:

$$\begin{aligned}\mathcal{R}_{\rm eff}(c,v) &= \sup_{\xi\in\mathbb{R}^{i*}} \{v\cdot\xi - \mathcal{R}^*_{\rm eff}(c,\xi)\} = \sup_{\xi\in\mathbb{R}^{i*}} \Big\{v\cdot\xi - \mathcal{R}^*_{\rm sl}(c,\xi) - \chi_{\Gamma_{\rm fa}^\perp}(\xi)\Big\}\\ &= \inf_{v_1+v_2=v} \{\mathcal{R}_{\rm sl}(c,v_1) + \chi_{\Gamma_{\rm fa}}(v_2)\} = \inf_{v_2\in\Gamma_{\rm fa}} \{\mathcal{R}_{\rm sl}(c,v-v_2)\}\,,\end{aligned} \tag{3.4b}$$

where we have used $(\chi_{\Gamma_{\rm fa}})^* = \chi_{\Gamma_{\rm fa}^\perp}$ and the classical theorem on the Legendre-Fenchel transformation turning a sum into an infimal convolution (see [Att84, Prop. 3.4]).

To state our main result we now impose a non-trivial structural assumption that is crucial for our result and its proof. An analogous condition on the uniqueness of equilibria in each stoichiometric subset $\mathbf{C}^{\rm fa}_{\mathsf{q}}$ was used in [Mie17, Eqn. (17)]. We believe that the theory of EDP-convergence can be studied without this assumption, but then one has to refine the results and the solution technique suitably, see the counterexample in Remark 3.10.

Assumption 3.3 (Conditions on the fast equilibria $\mathscr{E}_{\rm fa}$)**.** *For all* $\mathsf{q} \in \mathbf{Q} := \big\{\, Q_{\rm fa}c \,\big|\, c \in \mathbf{C}\,\big\}$*, there is exactly one equilibrium of* $c' = \boldsymbol{R}_{\rm fa}(c)$ *in the invariant subset* $\mathbf{C}^{\rm fa}_{\mathsf{q}}$ *(cf.* (2.18)*), i.e.*

$$\textit{(UFEC)} \qquad \forall\, \mathsf{q} \in \mathbf{Q} :\quad \#\big(\mathbf{C}^{\rm fa}_{\mathsf{q}} \cap \mathscr{E}_{\rm fa}\big) \;=\; 1\,, \tag{3.5}$$

which is called the unique fast-equilibrium condition*. By* $\Psi : \mathbf{Q} \to \mathbf{C}$ *we denote the mapping such that* $\{\Psi(\mathsf{q})\} = \mathbf{C}^{\rm fa}_{\mathsf{q}} \cap \mathscr{E}_{\rm fa}$ *for all* $\mathsf{q} \in \mathbf{Q}$*.*

We further impose the following positivity assumption on Ψ*:*

$$\exists\, \overline{\mathsf{q}} \in \mathbf{Q}\ \forall\, \theta \in]0,1]\ \forall\, \mathsf{q} \in \mathbf{Q}\ \forall\, i \in I :\quad \Psi(\mathsf{q}{+}\theta\overline{\mathsf{q}})_i > 0 \ \ \textit{and}\ \ \Psi(\mathsf{q}{+}\theta\overline{\mathsf{q}})_i \geq \Psi(\mathsf{q})_i. \tag{3.6}$$

The positivity and monotonicity assumption (3.6) seems to be only technical and it is only used at one point, namely in Step 1 in the proof of Theorem 5.5. We expect that this assumption can be avoided by a more careful construction of recovery sequence.

In Section 3.3 we will show that one of possibly several equilibria in $\mathbf{C}^{\rm fa}_{\mathsf{q}}$ is always given as the minimizer of $\mathcal{E}$ on $\mathbf{C}^{\rm fa}_{\mathsf{q}}$. Thus, the assumption really means that this "thermodynamic equilibrium" is the only steady state. Our main Γ-convergence result reads as follows.

Theorem 3.4 (Γ-convergence)**.** *Consider a fast-slow DBRS* $(A, B, c_*, \widehat{\kappa}^\varepsilon)$ *as in* (2.14) *together with its cosh-type gradient structure* $(\mathbf{C}, \mathcal{E}, \mathcal{R}_\varepsilon)$ *as in Proposition 2.3 and the dissipation functional* $\mathfrak{D}_\varepsilon$ *defined in* (3.2)*. Moreover, let Assumption 3.3 be satisfied.*

Then we have $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M_E}} \mathfrak{D}_0$ *on* $\mathrm{L}^1([0,T],\mathbf{C})$ *conditioned to bounded energies, where* $\mathfrak{D}_0 : \mathrm{L}^1([0,T];\mathbf{C}) \to [0,\infty]$ *is defined as*

$$\mathfrak{D}_0(c) := \begin{cases} \int_0^T \big\{\mathcal{R}_{\rm eff}(c,\dot c) + \mathcal{S}_0(c)\big\}\,\mathrm{d}t & \text{for } c \in \mathrm{C}^0([0,T];\mathbf{C}) \text{ and } Q_{\rm fa}c \in \mathrm{W}^{1,1}([0,T];\mathbb{R}^{m_{\rm fa}}),\\ \infty & \text{otherwise,}\end{cases}$$

where $\mathcal{R}_{\rm eff}$ *and* $\mathcal{S}_0$ *are defined in* (3.4)*.*

The proof of this result is the content of Section 5.

We emphasize that the integrand of $\mathfrak{D}_0$ is (i) degenerate (non-coercive) in $\dot{\mathsf{q}}$ and (ii) singular (taking the value ∞). Concerning (i), we recall that the definition of $\mathcal{R}_{\text{eff}}$ in (3.4b) implies that $\mathcal{R}_{\text{eff}}(c,\cdot)$ vanishes on Γ_{fa}. In fact, it is only possible to control the time derivative of $t \mapsto Q_{\text{fa}}c(t) \in \mathbb{R}^{m_{\text{fa}}}$. Concerning (ii), we observe that $\mathcal{S}_0$ equals $+\infty$ outside of $\mathscr{E}_{\text{fa}}^{\circ}$, which is a manifold of dimension m_{fa}, and at each $c \in \mathscr{E}_{\text{fa}}^{\circ} \cap \mathbf{C}_+$ the subspaces $\mathrm{T}_c\mathscr{E}_{\text{fa}}^{\circ}$ and Γ_{fa} are transversal, see Section 4. Assumption 3.3 will be needed to avoid jump-type behavior which can occur otherwise, see the counterexample discussed in Remark 3.10.

We now come to our main result on the EDP-convergence with tilting for the cosh-type gradient systems $(\mathbf{C},\mathcal{E},\mathcal{R}_\varepsilon)$ towards the effective gradient system $(\mathbf{C},\mathcal{E},\mathcal{R}_{\text{eff}})$.

The theorem enables to establish our main result on EDP-convergence with tilting. The result is a direct consequence of the Γ-convergence stated in Theorem 3.4 and the general fact for the Boltzmann entropy that tilting is equivalent to changing the reference measure. In fact, introducing the relative Boltzmann entropy $\mathcal{H}(c\,|\,w) = \sum_{i=1}^{i_*} w_i \lambda_{\mathrm{B}}(c_i/w_i)$ we have $\mathcal{E}(c) = \mathcal{H}(c\,|\,c_*)$ and obtain, for all $\eta \in \mathbb{R}^{i_*}$, the relation

$$\mathcal{E}^\eta(c) = \mathcal{E}(c) - \eta\cdot c = \mathcal{H}(c\,|\,\mathbb{D}^\eta c_*) + E_\eta \quad \text{with } \mathbb{D}^\eta c := (\mathrm{e}^{\eta_i}c_i)_{i\in I} \text{ and } E_\eta = \sum_{i=1}^{i_*}(1-\mathrm{e}^{\eta_i})c_i^*. \tag{3.7}$$

Thus, we observe that tilting of a DBRS $(A,B,c_*,\widehat{\kappa}^\varepsilon)$ only changes the static property, namely the equilibrium c_* into $\mathbb{D}^\eta c_*$, while the dissipative properties encoded in the stoichiometric matrices A and B and the reaction coefficients $\widehat{\kappa}$ remain unchanged.

Theorem 3.5 (EDP-convergence with tilting)**.** *Under the assumptions of Theorem 3.4, the gradient systems $(\mathbf{C},\mathcal{E},\mathcal{R}_\varepsilon)$ EDP-converge with tilting to the gradient system $(\mathbf{C},\mathcal{E},\mathcal{R}_{\text{eff}})$.*

Proof. *Step 1. Simple EDP-convergence:* Since $\mathcal{E}_\varepsilon = \mathcal{E}$ is continuous we obviously have $\mathcal{E}_\varepsilon \xrightarrow{\mathrm{M}} \mathcal{E}$. Moreover, Theorem 3.4 provides $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M_E}} \mathfrak{D}_0$. Finally, the relation (3.4a) shows that the integrand of $\mathfrak{D}_0$ has the desired dual structure $\mathcal{R}_{\text{eff}}(c,\dot{c})+\mathcal{R}_{\text{eff}}^*(c,-\mathrm{D}\mathcal{E}(c))$. Thus, we have established the simple EDP-convergence of $(\mathbf{C},\mathcal{E},\mathcal{R}_\varepsilon)$ to the effective gradient system $(\mathbf{C},\mathcal{E},\mathcal{R}_{\text{eff}})$.

Step 2. EDP-convergence with tilting: We use that $\mathcal{E}^\eta = \mathcal{H}(\cdot\,|\,\mathbb{D}^\eta c_*) + E_\eta$ is of the same type as $\mathcal{E} = \mathcal{H}(\cdot\,|\,c_*)$ if we ignore the irrelevant constant energy shift. Clearly, the new fast-slow RRE (2.14) has the same A, B, κ_r, i_*, and hence Q_{fa}; only c_* is replaced by $\mathbb{D}^\eta c_*$. Thus, all structural assumptions are the same, and Theorem 3.4 is applicable for all $\eta \in \mathbb{R}^*$. In particular, the UFEC in (3.5) holds for the tilted DBRS by Corollary 3.8. Thus, $(\mathbf{C},\mathcal{E}^\eta,\mathcal{R}_\varepsilon)$ EDP-converges to $(\mathbf{C},\mathcal{E}^\eta,\mathcal{R}_{\text{eff}})$ according to Step 1. Since the effective dissipation potential $\mathcal{R}_{\text{eff}}$ is independent of $\eta \in \mathbb{R}^{i_*}$, we have shown EDP-convergence with tilting. □

3.3 Discussion of the UFEC and definition of $\mathscr{M}_{\text{sl}}$

Here we first prove properties of the function Ψ that provides the fast equilibria (see Assumption 3.3). Secondly, we show that UFEC is invariant under tilting.

The stoichiometric subsets $\mathbf{C}_{\mathsf{q}}^{\text{fa}} := \{\, c \in \mathbf{C} \,\big|\, Q_{\text{fa}}c = \mathsf{q} \,\}$ are the intersection of the affine subspace $\{\, y \in \mathbb{R}^{i_*} \,\big|\, Q_{\text{fa}}y = \mathsf{q} \,\}$ of dimension m_{fa} with the simplicial convex

cone $\mathbf{C} = [0,\infty[^{i_*}$. Hence, each $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ is a closed and convex simplex of dimension $m(\mathsf{q}) \in \{0,1,\dots,m_{\mathrm{fa}}\}$. The simplex-boundary $\partial\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ of such a simplex is the union of its boundary simplices of dimension $m(\mathsf{q})-1$. A two-dimensional n-gon has n intervals as boundary, and an interval has 2 points as boundary. For the case of a point, which is the only 0-dimensional simplex, we say that the boundary is empty. We say that an equilibrium $c \in \mathscr{E}_{\mathrm{fa}}$ is a *boundary equilibrium* if $c \in \partial\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$. Otherwise $c \in \mathscr{E}_{\mathrm{fa}}$ is called an *interior equilibrium*.

The following result provides an alternative construction of the mapping $\Psi : \mathbf{Q} \to \mathbf{C}$ that is independent of the UFEC (3.5). We observe that Ψ is defined for every fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$ and that Ψ only depends on $A^{\mathrm{fa}}-B^{\mathrm{fa}}$ and c_*. The first part of the next result is also shown in [MHM15, Prop. 2.1] or [DLZ18, Lem. 2.3].

Proposition 3.6 (Existence and continuity of interior equilibria)**.** *For a fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$ the energy $\mathcal{E}$ only depends on c_*, and Q_{fa} only on $\Gamma_{\mathrm{fa}} = \mathrm{im}(A^{\mathrm{fa}}-B^{\mathrm{fa}})$. For each $\mathsf{q} \in \mathbf{Q}$, denote by $\Psi(\mathsf{q})$ the unique minimizer of $\mathcal{E}$ on $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$. Then, $\Psi(\mathsf{q})$ is the only equilibrium of $\dot c = \boldsymbol{R}_{\mathrm{fa}}(c)$ that lies in the interior $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}} \setminus \partial\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$. Moreover, the mapping $\Psi : \mathbf{Q} \to \mathbf{C}$ is continuous, and $\Psi : \operatorname{int}\mathbf{Q} \to \operatorname{int}\mathbf{C}$ is analytic.*

Proof. Step 1. Uniqueness and existence of minimizer: The existence of a global minimizer follows from the coercivity of $\mathcal{E}$ and the closedness of $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$. The uniqueness follows from the convexity of $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ and the strict convexity of $\mathcal{E}$.

Step 2. Interior property: If $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ is a singleton $\{\widehat c\}$, then $\Psi(\mathsf{q}) = \widehat c$ automatically lies in the interior. If c^∂ is a point in the boundary and c° a point in the interior of $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$, then there is at least one $k \in I$ such that $c^\partial_k = 0$ and $c^\circ_k > 0$. Since $c_k \mapsto c^*_k \lambda_{\mathrm{B}}(c_k/c^*_k)$ has slope $-\infty$ at $c_k = 0$, we conclude that c^∂ cannot be a minimizer of $\mathcal{E} : c \mapsto \sum_i c^*_i \lambda_{\mathrm{B}}(c_i/c^*_i)$. Hence, $\widehat c = \Psi(\mathsf{q})$ lies in the interior of $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$.

Step 3. Unique equilibrium property: Since $\mathcal{E}$ is a strict Liapunov function for the RRE, the minimizer $\Psi(\mathsf{q})$ has to be an equilibrium.

For the uniqueness, we consider first the case $\dim(\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}) = m_{\mathrm{fa}}$,in which case interior points in $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ lie in $\mathbf{C}_+$. Hence, for any other equilibrium c_{e} in the interior of $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ the derivative $\mathrm{D}\mathcal{E}(c_{\mathrm{e}}) = \big(\log(c^{\mathrm{e}}_i/c^*_i)\big)_i$ is well-defined. Moreover, Lemma 2.4 implies $c_{\mathrm{e}}^{\alpha^r}/c_*^{\alpha^r} = c_{\mathrm{e}}^{\beta^r}/c_*^{\beta^r}$ for all $r \in R_{\mathrm{fa}}$. These two properties yield $\mathrm{D}\mathcal{E}(c_{\mathrm{e}}) \cdot \gamma^r = 0$ for $r \in R_{\mathrm{fa}}$. But $\mathrm{D}\mathcal{E}(c_{\mathrm{e}}) \in \Gamma_{\mathrm{fa}}^\perp$ and $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}} \subset c_{\mathrm{e}} + \Gamma_{\mathrm{fa}}$ guarantee that c_{e} minimizes the convex functional $\mathcal{E}$ on $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$, which yields $c_{\mathrm{e}} = \Psi(\mathsf{q})$.

If $\dim(\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}) = m(\mathsf{q}) < m_{\mathrm{fa}}$ then there exists $I_0 \subset I$ with $m_{\mathrm{fa}}-m(\mathsf{q})$ elements such that $\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}} \subset \big\{\, c \in \mathbf{C} \,\big|\, c_i = 0 \text{ for all } i \in I_0 \,\big\}$ and that for interior points $\widetilde c \in \mathbf{C}^{\mathrm{fa}}_{\mathsf{q}} \setminus \partial\mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$ we have $\widetilde c_i > 0$ for $i \notin I_0$. Hence, the above argument can be applied to the reduced system for $\widetilde c = (c_i)_{i \in I \setminus I_0}$, i.e. the components $c_i = 0$, $i \in I_0$ are simply ignored.

Step 4. Continuity of Ψ: Consider a sequence $\mathsf{q}_k \to q_\infty$ and let $c_k = \Psi(\mathsf{q}_k)$, then we have to show that $c_k \to c_\infty$. We set $\alpha_k = \mathcal{E}(c_k) = \min\big\{\, \mathcal{E}(c) \,\big|\, c \in \mathbf{C}^{\mathrm{fa}}_{\mathsf{q}_k} \,\big\}$ and choose a subsequence (k_l) such that $\alpha := \liminf_{k\to\infty} \alpha_k = \lim_{l\to\infty} \alpha_{k_l}$. By coercivity of $\mathcal{E}$ we know that (c_k) is bounded that there exists a further subsequence (not relabeled) with $c_{k_l} \to \widetilde c$ and $Q\widetilde c = \lim Qc_{k_l} = \lim \mathsf{q}_k = \mathsf{q}_\infty$. Hence, we obtain the estimate

$$\mathcal{E}(c_\infty) \le \mathcal{E}(\widetilde c) = \lim_{l\to\infty} \mathcal{E}(c_{k_l}) = \lim_{l\to\infty} \alpha_{k_l} = \alpha. \tag{3.8}$$

Moreover, our given c_∞ and each $\varepsilon > 0$ there exists a $\delta > 0$ such that $Q\big(B^{\mathbb{R}^{i_*}}_\varepsilon(c_\infty) \cap \mathbf{C}\big)$ contains the set $B^{\mathbb{R}^{m_{\mathrm{fa}}}}_\delta(\mathsf{q}_\infty) \cap \mathbf{Q}$. Thus, we find a sequence $(\widehat c_k)_{k\in\mathbb{N}}$ with $\widehat c_k \to c_\infty$ and

$Q\widehat{c}_k = \mathsf{q}_k \to \mathsf{q}_\infty$. Since $\mathcal{E}$ is continuous we conclude

$$\mathcal{E}(c_\infty) = \lim_{k\to\infty} \mathcal{E}(\widehat{c}_k) \geq \liminf_{k\to\infty} \mathcal{E}(c_k) = \alpha.$$

With (3.8) we conclude $\mathcal{E}(\widetilde{c}) = \mathcal{E}(c_\infty)$, which implies $c_k \to c_\infty = \Psi(\mathsf{q}_\infty)$, as desired.

Step 5. Analyticity of Ψ: For $\mathsf{q} \in \operatorname{int} \mathbf{Q}$ we have $\Psi(\mathsf{q}) \in \mathbf{C}_+ = \operatorname{int} \mathbf{C}$. Hence, $c = \Psi(\mathsf{q})$ can be characterized by the Lagrange principle for constrained minimizers using the Lagrange function $L(c,\lambda) = \mathcal{E}(c) - \mu \cdot (Q_{\mathrm{fa}}c - \mathsf{q})$ with $\mu \in \mathbb{R}^{m_{\mathrm{fa}}}$. This characterization leads to the equation $F(c,\mu) = (0,\mathsf{q})$, where

$$F(c,\mu) := \big(\mathrm{D}\mathcal{E}(c) - Q_{\mathrm{fa}}^\top \mu, Q_{\mathrm{fa}}c\big).$$

Obviously, $F : \mathbf{C}_+ \times \mathbb{R}^{m_{\mathrm{fa}}} \to \mathbb{R}^{i_*} \times \mathbb{R}^{m_{\mathrm{fa}}}$ is analytic, and we have $F(\Psi(\mathsf{q}), \widetilde{\mu}(\mathsf{q})) = (0,\mathsf{q})$ for a suitable $\widetilde{\mu}$. If we can show that $\mathrm{D}F(\Psi(\mathsf{q}),\mu)$ is invertible for all $\mathsf{q} \in \operatorname{int} \mathbf{Q}$, then the implicit function theorem implies that the mapping $\mathsf{q} \to (\Psi(\mathsf{q}), \widetilde{\mu}(\mathsf{q}))$ is analytic as well.

The Jacobian of $F(c,\mu)$ is given by $\mathrm{D}F(c,\mu) = \left(\begin{smallmatrix} \mathrm{D}^2\mathcal{E}(c) & -Q_{\mathrm{fa}}^\top \\ Q_{\mathrm{fa}} & 0 \end{smallmatrix}\right)$, and we prove that $\mathrm{D}F(c,\mu)$ is invertible by showing that its kernel is trivial. Let (w,η) be such that $\mathrm{D}F(c,\mu)(w,\eta)^\top = 0$. We conclude that $\mathrm{D}^2\mathcal{E}(c)w = Q_{\mathrm{fa}}^\top\eta$ and $Q_{\mathrm{fa}}w = 0$. Since c is positive, the Hessian $\mathrm{D}^2\mathcal{E}(c)$ is invertible, and hence, we have $Q_{\mathrm{fa}}\mathrm{D}^2\mathcal{E}(c)^{-1}Q_{\mathrm{fa}}^\top\eta = 0$. Multiplying η from the left and using that $\mathrm{D}^2\mathcal{E}(c)^{-1}$ is a positive matrix, we have $Q_{\mathrm{fa}}^\top\eta = 0$. Since $Q_{\mathrm{fa}}^\top$ is injective, we conclude that $\eta = 0$ which implies that also $w = 0$ due to $\mathrm{D}^2\mathcal{E}(c)w = Q_{\mathrm{fa}}^\top\eta = 0$. □

For later use we observe that by construction we have the relation

$$Q_{\mathrm{fa}}\Psi(\mathsf{q}) = \mathsf{q} \quad \text{for all } \mathsf{q} \in \mathbf{Q}. \tag{3.9}$$

A crucial role in our further analysis will be played by the image of Ψ, which we call the slow manifold:

$$\mathscr{M}_{\mathrm{sl}} := \operatorname{im}(\Psi) = \big\{\, \Psi(\mathsf{q}) \,\big|\, \mathsf{q} \in \mathbf{Q} \,\big\} \;\subset\; \mathbf{C}, \tag{3.10}$$

which is a closed set that is contained in the set of the fast equilibria $\mathscr{E}_{\mathrm{fa}}$ defined in (2.19). The UFEC in (3.5) is made to guarantee that $\mathscr{M}_{\mathrm{sl}}$ contains all the fast equilibria:

$$\text{(UFEC)} \iff \mathscr{E}_{\mathrm{fa}} = \mathscr{M}_{\mathrm{sl}}. \tag{3.11}$$

It is important to emphasize that $\mathscr{E}_{\mathrm{fa}}$ can be strictly bigger than $\mathscr{M}_{\mathrm{sl}}$, but by Proposition 3.6 these equilibria must be so-called boundary equilibria, i.e. they lie in $\partial\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}} \subset \partial\mathbf{C}$. (In the case that $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}} \subset \partial\mathbf{C}$ the equilibrium $\Psi(\mathsf{q})$ lies in the boundary of $\mathbf{C}$, but is not a boundary equilibrium!)

The equilibria on $\mathscr{M}_{\mathrm{sl}}$ are stable, since they are global minimizers of the Liapunov function $\mathcal{E}$ in their invariant subset. In contrast, possible boundary equilibria are always unstable, because starting near the equilibrium but in the interior of $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}}$ gives a solution moving towards $\Psi(\mathsf{q})$, see Figure 3.1. The UFEC may fail if one has autocatalytic reactions where the product $\alpha_i^r\beta_i^r$ is strictly positive for some $i \in I$; see the example treated in Remark 3.9.

The following simple result provides the characterization of the slow manifold $\mathscr{M}_{\mathrm{sl}}$ in terms of the potential force $\mathrm{D}\mathcal{E}(c)$ and the annihilator of the fast subspace Γ_{fa}.

Lemma 3.7. *Consider a fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$. Then for $c \in \mathbf{C}_+$ we have*

$$\mathrm{D}\mathcal{E}(c) \in \Gamma_{\mathrm{fa}}^\perp = \big\{\, \xi \in \mathbb{R}^{i_*} \,\big|\, \xi \cdot \gamma^r \text{ for } r \in R_{\mathrm{fa}} \,\big\} \quad \iff \quad c \in \mathscr{M}_{\mathrm{sl}}.$$

Proof. Using $\mathrm{D}\mathcal{E}(c) = \big(\log(c_i/c_i^*)\big)_{i\in I}$ we find, for all $r \in R_{\mathrm{fa}}$,

$$0 = \mathrm{D}\mathcal{E}(c)\cdot\gamma^r = \log\Big(\frac{c^{\alpha^r}}{c_*^{\alpha^r}}\,\frac{c_*^{\beta^r}}{c^{\beta^r}}\Big) \quad\Longleftrightarrow\quad \frac{c^{\alpha^r}}{c_*^{\alpha^r}} = \frac{c^{\beta^r}}{c_*^{\beta^r}}$$

With Proposition 3.6 and the definition of $\mathscr{M}_{\mathrm{sl}}$ in (3.10) we obtain the desired result. □

Finally, we show that the UFEC is invariant under tilting. This is a nice consequence of the fact that tilting in systems satisfying the DBC allows us easily to follow the changes in the set $\mathscr{E}_{\mathrm{fa}}$ of fast equilibria.

Corollary 3.8 (UFEC and tilting)**.** *Consider a fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$ and general tilt vectors $\eta \in \mathbb{R}^{i_*}$. Denote by $\mathscr{E}_{\mathrm{fa}}^\eta$ and $\mathscr{M}_{\mathrm{sl}}^\eta$ the set of equilibria and the slow manifold, respectively, for the fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, \mathbb{D}^\eta c_*, \kappa^{\mathrm{fa}})$. Then, the following holds:*

(a) $\mathscr{E}_{\mathrm{fa}}^\eta = \mathbb{D}^\eta\mathscr{E}_{\mathrm{fa}}^0$ and $\mathscr{M}_{\mathrm{sl}}^\eta = \mathbb{D}^\eta\mathscr{M}_{\mathrm{sl}}^0$,

(b) $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$ satisfies UFEC if and only if $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, \mathbb{D}^\eta c_*, \kappa^{\mathrm{fa}})$ does so.

Proof. By Lemma 2.4 the equilibria $c \in \mathscr{E}_{\mathrm{fa}}^0$ are given by the condition $\frac{c^{\alpha^r}}{c_*^{\alpha^r}} = \frac{c^{\beta^r}}{c_*^{\beta^r}}$ for all $r \in R_{\mathrm{fa}}$. However, changing c and c_* into $\mathbb{D}^\eta c$ and $\mathbb{D}^\eta c_*$, respectively, shows that the condition remains the same.

Moreover, for $c \in \mathbf{C}_+$ we have $\mathrm{D}\mathcal{E}^\eta(\mathbb{D}^\eta c) = \mathrm{D}\mathcal{E}(c)$ by construction. Since $c \in \mathbf{C}_+ \cap \mathscr{M}_{\mathrm{sl}}^0$ is equivalent to $\mathrm{D}\mathcal{E}(c) \in \Gamma_{\mathrm{fa}}^\perp$ we have $\mathbb{D}^\eta c \in \mathscr{M}_{\mathrm{sl}}^\eta$. By the continuity of $\Psi = \Psi^0$ and Ψ^η (see Proposition 3.6) we conclude $\mathbb{D}^\eta\mathscr{M}_{\mathrm{sl}}^0 \subset \mathscr{M}_{\mathrm{sl}}^\eta$. As $\mathbb{D}^\eta$ is invertible, we can revert the argument and arrive at $\mathbb{D}^\eta\mathscr{M}_{\mathrm{sl}}^0 = \mathscr{M}_{\mathrm{sl}}^\eta$. Thus, (a) is established.

With (a) we see that $\mathscr{E}_{\mathrm{fa}}^0 = \mathscr{M}_{\mathrm{sl}}^0$ is equivalent to $\mathscr{E}_{\mathrm{fa}}^\eta = \mathscr{M}_{\mathrm{sl}}^\eta$, and (b) is established as well. □

3.4 Examples and problems without the UFEC

In the following two remarks, we firstly provide a few examples where UFEC does not hold and secondly show that our main result in Theorem 3.4 fails without UFEC.

Remark 3.9 (Examples without UFEC). The simplest example of a RRE not satisfying the UFEC condition is the autocatalytic reaction $2X \rightleftharpoons X$, leading to the RRE $\dot c = \frac{1}{\varepsilon}(c - c^2)$, where $\Gamma = \Gamma_{\mathrm{fa}} = \mathbb{R}$ and $m = m_{\mathrm{fa}} = 0$. In particular, the fast stoichiometric subset $\mathbf{C} = \mathbf{C}_0^{\mathrm{fa}} = [0,\infty[$ contains the the interior equilibrium $c_* = 1$ and the boundary equilibrium $c = 0$.

Next, we consider two different fast systems for two species, the first with the single autocatalytic reaction $X_1 + X_2 \leftrightharpoons 2X_1$ and the second with two non-autocatalytic reactions $2X_1 \leftrightharpoons X_2$ and $X_1 \leftrightharpoons 2X_2$. The fast RREs read

$$c' = \boldsymbol{R}^{(1)}(c) = (c_1^2 - c_1c_2)\begin{pmatrix}-1\\1\end{pmatrix}, \qquad c' = \boldsymbol{R}^{(2)}(c) = (c_1^2 - c_2)\begin{pmatrix}-2\\1\end{pmatrix} + (c_1 - c_2^2)\begin{pmatrix}-1\\2\end{pmatrix}.$$

The conserved quantities are given by the matrices

$$Q_{\mathrm{fa}}^{(1)}c = c_1 + c_2 \in \mathbf{Q}^{(1)} = [0,\infty[\qquad \text{and} \qquad Q_{\mathrm{fa}}^{(2)}c = 0 \in \mathbf{Q}^{(2)} = \{0\}.$$

The functions Ψ for the minimizers of $\mathcal{E}$ over $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}}$ are given by $\Psi^{(1)}(\mathsf{q}) = (\mathsf{q}/2, \mathsf{q}/2)^\top$ and $\Psi^{(2)}(0) = (1,1)^\top$ leading to

$$\mathscr{M}_{\mathrm{sl}}^{(1)} = \big\{\,(z,z)^\top \,\big|\, z \ge 0\,\big\} \quad\text{and}\quad \mathscr{M}_{\mathrm{sl}}^{(2)} = \{(1,1)^\top\}\,.$$

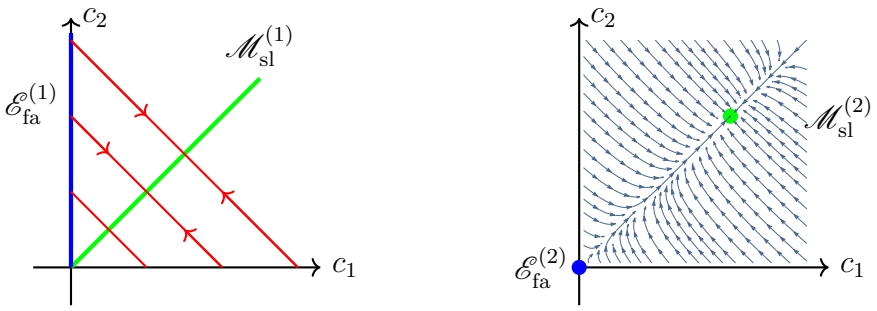

Figure 3.1: The slow manifolds $\mathscr{M}_{\mathrm{sl}}^{(k)}$ (green) are strictly contained in $\mathscr{E}_{\mathrm{fa}}^{(k)}$ (blue and green). The blue points are unstable, while the green points are stable. In the case (1) the invariant sets $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}}$ (red) are one-dimensional, while in case (2) we have $\mathbf{C}_0^{\mathrm{fa}} = \mathbf{C}$.

However, the set of fast equilibria is bigger in both cases:

$$\mathscr{E}_{\mathrm{fa}}^{(1)} = \mathscr{M}_{\mathrm{sl}}^{(1)} \dot\cup \big\{ (0,z) \,\big|\, z \geq 0 \big\} \quad \text{and} \quad \mathscr{E}_{\mathrm{fa}}^{(2)} = \mathscr{M}_{\mathrm{sl}}^{(2)} \dot\cup \{(0,0)^\top\}.$$

Figure 3.1 displays the invariant sets $\mathbf{C}_{\mathsf{q}}^{\mathrm{fa}}$, $\mathscr{M}_{\mathrm{sl}}$, and $\mathscr{E}_{\mathrm{fa}}$ for both cases.

To the knowledge of the authors there are currently no general sufficient conditions on the fast DBRS $(A^{\mathrm{fa}}, B^{\mathrm{fa}}, c_*, \kappa^{\mathrm{fa}})$ available that guarantee the validity of the UFEC. However, in many applications the number $\#(R_{\mathrm{fa}})$ of fast reactions is rather small such that an analysis of the fast RRE is easily done.

The next remark shows that Theorem 3.4 does not hold if the UFEC in (3.5) does not hold.

Remark 3.10 (A counterexample with jumps). We return to the first RRE $\dot c = \frac{1}{\varepsilon}(c - c^2)$ of the previous remark. The associated dissipation potential and slope functions are

$$\mathcal{R}_\varepsilon^*(c,\xi) = \frac{c^{3/2}}{\varepsilon}\, \mathsf{C}^*(\xi) \quad \text{and} \quad \mathcal{S}_\varepsilon(c) = \frac{2}{\varepsilon}\, c \left(c^{1/2}-1\right)^2.$$

Moreover, the dissipation functional $\mathfrak{D}_\varepsilon$ takes the form

$$\mathfrak{D}_\varepsilon(c) = \int_0^T \left\{ \frac{c^{3/2}}{\varepsilon}\, \mathsf{C}\Big(\frac{\varepsilon \dot c}{c^{3/2}}\Big) + \frac{2c}{\varepsilon}\big(c^{1/2}-1\big)^2 \Big) \right\} \mathrm{d}t.$$

Note that $c \equiv 0$ and $c \equiv 1$ yield $\mathfrak{D}_\varepsilon(c) = 0$. Moreover, fixing $t_* \in \,]0,T[$ the trajectories $\widetilde c^\varepsilon(t) = \mathrm{e}^{(t-t_*)/\varepsilon}/(1+\mathrm{e}^{(t-t_*)/\varepsilon})$ are exact solutions of the RRE $\dot c = \frac{1}{\varepsilon}(c-c^2)$, hence the energy-dissipation principle gives $\mathfrak{D}_\varepsilon(\widetilde c^\varepsilon) = \mathcal{E}(\widetilde c^\varepsilon(0)) - \mathcal{E}(\widetilde c^\varepsilon(T)) \leq \mathcal{E}(0) - \mathcal{E}(1) = 1$. Thus, the limit function $\widetilde c^0$ with $\widetilde c^0(t) = 0$ for $t < t_*$ and $\widetilde c^0(t) = 1$ for $t > t_*$ is not continuous but must satisfy $\mathfrak{D}_0(\widetilde c^0) \leq 1$, which is in contradiction to Theorem 3.4.

Indeed, using the Modica-Mortola approach as described in [Bra02, Sec. 6] (involving the estimate $\mathcal{R}_\varepsilon(c,\dot c) + \mathcal{R}_\varepsilon^*(c, -\mathrm{D}\mathcal{E}(c)) \geq -\mathrm{D}\mathcal{E}(c)\dot c$) it can be shown that $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma} \mathfrak{D}_0$ in $\mathrm{L}^1([0,T];\mathbb{R})$, where $\mathfrak{D}_0$ is finite only on piecewise constant functions taking values in $\{0,1\}$ only. Moreover, for these functions $\mathfrak{D}_0(c)$ equals the number of jumps times $\mathcal{E}(0) - \mathcal{E}(1) = 1$. The same was also observed in [Ste19].

4 The effective GS and the limiting equation

Here we present two different ways to derive the the limiting equation from our effective gradient system. The first one is in line with the coarse-graining approach developed

in [MiS19], where a lower-dimensional system is derived for the coarse-grained variable $\mathsf{q} = Q_{\mathrm{fa}}c$ and the restriction $c = \Psi(\mathsf{q})$ is built into the model. The second one follows [Bot03] and [DLZ18, Thm. 4.5], where the variable c is maintained and the constraint $c \in \mathscr{M}_{\mathrm{sl}}$ is realized by a suitable projection.

In both cases we start from the Γ-limit $\mathfrak{D}_0$ of the dissipation functionals $\mathfrak{D}_\varepsilon$. Using the energy-dissipation principle from Theorem 2.1 the limiting evolution can be recovered from

$$\mathcal{E}(c(T))+\mathfrak{D}_0(c;0,T) \le \mathcal{E}(c(0)), \;\; \mathfrak{D}(c;0,T) = \int_0^T \{\mathcal{R}_{\mathrm{eff}}(c,\dot c) + \mathcal{R}^*_{\mathrm{eff}}(c,-\mathrm{D}\mathcal{E}(c))\}\,\mathrm{d}t \;\; (4.1)$$

via the chain rule, which holds in the finite-dimensional space $\mathbf{C} \subset \mathbb{R}^{i_*}$.

Any solution satisfies the condition

$$\int_0^T \mathcal{S}_0(c(t))\,\mathrm{d}t \le \mathfrak{D}_0(c;0,T) = \int_0^T \{\mathcal{R}_{\mathrm{eff}}(c,\dot c)+\mathcal{R}^*_{\mathrm{eff}}(c,-\mathrm{D}\mathcal{E}(c))\}\,\mathrm{d}t \le \mathcal{E}(c(0))-\mathcal{E}(c(T)) < \infty,$$

where by the UFEC the function $\mathcal{S}_0$ assumes the value $+\infty$ for $c \notin \mathscr{M}_{\mathrm{sl}}$. Hence, the continuity of c implies that $c(t) \in \mathscr{M}_{\mathrm{sl}}$ for all $t \in [0,T]$. Thus, setting $\mathsf{q}(t) := Q_{\mathrm{fa}}c(t)$ and using the relation (3.9) we have $c(t) = \Psi(\mathsf{q}(t))$ for all $t \in [0,T]$. We recall that the properties

$$c \in \mathrm{C}^0([0,T];\mathbf{C}) \qquad \text{and} \qquad \mathsf{q} = Q_{\mathrm{fa}}c \in \mathrm{W}^{1,1}([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$$

are consequences of Theorem 3.4.

4.1 Coarse-graining approach

In this part we concentrate solely on the slow variables q and define

$$\mathsf{E}(\mathsf{q}) := \mathcal{E}(\Psi(\mathsf{q})) \quad \text{and} \quad \mathsf{R}^*(\mathsf{q},\zeta) := \mathcal{R}^*_{\mathrm{sl}}(\Psi(\mathsf{q}), Q_{\mathrm{fa}}^\top\zeta), \tag{4.2}$$

which defines a reduced gradient system $(\mathbf{Q},\mathsf{E},\mathsf{R})$ for the coarse-grained state $\mathsf{q} \in \mathbf{Q} \subset \mathbb{R}^{m_{\mathrm{fa}}}$. In particular, $\mathsf{R}^* : \mathbf{Q} \times \mathbb{R}^{m_{\mathrm{fa}}} \to [0,\infty]$ is a well-defined dual dissipation potential as $Q_{\mathrm{fa}}^\top : \mathbb{R}^{m_{\mathrm{fa}}} \to \mathbb{R}^{i_*}$.

The main result of this subsection will be that the gradient-flow equation for the reduced gradient system $(\mathbf{Q},\mathsf{E},\mathsf{R})$ is indeed the limiting equation and it has a simple representation in terms of $\boldsymbol{R}_{\mathrm{sl}}$, Q_{fa}, and Ψ:

$$\dot{\mathsf{q}} \;=\; \partial_\zeta \mathsf{R}^*(\mathsf{q},-\mathrm{D}\mathsf{E}(\mathsf{q})) \;=\; Q_{\mathrm{fa}}\boldsymbol{R}_{\mathrm{sl}}(\Psi(q)). \tag{4.3}$$

Thus, $(\mathbf{Q},\mathsf{E},\mathsf{R})$ provides an exact nonlinear coarse-graining in the sense of [MaM20, Sec. 6.1], where the relation $I_{m_{\mathrm{fa}}} = Q_{\mathrm{fa}}\mathrm{D}\Psi(\mathsf{q})$ simplifies the formula for R^* compared to [MaM20, Eq. (6.2)].

Remark 4.1. This theory is a nonlinear generalization of the coarse-graining theory developed in [MiS19], where $\dot{\widehat{c}} = MA_{\mathrm{sl}}N\widehat{c}$ is the coarse-grained equation. In our case the role of the reconstruction operator $N : \mathbb{R}^J \to \mathbb{R}^I$ is played by the nonlinear mapping $\Psi : \mathbf{Q} \to \mathbf{C}$, while the role of the coarse-graining operator $M : \mathbb{R}^I \to \mathbb{R}^J$ is our linear operator $Q_{\mathrm{fa}} : \mathbf{C} \to \mathbf{Q}$.

The following result provides first the justification of the second identity in (4.3), and then shows that this equation is indeed the limiting equation obtained from the energy-dissipation principle for $\mathcal{E}$ and $\mathfrak{D}_0$.

Proposition 4.2 (Reduced gradient structure)**.** *Let the DBRS $(A, B, c_*, \widehat{\kappa}^\varepsilon)$ be given as in Section 2.4 and satisfy the UFEC* (3.5)*, and let $(\mathbf{Q}, \mathsf{E}, \mathsf{R}^*)$ be defined as above. Then the following identities are valid:*

(a) For $\mathsf{q} \in \operatorname{int} \mathbf{Q}$ we have

$$Q_{\mathrm{fa}} \mathrm{D}\Psi(\mathsf{q}) = I_{m_{\mathrm{fa}}}, \quad \text{and,} \quad Q_{\mathrm{fa}}^\top \mathrm{D}\Psi(\mathsf{q})^\top \text{ is a projection onto } \operatorname{im}(Q_{\mathrm{fa}}^\top) = \Gamma_{\mathrm{fa}}^\perp \tag{4.4}$$

(b) For $\mathsf{q} \in \operatorname{int} \mathbf{Q}$ we have $\partial_\zeta \mathsf{R}^*(\mathsf{q}, -\mathrm{D}\mathsf{E}(\mathsf{q})) = Q_{\mathrm{fa}} \boldsymbol{R}_{\mathrm{sl}}(\Psi(q))$;

(c) the primal dissipation potential R takes the form

$$\mathsf{R}(\mathsf{q}, w) = \inf \big\{ \mathcal{R}_{\mathrm{sl}}(\Psi(\mathsf{q}), v) \,\big|\, Q_{\mathrm{fa}} v = w \big\} = \mathcal{R}_{\mathrm{eff}}(\Psi(\mathsf{q}), \widetilde{v}) \text{ whenever } Q_{\mathrm{fa}} \widetilde{v} = w\,;$$

(d) For $\mathsf{q} \in \operatorname{int} \mathbf{Q}$ we have $\mathsf{R}^*(\mathsf{q}, -\mathrm{D}\mathsf{E}(\mathsf{q})) = \mathcal{S}_{\mathrm{sl}}(\Psi(\mathsf{q})) =: \mathsf{S}(\mathsf{q})$;

(e) $\mathfrak{D}_0(\Psi(\mathsf{q})) = \int_0^T \big\{ \mathsf{R}(\mathsf{q}, \dot{\mathsf{q}}) + \mathsf{S}(\mathsf{q}) \big\} \,\mathrm{d}t$.

In part (e) it is crucial to observe that for differentiable $t \mapsto \mathsf{q}(t)$ we cannot guarantee that $t \mapsto c(t) = \Psi(\mathsf{q}(t))$ is differentiable as well, since $\mathsf{q}(t)$ need not remain in the interior of $\mathbf{Q}$. However, for $\mathfrak{D}_0$ we only need continuity of c and the differentiability of $t \mapsto Q_{\mathrm{fa}} c(t) = \mathsf{q}(t)$, where we used $\mathsf{q} = Q_{\mathrm{fa}} \Psi(\mathsf{q})$, see (3.9).

Proof. For part (a), we use that Ψ is differentiable in $\operatorname{int} \mathbf{Q}$. Differentiating the relation $Q_{\mathrm{fa}} \Psi(\mathsf{q}) = \mathsf{q}$ yields $Q_{\mathrm{fa}} \mathrm{D}\Psi(\mathsf{q}) = I_{m_{\mathrm{fa}}}$. In particular, this implies that $\mathrm{D}\Psi(\mathsf{q}) Q_{\mathrm{fa}}$ is a projection, and hence also its transpose $Q_{\mathrm{fa}}^\top \mathrm{D}\Psi(\mathsf{q})^\top$.

To show part (b) we first use the chain rule $\mathrm{D}\mathsf{E}(\mathsf{q}) = \mathrm{D}\Psi(\mathsf{q})^\top \mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))$. With Lemma 3.7 and part (a) we have that $\mathrm{D}\mathcal{E}(\Psi(\mathsf{q})) = Q_{\mathrm{fa}}^\top \mathrm{D}\Psi(\mathsf{q})^\top \mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))$, which yields

$$\begin{aligned} \partial_\zeta \mathsf{R}^*(\mathsf{q}, -\mathrm{D}\mathsf{E}(\mathsf{q})) &= Q_{\mathrm{fa}}^\top \mathrm{D}_\xi \mathcal{R}_{\mathrm{sl}}^*\big(\Psi(\mathsf{q}), -Q_{\mathrm{fa}}^\top \mathrm{D}\Psi(\mathsf{q})^\top \mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))\big) \\ &= Q_{\mathrm{fa}}^\top \mathrm{D}_\xi \mathcal{R}_{\mathrm{sl}}^*\big(\Psi(\mathsf{q}), -\mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))\big) \;=\; Q_{\mathrm{fa}} \boldsymbol{R}_{\mathrm{sl}}(\Psi(\mathsf{q})). \end{aligned}$$

For (c) we establish the relation $\mathsf{R}^* = \mathcal{L}\mathsf{R}$ via the Legendre transformation $\mathcal{L}$:

$$\begin{aligned} \big(\mathcal{L}\mathsf{R}(q, \cdot)\big)(\zeta) &= \sup \big\{ \zeta \cdot w - \mathsf{R}(\mathsf{q}, w) \,\big|\, w \in \mathbb{R}^{m_{\mathrm{fa}}} \big\} \\ &= \sup \Big\{ \zeta \cdot w + \sup \big\{ -\mathcal{R}_{\mathrm{sl}}(\Psi(\mathsf{q}), v) \,\big|\, Q_{\mathrm{fa}} v = w \big\} \,\Big|\, w \in \mathbb{R}^{m_{\mathrm{fa}}} \Big\} \\ &= \sup \big\{ \zeta \cdot w - \mathcal{R}_{\mathrm{sl}}(\Psi(\mathsf{q}), v) \,\big|\, Q_{\mathrm{fa}} v = w \big\} \\ &= \sup \big\{ \zeta \cdot Q_{\mathrm{fa}} v - \mathcal{R}_{\mathrm{sl}}(\Psi(\mathsf{q}), v) \,\big|\, v \in \mathbb{R}^{i_*} \big\} \;=\; \mathcal{R}_{\mathrm{sl}}^*(\Psi(\mathsf{q}), Q_{\mathrm{fa}}^\top \zeta) \;=\; \mathsf{R}^*(\mathsf{q}, \zeta). \end{aligned}$$

Part (d) follows similarly as part (b) by inserting $\mathrm{D}\mathsf{E}(\mathsf{q}) = \mathrm{D}\Psi(\mathsf{q})^\top \mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))$ and $\mathrm{D}\mathcal{E}(\Psi(\mathsf{q})) = Q_{\mathrm{fa}}^\top \mathrm{D}\Psi(\mathsf{q})^\top \mathrm{D}\mathcal{E}(\Psi(\mathsf{q}))$ into the definition of R^* via $\mathcal{R}_{\mathrm{sl}}^*$.

For part (e) we first observe that $\mathcal{S}_{\mathrm{sl}}(\Psi(\mathsf{q})) = \mathsf{S}(\mathsf{q})$ for all $q \in \mathbf{Q}$ by definition. For the rate part $\mathcal{R}_{\mathrm{eff}}(c, \dot{c})$ part (c) established that the dependence on $\dot{c}$ is only through $Q_{\mathrm{fa}} \dot{c}$. But relation (3.9) gives $\frac{\mathrm{d}}{\mathrm{d}t} Q_{\mathrm{fa}} \Psi(\mathsf{q}(t)) = \dot{\mathsf{q}}(t)$, and the relation $\mathcal{R}_{\mathrm{eff}}(c, \dot{c}) = \mathcal{R}_{\mathrm{eff}}(\Psi(\mathsf{q}), \mathrm{D}\Psi(\mathsf{q})\dot{\mathsf{q}}) = \mathsf{R}(\mathsf{q}, \dot{\mathsf{q}})$ holds even $q(t)$ touching the boundary of $\mathbf{Q}$. □

The next result shows that the reduced gradient-flow equation (4.3) indeed is the limiting equation for the fast-slow RRE (2.14) in the sense that for solutions $c^\varepsilon : [0, T] \to \mathbf{C}$ any accumulation point $\mathsf{q} : [0, T] \to \mathbf{Q}$ of the family $\big(Q_{\mathrm{fa}} c^\varepsilon\big)$ solves indeed (4.3). The assumptions on the initial conditions $c^\varepsilon(0)$ are special to avoid a potential jump at $t = 0$, see Section 2.4. The proof is based on the energy-dissipation principle and follows [Mie16, Thm. 3.3.3] or [MMP19, Lem. 2.8] with some special care because of the degeneracies and singularities of the limiting problem.

Proposition 4.3 (Reduced limiting equation). *Consider a fast-slow DBRS $(A, B, c_*, \widehat{\kappa}^\varepsilon)$ satisfying the UFEC (3.5) and let $c^\varepsilon : [0,T] \to \mathbb{R}^{i_*}$ be a family of solutions of the fast-slow RRE (2.14). If along a subsequence (not relabeled) we have $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T];\mathbf{C})$ and $c^\varepsilon(0) \to \overline{c}_0 \in \mathscr{M}_{\mathrm{sl}}$, then $Q_{\mathrm{fa}}c^\varepsilon \to \mathsf{q} := Q_{\mathrm{fa}}c^0$ weakly in $\mathrm{W}^{1,1}([0,T];\mathbf{Q})$ and strongly in $\mathrm{C}^0([0,T];\mathbf{Q})$, and q solves the reduced gradient-flow equation (4.3) with initial condition $\mathsf{q}(0) = Q_{\mathrm{fa}}\overline{c}_0$.*

Proof. The solutions c^ε satisfy the EDB $\mathcal{E}(c^\varepsilon(T)) + \mathfrak{D}_\varepsilon(c^\varepsilon) = \mathcal{E}(c^\varepsilon(0))$. Using $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T];\mathbb{R}^{i_*})$ and $\limsup_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(c^\varepsilon) \le \lim_{\varepsilon\to 0^+} \mathcal{E}(c^\varepsilon(0)) = \mathcal{E}(\overline{c}_0) < \infty$, we obtain $\mathsf{q}^\varepsilon := Q_{\mathrm{fa}}c^\varepsilon \to \mathsf{q}$ weakly in $\mathrm{W}^{1,1}([0,T];\mathbf{Q})$ and strongly in $\mathrm{C}^0([0,T];\mathbf{Q})$ by invoking Theorem 5.1(ii). Moreover, because of $\overline{c}_0 \in \mathscr{M}_{\mathrm{sl}}$ and $\mathsf{q}^\varepsilon(0) = Q_{\mathrm{fa}}c^\varepsilon(0) \to Q_{\mathrm{fa}}\overline{c}_0$ we have $\mathsf{q}(0) = Q_{\mathrm{fa}}\overline{c}_0$ and hence $\overline{c}_0 = \Psi(\mathsf{q}(0))$ and $\mathcal{E}(\overline{c}_0) = \mathsf{E}(\mathsf{q}(0))$. Passing to the limit $\varepsilon \to 0^+$ using the liminf estimate in $\mathfrak{D}_\varepsilon \overset{\Gamma_{\mathrm{E}}}{\to} \mathfrak{D}_0$ we arrive at

$$\mathsf{E}(\mathsf{q}(T)) + \mathfrak{D}_0(\Psi(\mathsf{q})) \le \mathcal{E}(c^0(T)) + \mathfrak{D}_0(c^0) \le \mathcal{E}(\overline{c}_0) = \mathsf{E}(\mathsf{q}(0)) .$$

Because $\mathfrak{D}_0(\Psi(\cdot))$ has the $\mathsf{R}\oplus\mathsf{R}^*$ structure (cf. Proposition 4.2(d+e)) the energy-dissipation principle shows that q solves the reduced RRE (4.3). □

4.2 The projection approach

By contrast to Section 4.1 above, in this section we maintain the variable c. First, we justify the limiting equation (2.20) with the constraint $c \in \mathscr{M}_{\mathrm{sl}}$ and the Lagrange multiplier $\lambda(t) \in \Gamma_{\mathrm{fa}}$. Secondly, we show that for positive solutions the evolution can be written as an ODE involving a suitable projection. Finally, we compare this to the reduced limiting equation (4.3).

Proposition 4.4 (Limiting equation with constraint). *For a fast-slow DBRS $(A, B, c_*, \widehat{\kappa}^\varepsilon)$ satisfying the UFEC (3.5) we consider a family $c^\varepsilon : [0,T] \to \mathbb{R}^{i_*}$ of solutions of the fast-slow RRE (2.14). If along a subsequence (not relabeled) we have $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T];\mathbf{C})$ and $c^\varepsilon(0) \to \overline{c}_0 \in \mathscr{M}_{\mathrm{sl}}$, then there exists $c \in \mathrm{C}^0([0,T];\mathbf{C})$ such that $c(t) = c^0(t)$ a.e. in $[0,T]$, $c(0) = \overline{c}_0$, $Q_{\mathrm{fa}}c \in \mathrm{W}^{1,1}([0,T];\mathbf{Q})$, and c solves the limiting equation with constraint:*

$$\dot{c}(t) = \boldsymbol{R}_{\mathrm{sl}}(c(t)) + \lambda(t), \quad \lambda(t) \in \Gamma_{\mathrm{fa}}, \quad c(t) \in \mathscr{M}_{\mathrm{sl}}. \tag{4.5}$$

Proof. We proceed as in the proof of Proposition 4.3 but stay with c rather than reducing to $\mathsf{q} = Q_{\mathrm{fa}}c$. The solutions c^ε satisfy the EDB $\mathcal{E}(c^\varepsilon(T)) + \mathfrak{D}_\varepsilon(c^\varepsilon) = \mathcal{E}(c^\varepsilon(0))$. Using $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T];\mathbb{R}^{i_*})$ and $\limsup_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(c^\varepsilon) \le \lim_{\varepsilon\to 0^+} \mathcal{E}(c^\varepsilon(0)) = \mathcal{E}(\overline{c}_0) < \infty$, we have $Q_{\mathrm{fa}}c^\varepsilon \to \mathsf{q}$ weakly in $\mathrm{W}^{1,1}([0,T];\mathbf{C})$ and strongly in $\mathrm{C}^0([0,T];\mathbb{R}^{i_*})$, see Theorem 5.1(ii). With this we define $c(t) = \Psi(\mathsf{q}(t))$ for $t \in [0,T]$ such that $c \in \mathrm{C}^0([0,T];\mathbf{C})$ and $Q_{\mathrm{fa}}c(t) = \mathsf{q}(t)$.

Passing to the limit $\varepsilon \to 0^+$ in the EDB we obtain $\mathcal{E}(c(T)) + \mathfrak{D}_0(c) \le \mathcal{E}(c(0))$, and the energy-dissipation principle gives the gradient-flow equation

$$\dot{c} \in \partial_\xi \mathcal{R}^*_{\mathrm{eff}}(c, -\mathrm{D}\mathcal{E}(c)) = \partial_\xi \Big(\mathcal{R}^*_{\mathrm{sl}}(c, -\mathrm{D}\mathcal{E}(c)) + \chi_{\Gamma_{\mathrm{fa}}^\perp}(-\mathrm{D}\mathcal{E}(c)) \Big). \tag{4.6}$$

For a linear subspace $Y \subset \mathbb{R}^{i_*}$ the set-valued convex subdifferential $\partial\chi_{Y^\perp}(\xi)$ equals Y for $\xi \in Y^\perp$ and $\emptyset$ otherwise, hence the last relation has the form

$$\dot{c} \in \partial_\xi \mathcal{R}^*_{\mathrm{sl}}(c, -\mathrm{D}\mathcal{E}(c)) + \Gamma_{\mathrm{fa}} = \boldsymbol{R}_{\mathrm{sl}}(c) + \Gamma_{\mathrm{fa}} \quad \text{and} \quad \mathrm{D}\mathcal{E}(c) \in \Gamma_{\mathrm{fa}}^\perp .$$

With Lemma 3.7 we can replace the last constraint by $c \in \mathscr{M}_{\rm sl}$, and (4.5) is established. □

To obtain an ODE of the form $\dot c = V(c)$ instead of the limiting equation (4.5) with constraint, we have to resolve the constraint $\mathrm{D}\mathcal{E}(c) \in \Gamma_{\rm fa}^\perp$. For any curve $s \to \widetilde c(s) \in \mathscr{M}_{\rm sl} \cap \mathbf{C}_+$ we have $\mathrm{D}\mathcal{E}(\widetilde c(s)) \in \Gamma_{\rm fa}^\perp$ and taking the derivative with respect to s, we find

$$\dot{\widetilde c}(s) \in \mathrm{T}_{\widetilde c(s)}\mathscr{M}_{\rm sl} \quad \text{and} \quad \mathrm{D}^2\mathcal{E}(\widetilde c(s))\dot{\widetilde c}(s) \in \Gamma_{\rm fa}^\perp.$$

Hence, for $c \in \mathscr{M}_{\rm sl} \cap \mathbf{C}_+$ the tangent space $\mathrm{T}_c\mathscr{M}_{\rm sl}$ of $\mathscr{M}_{\rm sl}$ at c is given by

$$\mathrm{T}_c\mathscr{M}_{\rm sl} = \big(\mathbb{H}(c)\big)^{-1}\Gamma_{\rm fa}^\perp \quad \text{with} \quad \mathbb{H}(c) := \mathrm{D}^2\mathcal{E}(c) = \mathrm{diag}(1/c_1, \dots, 1/c_{i_*}).$$

With this we obtain the following representation of the limiting equation, which matches that in [Bot03, Thm. 2(b)] and [DLZ18, Thm. 4.5]. Our result is more general, since we do not need to assume that the stoichiometric vectors $\big\{\, \gamma^r \,\big|\, r \in R_{\rm fa} \,\big\}$ are linearly independent.

Proposition 4.5 (Limiting equation for $c \in \mathbf{C}_+$)**.** *A curve $c : [0,T] \to \mathbf{C}_+$ is a solution* (4.5) *if and only if*

$$\dot c = \big(I - \mathbb{P}(c)\big)\, \boldsymbol{R}_{\rm sl}(c) \quad \textit{and} \quad c(0) \in \mathscr{M}_{\rm sl}. \tag{4.7}$$

where the projector $\mathbb{P}(c) \in \mathbb{R}^{i_* \times i_*}$ is defined via $\operatorname{im}\mathbb{P}(c) = \Gamma_{\rm fa}$ and $\ker\mathbb{P}(c) = \mathbb{H}(c)^{-1}\Gamma_{\rm fa}^\perp$.

Proof. Step 1. *Definition of the projector $\mathbb{P}(c)$:* The projector is uniquely defined if $Y_{\rm R} := \Gamma_{\rm fa}$ and $Y_{\rm K} := \mathbb{H}(c)^{-1}\Gamma_{\rm fa}^\perp$ provide a direct decomposition of $\mathbb{R}^{i_*}$. Assuming $v \in Y_{\rm R} \cap Y_{\rm K}$ we have $v \in \Gamma_{\rm fa}$ and $\mathbb{H}(c)v \in \Gamma_{\rm fa}^\perp$. This implies $v \cdot \mathbb{H}(c)v = 0$, but since $\mathbb{H}(c)$ is positive definite we arrive at $v = 0$. Hence, $Y_{\rm R} \cap Y_{\rm K} = \{0\}$. Obviously, $\dim Y_{\rm R} + \dim Y_{\rm K} = i_*$, so that $\mathbb{R}^{i_*} = Y_{\rm R} \oplus Y_{\rm K}$ is established.

Step 2. (4.7) $\Longrightarrow$ (4.5): We set $\lambda(t) = -\mathbb{P}(c(t))\boldsymbol{R}_{\rm sl}(c)$, and with (4.7) we obtain

$$\dot c(t) = \boldsymbol{R}_{\rm sl}(c(t)) - \mathbb{P}(c(t))\boldsymbol{R}_{\rm sl}(c(t)) = \boldsymbol{R}_{\rm sl}(c(t)) + \lambda(t) \quad \text{ with } \lambda(t) \in \Gamma_{\rm fa}.$$

Moreover, $\mathbb{P}(c(t))\dot c(t) = \mathbb{P}(c)(I - \mathbb{P}(c))\boldsymbol{R}_{\rm sl}(c) = 0$, which implies $\dot c \in \mathbb{H}(c)^{-1}\Gamma_{\rm fa}^\perp = \mathrm{T}_{c(t)}\mathscr{M}_{\rm sl}$. Hence, with $c(0) \in \mathscr{M}_{\rm sl}$ we obtain $c(t) \in \mathscr{M}_{\rm sl}$ for all $t \in [0,T]$, and (4.5) is established.

Step 3. (4.5) $\Longrightarrow$ (4.7): From $c(t) \in \mathscr{M}_{\rm sl}$ we obtain $\dot c(t) \in \mathrm{T}_{c(t)}\mathscr{M}_{\rm sl} = \mathbb{H}(c(t))^{-1}\Gamma_{\rm fa}^\perp$ and conclude $0 = \mathbb{P}(c)\dot c = \mathbb{P}(c)\boldsymbol{R}_{\rm sl}(c) + \mathbb{P}(c)\lambda$. Using $\lambda \in \operatorname{im}\mathbb{P}(c) = \Gamma_{\rm fa}$ we have $\mathbb{P}(c)\lambda = \lambda$ and find

$$\big(I - \mathbb{P}(c)\big)\, \boldsymbol{R}_{\rm sl}(c) = \boldsymbol{R}_{\rm sl}(c) - \mathbb{P}(c)\boldsymbol{R}_{\rm sl}(c) = \boldsymbol{R}_{\rm sl}(c) + \mathbb{P}(c)\lambda = \boldsymbol{R}_{\rm sl}(c) + \lambda = \dot c,$$

which is the desired equation (4.7). □

To compare the last result with the reduced limiting equation (4.3), we simply use the relation $c(t) = \Psi(\mathsf{q}(t))$ and the fact that Ψ is smooth on $\operatorname{int}\mathbf{Q}$. From this we obtain

$$\big(I - \mathbb{P}(c)\big)\, \boldsymbol{R}_{\rm sl}(c) \;=\; \dot c \;=\; \mathrm{D}\Psi(\mathsf{q})\dot{\mathsf{q}} \;=\; \mathrm{D}\Psi(\mathsf{q}(t))Q_{\rm fa}\boldsymbol{R}_{\rm sl}(\Psi(\mathsf{q})) \;=\; \mathrm{D}\Psi(\mathsf{q}(t))Q_{\rm fa}\boldsymbol{R}_{\rm sl}(c).$$

Thus, we can conclude that for $c = \Psi(\mathsf{q}) \in \mathscr{M}_{\rm sl}$ we have the identity

$$\big(I - \mathbb{P}(c)\big) \;=\; \mathrm{D}\Psi(\mathsf{q})Q_{\rm fa},$$

since the above identity must hold for all possible right-hand sides $\boldsymbol{R}_{\rm sl}$. This can also be shown by using the identity $c = \Psi(Q_{\rm fa}c)$ for all $c \in \mathscr{M}_{\rm sl}$ and taking derivatives in the direction $v \in \Gamma_{\rm fa}$ and $w \in \mathrm{T}_c\mathscr{M}_{\rm sl}$, respectively. In particular, this provides the explicit form of the projection of Proposition 4.2(a).

4.3 An example for the effective gradient system

In the following example we consider a system with $i_* = 5$ species and $r_* = 2$ bimolecular reactions, one fast and one slow. As a result we obtain a limiting equation with one reaction that is no longer of mass-action type but involves all species. Taking a further EDP limit (done only formally) we recover a trimolecular reaction of mass-action type again.

We consider the following two reactions

$$\text{fast:} \quad X_1 + X_2 \leftharpoons X_3 \qquad \text{and} \qquad \text{slow:} \quad X_3 + X_4 \rightleftharpoons X_5,$$

which give rise to the two stoichiometric vectors

$$\gamma^{\mathrm{fa}} = (1,1,-1,0,0)^\top \quad \text{and} \quad \gamma^{\mathrm{sl}} = (0,0,1,1,-1)^\top.$$

Assuming the steady state $c_* = (1,1,\varrho,1,1)^\top$ and the reaction coefficients $\widehat{\kappa}^\varepsilon = (\kappa^{\mathrm{fa}}/\varepsilon, \kappa^{\mathrm{sl}})$ the RRE (2.14) takes the form

$$\dot{c} = -\frac{\kappa^{\mathrm{fa}}\varrho^{1/2}}{\varepsilon}\big(c_1c_2 - c_3/\varrho\big)\gamma^{\mathrm{fa}} - \kappa^{\mathrm{sl}}\varrho^{1/2}\big(c_3c_4/\varrho - c_5\big)\gamma^{\mathrm{sl}}.$$

The slow manifold is $\mathscr{M}_{\mathrm{sl}} = \big\{\, c \in [0,\infty[^5 \;\big|\; c_1c_2 = c_3/\varrho \,\big\}$ and $\Gamma_{\mathrm{fa}} = \operatorname{span}\gamma^{\mathrm{fa}}$. With

$$Q_{\mathrm{fa}} = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

we obtain $\mathbf{Q} = \operatorname{im} Q_{\mathrm{fa}} = [0,\infty[^4$. For $\mathsf{q} \in \mathbf{Q}$ it is easy to compute $\Psi_\varrho(\mathsf{q})$ as a minimizer of $c \mapsto \mathcal{E}(c)$ under the constraint $Q_{\mathrm{fa}}c = \mathsf{q} = (q_1,...,q_4)$. We obtain

$$\begin{aligned} &\Psi_\varrho(\mathsf{q}) = \big(q_1 - a_\varrho(q_1,q_2),\ q_2 - a_\varrho(q_1,q_2),\ a_\varrho(q_1,q_2),\ q_3,\ q_4\big)^\top \in \mathbf{C} = [0,\infty[^5 \\ &\text{with } a_\varrho(q_1,q_2) = \frac{1}{2\varrho}\Big(1 + \varrho q_1 + \varrho q_2 - \sqrt{1+\varrho q_1+\varrho q_2)^2 - 4\varrho^2 q_1 q_2}\Big) \in \big[0, \min\{q_1,q_2\}\big]. \end{aligned}$$

In particular, the UFEC (3.5) holds. Moreover, the positivity and monotonicity condition (3.6) can be checked easily with $\overline{\mathsf{q}} = (1,1,1,1)^\top$. We see that $c(\theta) := \Psi_\varrho(\mathsf{q}+\theta\overline{\mathsf{q}})$ for $\theta \in]0,1]$ is given by

$$c(\theta) = \big(q_1+\theta - a_\varrho(q_1+\theta, q_2+\theta),\ q_2+\theta - a_\varrho(q_1+\theta,q_2+\theta),\ a_\varrho(q_1+\theta,q_2+\theta),\ q_3+\theta,\ q_4+\theta\big)^\top.$$

Clearly we have $c(\theta)_i > 0$, since $c(\theta)_i = 0$ would imply $q_i + \theta = 0$. Differentiating with respect to θ, we obtain

$$c'(\theta) = \big(1 - a'_\varrho[\theta], 1 - a'_\varrho[\theta], a'_\varrho[\theta], 1, 1\big)^\top \quad \text{with } a'_\varrho[\theta] = \frac{\varrho(c_1(\theta)+c_2(\theta))}{1+\varrho(c_1(\theta)+c_2(\theta))},$$

which implies that $c'(\theta)_i > 0$. Hence, $\Psi_\varrho(\mathsf{q}+\theta\overline{q})_i = c(\theta)_i \geq c(0)_i = \Psi(\mathsf{q})$, i.e. the monotonicity condition (3.6) holds.

We investigate the reduced system. First, we observe that the reduced limiting equation (4.3) is given by

$$\dot{\mathsf{q}} = Q_{\mathrm{fa}}\boldsymbol{R}_{\mathrm{sl}}(\Psi_\varrho(\mathsf{q})) = -\kappa^{\mathrm{sl}}\varrho^{1/2}\Big(\frac{a_\varrho(q_1,q_2)q_3}{\varrho} - q_4\Big)\,\widehat{\boldsymbol{\gamma}} \quad \text{with } \widehat{\boldsymbol{\gamma}} := Q_{\mathrm{fa}}\gamma^{\mathrm{sl}} = (1,1,1,-1)^\top. \tag{4.8}$$

Since a_ϱ is not a monomial, this RRE is no longer of mass-action type.

According to Section 4.1 the gradient structure $(\mathbf{Q}, \mathsf{E}_\varrho, \mathsf{R}_\varrho)$ for (4.8) is given via

$$\begin{aligned}\mathsf{E}_\varrho(\mathsf{q}) &= \mathcal{E}(\Psi_\varrho(\mathsf{q})) = \lambda_{\mathrm{B}}(q_1{-}a) + \lambda_{\mathrm{B}}(q_2{-}a) + \varrho\lambda_{\mathrm{B}}(a/\varrho) + \lambda_{\mathrm{B}}(q_3) + \lambda_{\mathrm{B}}(q_4)\Big|_{a=a_\varrho(q_1,q_2)},\\ \mathsf{R}^*_\varrho(\mathsf{q},\zeta) &= \mathcal{R}_{\mathrm{sl}}(\Psi_\varrho(\mathsf{q}), Q_{\mathrm{fa}}^\top\zeta) = \kappa^{\mathrm{sl}}\left(a_\varrho(q_1,q_2)\, q_3q_4\right)^{1/2} \mathsf{C}^*\big(\zeta_1{+}\zeta_2{+}\zeta_3{-}\zeta_4\big).\end{aligned}$$

The energy E_ϱ is no longer of Boltzmann type, because the previously uncoupled densities c_1, c_2, and c_3 are now constrained to lie on $\mathscr{M}_{\mathrm{sl}}$, i.e. $c_1c_2 = c_3$. Nevertheless, the form is close to a mass-action type for the trimolecular reaction $Y_1 + Y_2 + Y_3 \rightleftharpoons Y_4$.

To recover an exact trimolecular reaction of mass-action type, one has to perform another limit, namely $\varrho \to 0^+$, which means that the species X_3 is no longer observed, but still exists on a microscopic reaction pathway. For the limit $\varrho \to 0^+$ we simply observe the expansion

$$a_\varrho(q_1,q_2) = \varrho q_1q_2 + O(\varrho^2) \quad \text{for } \varrho \to 0^+,$$

which implies $\Psi_\varrho(q) \to \Psi_0(q) := (q_1, q_2, 0, q_3, q_4)^T$. If we additionally choose $\kappa^{\mathrm{sl}} = \overline{\kappa}/\varrho^{1/2}$ and insert the expansion for a_ϱ we obtain

$$\begin{aligned}\mathsf{E}_\varrho(\mathsf{q}) \;\to\; \mathsf{E}_0(\mathsf{q}) &= \sum_{j=1}^4 \lambda_{\mathrm{B}}(q_j),\\ \mathsf{R}^*_\varrho(\mathsf{q},\zeta) \to \mathsf{R}^*_0(q,\zeta) &= \overline{\kappa}\left(q_1q_2q_3q_4\right)^{1/2} \mathsf{C}^*\big(\zeta_1{+}\zeta_2{+}\zeta_3{-}\zeta_4\big).\end{aligned}$$

Clearly, this is the gradient system generating the RRE of the trimolecular reaction $X_1 + X_2 + X_4 \rightleftharpoons X_5$. Of course, it is possible to show that this convergence is again a EDP-convergence with tilting of the gradient systems $(\mathbf{Q}, \mathsf{E}_\varrho, \mathsf{R}_\varrho)$ to the effective system $(\mathbf{Q}, \mathsf{E}_0, \mathsf{R}_0)$.

5 Proof of Theorem 3.4

Here we will show the Γ-convergence of the dissipation functionals, namely $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M_E}} \mathfrak{D}_0$. As usual the proof consists in three parts: (i) compactness of the sequences (c^ε) satisfying $\mathfrak{D}_\varepsilon(c^\varepsilon) \le C$, (ii) the liminf estimate, and the (iii) the limsup estimate, which needs the construction of recovery sequences.

All the following results are derived under the assumptions of Theorem 3.4: The fast-slow DBRS $(A, B, c_*, \widehat{\kappa}^\varepsilon)$ satisfies the unique fast-equilibrium condition UFEC (3.5). For constructing the recovery sequence in Section 5.3, we need additionally the positivity and monotonicity assumption (3.6) for Ψ.

5.1 Compactness

In the definition of $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M_E}} \mathfrak{D}_0$ we consider sequences $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T];\mathbf{C})$ that additionally satisfy $\sup_{\varepsilon\in]0,1[,\ t\in[0,T]} \mathcal{E}(c^\varepsilon(t)) \le C$. The aim is to extract a strongly converging subsequence $c^\varepsilon \to c^0$, such that we can talk about pointwise convergence almost everywhere. This will be necessary in the liminf estimate because we cannot rely on convexity, in contrast to the linear theory developed in [MiS19]. The compactness is derived via two quite different arguments that complement each other and reflect the underlying

fast-slow structure, which is seen on the local level via the decomposition of $\mathrm{T}_c\mathbf{C} = \mathbb{R}^{i_*}$ in the direct sum of Γ_{fa} and $\mathrm{T}_c\mathscr{M}_{\mathrm{sl}}$, see Step 1 in the proof of Proposition 4.5. First, we derive time regularity for the slow part of the reactions. Secondly, we prove convergence towards the slow manifold which then provides the remaining information for the whole sequence.

Theorem 5.1 (Compactness via dissipation bound)**.** *Consider a family $(c^\varepsilon)_{\varepsilon>0}$ with $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^1([0,T];\mathbf{C})$, $\sup_{\varepsilon>0,\ t\in[0,T]} \mathcal{E}(c^\varepsilon(t)) \le M_{\mathrm{ener}} < \infty$, and $\mathfrak{D}_\varepsilon(c^\varepsilon) \le M_{\mathrm{diss}} < \infty$. Then, we have*
(i) $c^\varepsilon(\cdot)$ is bounded in $\mathrm{L}^\infty([0,T];\mathbf{C})$;
(ii) $Q_{\mathrm{fa}}c^\varepsilon \to Q_{\mathrm{fa}}c^0$ weakly in $\mathrm{W}^{1,1}([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$ and strongly in $\mathrm{C}^0([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$;
(iii) $c^0(t) = \widetilde{c}(t) := \Psi(Q_{\mathrm{fa}}c^0(t)) \in \mathscr{M}_{\mathrm{sl}}$ for a.a. $t \in [0,T]$, and, in particular $\widetilde{c} \in \mathrm{C}^0([0,T],\mathbf{C})$;
(iv) $c^\varepsilon \to c^0$ in $\mathrm{L}^p([0,T];\mathbf{C})$ strongly for all $p \in [1,\infty[$.

We emphasize that c^0 and $\widetilde{c}$ may be different, and this happens even for solutions, if near $t = 0$ a jump develops such that (cf. Section 2.4)

$$\lim c^\varepsilon(0) =: c_0 \ \neq\ \overline{c}_0 := \lim_{\tau\to 0^+} \Big(\lim_{\varepsilon\to 0^+} c^\varepsilon(\tau) \Big).$$

Before giving the detailed proof we provide two preliminary results that underpin the two complementary arguments of the proof.

For deriving bounds on the time derivatives, one heuristically sees that for fixed (c,ξ) we have $\mathcal{R}^*_\varepsilon(c,\xi) \nearrow \mathcal{R}^*_{\mathrm{eff}}(c,\xi)$ as $\varepsilon \to 0$. By duality, this implies $\mathcal{R}_\varepsilon(c,v) \searrow \mathcal{R}_{\mathrm{eff}}(c,v)$. This already shows that control of time derivatives has to be obtained from $\mathcal{R}_{\mathrm{eff}}(c,\cdot)$, which only controls $Q_{\mathrm{fa}}\dot{c}$ because $\mathcal{R}_{\mathrm{eff}}(c,v) = \mathcal{R}_{\mathrm{eff}}(c,w)$ if $Q_{\mathrm{fa}}v = Q_{\mathrm{fa}}w$, see (3.4b).

Proposition 5.2 (Effective dissipation potential)**.** *For all $\varepsilon > 0$ we have $\mathcal{R}_\varepsilon(c,v) \ge \mathcal{R}_{\mathrm{eff}}(c,v)$ for all $(c,v) \in \mathbf{C} \times \mathbb{R}^{i_*}$. Moreover, $\mathcal{R}_{\mathrm{eff}}$ takes the form*

$$\mathcal{R}_{\mathrm{eff}}(c,v) = \widetilde{\mathcal{R}}(c,Q_{\mathrm{fa}}v) \quad \text{where } \widetilde{\mathcal{R}}(c,\mathsf{q}) := \sup\big\{\, \zeta\cdot\mathsf{q} - \mathcal{R}^*_{\mathrm{sl}}(c,Q_{\mathrm{fa}}^\top\zeta) \,\big|\, \zeta \in \mathbb{R}^{m_{\mathrm{fa}}} \,\big\}.$$

Proof. We first use the standard relation from linear algebra: $\mathrm{im}(Q_{\mathrm{fa}}^\top) = \big(\ker(Q_{\mathrm{fa}})\big)^\perp = \Gamma_{\mathrm{fa}}^\perp$. By construction of Γ_{fa} we have $\mathcal{R}^*_{\mathrm{fa}}(c,\xi) = 0$ for $\xi \in \Gamma_{\mathrm{fa}}^\perp$ and obtain

$$\mathcal{R}^*_\varepsilon(c,\xi) = \mathcal{R}^*_{\mathrm{sl}}(c,\xi) + \frac{1}{\varepsilon}\mathcal{R}^*_{\mathrm{fa}}(c,\xi) \le \mathcal{R}^*_{\mathrm{eff}}(c,\xi) := \mathcal{R}^*_{\mathrm{sl}}(c,\xi) + \chi_{\Gamma_{\mathrm{fa}}^\top}(\xi) = \mathcal{R}^*_{\mathrm{sl}}(c,\xi) + \chi_{\mathrm{im}\,Q_{\mathrm{fa}}^\top}(\xi).$$

Applying the Legendre-Fenchel transformation we obtain

$$\begin{aligned}\mathcal{R}_\varepsilon(c,v) \ge \mathcal{R}_{\mathrm{eff}}(c,v) &= \sup\big\{\, v\cdot\xi - \mathcal{R}^*_{\mathrm{sl}}(c,\xi) \,\big|\, \xi \in \mathrm{im}(Q_{\mathrm{fa}}^\top) \,\big\} \\ &= \sup\big\{\, v\cdot Q_{\mathrm{fa}}^\top\zeta - \mathcal{R}^*_{\mathrm{sl}}(c,Q_{\mathrm{fa}}^\top\zeta) \,\big|\, \zeta \in \mathbb{R}^{m_{\mathrm{fa}}} \,\big\} = \widetilde{\mathcal{R}}(c,Q_{\mathrm{fa}}v),\end{aligned}$$

which provides the desired estimate as well as the representation via $\widetilde{\mathcal{R}}$. □

The second result concerns the convergence of points towards the slow manifold $\mathscr{M}_{\mathrm{sl}}$, and the crucial property here is the UFEC (3.5) that guarantees the relation

$$\big\{\, \Psi(\mathsf{q}) \,\big|\, \mathsf{q} \in \mathbf{Q} \subset \mathbb{R}^{m_{\mathrm{fa}}} \,\big\} =: \mathscr{M}_{\mathrm{sl}} \ \overset{!!}{=}\ \mathscr{E}_{\mathrm{fa}} \overset{\text{Lemma 2.4}}{=} \big\{\, c \in \mathbf{C} \,\big|\, \mathcal{S}_{\mathrm{fa}}(c) = 0 \,\big\}.$$

Lemma 5.3 (Convergence towards $\mathscr{M}_{\mathrm{sl}}$)**.** *For bounded sequences $(c^n)_{n\in\mathbb{N}}$ in $\mathbf{C}$ we have*

$$Q_{\mathrm{fa}}c^n \to \mathsf{q} \text{ and } \mathcal{S}_{\mathrm{fa}}(c^n)\to 0 \quad \Longrightarrow \quad c^n \to \Psi(\mathsf{q}). \tag{5.1}$$

Proof. Without loss of generality we may assume $c^n \to \overline{c}$. Hence we have $Q_{\mathrm{fa}}c^n \to Q_{\mathrm{fa}}\overline{c} = \mathsf{q}$. Moreover, the continuity of $\mathcal{S}_{\mathrm{fa}}$ gives $0 = \lim \mathcal{S}_{\mathrm{fa}}(c^n) = \mathcal{S}_{\mathrm{fa}}(\overline{c})$. Thus, we have $\overline{c} \in \mathscr{E}_{\mathrm{fa}} \cap \mathbf{C}^{\mathrm{fa}}_{\mathsf{q}}$. Now, the UFEC (see (3.11)) gives $\overline{c} = \Psi(\mathsf{q})$ which is the desired result. □

We are now ready to establish the main compactness result.

Proof of Theorem 5.1. Part (i): From the energy bound $\mathcal{E}(c^\varepsilon(t)) \le M_{\mathrm{ener}} < \infty$ and the coercivity of $\mathcal{E}$ we obtain an L^∞ bound for c^ε, namely $0 \le c_j^\varepsilon(t) \le |c^\varepsilon(t)| \le \|c^\varepsilon\|_{\mathrm{L}^\infty} \le M_{\mathrm{ener}}$.

Part (ii): To provide a lower bound on $\mathcal{R}_{\mathrm{eff}}$ we first observe an upper bound on $\mathcal{R}^*_{\mathrm{sl}}$, namely

$$\mathcal{R}^*_{\mathrm{sl}}(c^\varepsilon, Q_{\mathrm{fa}}^\top\zeta) \le \sum_{r\in R_{\mathrm{sl}}} \kappa_r M_{\mathrm{ener}}^{(\alpha^r+\beta^r)/2}\, \mathsf{C}^*\Big(\gamma^r\cdot Q_{\mathrm{fa}}^\top\zeta\Big) \le b_M \mathsf{C}^*\big(b_Q|\zeta|\big) \quad \text{with } b_Q = \max_{r\in R_{\mathrm{sl}}}|Q_{\mathrm{fa}}\gamma^r|,$$

where we used $0 \le c_j^\varepsilon \le M_{\mathrm{ener}}$ from part (i). Using the Legendre-Fenchel transformation and Proposition 5.2 we obtain the lower bound

$$\mathcal{R}_\varepsilon(c^\varepsilon, v) \ge \widetilde{\mathcal{R}}(c^\varepsilon, Q_{\mathrm{fa}}v) \ge \sup\big\{\, Q_{\mathrm{fa}}v\cdot\zeta - b_M\mathsf{C}^*(b_Q|\zeta|) \,\big|\, \zeta\in\mathbb{R}^{m_{\mathrm{fa}}}\,\big\} \;=\; b_M\,\mathsf{C}\Big(\frac{|Q_{\mathrm{fa}}v|}{b_M b_Q}\Big).$$

Using the bound M_{diss} for the dissipation functionals, the family satisfies

$$\int_0^T \mathsf{C}\bigg(\frac{|Q_{\mathrm{fa}}\dot c^\varepsilon(t)|}{b_M b_Q}\bigg)\,\mathrm{d}t \le \int_0^T \frac{1}{b_M}\mathcal{R}_\varepsilon\big(c^\varepsilon(t),\dot c^\varepsilon(t)\big)\,\mathrm{d}t \le \frac{1}{b_M}\mathfrak{D}_\varepsilon(c^\varepsilon) \le M_{\mathrm{diss}}/b_M.$$

Since $\mathsf{C}(s) \ge \frac12|s|\log(1+|s|)$ for all $s\in\mathbb{R}$ (cf. [MiS19, Eqn. (A.2)]) we have a uniform superlinear bound for $Q_{\mathrm{fa}}\dot c^\varepsilon$. Thus, there exists a subsequence (not relabeled) such that $Q_{\mathrm{fa}}\dot c^\varepsilon \rightharpoonup \mathsf{w}$ in $\mathrm{L}^1([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$. Moreover, $Q_{\mathrm{fa}}c^\varepsilon$ is equicontinuous (cf. [MiS19, Prop. 5.9]), which implies $Q_{\mathrm{fa}}c^\varepsilon \to \mathsf{q}^0$ in $\mathrm{C}^0([0,T];\mathbf{Q})$.

Because of $c^\varepsilon \rightharpoonup c^0$ we conclude $\mathsf{q}^0 = Q_{\mathrm{fa}}c^0 \in \mathrm{W}^{1,1}([0,T];\mathbf{Q})$ and $\dot{\mathsf{q}} = \mathsf{w}$. Since the limit is unique, we also know that the whole family converges.

Part (iii): The dissipation bound gives the estimate $\int_0^T \mathcal{S}_{\mathrm{fa}}(c^\varepsilon(t))\,\mathrm{d}t \le \varepsilon\, M_{\mathrm{diss}}$. Using $\mathcal{S}_{\mathrm{fa}}(c)\ge 0$ this implies that $f_\varepsilon = \mathcal{S}_{\mathrm{fa}}\circ c^\varepsilon$ converges to 0 in $\mathrm{L}^1([0,T])$. Thus, we may choose a subsequence (not relabeled) such that $f_\varepsilon(t)\to 0$ a.e. in $[0,T]$.

By the continuity $\mathcal{S}_{\mathrm{fa}}$ and $|c^\varepsilon(t)| \le M_{\mathrm{ener}}$ we also know that $(f_\varepsilon(t))_{\varepsilon\in]0,1[}$ is bounded, while part (ii) provides the convergence $Q_{\mathrm{fa}}c^\varepsilon(t) \to \mathsf{q}^0(t) = Q_{\mathrm{fa}}c^0(t)$. Hence, Lemma 5.3 guarantees $c^\varepsilon(t) \to \widetilde{c}(t) := \Psi(Q_{\mathrm{fa}}c^0(t))$ a.e. in $[0,T]$. By $c^\varepsilon \rightharpoonup c^0$ we have $c^0(t) = \widetilde{c}(t)$ a.e.

Since Ψ is continuous by Proposition 3.6, also $\widetilde{c} = \Psi(Q_{\mathrm{fa}}c^0)$ is continuous.

Part (iv): This follows via part (i), the pointwise a.e. convergence established in the proof of part (iii), and from the dominated-convergence theorem. □

5.2 Liminf estimate

The liminf estimate follows in a straightforward manner by using the fact that the velocity part $\mathcal{R}_\varepsilon$ in $\mathfrak{D}_\varepsilon$ satisfies the monotonicity $\mathcal{R}_\varepsilon \ge \mathcal{R}_{\mathrm{eff}}$, see Proposition 5.2, and that the slope part $\mathcal{S}_\varepsilon$ takes the simple form $\mathcal{S}_{\mathrm{sl}} + \frac{1}{\varepsilon}\mathcal{S}_{\mathrm{fa}}$.

Theorem 5.4 (Liminf estimate). *Let $(c^\varepsilon)_{\varepsilon>0}$ with $c^\varepsilon \rightharpoonup c^0$ in $\mathrm{L}^1([0,T];\mathbf{C})$ as in Theorem 5.1 we have the estimate $\mathfrak{D}_0(c^0) \le \liminf_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(c^\varepsilon)$.*

Proof. We may assume that $\alpha_* := \liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) < \infty$, since otherwise the desired estimate is trivially satisfied. This implies $\mathcal{S}_{\mathrm{fa}}(c^0(t)) = 0$ a.e. in $[0,T]$ as in the previous proof. We define the functional

$$\mathfrak{I}(c,\mathsf{q}) := \int_0^T \mathcal{F}(c(t),\mathsf{q}(t))\,\mathrm{d}t \quad \text{with } \mathcal{F}(c,\mathsf{w}) = \widetilde{\mathcal{R}}(c,\mathsf{w}) + \mathcal{S}_{\mathrm{sl}}(c).$$

Then, using $\mathcal{R}_\varepsilon \ge \mathcal{R}_{\mathrm{eff}}$ and $\mathcal{S}_\varepsilon \ge \mathcal{S}_{\mathrm{sl}}$, we have

$$\mathfrak{D}_\varepsilon(c^\varepsilon) \ge \mathfrak{I}(c^\varepsilon, Q_{\mathrm{fa}}\dot{c}^\varepsilon) \quad \text{and} \quad \mathfrak{D}_0(c^0) = \mathfrak{I}(c^0, Q_{\mathrm{fa}}\dot{c}^0),$$

where the last identity follows from the construction of the density $\mathcal{F}$ via $\widetilde{\mathcal{R}}$ and $\mathcal{S}_{\mathrm{sl}}$, and $\mathcal{S}_0(c(t)) = \mathcal{S}_{\mathrm{sl}}(c(t))$ a.e. because of $\mathcal{S}_{\mathrm{fa}}(c^0(t)) = 0$.

Thus, it suffices to show the lower semicontinuity $\mathfrak{I}(c^0, Q_{\mathrm{fa}}\dot{c}^0) \le \liminf_{\varepsilon\to 0^+} \mathfrak{I}(c^\varepsilon, Q_{\mathrm{fa}}\dot{c}^\varepsilon)$. Using the strong convergence $c^\varepsilon \to c^0$ in $\mathrm{L}^p([0,T];\mathbf{C})$ and the weak convergence $Q_{\mathrm{fa}}\dot{c}^\varepsilon \rightharpoonup Q_{\mathrm{fa}}\dot{c}^0$ in $\mathrm{L}^1([0,T];\mathbb{R}^{m_{\mathrm{fa}}})$, see Theorem 5.1(ii+iv), this follows by Ioffe's theorem (cf. [FoL07, Thm. 7.5] if we know that $\mathcal{F} : \mathbf{C}\times\mathbb{R}^{m_{\mathrm{fa}}} \to [0,\infty]$ is lower semicontinuous. However, the lower semicontinuity of $(c,\mathsf{w}) \mapsto \mathcal{F}(c,\mathsf{w}) = \widetilde{\mathcal{R}}(c,\mathsf{w}) + \mathcal{S}_{\mathrm{sl}}(c)$ follows immediately from the continuity of $\mathcal{S}_{\mathrm{sl}}$ and the by Legendre transforming the continuous function $(c,\zeta) \mapsto \mathcal{R}^*_{\mathrm{sl}}(c, Q_{\mathrm{fa}}^\top\zeta)$.

This finishes the proof of Theorem 5.4. □

5.3 Construction of the recovery sequence

In this section we construct the recovery sequence which completes the proof of the Mosco convergence $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M_E}} \mathfrak{D}_0$ with energy constraint. Below in Step 1, we will need the positivity and monotonicity condition (3.6) for $\theta \mapsto \Psi(\mathsf{q}+\theta\overline{\mathsf{q}})$.

Theorem 5.5 (Limsup estimate). *Let $c^0 \in \mathrm{L}^1([0,T];\mathbf{C})$ with $\sup_{t\in[0,T]} \mathcal{E}(c^0(t)) < \infty$. Then there exists a family $(c^\varepsilon)_{\varepsilon\in]0,1]}$ with $\sup_{t\in[0,T],\ \varepsilon\in]0,1]} \mathcal{E}(c^\varepsilon(t)) \le M_{\mathrm{ener}} < \infty$, $c^\varepsilon \to c^0$ strongly in $\mathrm{L}^1([0,T];\mathbf{C})$, and $\lim_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) = \mathfrak{D}_0(c^0)$.*

Proof. We prove the theorem in several steps. In Steps 1 and 2 we show that it is sufficient to consider $c^0 \in \mathrm{W}^{1,\infty}([0,T];\mathbf{C})$ with $c^0_j(t) \ge \underline{c} > 0$, where we only work in $\mathfrak{D}_0$ which has the advantage that $\mathcal{R}_{\mathrm{eff}}(c,\dot{c})$ only depends on $(\mathsf{q},\dot{\mathsf{q}}) = (Q_{\mathrm{fa}}c, Q_{\mathrm{fa}}\dot{c})$, see Section 4.1. In Step 3 we construct a recovery sequence, and in Step 4 we conclude with a diagonal argument.

Step 0: To start with we may assume $\mathfrak{D}_0(c^0) < \infty$. Indeed, if $\mathfrak{D}_0(c^0) = \infty$, then we choose $c^\varepsilon = c^0$ and Theorem 5.4 gives $\liminf_{\varepsilon\to 0} \mathfrak{D}_\varepsilon(c^\varepsilon) \ge \mathfrak{D}_0(c^0) = \infty$, which means $\mathfrak{D}_\varepsilon(c^\varepsilon) \to \infty$ as desired.

Step 1. Reducing to positive curves c^0: For c^0 with $\mathfrak{D}_0(c^0) < \infty$ we know that $Q_{\mathrm{fa}}c^0 \in \mathrm{W}^{1,1}([0,T];\mathbf{Q})$ and $c^0 \in \mathrm{C}^0([0,T];\mathbf{C})$ after choosing the continuous representative $c^0 = \widetilde{c}$, see Theorem 5.1. Exploiting the positivity and monotonicity condition (3.6) we now set

$$\underline{c}^l(t) := \Psi\big(\mathsf{q}(t) + \theta_l\,\overline{\mathsf{q}}\big) \quad \text{with } \theta_l = \frac{1}{l+1} \in]0,1[\quad \text{for all } t\in[0,T].$$

By this condition, we know that $\underline{c}^l(t)$ lies in $\mathbf{C}_+$ for all $t \in [0,T]$, such that the continuity of $\underline{c}^l$ guarantees that for each l there exists a $\delta_l > 0$ such that $\underline{c}^l_i(t) \geq \delta_l$ for all $i \in I$ and $t \in [0,T]$.

By the continuity of Ψ we have $\underline{c}^l \to c^0$ uniformly and hence strongly in $\mathrm{L}^1([0,T];\mathbf{C})$. We now show

$$\mathfrak{D}_0(\underline{c}^l) = \int_0^T \big\{ \mathcal{R}_{\mathrm{eff}}(\underline{c}^l(t), \dot{\underline{c}}^l(t)) + \mathcal{S}_0(\underline{c}^l(t)) \big\} \,\mathrm{d}t \;\to\; \mathfrak{D}_0(c^0) \quad \text{as} \quad l \to 0. \tag{5.2}$$

For the second part, we use $\underline{c}^l(t) \in \mathscr{M}_{\mathrm{sl}}$ by construction via Ψ, and the continuity of $\mathcal{S}_{\mathrm{sl}}$ yields $\mathcal{S}_0(\underline{c}^l(t)) = \mathcal{S}_{\mathrm{sl}}(\underline{c}^l(t)) \to \mathcal{S}_{\mathrm{sl}}(c^0(t)) = \mathcal{S}_0(c^0(t))$ uniformly in $[0,T]$.

For the first part we use (i) the special form of $\mathcal{R}_{\mathrm{eff}}$ derived in Proposition 5.2, namely $\mathcal{R}_{\mathrm{eff}}(c,v) = \widetilde{\mathcal{R}}(c, Q_{\mathrm{fa}} v)$, where $\widetilde{\mathcal{R}}(c,\cdot)$ is the Legendre transform of $\mathcal{R}^*_{\mathrm{sl}}(c, Q^\top \cdot)$. Moreover, the cosh-type dual dissipation potential $\mathcal{R}^*_{\mathrm{sl}}$ as defined in (2.6b) or (2.14) enjoys (ii) a monotonicity property namely $\mathcal{R}^*_{\mathrm{sl}}(c,\xi) \leq \mathcal{R}^*_{\mathrm{sl}}(\widetilde{c},\xi)$ or equivalently $\mathcal{R}_{\mathrm{sl}}(c,v) \geq \mathcal{R}_{\mathrm{sl}}(\widetilde{c},v)$ if $c \leq \widetilde{c}$ componentwise. This can be exploited because of the monotonicity condition (3.6) using $\underline{c}^l(t) \geq c^0(t)$ componentwise. With $Q_{\mathrm{fa}}\, \dot{\underline{c}}^l(t) = \dot{\mathsf{q}}(t)$ for all $l \in \mathbb{N}$ we obtain

$$\int_0^T \mathcal{R}_{\mathrm{eff}}(\underline{c}^l, \dot{\underline{c}}^l(t)) \,\mathrm{d}t \overset{\text{(i)}}{=} \int_0^T \widetilde{\mathcal{R}}(\underline{c}^l, \dot{\mathsf{q}}(t)) \,\mathrm{d}t \xrightarrow{\text{(ii)}} \int_0^T \widetilde{\mathcal{R}}(c^0, \dot{\mathsf{q}}(t)) \,\mathrm{d}t \overset{\text{(i)}}{=} \int_0^T \mathcal{R}_{\mathrm{eff}}(c^0, \dot{c}^0) \,\mathrm{d}t,$$

where the convergence $\xrightarrow{\text{(ii)}}$ follows from the dominated-convergence theorem, since the integrands on the left-hand side are bounded by that on the right-hand side and we have pointwise convergence. With this we have established the desired convergence (5.2).

Step 2. Reducing to bounded derivative $\dot{\mathsf{q}} = Q_{\mathrm{fa}} \dot{c}$*:* Because of Step 1, we can now assume

$$c^0(t) \in \mathbf{C}_\delta := \big\{ c \in \mathbf{C} \,\big|\, |c| \leq 1/\delta, c_i \geq \delta \text{ for all } i \in I \big\} \;\text{ for all } t \in [0,T]$$

where $\delta > 0$. Moreover, as in [MiS19, Step 2(b) of proof of Thm. 5.12] we find Λ^* such that

$$c, \widetilde{c} \in \mathbf{C}_\delta \text{ and } |c - \widetilde{c}| \leq \alpha < \frac{1}{2\Lambda^*} \quad \Longrightarrow \quad \widetilde{\mathcal{R}}(\widetilde{c}, \mathsf{w}) \;\leq\; (1+\Lambda^*\alpha)\, \widetilde{\mathcal{R}}(c, \mathsf{w}).$$

With this we can estimate $\mathcal{R}^*_{\mathrm{sl}}(c,\cdot)$ from below and hence $\mathcal{R}_{\mathrm{eff}}$ from above. Moreover, we can use the Lipschitz continuity of $c \mapsto \mathcal{R}^*_\varepsilon$.

For $\mathsf{q}(t) = Q_{\mathrm{fa}} c^0 \in \mathrm{W}^{1,1}([0,T];\mathbf{Q})$ we define the piecewise affine interpolants $\widehat{\mathsf{q}}^k$ via

$$\widehat{\mathsf{q}}^k\big((n+\theta)2^{-k}T\big) = (1-\theta)\mathsf{q}\big(n2^{-k}T\big) + \theta \mathsf{q}\big((n+1)2^{-k}T\big) \text{ for } \theta \in [0,1],\ n \in \{0,\dots,2^k-1\}$$

and the piecewise constant interpolant $\overline{\mathsf{q}}^k\big((n+\theta)2^{-k}T\big) = \mathsf{q}(2^{-k}nT)$ for $\theta \in [0,1[$. We also set $\widehat{c}^k(t) = \Psi(\widehat{\mathsf{q}}^k(t))$ and $\overline{c}^k(t) = \Psi(\overline{\mathsf{q}}^k(t))$. By standard arguments we have

$$\|\overline{c}^k - \widehat{c}^k\|_{\mathrm{L}^\infty} + \|\widehat{c}^k - c^0\|_{\mathrm{L}^\infty} =: \alpha_k \to 0 \quad \text{for } k \to \infty.$$

As in Step 1 we again find $\int_0^T \mathcal{S}_0(\widehat{c}^k(t)) \,\mathrm{d}t \to \int_0^T \mathcal{S}_0(c^0(t)) \,\mathrm{d}t$. To treat the velocity part we use both interpolants obtain the estimate

$$\begin{aligned}
\int_0^T \mathcal{R}_{\mathrm{eff}}(\widehat{c}^k, \dot{\widehat{c}}^k) \,\mathrm{d}t \;&=\; \int_0^T \widetilde{\mathcal{R}}(\widehat{c}^k, \dot{\widehat{\mathsf{q}}}^k) \,\mathrm{d}t \;\leq\; (1+\Lambda^*\alpha_k) \int_0^T \widetilde{\mathcal{R}}(\overline{c}^k, \dot{\widehat{\mathsf{q}}}^k) \,\mathrm{d}t \\
&\overset{\text{(J)}}{\leq} (1+\Lambda^*\alpha_k) \int_0^T \widetilde{\mathcal{R}}(\overline{c}^k, \dot{\mathsf{q}}) \,\mathrm{d}t \;\leq\; \int_0^T \widetilde{\mathcal{R}}(c^0, \dot{\mathsf{q}}) \,\mathrm{d}t \;=\; (1+\Lambda^*\alpha_k)^2 \int_0^T \mathcal{R}_{\mathrm{eff}}(c^0, \dot{c}^0) \,\mathrm{d}t,
\end{aligned}$$

where $\overset{(J)}{\leq}$ indicates the use of Jensen's inequality applied to the convex integrand $\widetilde{\mathcal{R}}(\overline{c}^k(t),\,\cdot\,)$, which is independent of t in the intervals $]2^{-k}nT, 2^{-k}(n+1)T[$. Combining this with the slope part and using $\alpha_k \to 0$ we obtain the desired estimate $\limsup_{k\to\infty} \mathfrak{D}_0(\widehat{c}^k) \leq \mathfrak{D}_0(c^0)$, which is of course a limit because of the liminf estimate in Theorem 5.4.

Step 3. The limsup for $\varepsilon \to 0^+$: By Steps 1 and 2 it is sufficient to consider $c^0 \in \mathrm{W}^{1,\infty}([0,T];\mathbf{C})$ with $c^0(t) = \Psi(\mathsf{q}(t)) \in \mathbf{C}_\delta$ for some $\delta > 0$. For these functions we can now use the constant recovery sequence $c^\varepsilon = c^0$, i.e. we will show

$$\mathfrak{D}_\varepsilon(c^0) = \int_0^T \big\{\mathcal{R}_\varepsilon(c^0,\dot{c}^0) + \mathcal{S}_\varepsilon(c^0)\big\}\,\mathrm{d}t \;\to\; \mathfrak{D}_0(c^0) = \int_0^T \big\{\mathcal{R}_{\mathrm{eff}}(c^0,\dot{c}^0) + \mathcal{S}_0(c^0)\big\}\,\mathrm{d}t \quad (5.3)$$

for $\varepsilon \to 0^+$. Because of $c^0(t) \in \mathscr{M}_{\mathrm{sl}}$ we have $\mathcal{S}_\varepsilon(c^0(t)) = \mathcal{S}_{\mathrm{sl}}(c^0(t)) = \mathcal{S}_0(c^0(t))$, so the second summand of the integral $\mathfrak{D}_\varepsilon(c^0)$ converges trivially.

Recall that $\Gamma = \operatorname{span}\big\{\,\gamma^r \,\big|\, r \in R = R_{\mathrm{sl}} \dot\cup R_{\mathrm{fa}}\,\big\}$ and define a projection $\mathbb{Q}$ on $\mathbb{R}^{i_*}$ with $\operatorname{im}\mathbb{Q} = \Gamma$ giving $\ker\mathbb{Q}^\top = \Gamma^\perp$. With this we can estimate the dual dissipation potential $\mathcal{R}_\varepsilon^*$ from below:

$$\mathcal{R}_\varepsilon^*(c,\xi) \;\geq\; \mathcal{R}_1^*(c,\xi) \geq b_*|\mathbb{Q}^\top\xi|^2.$$

To see this use $\mathsf{C}^*(\sigma) \geq \frac{1}{2}\sigma^2$ and $\big(c^{\alpha^r}c^{\beta^r}\big)^{1/2} \geq \delta^{(\alpha^r+\beta^r)/2}$ for all $r \in R$.

By Legendre-Fenchel transformation we obtain an upper bound for $\mathcal{R}_\varepsilon$, where we use $\dot{c}^0 \in \Gamma$, i.e. $\mathbb{Q}\dot{c}^0(t) = \dot{c}^0(t)$ (cf. Lemma 2.5):

$$\mathcal{R}_\varepsilon(c^0(t),\dot{c}^0(t)) \;\leq\; \mathcal{R}_1(c^0(t),\dot{c}^0(t)) \;\leq\; \frac{1}{4b_*}|\mathbb{Q}\dot{c}^0(t)|^2 \;=\; \frac{1}{4b_*}|\dot{c}^0(t)|^2.$$

From $c^0 \in \mathrm{W}^{1,\infty}([0,T];\mathbf{C})$ we see that $t \mapsto \mathcal{R}_1(c^0(t),\dot{c}^0(t))$ lies in $\mathrm{L}^\infty([0,T])$ and thus provides an integrable majorant for $t \mapsto \mathcal{R}_\varepsilon(c^0(t),\dot{c}^0(t))$. However, the convergence $\mathcal{R}_\varepsilon^*(c,\xi) \nearrow \mathcal{R}_0^* = \mathcal{R}_{\mathrm{sl}}^* + \chi_{\Gamma_{\mathrm{fa}}^\perp}$ for $\varepsilon \to 0^+$ implies $\mathcal{R}_\varepsilon(c,v) \searrow \mathcal{R}_{\mathrm{eff}}(c,v)$ for all $(c,v) \in \mathbf{C}_\delta \times \mathbb{R}^{i_*}$. Hence, Lebesgue's dominated convergence theorem gives

$$\int_0^T \mathcal{R}_\varepsilon(c^0(t),\dot{c}^0(t))\,\mathrm{d}t \;\to\; \int_0^T \mathcal{R}_{\mathrm{eff}}(c^0(t),\dot{c}^0(t))\,\mathrm{d}t \quad \text{for } \varepsilon \to 0^+,$$

and (5.3) is established.

Step 4. Diagonal sequence: The full recovery sequence for a general c^0 with $\mathfrak{D}_0(c^0) < \infty$ is obtained via $\mathsf{q}(t) = Q_{\mathrm{fa}}c^0(t)$ as a diagonal sequence $c^\varepsilon = \Psi\big(\widehat{\mathsf{q}}^{k(\varepsilon)}(t) + \theta_{l(\varepsilon)}\overline{\mathsf{q}}\big)$, where the functions $k(\varepsilon)$ and $l(\varepsilon)$ are suitably chosen such that $c^\varepsilon \to c^0$ strongly in $\mathrm{L}^1([0,T];\mathbf{C})$ and $\mathfrak{D}_\varepsilon(c^\varepsilon) \to \mathfrak{D}_0(c^0)$. It is also clear from the construction that $\|c^\varepsilon\|_{\mathrm{L}^\infty} \leq 1 + \|c^0\|_{\mathrm{L}^\infty}$ such that the uniform energy bound $\mathcal{E}(c^\varepsilon(t)) \leq M_{\mathrm{ener}}$ holds. □

Acknowledgments. The research was partially supported by Deutsche Forschungsgemeinschaft (DFG) through the Collaborative Research Center SFB 1114 "*Scaling Cascades in Complex Systems*" (Project no. 235221301), Subproject C05 "Effective models for materials and interfaces with multiple scales". The authors are grateful to Michiel Renger for helpful and stimulating discussions.

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Part 3

EDP-convergence for a linear reaction-diffusion system with fast reversible reaction

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This preprint has not undergone peer review or any post-submission improvements or corrections. The Version of Record of this article is published in *Calculus of Variations and Partial Differential Equations*, and is available online at https://doi.org/10.1007/s00526-021-02089-0.

EDP-convergence for a linear reaction-diffusion system with fast reversible reaction*

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Abstract

We perform a fast-reaction limit for a linear reaction-diffusion system consisting of two diffusion equations coupled by a linear reaction. We understand the linear reaction-diffusion system as a gradient flow of the free energy in the space of probability measures equipped with a geometric structure, which contains the Wasserstein metric for the diffusion part and cosh-type functions for the reaction part. The fast-reaction limit is done on the level of the gradient structure by proving EDP-convergence with tilting. The limit gradient system induces a diffusion system with Lagrange multipliers on the linear slow-manifold. Moreover, the limit gradient system can be equivalently described by a coarse-grained gradient system, which induces a diffusion equation with a mixed diffusion constant for the coarse-grained slow variable.

1 Introduction

Considering two species X_1 and X_2 which diffuse in a bounded medium $\Omega \subset \mathbb{R}^d$ and react linearly $X_1 \leftrightharpoons X_2$, the evolution of their concentrations $c = (c_1, c_2)$ can be described by the linear reaction-diffusion system

$$\begin{aligned} \dot{c_1} &= \delta_1 \Delta c_1 - (\tilde{\alpha} c_1 - \tilde{\beta} c_2) \\ \dot{c_2} &= \delta_2 \Delta c_2 + (\tilde{\alpha} c_1 - \tilde{\beta} c_2) \end{aligned} \tag{1.1}$$

complemented with no-flux boundary conditions and initial conditions, where $\delta_1, \delta_2 > 0$ are diffusion coefficients for species X_1 and X_2, respectively, and $\tilde{\alpha}, \tilde{\beta} > 0$ are reaction rates describing the reaction speed of the linear reaction $X_1 \leftrightharpoons X_2$. The aim of the paper is to investigate system (1.1) if the reaction is much faster than the diffusion. To do this, we introduce a small parameter $\varepsilon > 0$ and assume that the reaction rates are given by $\tilde{\alpha} = \frac{1}{\varepsilon}\sqrt{\frac{\alpha}{\beta}}$, $\tilde{\beta} = \frac{1}{\varepsilon}\sqrt{\frac{\beta}{\alpha}}$. Then, the system (1.1) can be rewritten in an ε-dependent

*Research supported by DFG via SFB 1114 (project no.235221301, subproject C05).

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reaction-diffusion system

$$\begin{aligned}\dot{c_1^\varepsilon} &= \delta_1 \Delta c_1^\varepsilon - \frac{1}{\varepsilon}\left(\sqrt{\frac{\alpha}{\beta}}c_1^\varepsilon - \sqrt{\frac{\beta}{\alpha}}c_2^\varepsilon\right)\\ \dot{c_2^\varepsilon} &= \delta_2 \Delta c_2^\varepsilon + \frac{1}{\varepsilon}\left(\sqrt{\frac{\alpha}{\beta}}c_1^\varepsilon - \sqrt{\frac{\beta}{\alpha}}c_2^\varepsilon\right)\ .\end{aligned} \tag{1.2}$$

Reaction systems and reaction-diffusion systems with slow and fast time scales have attracted a lot of attention in the last years [Eva80, HvdHP00, Bot03, BoP10, BoP11, BPR12, MuN11, MiS20, DDJ20, MPS20, PeR20]. Bothe and Hilhorst proved a fast-reaction limit $\varepsilon \to 0$ for (1.2) in the following form.

Theorem 1.1 ([BoH02]). *Let $\Omega \subset \mathbb{R}^d$ be a domain with Lipschitz boundary. Let c_1^ε and c_2^ε be weak solutions of (1.2) with no-flux boundary conditions $\nabla c_i^\varepsilon \cdot \nu = 0$ on $\partial\Omega$. Then $c_1^\varepsilon \to c_1$ and $c_2^\varepsilon \to c_2$ in $\mathrm{L}^2([0,T]\times\Omega)$ as $\varepsilon \to 0$ and we have $\frac{c_1}{\beta} = \frac{c_2}{\alpha}$. Moreover, defining the coarse-grained concentration $\hat{c} = c_1 + c_2$, then $\hat{c}$ solves the diffusion equation $\dot{\hat{c}} = \hat{\delta}\Delta\hat{c}$ with a new mixed diffusion coefficient $\hat{\delta} = \frac{\beta\delta_1 + \alpha\delta_2}{\alpha+\beta}$.*

Essentially, the proof uses the free-energy as a Lyapunov function to derive ε-uniform bounds on the concentrations c_i^ε and their gradients ∇c_i^ε, which is then used to prove convergence towards the slow manifold $\{c \in [0,\infty[^2 \mid \alpha c_1 = \beta c_2\}$. This proof also works for nonlinear reactions once ε-uniform L^∞-estimates are established (see [BoH02]). On the linear slow manifold, one easily verifies that the coarse grained concentration $\hat{c} := \frac{\alpha+\beta}{\beta}c_1 = \frac{\alpha+\beta}{\alpha}c_2 = c_1 + c_2$ solves $\dot{\hat{c}} = \hat{\delta}\Delta\hat{c}$ where $\hat{\delta} = \frac{\beta\delta_1+\alpha\delta_2}{\alpha+\beta}$ is the effective mixed diffusion coefficient.

In this work, we are not primary interested in convergence of solutions of system (1.2). Instead, we perform the fast-reaction limit on the level of the underlying variational structure, which then implies convergence of solutions as a byproduct. Our starting point is that reaction-diffusion systems such as (1.2) can be written as a gradient flow equation induced by a gradient system $(Q, \mathcal{E}, \mathcal{R}_\varepsilon^*)$, where the state space Q is the space of probability measures $Q = \mathrm{Prob}(\Omega \times \{1,2\})$ and the driving functional is the free-energy $\mathcal{E}(\mu) = \int_\Omega \sum_{j=1}^2 E_B\left(\frac{c_j}{w_j}\right) w_j \mathrm{d}x$ for measures $\mu = c\ \mathrm{d}x$, with the Boltzmann function $E_B(r) = r\log r - r + 1$ and the (in general space dependent) stationary measure $w = (w_1, w_2)^{\mathrm{T}}$. The dissipation potential $\mathcal{R}_\varepsilon^*$ that determines the geometry of the underlying space is given by two parts $\mathcal{R}_\varepsilon^* = \mathcal{R}_{\mathrm{diff}}^* + \mathcal{R}_{\mathrm{react},\varepsilon}^*$ describing the diffusion and reaction separately. Since the pioneering work of Otto and coauthors [JKO98, Ott01] it is known that diffusion has to be understood as a gradient system driven by the free-energy in the space of probability measures equipped with the Wasserstein distance. The corresponding dissipation potential $\mathcal{R}_{\mathrm{diff}}^*$ is quadratic and given by

$$\mathcal{R}_{\mathrm{diff}}^*(\mu,\xi) = \frac{1}{2}\int_\Omega \sum_{i=1}^2 \delta_i \left|\nabla\xi_i\right|^2\ \mathrm{d}\mu_i.$$

Later Mielke [Mie11] proposed a quadratic gradient structure also for reaction-diffusion systems with the same driving functional. Geometric properties of that gradient structure were investigated in [LiM13, GK*20]. Here, we are not interested in that gradient structure, but use a different, the so-called *cosh-type gradient structure*, where the reaction part is given by

$$\mathcal{R}_{\mathrm{react},\varepsilon}^*(\mu,\xi) = \frac{1}{\varepsilon}\int_\Omega \mathsf{C}^*(\xi_1(x) - \xi_2(x))\ \sqrt{\mathrm{d}\mu_1 \mathrm{d}\mu_2},$$

with $\mathsf{C}^*(r) = 4(\cosh(r/2)-1)$. Setting $\mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\text{diff}} + \mathcal{R}^*_{\text{react},\varepsilon}$, the reaction-diffusion system (1.2) can now be written as a gradient flow equation

$$\dot\mu = \partial_\xi \mathcal{R}^*_\varepsilon(\mu, -\mathrm{D}\mathcal{E}(\mu)).$$

Although there are many gradient structures for (1.2) (see e.g. [MiS20, Sect. 4]) and the cosh-type gradient structure entails several technical difficulties as defining a nonlinear kinetic relation and not inducing metric on Q, it nevertheless has several significant features. Historically, it has its origin in [Mar15] where, following thermodynamic considerations, chemical reactions are written in exponential terms. In recent years, the cosh-gradient structure has been derived via a large-deviation principle [MPR14, MP*17], and it was shown that it is stable under limit processes [LM*17] that are similar to our approach. Moreover, it does not explicitly depend on the stationary measure w, which allows for an rigorous distinction between the energetic and dissipative part [MiS20]. This is physically reasonable because a change of the energy by an external field should not influence the geometric structure of the underlying space.

The goal of the paper is to construct an effective gradient system $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$ and perform the limit $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon) \to (Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$ as $\varepsilon \to 0$. For this, we use the notion of *convergence of gradient systems in the sense of the energy-dissipation principle*, shortly called *EDP-convergence*. EDP-convergence was introduced in [DFM19] and further developed in [MMP20, MiS20] and is based on the dissipation functional

$$\mathfrak{D}^\eta_\varepsilon(\mu) = \int_0^T \mathcal{R}_\varepsilon(\mu, \dot\mu) + \mathcal{R}^*_\varepsilon(\mu, \eta - \mathrm{D}\mathcal{E}(\mu))\,\mathrm{d}t$$

which, for solutions μ of the gradient flow equation describes the total dissipation between initial time $\mathcal{E}(\mu(0))$ and final time $\mathcal{E}(\mu(T))$, and can now be defined for general trajectories $\mu \in \mathrm{L}^1([0,T], Q)$. The notion of EDP-convergence with tilting requires Γ-convergences of the energies $\mathcal{E}_\varepsilon \overset{\Gamma}{\to} \mathcal{E}_0$ and of the dissipation functionals $\mathfrak{D}^\eta_\varepsilon \overset{\Gamma}{\to} \mathfrak{D}^\eta_0$ in suitable topologies, such that for all tilts η the limit $\mathfrak{D}^\eta_0$ has the form $\mathfrak{D}^\eta_0(\mu) = \int_0^T \mathcal{R}_{\text{eff}}(\mu, \dot\mu) + \mathcal{R}^*_{\text{eff}}(\mu, \eta - \mathrm{D}\mathcal{E}_0(\mu))\,\mathrm{d}t$, see Section 2.2 for a precise definition. Importantly, the effective dissipation potential $\mathcal{R}_{\text{eff}}$ in the Γ-limit is independent of the tilts, hence allowing for extended energies. In our situation, the tilts η correspond to an external potential $V = (V_1, V_2)$ added to the energy $\mathcal{E}$. On the level of the PDE, the starting reaction-diffusion system is extended to a reaction-drift-diffusion system of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \operatorname{div}\left(\begin{pmatrix} \delta_1 \nabla c_1 \\ \delta_2 \nabla c_2 \end{pmatrix} + \begin{pmatrix} \delta_1 c_1 \nabla V_1 \\ \delta_2 c_2 \nabla V_2 \end{pmatrix}\right) + \frac{1}{\varepsilon}\begin{pmatrix} -\sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & \sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \\ \sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & -\sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}.$$

The main result of the paper is Theorem 4.3 which asserts tilt EDP-convergence of $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$ to $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$ as $\varepsilon \to 0$ where the effective dissipation potential is given by

$$\mathcal{R}^*_{\text{eff}} = \mathcal{R}^*_{\text{diff}} + \chi_{\{\xi_1 = \xi_2\}},$$

where χ_A is the characteristic function of convex analysis taking values zero in A and infinity otherwise. The effective dissipation potential describes diffusion but restricts the chemical potential $\xi = (\xi_1, \xi_2)$ to a linear submanifold. The induced gradient flow equation of the gradient system $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$ is then given by a system of drift-diffusion

equations on a linear submanifold with a space and time dependent Lagrange multiplier λ

$$\begin{aligned} \dot{c_1} &= \operatorname{div}\left(\delta_1 \nabla c_1 + \delta_1 c_1 \nabla V_1\right) - \lambda \\ \dot{c_2} &= \operatorname{div}\left(\delta_2 \nabla c_2 + \delta_2 c_2 \nabla V_2\right) + \lambda \end{aligned} \quad , \quad \frac{c_1}{\beta \mathrm{e}^{-V_1}} = \frac{c_2}{\alpha \mathrm{e}^{-V_2}} \ .$$

Moreover, as an immediate consequence of Theorem 4.3, we obtain that the effective gradient flow equation can be equivalently described as a drift-diffusion equation of the coarse-grained concentration $\hat{c}$, see Proposition 4.5. Introducing the mixed diffusion coefficient $\hat{\delta}^V = \frac{\delta_1 \beta \mathrm{e}^{-V_1} + \delta_2 \alpha \mathrm{e}^{-V_2}}{\beta \mathrm{e}^{-V_1} + \alpha \mathrm{e}^{-V_2}}$ and the mixed potential $\hat{V} = -\log(\frac{\beta}{\alpha+\beta}\mathrm{e}^{-V_1} + \frac{\alpha}{\alpha+\beta}\mathrm{e}^{-V_2})$, we obtain

$$\hat{c} = \operatorname{div}\left(\hat{\delta}^V \nabla \hat{c} + \hat{\delta}^V \hat{c} \nabla \hat{V}\right),$$

which is in accordance with [BoH02] in the potential-free case $V = \text{const}$. Moreover, we obtain a natural coarse-grained gradient structure $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$, where $\hat{Q} = \mathrm{Prob}(\Omega)$ is the coarse-grained state space and $\hat{\mathcal{E}}, \hat{\mathcal{R}}^*$ are the coarse-grained energy functional and dissipation potential, respectively. Interestingly, this coarse-grained gradient structure $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$ contains the same information as the effective gradient structure $(Q, \mathcal{E}, \mathcal{R}^*_{\mathrm{eff}})$, although defined on a smaller state space, see Proposition 4.5.

The result on tilt EDP-convergence is an immediate consequence of the Γ-convergence result of the dissipation functional $\mathfrak{D}^\eta_\varepsilon$ (Theorem 5.12). The primal dissipation potential $\mathcal{R}_\varepsilon$ is given by an infimal sum consisting of diffusion fluxes and reaction fluxes coupled via a generalized continuity equation, see Section 3.3. Theorem 5.12 follows from the following observations: $\mathcal{R}^*_\varepsilon$ converges monotonically to a singular limit $\mathcal{R}^*_{\mathrm{eff}}$, the primal dissipation potentials $\mathcal{R}_\varepsilon$ degenerate. It is not possible to control the rates of $\dot{\mu}_1$ and $\dot{\mu}_2$ separately by $\mathcal{R}_\varepsilon$, since the reaction flux between both species may become unbounded. Instead, it is possible to prove compactness for the sum (or slow variable) $\mu_1 + \mu_2$ by $\mathcal{R}_\varepsilon$, and proving convergence towards the slow-manifold where an equilibration takes place, i.e. $\alpha c_1^\varepsilon - \beta c_2^\varepsilon \to 0$. The two pieces of complementary information provide strong convergence of the densities c^ε in $\mathrm{L}^1([0,T] \times \Omega)$. This procedure has been already successfully applied for linear and nonlinear reaction systems [MiS20, MPS20] and is here applied to a space-dependent evolution system. A posteriori we conclude that the limit measure μ^0 has indeed an absolutely continuous representative using results from [AGS05]. The construction of the recovery sequence relies on the fact that the limit dissipation functional can be equivalently written as a functional of coarse-grained variables. Only the reaction flux, which is present for positive $\varepsilon > 0$ and hidden for $\varepsilon = 0$, has to be reconstructed. One observes that diffusion causes the reaction flux on an infinitesimally small scale. Since the dissipation functional considers also fluctuations which may be not strictly positive and not smooth in contrast to the solution of the linear reaction diffusion system (1.2), the construction of a recovery sequence is completed by a suitable approximation argument.

Let us finally mention, that the same results can also be established for reaction-diffusion systems, where more than two species are involved. Applying the coarse-graining and reconstruction machinery as developed in [MiS20], a similar Γ-convergence result for the dissipation functional can be proved. For notational convenience we restrict to the two-species situation and briefly discuss the multi-species case in Section 6. We refer also to [Ste21], where coarse-graining and reconstruction for concentrations as well as the fluxes is developed.

2 Gradient structures

2.1 Gradient systems and the energy-dissipation principle

Let us briefly recall what we mean with a gradient system. Following [Mie16], we call a triple $(Q, \mathcal{E}, \mathcal{R})$ a *gradient system* if

(1) Q is a closed convex subset of a Banach space X

(2) $\mathcal{E} : Q \to \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ is a functional (such as the free energy)

(3) $\mathcal{R} : Q \times X \to \mathbb{R}_\infty$ is a dissipation potential, which means that for any $u \in Q$ the functional $\mathcal{R}(u, \cdot) : X \to \mathbb{R}_\infty$ is lower semicontinuous (lsc), nonnegative and convex, and it satisfies $\mathcal{R}(u, 0) = 0$.

We define the dual dissipation potential $\mathcal{R}^* : Q \times X^* \to [0, \infty]$ using the Legendre transform via

$$\mathcal{R}^*(u, \xi) = (\mathcal{R}(u, \cdot))^*(\xi) = \sup_{v \in X} \{\langle v, \xi\rangle - \mathcal{R}(u, v)\} \ .$$

The gradient system is uniquely described by $(Q, \mathcal{E}, \mathcal{R})$ or, equivalently by $(Q, \mathcal{E}, \mathcal{R}^*)$ and, in particular, in this paper we use the second representation.

The dynamics of a gradient system can be formulated in different ways as an equation in X, in $\mathbb{R}$ or in X^* (the dual Banach space of X), respectively:

(1) **Force balance in X^*:** $0 \in \partial_{\dot u} \mathcal{R}(u, \dot u) + \mathrm{D}\mathcal{E}(u) \in X^*$,

(2) **Power balance in $\mathbb{R}$:** $\mathcal{R}(u, \dot u) + \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u)) = -\langle \mathrm{D}\mathcal{E}(u), \dot u\rangle$,

(3) **Rate equation in X:** $\dot u \in \partial_\xi \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u)) \in X$.

(Here, ∂ denotes the subdifferential of convex analysis.) Equations (1) and (3) are called *gradient flow equation* associated with $(Q, \mathcal{E}, \mathcal{R}^*)$. The equivalent formulations rely on the following fact: Let X be a reflexive Banach space and $\Psi : X \to \mathbb{R}_\infty$ be a proper, convex and lsc. Then for every $\xi \in X^*$ and $v \in X$ the following five statements, the so-called *Legendre-Fenchel-equivalences*, are equivalent:

$$\begin{array}{ccccc} v \in \mathrm{Argmin}_{w\in X}(\Psi(w) - \langle \xi, w\rangle) & & \Leftrightarrow & & \Psi(v) + \Psi^*(\xi) = \langle \xi, v\rangle \\ \Leftrightarrow & & & & \Leftrightarrow \\ v \in \partial\Psi^*(\xi) & & \Psi(v) + \Psi^*(\xi) = \langle \xi, v\rangle & & \xi \in \mathrm{Argmin}_{\eta\in X^*}(\Psi^*(\eta) - \langle \eta, v\rangle) \\ & & \Leftrightarrow & & \end{array}$$

Especially the second dynamic formulation, the power balance (2), is interesting for us. Integrating the power balance (2) in time form 0 to T and using the chain rule for the time-derivative of $t \mapsto \mathcal{E}(u(t))$, we get another equivalent formulation of the dynamics of the gradient system, which is called *Energy-Dissipation-Balance*:

$$\text{(EDB)} \qquad \mathcal{E}(u(T)) + \int_0^T [\mathcal{R}(u, \dot u) + \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u))]\,\mathrm{d}t = \mathcal{E}(u(0)). \tag{2.1}$$

Equation (EDB) compares the energy of the system at time $t = 0$ and at time $t = T$, the difference is described by the total dissipation from $t = 0$ to $t = T$. This gives rise to another definition: We define the *De Giorgi dissipation functional* as

$$\mathfrak{D}(u) = \int_0^T [\mathcal{R}(u, \dot u) + \mathcal{R}^*(u, -\mathrm{D}\mathcal{E}(u))]\,\mathrm{d}t,$$

for $u \in \mathrm{W}^{1,1}([0,T],Q)$ and extend it to infinity otherwise. The following *energy-dissipation principle* provides the definition for solutions of the gradient flow equation, see e.g. [AGS05, Prop. 1.4.1], [AM*12, Def. 1.1], [MMP20, Thm 2.5].

Definition 2.1. We say $u \in \mathrm{W}^{1,1}([0,T],Q)$ is a solution of the gradient flow equation (1) or (3) induced by the gradient system $(Q,\mathcal{E},\mathcal{R}^*)$, if $\mathcal{E}(u(0)) < \infty$ and the energy-dissipation balance holds.

2.2 Definition of EDP-convergence

The definition of EDP-convergence for gradient systems relies on the notion of Γ-convergence for functionals (cf. [Dal93]). If Y is a Banach space and $I_\varepsilon : Y \to \mathbb{R}_\infty$ we write $I_\varepsilon \xrightarrow{\Gamma} I_0$ and $I_\varepsilon \xrightarrow{\Gamma^-} I_0$ for Γ-convergence in the strong and weak topology, respectively. If both holds this is called Mosco-convergence and written as $I_\varepsilon \xrightarrow{\mathrm{M}} I_0$.

For families of gradient systems $(X,\mathcal{E}_\varepsilon,\mathcal{R}_\varepsilon)$, three different levels of EDP-convergence are introduced and discussed in [DFM19, MMP20], called simple EDP-convergence, EDP-convergence with tilting and contact EDP-convergence with tilting. EDP-convergence with tilting is the strongest notion, since it implies the other two notions. Here we will only use the first two notions. For all three notions the choice of weak or strong topology is still to be decided according to the specific problem.

Definition 2.2 (Simple EDP-convergence)**.** A family of gradient structures $(Q,\mathcal{E}_\varepsilon,\mathcal{R}_\varepsilon)$ is said to *EDP-converge* to the gradient system $(Q,\mathcal{E}_0,\mathcal{R}_{\mathrm{eff}})$ if the following conditions hold:

1. $\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_0$ on $Q \subset X$;
2. $\mathfrak{D}_\varepsilon$ strongly Γ-converges to $\mathfrak{D}_0$ on $\mathrm{L}^1([0,T],Q)$ conditioned to bounded energies (we write $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma_{\mathrm{E}}} \mathfrak{D}_0$), i.e. we
   (a) (Liminf-estimate) For all strongly converging families $u_\varepsilon \to u$ in $\mathrm{L}^1([0,T],Q)$ which satisfy $\sup_{\varepsilon>0} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}_\varepsilon(u_\varepsilon(t)) < \infty$, we have $\liminf_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(u_\varepsilon) \geq \mathfrak{D}_0(u)$,
   (b) (Limsup-estimate) For all $\widetilde{u} \in \mathrm{L}^1([0,T],Q)$ there exists a strongly converging family $u_\varepsilon \to \widetilde{u}$ in $\mathrm{L}^1([0,T],Q)$ with $\sup_{\varepsilon>0} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}_\varepsilon(\widetilde{u}_\varepsilon(t)) < \infty$ such that we have $\limsup_{\varepsilon\to 0^+} \mathfrak{D}_\varepsilon(u_\varepsilon) \leq \mathfrak{D}_0(\widetilde{u})$.
3. There is an effective dissipation potential $\mathcal{R}_{\mathrm{eff}} : Q \times X \to \mathbb{R}_\infty$ such that $\mathfrak{D}_0$ takes the form of a dual sum, namely $\mathfrak{D}_0(u) = \int_0^T \{\mathcal{R}_{\mathrm{eff}}(u,\dot{u}) + \mathcal{R}^*_{\mathrm{eff}}(u,-\mathrm{D}\mathcal{E}_{\mathrm{eff}}(u))\}\mathrm{d}t$.

Similarly, one can also use weak Γ- or Mosco-convergence conditioned to bounded energy, which we will then write as $\mathfrak{D}_\varepsilon \xrightarrow{\Gamma_{\mathrm{E}}} \mathfrak{D}_0$ and $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}_{\mathrm{E}}} \mathfrak{D}_0$. In fact, for our fast-slow reaction systems we are going to prove $\mathfrak{D}_\varepsilon \xrightarrow{\mathrm{M}_{\mathrm{E}}} \mathfrak{D}_0$.

A general feature of EDP-convergence is that, under suitable conditions, solutions u of the gradient flow equation $\dot{u} = \partial_\xi \mathcal{R}^*_{\mathrm{eff}}(u,-\mathrm{D}\mathcal{E}_0(u))$ of the effective gradient system $(X,\mathcal{E}_0,\mathcal{R}_{\mathrm{eff}})$ are indeed limits of solutions u^ε of the gradient flow equation $\dot{u} = \partial_\xi \mathcal{R}^*_\varepsilon(u,-\mathrm{D}\mathcal{E}_\varepsilon(u))$, see e.g. [Bra14, Thm. 11.3], [MiS20, Lem. 3.4] and [MMP20, Lem. 2.8].

A strengthening of simple EDP-convergence is the so-called *EDP-convergence with tilting*. This notion involves the tilted energy functionals $\mathcal{E}_\varepsilon^\eta : Q \ni u \mapsto \mathcal{E}_\varepsilon(u) - \langle \eta, u\rangle$, where the tilt η (also called *external loading*) varies through the whole dual space X^*.

Definition 2.3 (EDP-convergence with tilting (cf. [MMP20, Def. 2. 14])**.** A family of gradient structures $(Q, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$ is said to *EDP-converge with tilting* to the gradient system $(Q, \mathcal{E}_0, \mathcal{R}_{\text{eff}})$, if for all tilts $\eta \in X^*$ we have $(Q, \mathcal{E}_\varepsilon^\eta, \mathcal{R}_\varepsilon)$ EDP-converges to $(Q, \mathcal{E}_\varepsilon^\eta, \mathcal{R}_{\text{eff}})$.

Clearly, we have that $\mathcal{E}_\varepsilon \overset{\Gamma}{\to} \mathcal{E}_0$ implies $\mathcal{E}_\varepsilon^\eta \overset{\Gamma}{\to} \mathcal{E}_0^\eta$ for all $\eta \in X^*$ (and similarly for weak Γ-convergence), since the linear tilt $u \mapsto -\langle \eta, u\rangle$ is weakly continuous. The main and nontrivial assumption is that additionally

$$\mathfrak{D}_\varepsilon^\eta : u \mapsto \int_0^T \big\{\mathcal{R}_\varepsilon(u, \dot u) + \mathcal{R}_\varepsilon^*(u, \eta - \mathrm{D}\mathcal{E}_\varepsilon(u))\big\}\mathrm{d}t$$

Γ-converges in $\mathrm{L}^1([0,T], Q)$ to $\mathfrak{D}_0^\eta$ for all $\eta \in X^*$ and that this limit $\mathfrak{D}_0^\eta$ is given in $\mathcal{R} \oplus \mathcal{R}^*$-form with $\mathcal{R}_{\text{eff}}$ via

$$\mathfrak{D}_0^\eta(u) = \int_0^T \big\{\mathcal{R}_{\text{eff}}(u, \dot u) + \mathcal{R}_{\text{eff}}^*(u, \eta - \mathrm{D}\mathcal{E}_{\text{eff}}(u))\big\}\mathrm{d}t.$$

The main point is that $\mathcal{R}_{\text{eff}}$ remains independent of $\eta \in X^*$. We refer to [MMP20] for a discussion of this and the other two notions of EDP-convergence.

3 Gradient system of reaction-diffusion systems

In this section, we present the gradient system $(Q, \mathcal{E}, \mathcal{R}_\varepsilon^*)$, which induces the reaction-diffusion system (1.2). In Section 3.2 we derive the gradient flow equation of the gradient system including general tilts of the energy. In Section 3.3 we compute the primal dissipation potential $\mathcal{R}_\varepsilon$, which is only implicitly given via a infimal-convolution, and the total dissipation functional $\mathfrak{D}_\varepsilon^\eta$, which will be the main object of interest in Section 4. In Section 3, the computations are basically formal; the precise functional analytic setting is presented in Section 4 which also includes the Γ-convergence and EDP-convergence result.

3.1 Gradient structure for the linear reaction system

Although a gradient system induces a unique gradient flow equation, a general evolution equation can often be described by many different gradient systems. The choice of the gradient structure is a question of modeling since it adds thermodynamic information to the system, which is not inherent in the evolution equation itself. Here, we follow the pioneering work of Otto and coauthors [JKO98, Ott01] who showed that certain diffusion type equations can be understood as a gradient flow equation of the free energy in the space of probability measures equipped with the Wasserstein distance. Later Mielke proposed a gradient structure for a reaction diffusion system satisfying detailed balance [Mie11]. For a system with two species with a reversible reaction detailed balance is always satisfied. For the reaction part, we use the gradient structure which has been derived via a large-deviation principle from a microscopic Markov process in [MPR14]. We refer also to [Ren18], where our choice of gradient structure has been formally derived.

The gradient system $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$ is defined as follows: The state space is the space of probability measure on $Q \times \{1,2\}$

$$Q := \mathrm{Prob}(\Omega \times \{1,2\}) = \{\mu = (\mu_1, \mu_2) \in \mathbb{R}^2 : \mu_i \in \mathcal{M}(\Omega),\ \mu_i \geq 0,\ \sum_{i=1}^2 \mu_i(\Omega) = 1\},$$

where we assume that $\Omega \subset \mathbb{R}^d$ is a compact domain with normalized mass $|\Omega| = 1$. The driving energy functional $\mathcal{E} : Q \to \mathbb{R}_\infty := \mathbb{R} \cup \{\infty\}$ is the free-energy of the reaction-diffusion system. It is finite for measures $\mu = (\mu_1, \mu_2)$ with Lebesgue density $c = (c_1, c_2)$ only and has the form

$$\mathcal{E}(\mu) := \begin{cases} \int_\Omega \sum_{j=1}^2 E_B\left(\frac{c_j}{w_j}\right) w_j \mathrm{d}x, & \text{if } \mu = c \cdot \mathrm{d}x \\ \infty, & \text{otherwise.} \end{cases} \tag{3.1}$$

where the Boltzmann function is defined as $E_B(r) = r \log r - r + 1$ and the positive stationary measure is given by $w = \frac{1}{\alpha+\beta}(\beta, \alpha)^{\mathrm{T}}$. Note that the stationary measure w as well as the energy $\mathcal{E}$ is ε-independent. The derivative of the energy $\mathcal{E}$ is only defined in its domain, i.e. for measures with Lebesgue density c, and has the form

$$\mathrm{D}\mathcal{E}(\mu) = \sum_{j=1}^2 (\log c_j - \log w_j) = \sum_{j=1}^2 \left(\log \frac{c_j}{w_j}\right) .$$

As the equation splits into a diffusion and reaction part, so does the dual dissipation functional. We define

$$\mathcal{R}^*_\varepsilon(\mu, \xi) := \mathcal{R}^*_{\mathrm{diff}}(\mu, \xi) + \mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu, \xi)$$

where

$$\mathcal{R}^*_{\mathrm{diff}}(\mu, \xi) := \frac{1}{2} \int_\Omega \sum_{j=1}^2 \delta_j |\nabla \xi_j(x)|^2 \mathrm{d}\mu_j,$$
$$\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu, \xi) := \frac{1}{\varepsilon} \int_\Omega \mathsf{C}^*(\xi_1(x) - \xi_2(x))\ \mathrm{d}\sqrt{\mu_1\mu_2},$$

where we use the cosh-function $\mathsf{C}^*(x) = 4\,(\cosh(x/2) - 1)$ and for measures μ with Lebesgue density c we have $\mathrm{d}\sqrt{\mu_1\mu_2} := \sqrt{c_1 c_2}\mathrm{d}x$.

The diffusion part $\mathcal{R}^*_{\mathrm{diff}}$ induces the Wasserstein distance on Q. The ε-dependent reaction part $\mathcal{R}^*_{\mathrm{react},\varepsilon}$ forces the evolution close to a linear submanifold given by

$$\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu, -\mathrm{D}\mathcal{E}(\mu)) = 0 \Leftrightarrow \alpha c_1 - \beta c_2 = 0\,.$$

Note, that since $\mathcal{R}^*_{\mathrm{react},\varepsilon}$ is not 2-homogeneous, it does not define a metric on Q. We refer to [PR*20] which treats similar and general dissipation potentials and understands them as generalized transport costs on discrete spaces. Note that $\mathcal{R}^*_\varepsilon$ does not depend on the stationary measure w explicitly, as highlighted in [MiS20].

3.2 The tilted gradient flow equation

In this section, we derive the gradient flow equation of the gradient system $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$. To exploit the full information of the dissipation potential, we consider general tilted energies. First, we present how a change of energy by a linear tilt corresponds to a change of stationary measure, and secondly, we compute the induced gradient flow equation.

Let us first consider two free energies (3.1) with different stationary measures $w, \widetilde{w}$, which may be space dependent but are assumed to be positive. Assuming a density $\mu = c\,\mathrm{d}x$ and using $\sum_i \int_\Omega w_i \mathrm{d}x = \sum_i \int_\Omega c_i \mathrm{d}x = 1$ (where we used $|\Omega| = 1$), we have

$$\mathcal{E}(\mu) = \sum_{i=1}^2 \int_\Omega E_B\left(\frac{c_i}{w_i}\right) w_i \mathrm{d}x = \sum_{i=1}^2 \int_\Omega \{c_i \log c_i - c_i \log w_i\}\,\mathrm{d}x.$$

In particular, we conclude that $\widetilde{\mathcal{E}}(\mu) + \sum_{i=1}^2 \int_\Omega c_i \log \widetilde{w}_i \mathrm{d}x = \mathcal{E}(\mu) + \sum_{i=1}^2 \int_\Omega c_i \log w_i \mathrm{d}x$ which implies

$$\widetilde{\mathcal{E}}(\mu) = \mathcal{E}(\mu) + \sum_{i=1}^2 \int_\Omega c_i \log\left(\frac{w_i}{\widetilde{w}_i}\right)\mathrm{d}x.$$

Hence, changing the underlying stationary measure corresponds to a linear tilt of the energy by a two component potential $V = (V_1, V_2)$ where $V_i = \log\left(\frac{w_i}{\widetilde{w}_i}\right)$. On the other hand, a tilted energy has a different stationary measure as its minimum. To compute the new stationary measure, we introduce tilted energies

$$\mathcal{E}^V(\mu) := \mathcal{E}(\mu) + \sum_{i=1}^2 \int_\Omega V_i \mathrm{d}\mu_i,$$

where $V \in \mathrm{C}^1(\Omega, \mathbb{R}^2)$ is a two component smooth potential. Moreover, we introduce $\eta_i := \mathrm{e}^{-V_i}$ and clearly, we have $\eta_i > 0$ on $\Omega \subset \mathbb{R}^d$. We compute the stationary state w^V by minimizing $\mathcal{E}^V$ on the space $Q = \mathrm{Prob}(\Omega \times \{1,2\})$. We obtain the space dependent stationary measure

$$w_i^V = \frac{1}{Z} w_i \mathrm{e}^{-V_i}, \text{ where } Z := \sum_{i=1}^2 \int_\Omega w_i \mathrm{e}^{-V_i}\mathrm{d}x\ . \tag{3.2}$$

Next, we compute the tilted gradient flow equation $\dot{c} = \partial_\xi \mathcal{R}^*_\varepsilon(\mu, -\mathrm{D}\mathcal{E}^V(\mu))$, which is induced by the gradient system $(Q, \mathcal{E}^V, \mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\mathrm{diff}} + \mathcal{R}^*_{\mathrm{react},\varepsilon})$. First, we observe that $\mathcal{E}(\mu) < \infty$ if and only if $\mathcal{E}^V(\mu) < \infty$. Inserting $\xi_i = \left(-\mathrm{D}\mathcal{E}^V(\mu)\right)_i$ into $\partial_\xi \mathcal{R}^*_{\mathrm{diff},\varepsilon}(\mu, \xi)$, we see that

$$\partial_\xi \mathcal{R}^*_{\mathrm{diff}}(\mu, \cdot)|_{\xi = -\mathrm{D}\mathcal{E}^V(\mu)} = -(\mathrm{div}(\delta_i c_i \nabla(-\log(c_i/w_i) - V_i))_{i=1,2} = \mathrm{div}\left(\delta_i \nabla c_i + \delta_i c_i \nabla V_i\right)_{i=1,2},$$

which is a system of two uncoupled drift-diffusion equations or Fokker-Planck equations for the concentrations c_i where the fluxes are given by a diffusion part $-\delta_i \nabla c_i$ and a drift part $-\delta_i c_i \nabla V_i$.

For the reaction part of the dual dissipation potential, we insert $\xi_i = \left(-\mathrm{D}\mathcal{E}^V(\mu)\right)_i$ into $\partial_\xi \mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu, -\mathrm{D}\mathcal{E}^V(\mu))$. On readily verifies the identity $(\mathsf{C}^*)'(\log p - \log q) = \frac{p-q}{\sqrt{pq}}$ for the cosh-function and conclude

$$\sqrt{c_1 c_2}\,(\mathsf{C}^*)'(\xi_1(x) - \xi_2(x))|_{\xi = -\mathrm{D}\mathcal{E}^V(\mu)} = \sqrt{c_1 c_1}\frac{\frac{c_2}{w_2\eta_2} - \frac{c_1}{w_1\eta_1}}{\sqrt{\frac{c_1}{w_1\eta_1}\frac{c_2}{w_2\eta_2}}} = \sqrt{w_1\eta_1 w_2\eta_2}\left(\frac{c_2}{w_2\eta_2} - \frac{c_1}{w_1\eta_1}\right).$$

Hence, we get

$$\partial_{\xi_1}\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu,\cdot)|_{\xi=-\mathrm{D}\mathcal{E}^V(\mu)} = -\partial_{\xi_2}\mathcal{R}^*_{\mathrm{react}}(\mu,\cdot)|_{\xi=-\mathrm{D}\mathcal{E}^V(\mu)} = \frac{1}{\varepsilon}\left(\sqrt{\frac{\beta}{\alpha}}\sqrt{\frac{\eta_1}{\eta_2}}c_2 - \sqrt{\frac{\alpha}{\beta}}\sqrt{\frac{\eta_2}{\eta_1}}c_1\right),$$

which is linear in $c=(c_1,c_2)$. In vector notation, we get a tilted Markov generator of the form

$$\partial_\xi\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu,-\mathrm{D}\mathcal{E}^V(\mu)) = \frac{1}{\varepsilon}\begin{pmatrix} -\sqrt{\frac{\alpha}{\beta}\frac{\eta_2}{\eta_1}} & \sqrt{\frac{\beta}{\alpha}\frac{\eta_1}{\eta_2}} \\ \sqrt{\frac{\alpha}{\beta}\frac{\eta_2}{\eta_1}} & -\sqrt{\frac{\beta}{\alpha}\frac{\eta_1}{\eta_2}}\end{pmatrix} c = \frac{1}{\varepsilon}\begin{pmatrix} -\sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & \sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \\ \sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & -\sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}}\end{pmatrix} c$$

which has the space dependent stationary measure

$$w^V = \frac{1}{Z(\alpha+\beta)}(\beta\eta^1,\alpha\eta^2)^{\mathrm{T}} = \frac{1}{Z}(w_1\mathrm{e}^{-V_1},w_2\mathrm{e}^{-V_2})^{\mathrm{T}}.$$

Summarizing, the tilted evolution equation has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}c_1\\c_2\end{pmatrix} = \mathrm{div}\left(\begin{pmatrix}\delta_1\nabla c_1\\ \delta_2\nabla c_2\end{pmatrix} + \begin{pmatrix}\delta_1 c_1\nabla V_1\\ \delta_2 c_2\nabla V_2\end{pmatrix}\right) + \frac{1}{\varepsilon}\begin{pmatrix} -\sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & \sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}} \\ \sqrt{\frac{\alpha}{\beta}}\mathrm{e}^{\frac{V_1-V_2}{2}} & -\sqrt{\frac{\beta}{\alpha}}\mathrm{e}^{\frac{V_2-V_1}{2}}\end{pmatrix}\begin{pmatrix}c_1\\c_2\end{pmatrix}, \tag{3.3}$$

which is a linear reaction-drift-diffusion system with space dependent reaction rates. In the special case without external forcing $V=\mathrm{const}$, we get the linear reaction diffusion system (1.2). Note that the reaction part still inherits symmetry since the product of the off-diagonal elements is constant in space. In particular, not all general linear reaction-drift-diffusion system with space dependent reaction rates for two species can be expressed in the form (3.3) and are induced by the gradient system $(Q,\mathcal{E}^V,\mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\mathrm{diff}}+\mathcal{R}^*_{\mathrm{react},\varepsilon})$.

3.3 The dissipation functional

In this section, we compute the dissipation functional $\mathfrak{D}_\varepsilon$, which consists of two parts: the velocity part given by the primal dissipation potential $\mathcal{R}_\varepsilon$ and the slope-part (sometimes also called *Fisher information*) $\mathcal{R}^*_\varepsilon(\mu,-\mathrm{D}\mathcal{E}(\mu))$. Here, all computations are formal and we always assume that the measure μ has a Lebesgue density c. The precise functional analytic setting is presented in the Section 4.

The primal dissipation potential $\mathcal{R}_\varepsilon$, given by the Legendre transform of the dual dissipation potential $\mathcal{R}^*_\varepsilon = \mathcal{R}^*_{\mathrm{diff}}+\mathcal{R}^*_{\varepsilon,\mathrm{react}}$, can be computed via inf-convolution of $\mathcal{R}_{\mathrm{diff}}$ and $\mathcal{R}_{\mathrm{react},\varepsilon}$. First, we compute both primal dissipation potentials separately. To do this, we introduce the following notation: For a convex, lsc. function $\mathsf{F}: X\to[0,\infty]$ on a reflexive and separable Banach space X with Legendre dual F^*, we define the function $\widetilde{\mathsf{F}}:[0,\infty[\times X\to[0,\infty]$ by

$$\widetilde{\mathsf{F}}(a,x) := (a\,\mathsf{F}^*(\cdot))^*(x) = \begin{cases} a\,\mathsf{F}\left(\frac{1}{a}\,x\right) & \text{for } a>0\,,\\ \chi_0(x) & \text{for } a=0\,.\end{cases}$$

Introducing the quadratic function $\mathsf{Q}(x)=\frac{1}{2}|x|^2$ on $\mathbb{R}^d$, the primal dissipation potential of the diffusion part $\mathcal{R}^*_{\mathrm{diff}}$ is given by

$$\mathcal{R}_{\mathrm{diff}}(\mu, v) = \sum_{j=1}^{2} \int_\Omega \widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right) \mathrm{d}x,$$

where J_j is, by definition, the unique solution of the elliptic equation $v_j + \mathrm{div} J_j = 0$ with $J \cdot \nu = 0$ on $\partial\Omega$. For positive c_j, we have $\widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right) = \frac{1}{2}\frac{|J_j|^2}{\delta_j c_j}$.

The primal dissipation potential of the reaction part is

$$\mathcal{R}_{\mathrm{react},\varepsilon}(\mu, b) = \begin{cases} \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1 c_2}}{\varepsilon}, b_2\right) \mathrm{d}x, & \text{for } b_1 + b_2 = 0 \\ \infty & \text{for } b_1 + b_2 \neq 0 \end{cases},$$

where $\mathsf{C} = (\mathsf{C}^*)^*$ is the Legendre transform of the cosh-function $\mathsf{C}^*(x) = 4\left(\cosh(x/2) - 1\right)$. In the following, we use the inequality

$$\frac{1}{2}|r| \cdot \log(|r| + 1) \leq \mathsf{C}(r) \leq 2|r| \cdot \log(|r| + 1), \tag{3.4}$$

which, in particular, implies that the Orlicz class for $A \subset \mathbb{R}^d$ given by

$$\widetilde{\mathrm{L}}^{\mathsf{C}}(A) := \{u \in \mathrm{L}^1(A) : \int_A \mathsf{C}(u)\mathrm{d}x < \infty\},$$

is, in fact, a Banach space $\widetilde{\mathrm{L}}^{\mathsf{C}}(A) = \mathrm{L}^{\mathsf{C}}(A)$ with the norm $\|u\|_{\mathsf{C}} = \sup_{\int_A \mathsf{C}^*(v) \leq 1} \left|\int_A uv \ \mathrm{d}x\right|$.

Importantly, functions $\widetilde{\mathsf{Q}}$, $\widetilde{\mathsf{C}}$ as well as the functionals $\mathcal{R}_{\mathrm{diff}}, \mathcal{R}_{\mathrm{react},\varepsilon}$ are convex on their domain of definition.

The primal dissipation potential $\mathcal{R}_\varepsilon$ is the inf-convolution of $\mathcal{R}_{\mathrm{diff}}$ and $\mathcal{R}_{\mathrm{react},\varepsilon}$, and is given by

$$\begin{aligned} &\mathcal{R}_\varepsilon(\mu, v) = \inf_{v = u_1 + u_2} \left\{\mathcal{R}_{\mathrm{diff}}(\mu, u_1) + \mathcal{R}_{\mathrm{react},\varepsilon}(\mu, u_2)\right\} \\ &= \inf_{J,b} \left\{ \sum_{j=1}^{2} \int_\Omega \widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right) \mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\tfrac{\sqrt{c_1 c_2}}{\varepsilon}, b_2(x)\right) \mathrm{d}x : \left\{ \begin{array}{c} v_1 = -\mathrm{div} J_1 + b_1 \\ v_2 = -\mathrm{div} J_2 + b_2 \\ b_1 + b_2 = 0 \end{array} \right\} \right\}. \end{aligned}$$

In time-integrated form we get for $v = \dot{\mu}$ that

$$\begin{aligned} &\int_0^T \mathcal{R}_\varepsilon(\mu, \dot{\mu}) \ \mathrm{d}t = \inf_{v = v_1 + v_2} \int_0^T \left\{\mathcal{R}_{\mathrm{diff}}(\mu, v_1) + \mathcal{R}_{\mathrm{react},\varepsilon}(\mu, v_2)\right\} \mathrm{d}t \\ &= \inf_{J,b} \left\{ \int_0^T \left\{ \sum_{j=1}^{2} \int_\Omega \widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right) \mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\tfrac{\sqrt{c_1 c_2}}{\varepsilon}, b_2(x)\right) \right\} \mathrm{d}x \ \mathrm{d}t : \ (c, J, b) \in (\mathrm{gCE}) \right\}. \end{aligned}$$

where we introduce the notation of a (linear) generalized continuity equation

$$(c, J, b) \in (\mathrm{gCE}) \quad \Leftrightarrow \quad \left\{ b_1 + b_2 = 0 \text{ and } \left\{ \begin{array}{c} \dot{c}_1 = -\mathrm{div} J_1 + b_1 \\ \dot{c}_2 = -\mathrm{div} J_2 + b_2 \end{array} \right\} \right\}.$$

Without the reaction part, $\int_0^T \mathcal{R}_\varepsilon \mathrm{d}t$ is the dynamic formulation à la Benamou-Brenier of the Wasserstein distance in Q [BeB00], which can be equivalently written in the form

$$\mathcal{W}_2(\mu_0, \mu_1)^2 = \inf \left\{ \int_0^1 \int_\Omega \sum_{j=1}^{2} \delta_j |v_j|^2 \mathrm{d}\mu_j : \dot{\mu}_j + \mathrm{div}(\mu_j v_j) = 0, \ \mu_{j,0} = \mu_0, \ \mu_{j,1} = \mu_1 \right\}$$

expressed in terms of transport velocities $v_j = J_j/c_j$. The Wasserstein distance can be interpreted as a cost in transporting mass from one measure μ_0 to μ_1. In our situation $\int_0^T \mathcal{R}_\varepsilon \mathrm{d}t$ is jointly convex in c, J and b and corresponds to modified cost function which also takes the reaction fluxes into account. The optimal diffusion fluxes J_j and reaction fluxes b_j have to satisfy the generalized continuity equation. Note that $\int_0^T \mathcal{R}_\varepsilon \mathrm{d}t$ does not induce a metric on Q since the reaction part is not quadratic.

Next, we compute the tilted slope part $\mathcal{R}_\varepsilon^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu))$. To do this, we introduce the relative densities ρ^V of μ w.r.t. the stationary measure $w^V \mathrm{d}x$, i.e. $\rho_j^V = \frac{\mathrm{d}\mu}{w_j^V \mathrm{d}x} = \frac{c_j}{w_j^V}$, where by (3.2) the stationary measure is $w_j^V = \frac{1}{Z} w_i \mathrm{e}^{-V_j}$. Since $V \in \mathrm{C}^1(\Omega, \mathbb{R}^2)$ and $\Omega \subset \mathbb{R}^d$ is compact, μ is absolutely continuous w.r.t. the Lebesgue measure $\mathrm{d}x$ if and only if it is w.r.t. the stationary measure $w^V \mathrm{d}x$, . Inserting $\xi = -\mathrm{D}\mathcal{E}^V(\mu) = -(\log(c_i/w_i)+V_i)_{i=1,2}$ in the dual dissipation potential $\mathcal{R}_\varepsilon^*$, we get for the diffusive part

$$\mathcal{R}_{\mathrm{diff}}^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu)) = \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j c_j |\nabla \left(\log c_j/w_j + V_j\right)|^2 \mathrm{d}x.$$

Using $w_j^V = \frac{1}{Z} w_j \mathrm{e}^{-V_j}$, a short calculation shows $\delta_j c_j \left|\nabla \left(\log c_j/w_j + V_j\right)\right|^2 = \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V}$. Hence, we have

$$\mathcal{R}_{\mathrm{diff}}^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu)) = \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V} \mathrm{d}x.$$

For the reaction part, we use the identity $\mathsf{C}^*(\log p - \log q) = 2\frac{\left(\sqrt{p}-\sqrt{q}\right)^2}{\sqrt{pq}}$ and get

$$\begin{aligned}\mathcal{R}_{\mathrm{react},\varepsilon}^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu)) &= 2\int_\Omega \frac{1}{\varepsilon}\sqrt{c_1 c_2}\frac{\left(\sqrt{c_1/\eta_1 w_1} - \sqrt{c_2/\eta_2 w_2}\right)^2}{\sqrt{c_1 c_2/\eta_1 w_1 \eta_2 w_2}}\mathrm{d}x \\ &= \frac{2}{\varepsilon}\int_\Omega \sqrt{w_1^V w_2^V}\left(\sqrt{\rho_1^V} - \sqrt{\rho_2^V}\right)^2 \mathrm{d}x.\end{aligned}$$

Summarizing, the total dissipation functional is

$$\begin{aligned}\mathfrak{D}_\varepsilon^V(\mu) &= \int_0^T \mathcal{R}_\varepsilon(\mu, \dot\mu) + \mathcal{R}_\varepsilon^*(\mu, -V - \mathrm{D}\mathcal{E}(\mu))\mathrm{d}t \qquad (3.5)\\ &= \inf_{(c,J,b)\in(\mathrm{gCE})}\left\{\int_0^T\left\{\int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right)\mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1 c_2}}{\varepsilon}, b_2(x)\right)\mathrm{d}x\right\}\mathrm{d}t\right\} + \\ &\quad + \int_0^T\left\{\frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V}\mathrm{d}x + \frac{2}{\varepsilon}\int_\Omega \sqrt{w_1^V w_2^V}\left(\sqrt{\rho_1^V} - \sqrt{\rho_2^V}\right)^2 \mathrm{d}x\right\}\mathrm{d}t\,.\end{aligned}$$

4 EDP-convergence result

In this section we state the EDP-convergence result for the gradient systems $(Q, \mathcal{E}, \mathcal{R}_\varepsilon^*)$ to $(Q, \mathcal{E}, \mathcal{R}_{\mathrm{eff}}^*)$ and discuss the properties of the effective gradient system $(Q, \mathcal{E}, \mathcal{R}_{\mathrm{eff}}^*)$. Since the energy $\mathcal{E}$ is ε-independent the major challenge is to prove Γ-convergence of the dissipation functional $\mathfrak{D}_\varepsilon^V$, which is a functional defined on the space of trajectories

in the state space Q. To be mathematical precise, we first fix the functional analytic setting.

The state space $Q = \mathrm{Prob}(\Omega \times \{1,2\})$ is equipped with the p-Wasserstein distance $d_{\mathcal{W}_p}$, where in our situation either $p = 1$ or $p = 2$. Recall that for any compact euclidean subspace $E \subset \mathbb{R}^k$ the p-Wasserstein distance is defined on the space of probability measures $\mathrm{Prob}(E)$ by

$$d_{\mathcal{W}_p}(\mu^1, \mu^2)^p = \min_{\gamma \in \Gamma(\mu^1, \mu^2)} \int_E |x - y|^p \mathrm{d}\gamma(x, y),$$

where $\Gamma(\mu^1, \mu^2)$ is the set of all transport plans with marginals μ^1 and μ^2 (see e.g. [AGS05]). The p-Wasserstein distance $d_{\mathcal{W}_p}$ metrizises the weak*-topology of measures, i.e. convergence tested against continuous functions on E. In the following we will consider either $E = \Omega$ or $E = \Omega \times \{1,2\}$.

To define the topology in the space of trajectories on Q, we start very coarse, where we understand the trajectories on Q as measures in space and time. We denote the space of trajectories by $\mathrm{L}^\infty_w([0,T], Q)$ equipped with the weak*-measureability. The weak*-convergence is defined as usual by

$$\mu^\varepsilon(\cdot) \to \mu^0(\cdot) \ :\Leftrightarrow\ \forall i \in \{1,2\}\,,\ \forall \phi \in \mathrm{C}^\infty(\Omega \times [0,T]) : \int_0^T \int_\Omega \phi \mathrm{d}\mu_i^\varepsilon(x)\mathrm{d}t \to \int_0^T \int_\Omega \phi \mathrm{d}\mu_i^0(x)\mathrm{d}t.$$

A finer topology, which enables to prove compactness and evaluate the effective dissipation functional is then given by the a priori bounds

$$\sup_{\varepsilon \in]0,1]} \mathfrak{D}_\varepsilon^V(\mu^\varepsilon) \leq C, \qquad \sup_{\varepsilon \in]0,1]} \operatorname*{ess\,sup}_{t \in [0,T]} \mathcal{E}(\mu^\varepsilon(t)) \leq C.$$

In fact, as presented in Section 5.1, these bounds provide that the measures μ^ε have Lebesgue densities c^ε which converge strongly in $\mathrm{L}^1([0,T] \times \Omega, \mathbb{R}^2_{\geq 0})$. Moreover, the limiting coarse-grained measure $\hat{\mu}^0 = \mu_1^0 + \mu_2^0$ has an representative which is absolutely continuous in time with values in $(\mathrm{Prob}(\Omega), d_{\mathcal{W}_2})$, i.e. there is a function $m \in \mathrm{L}^1([0,T]$ such that for all $t, s \in [0,T]$ with $s \leq t$ we have

$$d_{\mathcal{W}_2}\left(\hat{\mu}^0(s), \hat{\mu}^0(t)\right) \leq \int_s^t m(r)\mathrm{d}r.$$

Each component μ_i^0, $i = 1,2$ is not a trajectory in the space of probability measure, but in the space of non-negative Radon measures. Proposition 5.11 shows that μ_i^0 is absolutely continuous in time with values in $(\mathcal{M}_+(\Omega), d_{\mathcal{W}_1})$ exploiting the dual formulation of the 1-Wasserstein distance (see e.g. [Edw11]). This compactness result is comparable to the result of Bothe and Hilhorst [BoH02], where also strong convergence of solutions $c = (c_1, c_2)$ is proved. In particular, similar to the space independent situation in [MiS20, Ste19, MPS20] one cannot guarantee that $\mu^\varepsilon(t) \to \mu^0(t)$ in Q for all times $t \in [0,T]$ as jumps in time cannot be excluded. Instead the limit $\mu^0 = c^0\,\mathrm{d}x$ has an absolutely continuous representative.

4.1 Main theorem

Let us state our main EDP-convergence result. For doing this, we define for $V \in \mathrm{C}^1(\Omega, \mathbb{R}^2)$ the total dissipation functional on $\mathrm{L}^\infty_w([0,T], Q)$ as

$$\mathfrak{D}_\varepsilon^V(\mu) = \begin{cases} \int_0^T \left\{\mathcal{R}_\varepsilon(\mu, \dot{\mu}) + \mathcal{R}_\varepsilon^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu))\right\} \mathrm{d}t, & \mu \in \mathrm{AC}([0,T], Q), \mu = c\,\mathrm{d}x \text{ a.e. in } [0,T] \\ \infty & \text{otherwise.} \end{cases}$$

If $\mu = c\,\mathrm{d}x$ a.e. in $[0,T]$, then the dissipation functional is given by

$$\begin{aligned}
&\int_0^T \mathcal{R}_\varepsilon(\mu,\dot\mu) + \mathcal{R}^*_\varepsilon(\mu, -V - \mathrm{D}\mathcal{E}(\mu))\mathrm{d}t \\
&= \inf_{(c,J,b)\in(\mathrm{gCE})} \left\{ \int_0^T \left\{ \int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}(\delta_j c_j, J_j)\mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2(x)\right)\mathrm{d}x \right\}\,\mathrm{d}t \right\} + \\
&\quad + \int_0^T \left\{ \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V}\mathrm{d}x + \frac{2}{\varepsilon}\int_\Omega \sqrt{w_1^V w_2^V}\left(\sqrt{\rho_1^V} - \sqrt{\rho_2^V}\right)^2 \mathrm{d}x \right\}\,\mathrm{d}t, \qquad (4.1)
\end{aligned}$$

where the infimum is taken over all Borel fluxes $J_j \in \mathcal{M}([0,T]\times\Omega,\mathbb{R}^d), b_j \in \mathcal{M}([0,T]\times\Omega,\mathbb{R})$ which satisfy the generalized continuity equation (gCE) in the sense of distributions, i.e.

$$\begin{aligned}
&\forall j = 1,2\ \forall \phi \in \mathrm{C}_c^\infty([0,T]\times\Omega): \int_0^T\int_\Omega \dot\phi c_j - \nabla\phi\cdot J_j \mathrm{d}x\mathrm{d}t = -\int_0^T\int_\Omega b_j\phi\mathrm{d}x\mathrm{d}t,\\
&\quad J\cdot\nu = 0 \ \text{ on } \partial\Omega.
\end{aligned}$$

Remark 4.1. Strictly speaking, the functions $\widetilde{\mathsf{Q}}$ and $\widetilde{\mathsf{C}}$ are not defined for measures J_j,b_j and hence, the formula for the dissipation functional (3.5) is a priori not correct. In fact, introducing the related functional as in Lemma 5.2, the dissipation functional can be expressed via the densities of J_j, b_j. These densities are in $\mathrm{L}^1([0,T]\times\Omega)$ as Lemma 5.1 shows. For notational convenience, we identify the measures with their Lebesgue densities and stick to the above expression (3.5). In Lemma 5.7, we, in fact, show compactness for the sequence of measures J_i^ε.

The main result is the Γ-convergence of $\mathfrak{D}_\varepsilon^V$ to the effective dissipation functional $\mathfrak{D}_0^V$ which is defined by

$$\mathfrak{D}_0^V(\mu) = \begin{cases} \int_0^T \mathcal{R}_{\mathrm{eff}}(\mu,\dot\mu) + \mathcal{R}^*_{\mathrm{eff}}(\mu, -\mathrm{D}\mathcal{E}^V(\mu))\mathrm{d}t, & \text{if } \mu \in \mathrm{AC}([0,T],Q), \mu = c\,\mathrm{d}x \text{ a.e. in } [0,T] \\ \infty & \text{otherwise.}\end{cases}$$

where

$$\mathcal{R}^*_{\mathrm{eff}}(\mu,\xi) = \mathcal{R}^*_{\mathrm{diff}}(\mu,\xi) + \chi_{\{\xi_1=\xi_2\}}(\xi), \quad \mathcal{R}_{\mathrm{eff}}(\mu,v) = \left(\mathcal{R}_{\mathrm{eff}}(\mu,\cdot)\right)^*(v). \qquad (4.2)$$

Theorem 4.2. *Let $V \in \mathrm{C}^1(\Omega,\mathbb{R}^2)$. On $\mathrm{L}^\infty_w([0,T],Q)$, we have Γ-convergence constraint to bounded energies of $\mathfrak{D}_\varepsilon^V$, i.e. $\mathfrak{D}_\varepsilon^V \xrightarrow{\Gamma_E} \mathfrak{D}_0^V$ where*

$$\mathfrak{D}_0^V(\mu) = \begin{cases} \int_0^T \mathcal{R}_{\mathrm{eff}}(\mu,\dot\mu) + \mathcal{R}^*_{\mathrm{eff}}(\mu, -V - \mathrm{D}\mathcal{E}(\mu))\mathrm{d}t, & \mu \in \mathrm{AC}([0,T],Q), \mu = c\,\mathrm{d}x \text{ a.e. } [0,T] \\ \infty & \text{otherwise}\end{cases} \qquad (4.3)$$

with

$$\begin{aligned}
&\mathcal{R}^*_{\mathrm{eff}}(\mu,\xi) = \mathcal{R}^*_{\mathrm{diff}}(\mu,\xi) + \chi_{\{\xi_1=\xi_2\}}(\xi),\\
&\mathcal{R}_{\mathrm{eff}}(\mu,v) = \inf_{u+\tilde u = v}\left\{\mathcal{R}_{\mathrm{diff}}(\mu,\tilde u) + \chi_0(u_1+u_2)\right\} = \\
&\qquad = \inf\left\{ \sum_{j=1}^2 \int_\Omega \widetilde{\mathsf{Q}}(\delta_j c_j, J_j)\mathrm{d}x : u_1+u_2 = 0, \left\{ \begin{array}{l} v_1 = -\mathrm{div}J_1 + u_1 \\ v_2 = -\mathrm{div}J_2 + u_2 \end{array}\right\}\right\}.
\end{aligned}$$

The theorem states that the limit dissipation functional is again of $\mathcal{R} \oplus \mathcal{R}^*$-form with an effective dissipation potential $\mathcal{R}^*_{\text{eff}}$. The effective dissipation potential $\mathcal{R}^*_{\text{eff}}$ consists again of two terms describing the diffusion and a coupling, which forces the chemical potential $-\mathrm{D}\mathcal{E}^V$ to equilibration. This equilibration provides the microscopic equilibria of the densities ρ^V defining the slow manifold of the evolution.

In the Section 5, we will present the detailed proof of this Γ-convergence result. In this section, we discuss the effective gradient system and its induced gradient flow equation. As we will see the associated gradient flow equation can be understood as an evolution equation on Q and also on a smaller state space $\hat{Q} := \mathrm{Prob}(\Omega)$ of coarse-grained variables.

As an immediate consequence, Theorem 4.2 implies that $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$ EDP-converges with tilting to $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$.

Theorem 4.3. *Let $\mathcal{R}^*_{\text{eff}}$ be defined by (4.2). Then the gradient system $(Q, \mathcal{E}, \mathcal{R}^*_\varepsilon)$ EDP-converges with tilting to $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$.*

Proof. The energy $\mathcal{E}$ is ε-independent and lsc. on Q. Hence, it Γ-converges to itself. Theorem 4.2 implies that $\mathfrak{D}^V_\varepsilon$ Γ-converges to $\mathfrak{D}^V_0$ and $\mathfrak{D}^V_0$ is of $\mathcal{R} \oplus \mathcal{R}^*$ structure, where the effective dissipation potential $\mathcal{R}_{\text{eff}}$ is independent of the tilts $\eta = V$. Hence, EDP-convergence with tilting is established. □

4.2 Effective gradient flow equation

In this section, we discuss the effective gradient flow equation that is associated by the limit gradient structure $(Q, \mathcal{E}, \mathcal{R}^*_{\text{eff}})$. Similar to the space-independent situation in [MiS20, MPS20] the limit gradient structure can also be equivalently understood as a gradient structure on a smaller coarse-grained space of slow variables $\hat{Q}$. In particular, we obtain an effective gradient flow equation on the original state space Q with a Lagrange multiplier ensuring the projection on the slow manifold, and, moreover, an effective gradient flow equation in coarse-grained variables. First, we discuss the effective gradient flow equation with Lagrange multipliers, and secondly, the coarse-grained gradient structure and its induced gradient flow equation. Throughout the section the potential $V \in \mathrm{C}^1(\Omega, \mathbb{R}^2)$ is fixed.

4.2.1 Gradient flow equation with Lagrange multipliers

For being brief, the calculations in this section are rather formal. The effective dissipation potential $\mathcal{R}^*_{\text{eff}} = \mathcal{R}^*_{\text{diff}} + \chi_{\{\xi_1 = \xi_2\}}$ consists of two parts: the first describes the dissipation of the evolution and the second provides the linear constraint of being on the slow manifold and also the corresponding Lagrange multiplier. The evolution equation is given by

$$\dot{\mu} \in \partial_\xi \mathcal{R}^*_{\text{eff}}(\mu, -V - \mathrm{D}\mathcal{E}(\mu)) = \partial_\xi \left\{ \mathcal{R}^*_{\text{diff}}(\mu, -V - \mathrm{D}\mathcal{E}(\mu)) + \chi_{\{\xi_1 = \xi_2\}}(-V - \mathrm{D}\mathcal{E}(\mu)) \right\}.$$

Following [EkT76], the subdifferential of a sum is given by the sum of the subdifferential, if one term is continuous, which holds for the first term. For the second term, the subdifferential of the characteristic function is only definite in its domain, i.e. if

$$-V_1 - \mathrm{D}\mathcal{E}(\mu)_1 = -V_2 - \mathrm{D}\mathcal{E}(\mu)_2,$$

which implies that $\mu = c\mathrm{d}x$ and that their densities satisfy the relation $\frac{c_1}{\beta \mathrm{e}^{-V_1}} = \frac{c_2}{\alpha \mathrm{e}^{-V_2}}$ defining the linear slow manifold. Moreover, on its domain we have for the subdifferential that $\partial \chi_{\{\xi_1=\xi_2\}} = \mathcal{M}(\Omega)\begin{pmatrix}1\\-1\end{pmatrix}$. Hence, we conclude that

$$\dot{\mu} \in \partial_\xi \left\{\mathcal{R}^*_{\mathrm{diff}}(\mu, -V - \mathrm{D}\mathcal{E}(\mu))\right\} + \mathcal{M}(\Omega)\begin{pmatrix}1\\-1\end{pmatrix}, \quad \frac{c_1}{\beta \mathrm{e}^{-V_1}} = \frac{c_2}{\alpha \mathrm{e}^{-V_2}} ,$$

which implies the gradient flow equation on the slow manifold with a Lagrange multiplier $\lambda = (\lambda_1, \lambda_2)$ for the densities of the form

$$\begin{cases} \dot{c_1} = \mathrm{div}\left\{\delta_1 \nabla c_1 + \delta_1 c_1 \nabla V_1\right\} + \lambda_1(t,x) \\ \dot{c_2} = \mathrm{div}\left\{\delta_2 \nabla c_2 + \delta_2 c_2 \nabla V_2\right\} + \lambda_2(t,x) \end{cases}, \quad \lambda_1 + \lambda_2 = 0, \quad \frac{c_1}{\beta \mathrm{e}^{-V_1}} = \frac{c_2}{\alpha \mathrm{e}^{-V_2}} . \tag{4.4}$$

4.2.2 Coarse-grained gradient structure and its gradient flow equation

Now, we discuss the effective gradient structure $(Q, \mathcal{E}, \mathcal{R}^*_{\mathrm{eff}})$ in the slow coarse-grained variables. To do this, we introduce the coarse grained probability measure $\hat{\mu} = \mu_1 + \mu_2$ on Ω and the corresponding concentrations $\hat{c} := c_1 + c_2$. Moreover, we define the equilibrated densities $\hat{\rho}^V = \rho_1^V = \rho_2^V$ and the coarse-grained stationary measure $\hat{w}^V = w_1^V + w_2^V$, for which we get $\hat{c} = \rho_1^V w_1^V + \rho_2^V w_2^V = \hat{\rho}^V(w_1^V + w_2^V) = \hat{\rho}^V \hat{w}^V$. We introduce the coarse-grained diffusion coefficient $\hat{\delta}^V = \frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}$.

With this notation, we may define the coarse-grained gradient structure $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$. On the state space $\hat{Q} = \mathrm{Prob}(\Omega)$, we define

$$\begin{aligned} \hat{\mathcal{R}}^*(\hat{\mu}, \hat{\xi}) &:= \mathcal{R}^*_{\mathrm{eff}}\left(\left(\frac{w_1^V}{w_1^V + w_2^V}\hat{\mu}, \frac{w_2^V}{w_1^V + w_2^V}\hat{\mu}\right), (\hat{\xi}, \hat{\xi})\right) = \frac{1}{2}\int_\Omega \hat{\delta}^V |\nabla \hat{\xi}|^2 \mathrm{d}\hat{\mu} , \\ \hat{\mathcal{E}}(\hat{\mu}) &:= \mathcal{E}^V\left(\frac{w_1^V}{w_1^V + w_2^V}\hat{\mu}, \frac{w_2^V}{w_1^V + w_2^V}\hat{\mu}\right) . \end{aligned} \tag{4.5}$$

Introducing the coarse-grained potential $\hat{V} = -\log(w_1^V + w_2^V) - \log Z = -\log(\hat{w}^V) - \log Z = -\log\left(w_1 \mathrm{e}^{-V_1} + w_2 \mathrm{e}^{-V_2}\right)$, for which the exponential is given by the weighted arithmetic mean of the exponentials e^{-V_1} and e^{-V_2}, i.e. $\mathrm{e}^{-\hat{V}} = w_1 \mathrm{e}^{-V_1} + w_2 \mathrm{e}^{-V_2}$ (we used that $w_1 + w_2 = 1$). Easy calculations show that the energy has for the explicit form

$$\hat{\mathcal{E}}(\hat{\mu}) = \int_\Omega \hat{\mu}\log\hat{\mu} + \hat{\mu}\hat{V}\mathrm{d}x.$$

The coarse-grained dissipation functional is defined by

$$\hat{\mathfrak{D}}(\hat{\mu}) = \int_0^T \hat{\mathcal{R}}(\hat{\mu}, \dot{\hat{\mu}}) + \hat{\mathcal{R}}^*(\hat{\mu}, -\mathrm{D}\hat{\mathcal{E}}(\hat{\mu}))\mathrm{d}t,$$

which incorporates the tilt via the coarse-grained variables. Note, that the coarse-grained dissipation potential $\hat{\mathcal{R}}^*$ depends explicitly on the tilt V via the diffusion coefficient δ^V. This is not a contradiction to tilt-EDP convergence (Theorem 4.3), because in original variables the effective dissipation potential (4.3) is indeed independent of the tilts. The tilts dependence of $\hat{\mathcal{R}}^*$ originates from the energy and tilt dependent slow manifold.

To relate the dissipation functional $\mathfrak{D}_0^V$ with the coarse grained dissipation functional $\hat{\mathfrak{D}}$, we first show that also an equilibration of the fluxes occurs. To do this the following convexity property is important.

Lemma 4.4. *Let X a separable and reflexive Banach space and let $\mathsf{F} : X \to \mathbb{R}_\infty$ be convex and lsc. Then for the function $\widetilde{\mathsf{F}} : [0,\infty[\times X \to \mathbb{R}_\infty$, we have*

$$\widetilde{\mathsf{F}}\left(\sum_{i=1}^I a_i, \sum_{i=1}^I x_i\right) \leq \sum_{i=1}^I \widetilde{\mathsf{F}}(a_i, x_i).$$

If F is strictly convex then equality holds if and only if $(a_i, x_i) = (0,0)$ whenever $a_i = 0$ or $x_i/a_i = x_j/a_j$ whenever $a_i, a_j > 0$. Moreover, if $\mathsf{F}(0) = 0$, we have the following monotonicity property

$$\widetilde{\mathsf{F}}(a_1, x) \leq \widetilde{\mathsf{F}}(a_2, x), \quad \text{if } a_1 \geq a_2.$$

Proof. Let pairs (a_i, x_i) for $i = 1, \dots, I$ be given. If $a_i = 0$, then either $x_i = 0$ and the claim has to be shown for $I-1$ -number of pairs, or $x_i \neq 0$ and the right-hand side is ∞ meaning that the claim is trivial. So let us assume that $a_i > 0$ for all $i = 1 \dots, I$. Then $\widetilde{\mathsf{F}}(a_i, x_i) = a_i \mathsf{F}(x_i/a_i)$ and the claim is equivalent to

$$\sum_{i=1}^I \frac{a_i}{\sum_{i=1}^I a_i} \mathsf{F}(x_i/a_i) \geq \mathsf{F}\left(\sum_{i=1}^I \frac{a_i}{\sum_{i=1}^I a_i} \frac{x_i}{a_i}\right) = \mathsf{F}\left(\frac{\sum_{i=1}^I x_i}{\sum_{i=1}^I a_i}\right),$$

which holds since F is convex. If F is strictly convex then we immediately observe that whenever $a_i, a_j > 0$ we have $\frac{x_i}{a_i} = \frac{x_j}{a_j}$, and whenever $a_i = 0$ that also $x_i = 0$.

To see the monotonicity property, we observe that $\widetilde{\mathsf{F}}(a, 0) = 0$ for all $a \geq 0$. Hence, we have

$$\widetilde{\mathsf{F}}(a_1 + a_2, x) \leq \widetilde{\mathsf{F}}(a_1, x) + \widetilde{\mathsf{F}}(a_2, 0) = \widetilde{\mathsf{F}}(a_1, x),$$

which proves the claim. □

Recalling formula (4.3) of the effective dissipation functional $\mathfrak{D}_0^V$ and using the above lemma, we observe that the velocity part of the dissipation functional $\mathfrak{D}_0^V$ can now be estimated. In particular, we will see that the limit dissipation functional $\mathfrak{D}_0^V$ can be equivalently expressed in coarse-grained variables $(\hat{\mu}, \hat{J})$ by using that an equilibration of concentrations also provides an equilibration of the corresponding fluxes. In the reconstruction strategy in Section 5.3 this equilibration is explicitly used (see 4.10 and (5.3)).

Proposition 4.5. *Let $\mu \in \mathrm{AC}([0,T], Q)$ with $\mathfrak{D}_0^V(\mu) < \infty$ and $\operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}(\mu(t)) < \infty$. Then the following holds:*

1. *We have $\mathfrak{D}_0^V(\mu) = \hat{\mathfrak{D}}(\hat{\mu})$ where $\hat{\mu} = \mu_1 + \mu_2$ and*

$$\begin{aligned}\hat{\mathfrak{D}}(\hat{\mu}) &= \int_0^T \hat{\mathcal{R}}(\hat{\mu}, \dot{\hat{\mu}}) + \hat{\mathcal{R}}^*(\hat{\mu}, -\mathrm{D}\hat{\mathcal{E}}(\hat{\mu}))\, \mathrm{d}t \\ &= \inf_{\hat{J}:\dot{\hat{\mu}}+\mathrm{div}\hat{J}=0} \left\{ \int_0^T \int_\Omega \widetilde{\mathsf{Q}}(\hat{\delta}^V \hat{c}, \hat{J}) + \frac{\hat{\delta}\hat{w}^V}{2} \frac{|\nabla \hat{\rho}^V|^2}{\hat{\rho}^V}\, \mathrm{d}x\mathrm{d}t \right\}.\end{aligned}$$

2. The chain-rule holds for $[0,T] \ni t \mapsto \hat{\mathcal{E}}(\hat{\mu}(t)) \in \mathbb{R}$, i.e. we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathcal{E}}(\hat{\mu}(t)) = \langle \mathrm{D}\hat{\mathcal{E}}(\hat{\mu}(t)), \dot{\hat{\mu}}(t)\rangle \ .$$

3. The gradient flow equation of the gradient system $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$ is given by

$$\dot{\hat{c}} = -\mathrm{div}\left(\hat{\delta}^V \hat{c}\, \nabla\left(-\mathrm{D}\hat{\mathcal{E}}(\hat{\mu})\right)\right) = \mathrm{div}\left(\hat{\delta}^V \nabla \hat{c} + \hat{\delta}^V \hat{c} \nabla \hat{V}\right), \tag{4.6}$$

with the potential $\hat{V} = -\log \hat{w}^V$ and stationary measure $\hat{w}^V$.

Equation (4.6) shows that the coarse-grained gradient flow equation induced by $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$ is a drift-diffusion equation of the coarse-grained concentration $\hat{c}$ with mixed diffusion constant $\hat{\delta}^V$. In particular, in the tilt free case we have $\hat{\delta}^{V=\mathrm{const}} = \frac{\beta\delta_1 + \alpha\delta_2}{\alpha+\beta}$, and we recover the result of [BoH02].

Proof. To prove Part 1, we first observe that the bounded energy and dissipation for the trajectory μ implies that we have $\frac{c_1}{w_1^V} = \frac{c_2}{w_2^V}$ a.e. in $[0,T]\times\Omega$. Using $\hat{c} = c_1 + c_2$ for the densities, we get $\hat{c} = \frac{w_1^V + w_2^V}{w_1^V} c_1 = \frac{w_1^V + w_2^V}{w_2^V} c_2$. The Fisher information $\mathcal{S}_0^V(\mu) := \mathcal{R}^*_{\mathrm{eff}}(\mu, -V - \mathrm{D}\mathcal{E}(\mu))$ has the form

$$\mathcal{S}_0^V(\mu) = \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V}\mathrm{d}x = \frac{1}{2}\int_\Omega \left(\frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}\right)\left(w_1^V + w_2^V\right)\frac{|\nabla \hat{\rho}^V|^2}{\hat{\rho}^V}\mathrm{d}x \tag{4.7}$$

$$= \frac{1}{2}\int_\Omega \hat{\delta}^V \hat{w}^V \frac{|\nabla \hat{\rho}^V|^2}{\hat{\rho}^V}\mathrm{d}x = \hat{\mathcal{R}}^*(\hat{\mu}, -\mathrm{D}\hat{\mathcal{E}}(\hat{\mu})). \tag{4.8}$$

Lemma 4.4 provides that also an equilibration of the fluxes occurs. Indeed, defining the coarse-grained flux $\hat{J} = J_1 + J_2$, we conclude

$$\frac{|J_1|^2}{\delta_1 c_1} + \frac{|J_2|^2}{\delta_2 c_2} \geq \frac{|J_1 + J_2|^2}{\delta_1 c_1 + \delta_2 c_2} = \frac{|\hat{J}|^2}{\frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}\hat{c}} = \frac{|\hat{J}|^2}{\hat{\delta}\hat{c}}, \tag{4.9}$$

where $\hat{\delta}^V := \frac{\delta_1 w_1^V + \delta_2 w_2^V}{w_1^V + w_2^V}$. Equality holds if and only if $(J_1, c_1) = 0$ or $(J_2, c_2) = 0$ or $J_1/\delta_1 c_1 = J_2/\delta_2 c_2 = \hat{J}/\hat{\delta}^V \hat{c}$. The last condition is equivalent to

$$\hat{J} = \frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V} J_1 = \frac{\delta_2 w_2^V}{\delta_1 w_1^V + \delta_2 w_2^V} J_2 \ , \tag{4.10}$$

which provides an explicit formula for the coarse-grained diffusion flux.

For the dissipation functional that means

$$\mathfrak{D}_0^V(\mu) = \inf_{(c,J,b)\in(\mathrm{gCE})} \int_0^T \left\{ \int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}(\delta_j c_j, J_j)\mathrm{d}x + \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{|\nabla \rho_j|^2}{\rho_j}\mathrm{d}x \right\}\mathrm{d}t$$

$$\geq \inf_{\dot{\hat{c}} + \mathrm{div}\hat{J} = 0} \int_0^T \left\{ \int_\Omega \widetilde{\mathsf{Q}}\left(\hat{\delta}\hat{c}, \hat{J}\right)\mathrm{d}x + \frac{1}{2}\int_\Omega \hat{\delta}\hat{w}^V \frac{|\nabla \hat{\rho}|^2}{\hat{\rho}}\mathrm{d}x \right\}\mathrm{d}t. \tag{4.11}$$

To prove equality, we first observe that $\hat{J}, J_1, J_2$ satisfy the same boundary conditions. Moreover, the explicitly derived reaction flux b_1, b_2 from (5.3) shows that the reconstructed fluxes (J_1, J_2) from coarse-grained flux $\hat{J}$ is admissible. Hence, we obtain equality

$$\mathfrak{D}_0^V(\mu) = \inf_{\dot{\hat{c}}+\operatorname{div}\hat{J}=0} \int_0^T \left\{ \frac{1}{2}\int_\Omega \mathsf{Q}\left(\hat{\delta}\hat{c}, \hat{J}\right) \mathrm{d}x + \frac{1}{2}\int_\Omega \hat{\delta}\hat{w}^V \frac{|\nabla\hat{\rho}|^2}{\hat{\rho}} \mathrm{d}x \right\} \mathrm{d}t,$$

which proves the first part.

For the chain-rule in Part 2, we refer to the proof [FrL21, Lem 4.8] since we consider the pure diffusive situation. The proof uses a time-regularization argument and convexity of the Fisher-information following the ideas of [MRS13, Prop. 2.4].

For Part 3, we compute the evolution equation that is induced by the gradient system is $(\hat{Q}, \hat{\mathcal{E}}, \hat{\mathcal{R}}^*)$. We have

$$\begin{aligned}
\partial_{\hat{\xi}}\hat{\mathcal{R}}^*(\hat{\mu}, \hat{\xi}) &= -\operatorname{div}\left(\hat{\delta}^V \hat{c} \nabla \hat{\xi}\right), \\
\mathrm{D}\hat{\mathcal{E}}(\hat{\mu}) &= \log\hat{\mu} + 1 - \log\hat{w}^V - \log Z, \\
\nabla\left(-\mathrm{D}\hat{\mathcal{E}}(\hat{\mu})\right) &= -\frac{\nabla\hat{\mu}}{\hat{\mu}} + \frac{\nabla\hat{w}^V}{\hat{w}^V} = -\frac{\nabla\hat{\mu}}{\hat{\mu}} - \nabla\hat{V},
\end{aligned}$$

which results in

$$\dot{\hat{c}} = -\operatorname{div}\left(\hat{\delta}^V \hat{c}\, \nabla\left(-\mathrm{D}\mathsf{E}(\hat{\mu})\right)\right) = \operatorname{div}\left(\hat{\delta}^V \nabla\hat{c} + \hat{\delta}^V \hat{c} \nabla\hat{V}\right).$$

□

Note that the coarse-grained gradient flow equation (4.6) is equivalent to the gradient flow equation with Lagrange multipliers (4.4). Indeed, adding both equations in (4.4) together and using that the original concentrations can be expressed by the coarse-grained concentrations via

$$c_i = \frac{w_i \mathrm{e}^{-V_i}}{w_1\mathrm{e}^{-V_1} + w_2\mathrm{e}^{-V_2}}\hat{c}, \tag{4.12}$$

the coarse-grained gradient flow equation (4.6) with the drift term $\hat{\delta}^V\hat{c}\nabla\hat{V}$ can be readily derived. Conversely, using (4.12), we see that $c = (c_1, c_2)$ are on the slow manifold and satisfy (4.4). The corresponding Lagrange multipliers $\lambda = (\lambda_1, \lambda_2)$ can be explicitly calculated. Introducing the difference of the diffusion constants $\overline{\delta} = \delta_1 - \delta_2$ and the potentials $\overline{V} = V_1 - V_2$, we have

$$\begin{aligned}
\lambda_1 &= \frac{w_2\mathrm{e}^{-V_2}}{w_1\mathrm{e}^{-V_1} + w_2\mathrm{e}^{-V_2}} \left(-\overline{\delta}\Delta c_1 + \left(\delta_2\nabla\overline{V} - \overline{\delta}\nabla V_1\right)\cdot\nabla c_1 + c_1\left\{\delta_2\nabla\overline{V}\,\nabla V_1 - \overline{\delta}\Delta V_1\right\}\right) \\
\lambda_2 &= \frac{w_1\mathrm{e}^{-V_1}}{w_1\mathrm{e}^{-V_1} + w_2\mathrm{e}^{-V_2}} \left(\overline{\delta}\Delta c_2 + \left(-\delta_1\nabla\overline{V} + \overline{\delta}\nabla V_2\right)\cdot\nabla c_2 + c_2\left\{-\delta_1\nabla\overline{V}\,\nabla V_2 + \overline{\delta}\Delta V_2\right\}\right).
\end{aligned}$$

We observe that the Lagrange multiplier λ_i has the same regularity as the right-hand side of the evolution of c_i. Moreover, both evolution equations are completely uncoupled but contain a linear annihilation/creation term, which depends on the potential $V = (V_1, V_2)$ and the diffusion coefficient $\delta = (\delta_1, \delta_2)$. A lengthy calculation shows that indeed we have $\lambda_1 + \lambda_2 = 0$.

5 Proof of Γ-convergence

In this section we prove the Γ-convergence result of Theorem 4.2. As usual, we prove Γ-convergence in three steps: First deriving compactness, secondly establishing the liminf-estimate by exploiting the compactness, thirdly constructing the recovery sequence for the limsup-estimate.

In the following the next lemma will be useful.

Lemma 5.1. *Let $\mathsf{F} : \mathbb{R}^k \to [0, \infty[$ be a convex, lsc. function of superlinear growth, i.e. $\mathsf{F}(r)/r \to \infty$ as $r \to \infty$. Then there is a constant $k_{\mathsf{F}} > 0$ such that for any measurable functions $W : \Omega \to \mathbb{R}^k$ and $\rho : \Omega \to \mathbb{R}_{\geq 0}$ it holds*

$$\int_\Omega |W| \mathrm{d}x \leq \int_\Omega \widetilde{\mathsf{F}}(\rho, W) \mathrm{d}x + k_{\mathsf{F}} \int_\Omega \rho \mathrm{d}x \ .$$

Proof. Let W and ρ be given. We define three measurable subsets of Ω:

$$\Omega_0 = \{x : \rho(x) = 0\},\ \Omega_1 = \{x : \rho \neq 0, \tfrac{1}{\rho}|W| \leq \mathsf{F}(\tfrac{1}{\rho}W)\},\ \Omega_2 = \{x : \rho \neq 0, \tfrac{1}{\rho}|W| > \mathsf{F}(\tfrac{1}{\rho}W)\}.$$

Since F is superlinear, there is a constant $k_{\mathsf{F}} > 0$ such that on Ω_2 it holds $W/\rho \leq k_{\mathsf{F}}$. Hence we can estimate

$$\begin{aligned}
\int_\Omega |W| \mathrm{d}x &\leq \int_{\Omega_0} |W| \mathrm{d}x + \int_{\Omega_1} \frac{|W|}{\rho} \rho \mathrm{d}x + \int_{\Omega_2} \frac{|W|}{\rho} \rho \mathrm{d}x \\
&\leq \int_{\Omega_0} \widetilde{\mathsf{F}}(\rho, W) \mathrm{d}x + \int_{\Omega_1} \mathsf{F}(\tfrac{1}{\rho}W) \rho \mathrm{d}x + k_{\mathsf{F}} \int_{\Omega_2} \rho \mathrm{d}x \\
&\leq \int_\Omega \widetilde{\mathsf{F}}(\rho, W) \mathrm{d}x + k_{\mathsf{F}} \int_\Omega \rho \mathrm{d}x \ .
\end{aligned}$$

□

Moreover, we need the following classical lemma. It guarantees the necessary regularity for the limits, and moreover, it provides the desired liminf-estimate.

Lemma 5.2 (AGS05-Lemma 9.4.3, [AGS05])**.** *Let $F : [0, \infty[\to [0, \infty]$ be a proper, lsc, convex function with superlinear growth. We define the related functional*

$$\mathcal{F}(\mu, \gamma) = \begin{cases} \int_A F(\frac{\mathrm{d}\mu}{\mathrm{d}\gamma}) \mathrm{d}\gamma, & \text{if } \ \mu \ll \gamma, \\ \infty, & \text{otherwise.} \end{cases}$$

Let $\mu^\varepsilon, \gamma^\varepsilon \in \mathrm{Prob}(A)$ be two sequences with $\mu^\varepsilon \overset{*}{\rightharpoonup} \mu^0$ and $\gamma^\varepsilon \overset{*}{\rightharpoonup} \gamma^0$. Then

$$\liminf_{\varepsilon \to 0} \mathcal{F}(\mu^\varepsilon, \gamma^\varepsilon) \geq \mathcal{F}(\mu^0, \gamma^0).$$

In particular, if the left-hand side is finite then for the limits it holds $\mu^0 \ll \gamma^0$.

5.1 Compactness

In this section, we derive the required compactness for proving the liminf-estimate in Section 5.2.

Recall that for given potential $V \in \mathrm{C}^1(\Omega, \mathbb{R}^2)$ the dissipation functional $\mathfrak{D}_\varepsilon^V$ is defined on the space of trajectories equipped with the weak topology, i.e. $\mu^\varepsilon \to \mu^0 \in \mathrm{L}^\infty_w([0,T],Q)$ if and only if it holds

$$\forall i \in \{1,2\}\,,\ \forall \phi \in \mathrm{C}_0^\infty(\Omega \times [0,T]): \quad \int_0^T \int_\Omega \phi \mathrm{d}\mu_i^\varepsilon(x)\mathrm{d}t \to \int_0^T \int_\Omega \phi \mathrm{d}\mu_i^0(x)\mathrm{d}t\ .$$

In the following we want to derive compactness for a sequence $(\mu^\varepsilon)_{\varepsilon>0}$ of trajectories, satisfying the a priori bounds

$$\sup_{\varepsilon>0} \operatorname*{ess\,sup}_{t\in[0,T]} \mathcal{E}(\mu^\varepsilon(t)) \le C, \qquad \sup_{\varepsilon>0} \mathfrak{D}_\varepsilon^V(\mu^\varepsilon) \le C, \tag{5.1}$$

where the total dissipation functional is

$$\mathfrak{D}_\varepsilon^V(\mu) = \begin{cases} \int_0^T \mathcal{R}_\varepsilon(\mu,\dot\mu) + \mathcal{R}_\varepsilon^*(\mu, -\mathrm{D}\mathcal{E}^V(\mu))\mathrm{d}t, & \mu \in \mathrm{AC}([0,T],Q), \mu = c\,\mathrm{d}x \text{ a.e. in } [0,T] \\ \infty & \text{otherwise,} \end{cases}$$

and for $\mu = c\,\mathrm{d}x$ we have

$$\begin{aligned} &\int_0^T \mathcal{R}_\varepsilon(\mu,\dot\mu) + \mathcal{R}_\varepsilon^*(\mu, -V - \mathrm{D}\mathcal{E}(\mu))\mathrm{d}t \\ &= \inf_{(c,J,b)\in(\mathrm{gCE})} \left\{ \int_0^T \left\{ \int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}\left(\delta_j c_j, J_j\right)\mathrm{d}x + \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2(x)\right)\mathrm{d}x \right\}\ \mathrm{d}t \right\} +, \\ &+ \int_0^T \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{\left|\nabla \rho_j^V\right|^2}{\rho_j^V}\mathrm{d}x + \frac{2}{\varepsilon}\int_\Omega \sqrt{w_1^V w_2^V}\left(\sqrt{\rho_1^V} - \sqrt{\rho_2^V}\right)^2 \mathrm{d}x\ \ \mathrm{d}t\ . \end{aligned} \tag{5.2}$$

Using the bound of the dissipation functional $\mathfrak{D}_\varepsilon^V(\mu^\varepsilon) \le C$, we conclude that there are diffusive fluxes $J^\varepsilon = (J_1^\varepsilon, J_2^\varepsilon)$ and reaction fluxes $b^\varepsilon = (b_1^\varepsilon, b_2^\varepsilon)$ such that $J_i^\varepsilon \in \mathcal{M}(\Omega,\mathbb{R}^d)$, $b_i^\varepsilon \in \mathcal{M}(\Omega,\mathbb{R})$ and $(\mu^\varepsilon, J^\varepsilon, b^\varepsilon)$ satisfies the continuity equation

$$(c,J,b) \in (\mathrm{gCE}) \quad \Leftrightarrow \quad \left\{ b_1 + b_2 = 0 \text{ and } \left\{ \begin{array}{l} \dot c_1 = -\mathrm{div} J_1 + b_1 \\ \dot c_2 = -\mathrm{div} J_2 + b_2 \end{array} \right\} \right\}.$$

Moreover, we get bounds:

$$\begin{aligned} i=1,2: \quad &\int_0^T \int_\Omega \frac{|\nabla \rho_i^{V,\varepsilon}|^2}{\rho_i^{V,\varepsilon}}\mathrm{d}x\mathrm{d}t \le C, \quad \int_0^T \int_\Omega \widetilde{\mathsf{Q}}\left(c_i^\varepsilon, J_i^\varepsilon\right)\mathrm{d}x\mathrm{d}t \le C, \\ &\int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1^\varepsilon c_2^\varepsilon}}{\varepsilon}, b_2^\varepsilon(x)\right)\mathrm{d}x\mathrm{d}t \le C, \quad \frac{1}{\varepsilon}\int_0^T \int_\Omega \left(\sqrt{\rho_1^{V,\varepsilon}} - \sqrt{\rho_2^{V,\varepsilon}}\right)^2 \mathrm{d}x\mathrm{d}t \le C\ . \end{aligned}$$

Remark 5.3. Following [Man07] a distributional solution (μ, J, B) of the generalized continuity equation $\dot\mu = -\mathrm{div} J + B$ satisfying $\int_0^T \int_\Omega |B| + |J| \mathrm{d}x < \infty$ can be assumed to be absolutely continuous. The bounds can be obtained easily using Lemma 5.1 for fixed $\varepsilon > 0$.

Although the functional is convex in the concentration c and in the fluxes J and b, weak convergence would be sufficient to prove a liminf-estimate using a Joffe-type

argument. But, comparing the situation with the evolution equation, we aim in proving even strong convergence for the densities $c^\varepsilon \to c^0$ in $\mathrm{L}^1([0,T]\times\Omega,\mathbb{R}^2_{\geq 0})$. This is done in two steps: First, compactness of coarse-grained variables, and secondly, convergence towards the slow manifold is shown, which together implies strong compactness. This strategy has successfully been applied already in the space-independent case in [MiS20, MPS20]. Moreover, we show that the limit trajectory $\mu^0 = c^0\mathrm{d}x$ has a representative which is in $\mathrm{AC}([0,T],Q)$. Note that it is not possible to prove pointwise convergence $\mu^\varepsilon(t) \overset{*}{\rightharpoonup} \mu^0(t)$ for all $t\in[0,T]$. Instead, pointwise convergence is only shown for the coarse-grained variables $\hat\mu^\varepsilon := \mu_1^\varepsilon + \mu_2^\varepsilon$.

First, we derive weak compactness in space-time, which immediately follows from the uniform bound in ε and time on the energy.

Lemma 5.4 (Very Weak compactness in space-time)**.** *Let $(\mu^\varepsilon)_{\varepsilon>0}$, $\mu^\varepsilon \in \mathrm{L}^\infty_w([0,T],Q)$ satisfy $\sup_{\varepsilon>0}\operatorname*{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^\varepsilon(t)) \leq C$. Then for a.e. $t\in[0,T]$ the measure $\mu^\varepsilon(t,\cdot)$ has a Lebesgue density $c^\varepsilon(t,\cdot)$. Moreover, there is a subsequence (not relabeled), such that their densities c^ε are uniformly integrable in $\Omega\times[0,T]\times\{1,2\}$ and hence, c_i^ε converges weakly in $\mathrm{L}^1([0,T]\times\Omega)$ to c_i^0 for $i=1,2$.*

Proof. The bound on the energy implies that a.e. $t\in[0,T]$ the measure $\mu^\varepsilon(t,\cdot)$ has a Lebesgue density $c^\varepsilon(t,\cdot)$. Moreover, the functional $\mu\mapsto\int_0^T\mathcal{E}(\mu)\mathrm{d}t$ is superlinear and convex. Hence, it follows by the Theorem of de Valleé -Poussin that μ^ε are uniformly integrable and hence, μ_i^ε converges weakly in $\mathrm{L}^1([0,T]\times\Omega)$ to μ_i^0. □

In the following, we are going to derive compactness for the concentrations c_i^ε and the diffusive fluxes J_i^ε. It is not possible to get compactness for the fast reaction flux b_2^ε by bounding the dissipation functional. In particular, pointwise convergence for the measures $\mu^\varepsilon(t)$ cannot be achieved.

Remark 5.5. To see that compactness for the fast reaction flux b_2^ε is not possible obtain, we set $\rho^\varepsilon = 1$ constant in $[0,T]\times\Omega\times\{1,2\}$ and $b_2^\varepsilon = b^\varepsilon$ constant in $[0,T]\times\Omega$. Then, a bound means on the dissipation functional implies a bound

$$\infty > \int_0^T\int_\Omega \mathsf{C}\left(\frac{\sqrt{c_1^\varepsilon c_2^\varepsilon}}{\varepsilon}, b_2^\varepsilon(x)\right)\mathrm{d}x \approx \mathsf{C}(\frac{1}{\varepsilon},b^\varepsilon) = \frac{1}{\varepsilon}\mathsf{C}(\varepsilon b^\varepsilon) \approx |b^\varepsilon|\log(\varepsilon|b^\varepsilon|+1).$$

Setting $b^\varepsilon = -\log\varepsilon$, we easily see that $|b^\varepsilon|\log(\varepsilon|b^\varepsilon|+1)\to 0$ as $\varepsilon\to 0$, however, $b^\varepsilon\to\infty$. Hence, it is not possible to obtain compactness for the fast reaction flux b_i^ε. Later in Lemma 5.14 the "converse" statement is proved: If $\iint\mathsf{C}(b)\mathrm{d}x\mathrm{d}t<\infty$ then $\iint\mathsf{C}(\frac{1}{\varepsilon},b)\mathrm{d}x\mathrm{d}t\to 0$.

Next, we are going to derive time-regularity for the sequence $(\mu^\varepsilon)_{\varepsilon>0}$ in proving compactness for the coarse-grained trajectories $\hat\mu^\varepsilon = \mu_1^\varepsilon + \mu_2^\varepsilon$. In particular, we are able to prove pointwise convergence in time.

Lemma 5.6 (Time Regularity of μ^ε)**.** *Let $(\mu^\varepsilon)_{\varepsilon>0}$, $\mu^\varepsilon\in\mathrm{L}^\infty_w([0,T],Q)$ satisfying the a priori bounds* (5.1)*. Then the curves $t\mapsto\hat\mu^\varepsilon := \mu_1^\varepsilon(t)+\mu_2^\varepsilon(t)$ have ε-uniform bounded total variation in the space* $\mathrm{Prob}(\Omega)$ *equipped with the 1-Wasserstein distance, i.e.*

$$\|\hat\mu^\varepsilon\|_{TV} := \sup\left\{\sum_{k=1}^K \mathcal{W}_1(\hat\mu^\varepsilon(t_k),\hat\mu^\varepsilon(t_{k-1})) \ :\ 0=t_0<\cdots<t_k<\cdots<t_K=T\right\}.$$

In particular, by Helly's selection principle, we conclude pointwise convergence $\hat{\mu}^\varepsilon(t) := \mu_1^\varepsilon(t) + \mu_2^\varepsilon(t) \overset{*}{\rightharpoonup} \hat{\mu}^0(t) := \mu_1^0(t) + \mu_2^0(t)$ *for all* $t \in [0,T]$ *in* $\mathrm{Prob}(\Omega)$ *along a suitable subsequence.*

Proof. We exploit the dual formulation of the L^1-Wasserstein distance, i.e. integrating against Lipschitz functions (see e.g. [AGS05]). Take $\phi \in \mathrm{C}^1(\Omega \times \{1,2\})$ with $\|\phi\|_{\mathrm{W}^{1,\infty}(\Omega)} \leq 1$ and $\phi = (\hat{\phi}, \hat{\phi})$. Using the continuity equations

$$\left\{ b_1 + b_2 = 0 \text{ and } \left\{ \begin{array}{l} \dot{c}_1 = -\mathrm{div} J_1 + b_1 \\ \dot{c}_2 = -\mathrm{div} J_2 + b_2 \end{array} \right\} \right\},$$

we conclude for all $[t_1, t_2] \subset [0,T]$ that

$$\begin{aligned} \int_\Omega \phi \cdot (\mathrm{d}\mu^\varepsilon(t_2) - \mathrm{d}\mu^\varepsilon(t_1)) &= \int_{t_1}^{t_2} \langle \phi, \dot{\mu}^\varepsilon \rangle \mathrm{d}t \\ &\leq \int_{t_1}^{t_2} \int_\Omega \nabla \hat{\phi} \cdot (J_1^\varepsilon + J_2^\varepsilon) \ \mathrm{d}x \ \mathrm{d}t \leq \int_{t_1}^{t_2} \int_\Omega \sum_{i=1}^2 |J_i^\varepsilon| \ \mathrm{d}x \ \mathrm{d}t. \end{aligned}$$

By the bound on the dissipation functional, we obtain ε-uniform bounds on the term $\int_{t_1}^{t_2} \int_\Omega \mathsf{Q}(\delta_j c_j, J_j) \mathrm{d}x \mathrm{d}t$. Moreover, we have $\int_\Omega \rho_j^\varepsilon \leq 1$ for all $t \in [0,T]$. Hence by Lemma 5.1 we conclude an ε-uniform bound on each addend $\int_{t_1}^{t_2} \int_\Omega \sum_{i=1}^2 |J_i^\varepsilon| \ \mathrm{d}x \ \mathrm{d}t$, which by summing up implies that $\|\hat{\mu}^\varepsilon\|_{TV}$ is ε-uniformly bounded. □

Next, the compactness result from Lemma 5.2 is used in order to prove compactness for the fluxes and spatial regularity.

Lemma 5.7 (Regularity for the fluxes and spatial regularity)**.** *Let* $(\mu^\varepsilon)_{\varepsilon>0}$ *with* $\mu^\varepsilon \in \mathrm{L}^\infty_w([0,T], Q)$ *satisfying the a priori bounds* (5.1)*. Then the corresponding diffusive fluxes* $J^\varepsilon : [0,T] \times \Omega \to \mathbb{R}^2$ *converge weakly-star* $J^\varepsilon \overset{*}{\rightharpoonup} J^0$ *in* $\mathcal{M}([0,T] \times \Omega \times \{1,2\})$ *and* $J_j^0 \ll \mu_j^0$*. Moreover* $\nabla \rho^{V,\varepsilon} \overset{*}{\rightharpoonup} \nabla \rho^{V,0}$ *in* $\mathcal{M}([0,T] \times \Omega \times \{1,2\})$ *and* $\nabla \rho_j^0 \ll \mu_j^0$*. In particular, we conclude that* ρ_j^ε *is uniformly bounded in* $\mathrm{L}^1([0,T], \mathrm{W}^{1,1}(\Omega))$*, which also implies that* $\hat{c}^\varepsilon$ *is uniformly in* $\mathrm{L}^1([0,T], \mathrm{W}^{1,1}(\Omega))$*.*

Proof. By the bound on the dissipation functional, we get (after extracting a suitable subsequence of $\varepsilon \to 0$) that $J^\varepsilon \overset{*}{\rightharpoonup} J^0$. Moreover, we have $\int_0^T \int_\Omega \frac{|J_j^\varepsilon|^2}{\rho_j^\varepsilon} \mathrm{d}x \leq C$ and $\rho_j^\varepsilon \overset{*}{\rightharpoonup} \rho_j^0$. Hence applying the Lemma 5.2, we conclude that $J_j^0 \ll \mu_j^0$. Similarly, we conclude compactness for the gradients $\nabla \rho^{V,\varepsilon}$. The only thing that remains is to identify the limit. But this is clear by definition of the weak derivatives, i.e. integrating against smooth test functions, because this is captured in the weak star convergence. Lemma 5.1 implies that ρ_j^ε is uniformly bounded in $\mathrm{L}^1([0,T], \mathrm{W}^{1,1}(\Omega))$. □

The spatial regularity and the temporal regularity provides a compactness result by a BV-generalization of the Aubin-Lions-Simon Lemma.

Theorem 5.8 ([BaP86, HPR18])**.** *Let* X, Y, Z *be Banach spaces such that* X *is compactly embedded in* Y*, and* Y *is continuously in* Z^**. Let* u^ε *be a bounded sequence in* $\mathrm{L}^1([0,T], X)$ *and in* $BV([0,T], Z^*)$*. Then (up to a sequence)* u^ε *strongly converges in* $\mathrm{L}^1([0,T], Y)$*.*

In our situation we immediately conclude that $\hat{c}^\varepsilon$ converges strongly.

Corollary 5.9 (Strong convergence of coarse-grained variables)**.** *Let $(\mu^\varepsilon)_{\varepsilon>0}$ with $\mu^\varepsilon \in \mathrm{L}^\infty_w([0,T],Q)$ satisfying the a priori bounds* (5.1)*. Then the coarse-grained densities $\hat{c^\varepsilon}$ converge strongly in $\mathrm{L}^1([0,T]\times\Omega)$.*

Proof. Lemma 5.6 provides that $\hat{c}^\varepsilon$ is bounded in $BV([0,T],\mathrm{W}^{1,\infty}(\Omega)^*)$ and Lemma 5.7 provides that $\hat{c}^\varepsilon$ is bounded in $\mathrm{L}^1([0,T],\mathrm{W}^{1,1}(\Omega))$. Since the embedding $\mathrm{W}^{1,1}(\Omega)\subset\mathrm{L}^1(\Omega)$ is compact and the embedding $\mathrm{L}^1(\Omega)\subset\mathrm{W}^{1,\infty}(\Omega)^*$ is continuous, Theorem 5.8 yields that the sequence $\hat{c^\varepsilon}$ is compact in $\mathrm{L}^1([0,T]\times\Omega)$. □

It is also clear that we get convergence towards the fast manifold, which results from the Fisher information of the fast reaction.

Lemma 5.10 (Convergence towards microscopic equilibrium and strong compactness)**.** *Let $(\mu^\varepsilon)_{\varepsilon>0}$, $\mu^\varepsilon\in\mathrm{L}^\infty_w([0,T],Q)$ satisfying the a priori bounds* (5.1)*. Then there is a subsequence such that $c^\varepsilon\to c^0$ strongly in $\mathrm{L}^1([0,T]\times\Omega)$ and, moreover, it holds $\rho_1^{V,0}=\rho_2^{V,0}$ a.e. in $[0,T]\times\Omega$.*

Proof. The bound on the dissipation functional provides $\int_0^T\int_\Omega\left(\sqrt{\rho_1^{V,\varepsilon}}-\sqrt{\rho_2^{V,\varepsilon}}\right)^2\mathrm{d}x\mathrm{d}t\leq C\varepsilon$. Hence, we conclude $\|\sqrt{\rho_1^{V,\varepsilon}}-\sqrt{\rho_2^{V,\varepsilon}}\|_{\mathrm{L}^2([0,T]\times\Omega)}\to 0$ as $\varepsilon\to 0$. In particular, we conclude that $\rho_1^{V,0}=\rho_2^{V,0}$. The strong convergence towards the slow manifold provides strong convergence for the whole sequence. Indeed, using Cauchy-Schwartz inequality and $x-y=\left(\sqrt{x}-\sqrt{y}\right)\left(\sqrt{x}+\sqrt{y}\right)$, we have

$$\|\rho_1^{V,\varepsilon}-\rho_2^{V,\varepsilon}\|_{\mathrm{L}^1([0,T]\times\Omega)}\leq\|\sqrt{\rho_1^{V,\varepsilon}}-\sqrt{\rho_2^{V,\varepsilon}}\|_{\mathrm{L}^2([0,T]\times\Omega)}\|\sqrt{\rho_1^{V,\varepsilon}}+\sqrt{\rho_2^{V,\varepsilon}}\|_{\mathrm{L}^2([0,T]\times\Omega)}.$$

The last term can be estimated by the AM-GM inequality

$$\|\sqrt{\rho_1^{V,\varepsilon}}+\sqrt{\rho_2^{V,\varepsilon}}\|^2_{\mathrm{L}^2([0,T]\times\Omega)}=\int_0^T\int_\Omega\rho_1^{V,\varepsilon}+\rho_2^{V,\varepsilon}+2\sqrt{\rho_1^{V,\varepsilon}\rho_2^{V,\varepsilon}}\mathrm{d}x\mathrm{d}t\leq 2\int_0^T\int_\Omega\left(\rho_1^{V,\varepsilon}+\rho_2^{V,\varepsilon}\right)\mathrm{d}x\mathrm{d}t,$$

and the right-hand side is bounded since $\mu(t)\in Q$ for $t\in[0,T]$. Hence, we conclude that $\|\rho_1^{V,\varepsilon}-\rho_2^{V,\varepsilon}\|_{\mathrm{L}^1([0,T]\times\Omega)}\to 0$ as $\varepsilon\to 0$.

Using this convergence, we have that also $c_i^\varepsilon\to c_i^0$ strongly in $\mathrm{L}^1([0,T]\times\Omega)$. Indeed, we have

$$\begin{aligned}
c_i^\varepsilon-w_i^V\frac{c_1^0+c_2^0}{w_1^V+w_2^V}&=w_i^V\left(\frac{c_i^\varepsilon}{w_i^V}-\frac{c_1^0+c_2^0}{w_1^V+w_2^V}\right)\\
&=w_i^V\left(\frac{c_i^\varepsilon}{w_i^V}-\frac{c_1^\varepsilon+c_2^\varepsilon}{w_1^V+w_2^V}+\frac{c_1^\varepsilon+c_2^\varepsilon}{w_1^V+w_2^V}-\frac{c_1^0+c_2^0}{w_1^V+w_2^V}\right)\\
&=(-1)^i\left(\frac{\frac{c_2^\varepsilon}{w_2^V}-\frac{c_1^\varepsilon}{w_1^V}}{w_1^Vw_2^V\left(w_1^V+w_2^V\right)}\right)+\frac{w_i^V}{w_1^V+w_2^V}\left(c_1^\varepsilon+c_2^\varepsilon-(c_1^0+c_2^0)\right),
\end{aligned}$$

and both terms converge strongly to zero as $\varepsilon\to 0$ by convergence of $\hat{c}^\varepsilon\to\hat{c}^0$ and $\rho_1^{V,\varepsilon}-\rho_2^{V,\varepsilon}\to 0$. □

Finally, we show that the limit $\mu^0=c^0\mathrm{d}x$ has an absolutely continuous representative in the space of probability measures. To do this, we exploit the characterization of absolutely continuous curves as solutions of the continuity equation following [AGS05].

Proposition 5.11. *Let $(\mu^\varepsilon)_{\varepsilon>0}$, $\mu^\varepsilon \in \mathrm{L}^\infty([0,T],Q)$ satisfying the a priori bounds (5.1) and let c^0 be the limit of the densities c^ε. Then the coarse-grained slow variable $\hat{\mu} = \mu_1^0+\mu_2^0 = (c_1^0+c_2^0)\,\mathrm{d}x \in \mathrm{L}^\infty_w([0,T],\mathrm{Prob}(\Omega))$ has a representative (in time), which is absolutely continuous in the space of probability measures equipped with the 2-Wasserstein metric. Moreover, each component μ_i^0 has an absolutely continuous representative (in time), which is absolutely continuous in the space of non-negative Radon measures equipped with the 1-Wasserstein metric.*

Proof. The coarse-grained measures $\hat{\mu}^\varepsilon$ satisfy continuity equation $\dot{\hat{\mu}}^\varepsilon + \mathrm{div}(\hat{J}^\varepsilon) = 0$ in the sense of distributions where $\hat{J}^\varepsilon = J_1^\varepsilon + J_2^\varepsilon$ is the coarse-grained diffusion flux. Since the linear continuity equation is stable under weak convergence, we conclude that also the limits satisfy the same continuity equation $\dot{\hat{\mu}}^0 + \mathrm{div}(\hat{J}^0) = 0$, where $\hat{J}^0$ is the weak*-limit of $\hat{J}^\varepsilon$ (see Lemma 5.7). Using (4.9), the bound on the dissipation functional implies a bound $\int_0^T \int_\Omega \mathsf{Q}(\hat{c}^0,\hat{J}^0)\mathrm{d}x\mathrm{d}t < \infty$. Let us define the transport velocity $\hat{v} \in \mathcal{M}([0,T]\times\Omega,\mathbb{R})$

$$\hat{v} = \begin{cases} \frac{\hat{J}}{\hat{c}} & \text{for } \hat{c}>0 \\ 0 & \text{for } \hat{c}=0 \end{cases}.$$

Then $\int_0^T\int_\Omega \mathsf{Q}(\hat{c},\hat{J})\mathrm{d}x\mathrm{d}t = \frac{1}{2}\int_0^T\int_\Omega |\hat{v}|^2\hat{c}\mathrm{d}x\mathrm{d}t = \frac{1}{2}\int_0^T\int_\Omega |\hat{v}|^2\mathrm{d}\hat{\mu}\mathrm{d}t$ and the bound on the dissipation functional implies the bound on the Borel velocity field $\|\hat{v}\|_{\mathrm{L}^2(\hat{\mu})}<\infty$. Hence, by Theorem 8.3.1 from [AGS05] it follows that $t\mapsto\hat{\mu}(t)\in(\mathrm{Prob}(\Omega),d_{\mathcal{W}_2})$ has a continuous representative which is absolutely continuous.

To prove time-regularity for μ_i^0 for $i=1,2$, we first observe that $\mu_i^0 = \frac{w_i^V}{w_1^V+w_2^V}\hat{\mu}$ is a non-negative Radon measure. To show that it has an absolutely continuous representative, we proceed as in Lemma 5.6 and exploit the dual formulation of the 1-Wasserstein distance on the space of non-negative Radon measures, i.e. integrating against Lipschitz functions (see e.g. [Edw11]). Let $\phi\in\mathrm{C}^1(\Omega)$ with $\|\phi\|_{\mathrm{W}^{1,\infty}(\Omega)}\le 1$. Using the continuity equations $\dot{\hat{\mu}}^0+\mathrm{div}(\hat{J}^0)=0$, we conclude for all $[t_1,t_2]\subset[0,T]$ that

$$\begin{aligned}\int_\Omega \phi\cdot(\mathrm{d}\mu_i^0(t_2)-\mathrm{d}\mu_i^0(t_1)) &= \int_{t_1}^{t_2}\langle\phi,\dot{\mu}_i^0\rangle\mathrm{d}t = \int_{t_1}^{t_2}\langle\phi\frac{w_i^V}{w_1^V+w_2^V},\dot{\hat{\mu}}\rangle\mathrm{d}t \\ &\le \int_{t_1}^{t_2}\int_\Omega \nabla\left(\phi\frac{w_i^V}{w_1^V+w_2^V}\right)\cdot\hat{J}\;\mathrm{d}x\;\mathrm{d}t \le C\int_{t_1}^{t_2}\int_\Omega|\hat{J}|\;\mathrm{d}x\;\mathrm{d}t,\end{aligned}$$

where $C=C(w,V)$. The bound on the dissipation functional provides again that the right-hand side is bounded for each interval $[t_1,t_2]\subset[0,T]$. Summing up, we conclude that μ_i^0 has an absolutely continuous representative, which proves the claim. □

5.2 Liminf-estimate

In this section, we state and prove the liminf-estimate of the Γ-convergence result Theorem 4.2. Once the compactness is established the proof of the liminf-estimate is comparatively easy.

Theorem 5.12. *Let $\mu^\varepsilon\to\mu^0$ in $\mathrm{L}^\infty{}_w([0,T],Q)$ such that $\sup_{\varepsilon\in]0,1]}\sup_{t\in[0,T]}\mathcal{E}(\mu^\varepsilon)<\infty$. Then, we have the liminf-estimate*

$$\liminf_{\varepsilon\to0}\mathfrak{D}_\varepsilon(\mu^\varepsilon)\ge\mathfrak{D}_0(\mu^0),$$

where the limit dissipation functional is defined by

$$\mathfrak{D}_0^V(\mu)=\begin{cases}\int_0^T \mathcal{R}_{\mathrm{eff}}(\mu,\dot\mu)+\mathcal{R}^*_{\mathrm{eff}}(\mu,-\mathrm{D}\mathcal{E}^V(\mu))\mathrm{d}t, & \mu\in \mathrm{AC}([0,T],Q),\mu=c\,\mathrm{d}x \text{ a.e. in } [0,T]\\ \infty & \text{otherwise}\end{cases}$$

with

$$\begin{aligned}\mathcal{R}^*_{\mathrm{eff}}(\mu,\xi)&=\mathcal{R}^*_{\mathrm{diff}}(\mu,\xi)+\chi_{\{\xi_1=\xi_2\}}(\xi)\\ \mathcal{R}_{\mathrm{eff}}(\mu,v)&=\inf\left\{\sum_{j=1}^2\int_\Omega \widetilde{\mathsf{Q}}(\delta_j c_j,J_j)\mathrm{d}x : u_1+u_2=0,\left\{\begin{array}{c}v_1=-\mathrm{div}J_1+u_1\\ v_2=-\mathrm{div}J_2+u_2\end{array}\right\}\right\}.\end{aligned}$$

Proof. We may assume that $\mathfrak{D}_\varepsilon(\mu^\varepsilon)\le C<\infty$ (otherwise the claim is trivial). For the given curves $t\mapsto\mu^\varepsilon(t)\in Q$ take diffusive fluxes J^ε and reactive fluxes b^ε, which satisfy the generalized continuity equation

$$(c,J,b)\in(\mathrm{gCE})\quad\Leftrightarrow\quad\left\{b_1+b_2=0 \text{ and } \left\{\begin{array}{c}\dot c_1=-\mathrm{div}J_1+b_1\\ \dot c_2=-\mathrm{div}J_2+b_2\end{array}\right\}\right\},$$

and approximate the infimum in $\mathfrak{D}_\varepsilon(\mu^\varepsilon)$ arbitrarily close, i.e.

$$\mathfrak{D}_\varepsilon(\mu_\varepsilon)+\varepsilon\ge\int_0^T\mathcal{D}_\varepsilon(\mu_\varepsilon,J^\varepsilon,b^\varepsilon)\mathrm{d}t.$$

The integrand $\mathcal{D}_\varepsilon$ consists of a velocity and a slope part and both of them split into a reaction and a diffusion part:

$$\begin{aligned}\mathcal{D}_\varepsilon(\mu,J,b)&=\int_\Omega\sum_{j=1}^2\widetilde{\mathsf{Q}}\left(\delta_j c_j,J_j\right)\mathrm{d}x+\int_\Omega\widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon},b_2(x)\right)\mathrm{d}x+\\ &\quad+\frac12\int_\Omega\sum_{j=1}^2\delta_j w_j^V\frac{\left|\nabla\rho_j^V\right|^2}{\rho_j^V}\mathrm{d}x+\frac{2}{\varepsilon}\int_\Omega\sqrt{w_1^Vw_2^V}\left(\sqrt{\rho_1^V}-\sqrt{\rho_2^V}\right)^2\mathrm{d}x\\ &=:\mathcal{V}_{\mathrm{diff}}(\mu,J)+\mathcal{V}_{\mathrm{react},\varepsilon}(\mu,b)+\mathcal{S}_{\mathrm{diff}}(\mu)+\mathcal{S}_{\mathrm{react},\varepsilon}(\mu)\ .\end{aligned}$$

Clearly, we also have $\int_0^T\mathcal{D}_\varepsilon(\mu_\varepsilon,J^\varepsilon,b^\varepsilon)\mathrm{d}t\le C+\varepsilon<\infty$. By Lemma 5.10, we conclude compactness for the densities $c^\varepsilon\to c^0$ in $\mathrm{L}^1([0,T]\times\Omega\times\{1,2\})$ and by Lemma 5.7 that $J^\varepsilon\overset{*}{\rightharpoonup}J^0$ in $\mathcal{M}([0,T]\times\Omega\times\{1,2\})$. Using the lower-semicontinuity result from Lemma 5.2 (which implies the liminf-estimates for $\mathcal{V}_{\mathrm{diff}}$ and $\mathcal{S}_{\mathrm{diff}}$) and that $\mathcal{V}_{\mathrm{react},\varepsilon},\mathcal{S}_{\mathrm{react},\varepsilon}\ge0$, we obtain the estimate

$$\liminf_{\varepsilon\to0}\int_0^T\mathcal{D}_\varepsilon(\mu^\varepsilon)\mathrm{d}t\ge\int_0^T\left\{\int_\Omega\sum_{j=1}^2\widetilde{\mathsf{Q}}(\delta_jc_j^0,J_j^0)\mathrm{d}x+\frac12\int_\Omega\sum_{j=1}^2\delta_jw_j^V\frac{|\nabla\rho_j^0|^2}{\rho_j^0}\mathrm{d}x\right\}\mathrm{d}t.$$

Let us define $A_i^\varepsilon=\dot c_i^\varepsilon+\mathrm{div}J_i^\varepsilon$. We conclude convergence for $A_i^\varepsilon\to A_i^0$ in the sense of distributions, and, moreover, we have $A_1^\varepsilon+A_2^\varepsilon\to\dot c_1^0+\dot c_2^0+\mathrm{div}J_1^0+\mathrm{div}J_2^0=0$. Let us define $u_1:=A_0^2=\dot c_2^0+\mathrm{div}J_2^0$ and $u_2:=A_0^1=\dot c_1^0+\mathrm{div}J_1^0$. Then $u_1+u_2=0$, $A_1^0+u_1=0$ and $A_2^0+u_2=0$. In particular, we conclude the pointwise estimate

$$\int_\Omega\sum_{j=1}^2\widetilde{\mathsf{Q}}(\delta_jc_j^0,J_j^0)\mathrm{d}x\ge\inf_{(J,u)}\left\{\int_\Omega\sum_{j=1}^2\widetilde{\mathsf{Q}}(\delta_jc_j^0,J_j^0)\mathrm{d}x:\left\{\begin{array}{c}\dot c_1+\mathrm{div}J_1+u_1=0\\ \dot c_2+\mathrm{div}J_2+u_2=0\\ u_1+u_2=0\end{array}\right\}\right\},$$

which finally establishes the liminf-estimate

$$\liminf_{\varepsilon\to 0}\int_0^T \mathcal{D}_\varepsilon(\mu^\varepsilon)\mathrm{d}t \geq \mathfrak{D}_0^V(\mu).$$

□

5.3 Construction of the recovery sequence

In this section, we construct the recovery sequence for the functional $\mathfrak{D}_0^V$ to finish the Γ-convergence result in Theorem 4.2. To be precise, we will show the following:

Theorem 5.13. *Let $\mu^0 \in \mathrm{L}^\infty_w([0,T]\times\Omega,\mathbb{R}^2_{\geq 0})$ such that the a priori bounds $\mathfrak{D}_0^V(\mu^0)<\infty$ and $\operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^0(t))<\infty$ hold. Then there is a sequence $(\mu^\varepsilon)_{\varepsilon>0}$, $\mu^\varepsilon\in\mathrm{AC}([0,T],Q)$, $\sup_{\varepsilon>0}\ \operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^\varepsilon(t))<\infty$, such that the densities converge $c^\varepsilon\to c^0$ strongly in $\mathrm{L}^1([0,T]\times\Omega\times\{1,2\})$ and we have $\mathfrak{D}_\varepsilon^V(\mu^\varepsilon)\to\mathfrak{D}_0^V(\mu^0)$.*

Using Proposition 4.5, we see that the limit functionals do not contain more information than the functionals in coarse-grained variables and it holds $\mathfrak{D}_0^V(\mu^0)=\hat{\mathfrak{D}}(\hat{\mu}^0)$. Hence, we may reconstruct the dissipation functional with the corresponding diffusion and reaction flux (J,b) from the coarse-grained variables $(\hat{c},\hat{J})$.

The dissipation functional $\mathfrak{D}_0^V$ is defined on the space of general fluctuations around the solution of the evolution equation (1.2). These fluctuations are neither strictly positive nor smooth. The proof of the limsup-estimate is done in several steps, which are elaborated in the next lemmas. The bound $\mathfrak{D}_0^V(\mu^0)<\infty$ can be assumed without loss of generality because the other case is already treated in the liminf-estimate.

Proof of Theorem 5.13. We do the reconstruction in three steps using different approximation methods. We will do the following steps:

1. Proposition 5.21 shows that for $\mu^0=c^0\mathrm{d}x$ with sufficiently smooth and positive density c^0 the constant sequence $\mu^{\epsilon,\gamma}=\mu^0$ satisfies $|\mathfrak{D}_\varepsilon(\mu^{\epsilon,\gamma})-\mathfrak{D}_0(\mu^{\epsilon,\gamma})|\to 0$.

2. Lemma 5.15 overcomes the positivity assumption, i.e. it shows that for all $\mu^0=c^0\mathrm{d}x$ there is a positive c^γ such that $c^\gamma\to c^0$ and $\mathfrak{D}_0(\mu^\gamma)\to\mathfrak{D}_0(\mu^0)$ as $\gamma\to 0$.

3. A mollification argument as in [AGS05, Lemma 8.1.10] and stated in Lemma 5.20 allows us to overcome regularity by smoothing, which shows $\mathfrak{D}_0(\mu^{\epsilon,\gamma})\to\mathfrak{D}_0(\mu^\gamma)$ as $\epsilon\to 0$.

Hence, defining the recovery sequence $\mu^\varepsilon:=\mu^{\epsilon,\gamma}$, we have

$$\left|\mathfrak{D}_\varepsilon(\mu^\varepsilon)-\mathfrak{D}_0(\mu^0)\right|\leq|\mathfrak{D}_\varepsilon(\mu^{\epsilon,\gamma})-\mathfrak{D}_0(\mu^{\epsilon,\gamma})|+|\mathfrak{D}_0(\mu^{\epsilon,\gamma})-\mathfrak{D}_0(\mu^\gamma)|+\left|\mathfrak{D}_0(\mu^\gamma)-\mathfrak{D}_0(\mu^0)\right|,$$

where the first term tends to zero by the first reconstruction step, the second term tends to zero by the third reconstruction step and the third term tends to zero by the second reconstruction step, which in total proves the desired convergence. □

Before performing the three recovery steps in Section 5.3.2, we first illustrate the general idea of constructing the recovery sequence by forgetting about positivity and regularity issues for the first moment.

5.3.1 Construction of recovery sequence for smooth and positive measures

To show the general idea, let us firstly assume that the density of $\hat{\mu}$ is sufficiently smooth and positive, i.e. we assume that its Lebesgue density satisfies $\hat{c} \geq \frac{1}{C} > 0$ on $\Omega \times [0,T]$ and has a enough regularity that will be specified below. Let $\hat{J}$ be the diffusion flux which provides the minimum in $\hat{\mathfrak{D}}(\hat{\mu}^0) = \mathfrak{D}_0^V(\mu)$ and satisfies $\dot{\hat{c}} + \mathrm{div}(\hat{J}) = 0$. We define the reconstructed variables by

$$c_1 = \frac{w_1^V}{w_1^V + w_2^V}\hat{c}, \quad c_2 = \frac{w_2^V}{w_1^V + w_2^V}\hat{c}, \quad J_1 = \frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\hat{J}, \quad J_2 = \frac{\delta_2 w_2^V}{\delta_1 w_1^V + \delta_2 w_2^V}\hat{J}.$$
$$b_1 = \left(\frac{\delta_1 - \delta_2}{\delta_1 w_1^V + \delta_2 w_2^V}\frac{w_1^V w_2^V}{w_1^V + w_2^V}\right)\mathrm{div}\hat{J} + \hat{J}\cdot\nabla\left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right), \quad b_2 = -b_1. \tag{5.3}$$

The reconstructed concentrations c and diffusion fluxes $J = (J_1, J_2)$ are proportional to the coarse grained concentration $\hat{c}$ and diffusion flux $\hat{J}$, respectively. On the coarse-grained level, which considers only one species there is no reaction flux anymore. (This changes when considering large reaction-diffusion system as explained in Section 6). The reactive flux $b = (b_1, b_2)$ is given as a function of the coarse-grained diffusion flux $\hat{J}$, which means that in the limit the diffusion determines the hidden reaction.

Concerning regularity issues, we immediately observe the following. Since w^V is smooth and positive, c_1, c_2 have the same regularity as $\hat{c}$ and also J_1, J_2 have the same regularity as $\hat{J}$. Only the reaction fluxes b_i are a priori not well-defined (e.g. in L^1) if $\mathrm{div}\hat{J}$ and $\hat{J}$ are not regular enough. This means, that the reaction flux between the fast-connected species is not well-defined for general $\hat{J} \in \mathcal{M}(\Omega \times [0,T], \mathbb{R}^3)$. Note, that regularity assumptions for $\mathrm{div}\hat{J}$ are not needed if $\delta_1 = \delta_2$, i.e. if both species diffuse with the same diffusion constant. In particular, in this situation no regularization argument as in Lemma 5.20 is necessary. Moreover, no additional regularity for $\hat{J}$ is needed if $\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V} = \theta \in]0,1[$ is constant. This is equivalent to

$$V_1(x) - V_2(x) = \log\left(\frac{1-\theta}{\theta}\frac{\delta_1}{\delta_2}\frac{\beta}{\alpha}\right) = \mathrm{const},$$

which means that the potentials V_1, V_2 differ in a constant on Ω. In particular, this implies that for the coarse-grained potential $\hat{V}$ we have $\nabla\hat{V} = \nabla V_1 = \nabla V_2$. As we will see, enough regularity for $\hat{J}$ is already obtained from bounds on the dissipation functional. Of course, regularity properties for $\mathrm{div}\hat{J}$ and $\hat{J}$ are independent of each other.

So let us assume for the moment that b_i is well-defined. Then we conclude $(c, J, b) \in$ (gCE), because we have

$$\begin{aligned}
\dot{c}_1 + \mathrm{div}J_1 &= \frac{w_1^V}{w_1^V + w_2^V}\dot{\hat{c}} + \mathrm{div}\left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\hat{J}\right) = \\
&= \frac{w_1^V}{w_1^V + w_2^V}\dot{\hat{c}} + \hat{J}\cdot\nabla\left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right) + \left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right)\mathrm{div}\hat{J} \\
&= -\frac{w_1^V}{w_1^V + w_2^V}\mathrm{div}\hat{J} + \hat{J}\cdot\nabla\left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right) + \left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right)\mathrm{div}\hat{J} = b_1,
\end{aligned}$$

where we used that $(\hat{c}, \hat{J})$ solves $\dot{\hat{c}} + \mathrm{div}\hat{J} = 0$. Similarly, we see that $\dot{c}_2 + \mathrm{div}J_2 = b_2$ and, by definition, we have $b_1 + b_2 = 0$. Moreover, boundary properties of $\hat{J}$ remain for $J = (J_1, J_2)$.

Since $\frac{c_1}{w_1^V} = \frac{c_2}{w_2^V}$, we conclude that $\mathfrak{D}_\varepsilon^V(\mu) \leq \mathfrak{D}_0(\mu) + \int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \mathrm{d}x\mathrm{d}t$. That means, that for proving that the constant sequence $\mu^\varepsilon = \mu$ is a recovery sequence, it suffice to show that $\int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \mathrm{d}x\mathrm{d}t \to 0$ as $\varepsilon \to 0$. This is, in fact, shown in the next lemma under the assumption that $\mathrm{div}\hat{J}, \hat{J} \in \mathrm{L}^{\mathsf{C}}([0,T]\times\Omega)$. The proof basically uses the monotonicity property of the Legendre dual function $\widetilde{\mathsf{C}}(a_1, b) \leq \widetilde{\mathsf{C}}(a_2, b)$ as $a_1 \geq a_2$ (see Lemma 4.4), its superlinear growth and the dominated convergence theorem.

Lemma 5.14. *Let $\hat{c} \in \mathrm{L}^1(\Omega\times[0,T])$ with $\hat{c} \geq \frac{1}{C}$ a.e. in $[0,T]\times\Omega$ for a constant $C > 0$, and let $\hat{J} : \Omega \to \mathbb{R}^d$ satisfy $\mathrm{div}\hat{J}, |\hat{J}| \in \mathrm{L}^{\mathsf{C}}([0,T]\times\Omega)$. Then $\int_0^T\int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \mathrm{d}x\mathrm{d}t \to 0$ as $\varepsilon \to 0$.*

Proof. Since $\hat{c} \geq \frac{1}{C}$ a.e., Lemma 4.4 yields $\widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \leq \widetilde{\mathsf{C}}\left(\frac{1}{C\varepsilon}, b_2\right) = \frac{1}{C\varepsilon}\mathsf{C}(C\varepsilon b_2)$. Moreover, we have the estimate

$$\tfrac{1}{2}|r|\log(|r|+1) \leq \mathsf{C}(r) \leq 2|r|\log(|r|+1),$$

which implies

$$\int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \mathrm{d}x\mathrm{d}t \leq \tfrac{1}{C\varepsilon} \int_0^T \int_\Omega \mathsf{C}(C\varepsilon b_2)\,\mathrm{d}x\mathrm{d}t \leq \int_0^T \int_\Omega 2|b_2|\log(C\varepsilon|b_2|+1)\mathrm{d}x\mathrm{d}t.$$

By assumption, we have that $\mathrm{div}\hat{J}, |\hat{J}| \in \mathrm{L}^{\mathsf{C}}([0,T]\times\Omega)$. Since $V \in \mathrm{C}^1(\overline{\Omega})$ and the Orlicz space $\mathrm{L}^{\mathsf{C}}([0,T]\times\Omega)$ is a Banach space, we conclude that $b_2 \in \mathrm{L}^{\mathsf{C}}([0,T]\times\Omega)$. By the inequality for C, this implies that for $\varepsilon < \frac{1}{C}$, the right-hand side is bounded. We show that (for a subsequence) the integrand converges to zero pointwise a.e. in $[0,T]\times\Omega$. By the dominated convergence theorem, this would imply that $\int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1c_2}}{\varepsilon}, b_2\right) \mathrm{d}x\mathrm{d}t \to 0$ as $\varepsilon \to 0$.

To see that the integrand converges to zero pointwise, we firstly observe that $b_2 \in \mathrm{L}^{\mathsf{C}}([0,T]\times\Omega) \subset \mathrm{L}^1([0,T]\times\Omega)$, which means that

$$\int_0^T \int_\Omega \log(\varepsilon|b_2|+1)\mathrm{d}x\mathrm{d}t \leq \varepsilon \int_0^T \int_\Omega |b_2|\mathrm{d}x\mathrm{d}t \to 0.$$

Hence, (for a subsequence) $\log(\varepsilon|b_2|+1)$ converges pointwise to zero and, thus, also $|b_2|\log(C\varepsilon|b_2|+1)$. □

In fact, the above proof is quite robust and already suggests that the same convergence holds even if $\hat{c}^\varepsilon \to 0$ not to fast somewhere in $\Omega\times[0,T]$ and $\|b_\varepsilon^2\| \approx \varepsilon^{-\alpha}$ for some $\alpha > 0$. This is proved in Proposition 5.21.

In the following, we need to overcome the positivity assumption $\hat{c} \geq \frac{1}{C}$ and the regularity assumption for $\hat{J}$ and $\mathrm{div}\hat{J}$. The first is done by shifting the density $\hat{c}^\delta := \frac{1}{Z_\delta}(\hat{c}+\delta)$, $\delta > 0$; the necessary regularity of $\hat{J}$ is provided immediately by the bound on the dissipation functional; the regularity of $\mathrm{div}\hat{J}$ is achieved by smoothing using that $(\hat{c}, \hat{J})$ is a solution of the coarse-grained continuity equation $\dot{\hat{c}} + \mathrm{div}\hat{J} = 0$.

5.3.2 Auxiliary results for construction of recovery sequence for general measures

First, we show how to overcome the positivity assumption. This is done by a controlled positive shift.

Lemma 5.15. *For all $\mu^0 = c^0\,\mathrm{d}x$ satisfying $\mathfrak{D}_0^V(\mu^0) = \hat{\mathfrak{D}}(\hat{\mu}^0) < \infty$ there is a sequence $(\hat{c}^\gamma)$ of densities satisfying $\hat{c}^\gamma \geq \gamma$, $\hat{c}^\gamma \to \hat{c}$ in $\mathrm{L}^1([0,T]\times\Omega)$ such that for their corresponding measures we have $\hat{\mathfrak{D}}(\hat{\mu}^\gamma) = \mathfrak{D}_0(\mu^\gamma) \to \mathfrak{D}_0(\mu^0) = \hat{\mathfrak{D}}(\mu^0)$ as $\gamma \to 0$ and $\sup_{\gamma\in]0,1]} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}(\mu^\gamma(t)) < \infty$.*

Proof. For small $\gamma > 0$, we define $\hat{c}^\gamma := \frac{1}{Z_\gamma}(\hat{c} + 2\gamma)$, where $Z_\gamma = 1 + 2\gamma|\Omega| = 1 + 2\gamma > 0$ is the normalization factor such that $\int_\Omega \hat{c}^\gamma \mathrm{d}x = 1$. Hence, $Z_\gamma \searrow 1$, $\hat{c}^\gamma \to \hat{c}$, $\sup_{\gamma\in]0,1]} \operatorname{ess\,sup}_{t\in[0,T]} \mathcal{E}(\mu^\gamma(t)) < \infty$ and w.l.o.g. we assume that $\hat{c}^\gamma \geq \gamma$. Moreover, we define $\hat{J}^\gamma := \frac{1}{Z_\gamma}\hat{J}$. Clearly, $\hat{J}^\gamma \cdot \nu = 0$ on $\partial\Omega$ and $(\hat{c}^\gamma, \hat{J}^\gamma)$ solves the continuity equation $\dot{\hat{c}}^\gamma + \mathrm{div}\hat{J}^\gamma = 0$. We compute the terms in the dissipation functional $\mathfrak{D}_0^V(\mu^\gamma)$. We have $\hat{\rho}^{V,\gamma} = \frac{\hat{c}^\gamma}{w^V} = \frac{1}{Z_\gamma}\frac{\hat{c}+2\gamma}{w^V}$. Using the bounds $\sup_{x\in\overline{\Omega}} \left\{\nabla\left(1/w^V\right), w^V\right\} \leq C$, we get

$$\nabla\hat{\rho}^{V,\gamma} = \frac{1}{Z_\gamma}\left\{\nabla\left(\frac{\hat{c}}{w^V}\right) + 2\gamma\nabla\left(\frac{1}{w^V}\right)\right\} \quad\Rightarrow\quad \left|\nabla\hat{\rho}^{V,\gamma}\right| \leq \frac{1}{Z_\gamma}\left\{\left|\nabla\hat{\rho}^V\right| + 2\gamma C\right\}$$

Using the estimates $\frac{1}{a+\delta} \leq \frac{1}{a}$, $\frac{1}{Z_\gamma} \leq 1$ and the inequality $2xy \leq \sqrt{\gamma}x^2 + \frac{1}{\sqrt{\gamma}}y^2$ in the second estimate, we get the pointwise estimate

$$\begin{aligned}
\frac{|\nabla\hat{\rho}^{V,\gamma}|^2}{\hat{\rho}^{V,\gamma}} &= \frac{1}{Z_\gamma}\frac{\left(\left|\nabla\hat{\rho}^V\right| + 2\gamma C\right)^2}{\hat{\rho}^V + \frac{2\gamma}{w^V}} = \frac{1}{Z_\gamma}\frac{\left|\nabla\hat{\rho}^V\right|^2 + 4\gamma C\left|\nabla\hat{\rho}^V\right| + 4\gamma^2C^2}{\hat{\rho}^V + \frac{2\gamma}{w^V}}\\
&\leq \frac{\left|\nabla\hat{\rho}^V\right|^2}{\hat{\rho}^V} + 2\frac{2\gamma C\left|\nabla\hat{\rho}^V\right|}{\hat{\rho}^V + \frac{2\gamma}{w^V}} + \frac{4\gamma^2C^2}{\hat{\rho}^V + \frac{2\gamma}{w^V}}\\
&\leq \frac{\left|\nabla\hat{\rho}^V\right|^2}{\hat{\rho}^V} + \frac{1}{\hat{\rho}^V + \frac{2\gamma}{w^V}}\left(\sqrt{\gamma}\left|\nabla\hat{\rho}^V\right|^2 + \frac{1}{\sqrt{\gamma}}\left\{2\gamma C\right\}^2\right) + 2\gamma C^2 w^V\\
&\leq \frac{\left|\nabla\hat{\rho}^V\right|^2}{\hat{\rho}^V}(1+\sqrt{\gamma}) + 2\sqrt{\gamma}w^V C^2(1+\sqrt{\gamma}).
\end{aligned}$$

Hence, $\int_0^T\int_\Omega \delta^V w^V \frac{|\nabla\hat{\rho}^{V,\gamma}|^2}{\hat{\rho}^{V,\gamma}}\mathrm{d}x\mathrm{d}t \to \int_0^T\int_\Omega \delta^V w^V \frac{|\nabla\hat{\rho}^V|^2}{\hat{\rho}^V}\mathrm{d}x\mathrm{d}t$ as $\gamma \to 0$.

Similarly, we get

$$\int_0^T\int_\Omega \frac{|\hat{J}^\gamma|^2}{\hat{\delta}\hat{c}^\gamma}\mathrm{d}x\mathrm{d}t = \frac{1}{Z_\gamma}\int_0^T\int_\Omega \frac{|\hat{J}|^2}{\hat{\delta}\,(\hat{c}+2\gamma)}\mathrm{d}x\mathrm{d}t \leq \int_0^T\int_\Omega \frac{|\hat{J}|^2}{\hat{\delta}\hat{c}}\mathrm{d}x\mathrm{d}t,$$

which implies that $\int_0^T\int_\Omega \widetilde{\mathsf{Q}}(\hat{\delta}\hat{c}^\gamma, \hat{J}^\gamma)\mathrm{d}x\mathrm{d}t \leq \int_0^T\int_\Omega \widetilde{\mathsf{Q}}(\hat{\delta}\hat{c}, \hat{J})\mathrm{d}x\mathrm{d}t$. Hence, we conclude that $\hat{c}^\gamma \geq \gamma$, $\hat{c}^\gamma \to \hat{c}$ and $\hat{\mathfrak{D}}(\hat{c}^\gamma) \to \hat{\mathfrak{D}}(\hat{c})$ as $\gamma \to 0$. □

Next, we are going to show that the flux $b_1 = -b_2$ can be made sufficiently smooth, i.e. at least in L^{C} which would allow us to proceed similar as in Lemma 5.14.

Recalling the formula for the reconstructed flux, we have

$$b_2 = \left(\frac{\delta_1 - \delta_2}{\delta_1 w_1^V + \delta_2 w_2^V}\frac{w_1^V w_2^V}{w_1^V + w_2^V}\right)\mathrm{div}\hat{J} + \hat{J}\cdot\nabla\left(\frac{\delta_1 w_1^V}{\delta_1 w_1^V + \delta_2 w_2^V}\right) =: a_1\mathrm{div}\hat{J} + \hat{J}\cdot a_2$$

and $b_2 = -b_1$, where $a_1 \in \mathrm{C}^1(\overline{\Omega},\mathbb{R})$, $a_2 \in \mathrm{C}^0(\overline{\Omega},\mathbb{R}^d)$ such that $\sup_{x\in\overline{\Omega}}\{|a_1(x)|, |a_2(x)|\} \leq C$. In particular, the regularity of $b_1 = -b_2$ does not depend on a_1, a_2. We are going to prove that $\mathrm{div}\hat{J}$ and $\hat{J}$ have enough regularity. The regularity of $\hat{J}$ follows from the bound on the dissipation functional. The regularity of $\mathrm{div}\hat{J}$ is achieved by mollification.

First, we show that $\hat{J} \in \mathrm{L}^{\tilde{p}}([0,T]\times\Omega)$, for some $\tilde{p}>1$. Clearly, we have $\hat{J} \in \mathrm{L}^1([0,T]\times\Omega)$ by Lemma 5.1 and the bound on the dissipation functional. To improve the regularity of $\hat{J}$, we firstly improve the regularity of $\hat{c} \in \mathrm{L}^p([0,T]\times\Omega)$ which is provided from the bound on the dissipation functional $\mathfrak{D}_0$ and the energy functional $\mathcal{E}$. The bound on the energy yields $\hat{c} \in \mathrm{L}^\infty([0,T],\mathrm{L}^1(\Omega))$. The bound on the Fisher-information yields again by Lemma 5.1 that $\hat{c} \in \mathrm{L}^1([0,T],\mathrm{W}^{1,1}(\Omega))$ as in Lemma 5.7. By the Sobolev embedding theorem, we have the compact embedding $\mathrm{W}^{1,1}(\Omega)\subset \mathrm{L}^q(\Omega)$, where $1-\frac{1}{d}>\frac{1}{q} \Leftrightarrow q<\frac{d}{d-1}$. Thus $\hat{c}\in \mathrm{L}^\infty([0,T],\mathrm{L}^1(\Omega))\cap \mathrm{L}^1([0,T],\mathrm{L}^{\frac{d}{d-1}}(\Omega))$. Using the next classical interpolation result we get $\hat{c}\in \mathrm{L}^p([0,T]\times\Omega)$ for some $p>1$.

Theorem 5.16 (Theorem 5.1.2, [BeL76])**.** *Let X_1, X_2 be Banach spaces. Then for the complex interpolation spaces, it holds for any $\theta\in]0,1[$*

$$[\mathrm{L}^{p_1}([0,T],X_1),\mathrm{L}^{p_2}([0,T],X_2)]_\theta \simeq \mathrm{L}^{p_\theta}([0,T],[X,Y]_\theta),$$

where $\frac{1}{p_\theta}=\frac{1-\theta}{p_1}+\frac{\theta}{p_2}$.

In our particular situation, we have the following.

Lemma 5.17. *Let $\mu^0\in \mathrm{L}^\infty_w([0,T],Q)$ such that $\mathfrak{D}_0^V(\mu^0)<\infty$ and $\operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^0(t))<\infty$. Then the density $\hat{c}^0$ is in $\mathrm{L}^p([0,T]\times\Omega)$ with $p=\frac{d+1}{d}>1$.*

Proof. To apply Theorem 5.16, we first observe that the Lebesgue spaces form interpolation couples. In our situation we have $p_1=1, p_2=\infty$, $X_1=\mathrm{L}^{\frac{d}{d-1}}(\Omega), X_2=\mathrm{L}^1(\Omega)$. Hence, $p_\theta=\frac{1}{1-\theta}>1$. Moreover, $[X,Y]_\theta=[\mathrm{L}^q(\Omega),\mathrm{L}^1(\Omega)]_\theta\simeq \mathrm{L}^{q_\theta}(\Omega)$, where $\frac{1}{q_\theta}=\frac{1-\theta}{q}+\frac{\theta}{1}$. Setting $p_\theta=q_\theta$, we conclude $\frac{1-\theta}{1-2\theta}=q=\frac{d}{d-1}$. Solving $p_\theta=q_\theta$ for θ, we obtain $\theta=\frac{1}{1+d}$, and hence $p_\theta=q_\theta=\frac{d+1}{d}>1$. Summarizing, we conclude

$$\hat{c}\in \mathrm{L}^\infty([0,T],\mathrm{L}^1(\Omega)) \cap \mathrm{L}^1([0,T],\mathrm{W}^{1,1}(\Omega)) \subset \mathrm{L}^{\frac{d+1}{d}}([0,T]\times\Omega). \tag{5.4}$$

□

Remark 5.18. In particular, if $d=2$, then $\hat{c}\in \mathrm{L}^{3/2}([0,T]\times\Omega)$ and if $d=3$, then $\hat{c}\in \mathrm{L}^{4/3}([0,T]\times\Omega)$. Iterating the procedure, it is even possible to obtain $\hat{c}\in \mathrm{L}^{(d+2)/d}(([0,T]\times\Omega))$ for $d\geq 2$.

Knowing integrability of $\hat{c}$, we get also better integrability of the fluxes $\hat{J}\in \mathrm{L}^{\tilde{p}}([0,T]\times\Omega)$ for some $\tilde{p}>1$, which follows from the next lemma.

Lemma 5.19.

1. *We have for all $J\in\mathbb{R}^d$ and $c>0$ that*

$$\frac{|J|^2}{c}+\frac{1}{p}c^p \geq \left(1+\frac{1}{p}\right)|J|^{\frac{2p}{p+1}}.$$

2. *Let $\mu^0\in \mathrm{L}^\infty_w([0,T]\times\Omega,\mathbb{R}^2_{\geq 0})$ such that $\mathfrak{D}_0^V(\mu^0)<\infty$ and $\operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^0(t))<\infty$ and let $\hat{J}\in\mathcal{M}([0,T]\times\Omega,\mathbb{R}^d)$ be the corresponding diffusion flux satisfying the continuity equation. Then $\hat{J}\in \mathrm{L}^{\tilde{p}}([0,T]\times\Omega,\mathbb{R}^d)$ for $\tilde{p}=\frac{2d+2}{2d+1}>1$.*

Proof. For proving the first part, let us define for fixed $J \in \mathbb{R}^d$ the function $F :]0,\infty[\to \mathbb{R}$, $F(c) := \frac{|J|^2}{c} + \frac{1}{p}c^p$. Clearly, $F \geq 0$ and $F(c) \to \infty$ as $c \to 0$ or $c \to \infty$. We compute the minimum. We have $F'(c) = -|J|^2 c^{-2} + c^{p-1}$ and hence the critical point is at $c_0 = |J|^{2/(p+1)}$. Inserting c_0 into F we get $F(c) \geq F(c_0) = |J|^2 |J|^{-2/(p+1)} + \frac{1}{p}|J|^{2p/(p+1)} = (1+\frac{1}{p})|J|^{2p/(p+1)}$, which proves the claim.

For second part, we use that by Lemma 5.17 we have $\hat{c} \in \mathrm{L}^p([0,T]\times\Omega)$ for $p = \frac{d+1}{d}$. This implies by the first part that $\hat{J} \in \mathrm{L}^{\tilde{p}}([0,T]\times\Omega,\mathbb{R}^d)$ for $\tilde{p} = \frac{2\frac{d+1}{d}}{\frac{d+1}{d}+1} = \frac{2d+2}{2d+1}$. □

To obtain regularity for the whole reaction flux $b_1 = -b_2$, we have to get regularity also for $\mathrm{div}\hat{J}$. This is done by mollifying the solution $(\hat{c},\hat{J})$ of the continuity equation $\dot{\hat{c}} + \mathrm{div}\hat{J} = 0$ in time. We already now that $\hat{c} : [0,T] \to \mathrm{Prob}(\Omega)$ is continuous by Lemma 5.11. With a slight abuse of notation, we denote by $\hat{c}$ also a continuous continuation on $\mathbb{R}$ such that $\hat{c} \in \mathrm{L}^p(\mathbb{R},\mathrm{L}^p(\Omega))$. Now, we mollify in time and define $\hat{c}^\epsilon(t) = \int_{\mathbb{R}} \hat{c}(s)\psi_\epsilon(t-s)\mathrm{d}s$ where ψ_ϵ is a positive and symmetric mollifier. Analogously, we define $\hat{J}^\epsilon$ by convolution, i.e. $\hat{J}^\epsilon(t) = \int_{\mathbb{R}} \hat{J}(s)\psi_\epsilon(t-s)\mathrm{d}s$. Since the continuity equation is linear, the smoothed functions $(\hat{c}^\epsilon,\hat{J}^\epsilon)$ satisfy again the continuity equation with the same no-flux boundary conditions.

The next lemma shows that the dissipation functional can be approximated by mollifying $(\hat{c},\hat{J})$. This basically uses the convexity of $\hat{\mathfrak{D}}$ in $(\hat{c},\hat{J})$.

Lemma 5.20. *Let $\mu^0 \in \mathrm{L}^\infty_w([0,T]\times\Omega,\mathbb{R}^2_{\geq 0})$ such that the a priori bounds $\mathfrak{D}_0^V(\mu^0) < \infty$ and $\operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^0(t)) < \infty$ hold. Let $\hat{J} \in \mathcal{M}([0,T]\times\Omega,\mathbb{R}^d)$ be the corresponding diffusion flux satisfying the continuity equation. Let $\psi^\epsilon : \mathbb{R} \to \mathbb{R}$ be a positive and symmetric mollifier. Define $\hat{c}^\epsilon(t) = \int_{\mathbb{R}} \hat{c}(s)\psi_\epsilon(t-s)\mathrm{d}s$ and $\hat{J}^\epsilon(t) = \int_{\mathbb{R}} \hat{J}(s)\psi_\epsilon(t-s)\mathrm{d}s$. Then, we have $\sup_{\epsilon\in]0,1]} \operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^\varepsilon(t)) < \infty$ and*

$$\begin{aligned}\int_0^T \left\{ \int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}(\delta_j c_j^\epsilon, J_j^\epsilon)\mathrm{d}x + \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{|\nabla\rho_j^\epsilon|^2}{\rho_j^\epsilon}\mathrm{d}x \right\}\mathrm{d}t \\ \to \int_0^T \left\{ \int_\Omega \sum_{j=1}^2 \widetilde{\mathsf{Q}}(\delta_j c_j^0, J_j^0)\mathrm{d}x + \frac{1}{2}\int_\Omega \sum_{j=1}^2 \delta_j w_j^V \frac{|\nabla\rho_j^0|^2}{\rho_j^0}\mathrm{d}x \right\}\mathrm{d}t,\end{aligned} \tag{5.5}$$

which in particular, implies that $\mathfrak{D}_\varepsilon^V(\mu^\varepsilon) \to \mathfrak{D}_0^V(\mu^0)$.

Proof. The energy bound on μ^ϵ is trivially satisfied. The convergence for the dissipation functional (5.5) follows directly as the proof of Lemma 8.1.10 in [AGS05] since the integrand is convex in $(\hat{c},\hat{J})$. □

With these preparations, we are able to show the remaining step in the proof of Theorem 5.13. The next proposition shows in analogy to Lemma 5.14 that the contribution by the reaction flux b_2^ϵ to the dissipation functional $\mathfrak{D}_\varepsilon^V$ converges to zero as $\epsilon \to 0$.

Proposition 5.21. *Let $\mu^0 \in \mathrm{L}^\infty_w([0,T]\times\Omega,\mathbb{R}^2_{\geq 0})$ such that $\mathfrak{D}_0^V(\mu^0) = \hat{\mathfrak{D}}_0(\hat{\mu}) < \infty$ and $\operatorname{ess\,sup}_{t\in[0,T]}\mathcal{E}(\mu^0(t)) < \infty$ and let $\hat{J} \in \mathcal{M}([0,T]\times\Omega,\mathbb{R}^d)$ be the corresponding diffusion flux satisfying the continuity equation. Let $\psi^\epsilon : \mathbb{R} \to \mathbb{R}$ be a positive and symmetric mollifier, which is specified below. Let $\hat{c}^\epsilon, \hat{J}^\epsilon$ the mollified functions as in Lemma 5.20 and $\hat{c}^{\epsilon,\gamma}, \hat{J}^{\epsilon,\gamma}$ the mollified and shifted functions as in Lemma 5.15.*

Let ψ^ε be such that $\|\dot{\hat{c}}^\epsilon\|_{\mathrm{L}^{\tilde{p}}([0,T]\times\Omega)} \lesssim \frac{1}{\epsilon^\alpha}$ and $\gamma \geq C\epsilon^{1-\lambda}$ for $\epsilon \to 0$, where $\tilde{p}$ is the integrability exponent of the fluxes as in Lemma 5.19, $C > 0$ is a positive constant and $\lambda \in [0,1[$, $\alpha \in [0,1]$ satisfies the inequality $d+1 \leq \frac{\lambda}{2\alpha}$. Then, we have $|\mathfrak{D}_\varepsilon(\mu^{\epsilon,\gamma}) - \mathfrak{D}_0(\mu^{\epsilon,\gamma})| \to 0$.

Proof. First, we observe that for given $\hat{c}$ such a mollifier and these constants α, λ satisfying all the conditions can be easily constructed.

To prove the convergence, we follow the same strategy as in the proof of Lemma 5.14. Defining the reconstructed concentrations and fluxes as in (5.3), we observe that

$$|\mathfrak{D}_\varepsilon(\mu^{\epsilon,\gamma}) - \mathfrak{D}_0(\mu^{\epsilon,\gamma})| \leq \int_0^T \int_\Omega \widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1^{\epsilon,\gamma}c_2^{\epsilon,\gamma}}}{\varepsilon}, b_2^{\epsilon,\gamma}\right) \mathrm{d}x\mathrm{d}t\,.$$

Using the bound from below on $\hat{c}^\epsilon$, and the inequality $\log(x+1) \leq C_{\tilde{p}} x^{\tilde{p}-1}$, we get the estimate

$$\begin{aligned}\widetilde{\mathsf{C}}\left(\frac{\sqrt{c_1^{\epsilon,\gamma}c_2^{\epsilon,\gamma}}}{\varepsilon}, b_2^{\epsilon,\gamma}\right) &\leq \widetilde{\mathsf{C}}\left(C\epsilon^{-\lambda}, b_2^{\epsilon,\gamma}\right) \leq C\epsilon^{-\lambda}\mathsf{C}\left(C^{-1}\epsilon^\lambda b_2^{\epsilon,\gamma}\right)\\ &\leq 2C\epsilon^{-\lambda}|b_2^{\epsilon,\gamma}|C^{-1}\epsilon^\lambda \log\left(C^{-1}\epsilon^\lambda|b_2^{\epsilon,\gamma}|+1\right)\\ &\leq 2C_{\tilde{p}}|b_2^{\epsilon,\gamma}|C^{-\tilde{p}+1}\epsilon^{\lambda(\tilde{p}-1)}|b_2^{\epsilon,\gamma}|^{\tilde{p}-1} \leq \tilde{C}|b_2^{\epsilon,\gamma}|^{\tilde{p}}\epsilon^{\lambda(\tilde{p}-1)},\end{aligned}$$

where $\tilde{C} = \tilde{C}(C_{\tilde{p}}, C)$. By $\|\dot{c}^\epsilon\|_{\mathrm{L}^{\tilde{p}}([0,T]\times\Omega)} \lesssim \frac{1}{\epsilon^\alpha}$, we conclude that $\|\mathrm{div}\hat{J}^\epsilon\|_{\tilde{p}} \lesssim \frac{1}{\epsilon^\alpha}$, and by Lemma 5.19, we have $\hat{J}^\epsilon \in \mathrm{L}^{\tilde{p}}([0,T]\times\Omega)$. Together this implies that $\|b_2^\epsilon\|_{\mathrm{L}^{\tilde{p}}([0,T]\times\Omega)} \lesssim \frac{1}{\epsilon^\alpha}$. Hence, we get

$$|\mathfrak{D}_\varepsilon(\mu^{\epsilon,\gamma}) - \mathfrak{D}_0(\mu^{\epsilon,\gamma})| \lesssim \varepsilon^{\lambda(\tilde{p}-1)}\varepsilon^{-\tilde{p}\alpha} = \varepsilon^{-\frac{1}{2d+1}\{(2d+2)\alpha-\lambda\}}.$$

Choosing, $\lambda, \alpha \in [0,1[$ such that $d+1 \leq \frac{\lambda}{2\alpha}$, we conclude that the right-hand side converges to zero, which proves the claim. □

6 Remarks for reaction-diffusion systems involving more species

In the last section, we comment on linear reaction-diffusion systems involving more species. The evolution equation for concentrations $c \in \mathbb{R}^I_{\geq 0}$, $I \in \mathbb{N}$ is given by

$$\dot{c} = \mathrm{diag}(\delta_1, \dots, \delta_I)\Delta c + A^\varepsilon c$$

where $A^\varepsilon = A^S + \frac{1}{\varepsilon}A^F$ is a Markov generator (preserving positivity and total mass), which consists of a slow part and a fast part. The main assumption is the A^εsatisfies detailed balance with respect to its stationary measure w^ε. Similar to [MiS20, MPS20], we are going to assume that the stationary vector w^ε satisfies $w^\varepsilon \to w^0$ as $\varepsilon \to 0$ and that $w^0 > 0$. The positivity of the limit stationary measure w^0 means that in the limit the evolution respects all concentrations c_i and is not degenerate.

The gradient structure is defined on the state space

$$Q = \mathrm{Prob}(\Omega \times \{1, \cdots, I\}) := \{\mu = (\mu_1, \dots, \mu_I) \in \mathbb{R}^I : \mu_i \in \mathcal{M}(\Omega),\ \mu_i \geq 0,\ \mu_i(\Omega) = 1\}.$$

The driving energy functional $\mathcal{E}_\varepsilon : X \to \mathbb{R}_\infty$ has the form

$$\mathcal{E}_\varepsilon(\mu) = \begin{cases} \int_\Omega \sum_{j=1}^I E_B\left(\frac{c_j}{w_j^\varepsilon}\right) w_j^\varepsilon \mathrm{d}x, & \text{if } \mu = c\,\mathrm{d}x \\ \infty, & \text{otherwise.} \end{cases},$$

and the dual dissipation potential splits into two parts

$$\mathcal{R}^*(\mu,\xi) = \mathcal{R}^*_{\mathrm{diff}}(\mu,\xi) + \mathcal{R}^*_{\mathrm{react}}(\mu,\xi)$$
$$\mathcal{R}^*_{\mathrm{diff}}(\mu,\xi) = \frac{1}{2}\int_\Omega \sum_{j=1}^I \delta_j |\nabla \xi_j(x)|^2 \mathrm{d}\mu_j,\ \mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu,\xi) = \int_\Omega \sum_{i<j} \kappa_{ij}^\varepsilon \mathsf{C}^*(\xi_i(x) - \xi_j(x))\,\mathrm{d}\sqrt{\mu_i\mu_j},$$

where $\kappa_{ij}^\varepsilon := A_{ij}^\varepsilon \left(\frac{w_j^\varepsilon}{w_i^\varepsilon}\right)^{1/2}$. In particular, the reaction part of the dissipation potential splits into a fast part and a slow part

$$\mathcal{R}^*_{\mathrm{react},\varepsilon}(\mu,\xi) = \mathcal{R}^*_{\mathrm{slow},\varepsilon}(\mu,\xi) + \frac{1}{\varepsilon}\mathcal{R}^*_{\mathrm{fast},\varepsilon}(\mu,\xi)$$
$$\mathcal{R}^*_{\mathrm{xy},\varepsilon}(\mu,\xi) = \int_\Omega \sum_{i<j} \tilde{\kappa}_{ij}^\varepsilon\, \mathsf{C}^*(\xi_i(x) - \xi_j(x))\ \mathrm{d}\sqrt{\mu_i\mu_j}, \quad \mathrm{xy} \in \{\mathrm{slow}, \mathrm{fast}\},$$

where $\tilde{\kappa}_{ij}^\varepsilon$ are bounded and positive uniformly in $\varepsilon > 0$. In particular, we call a reaction and its flux b_{ij} slow if $A_{ij}^\varepsilon = O(1)$ and fast if $A_{ij}^\varepsilon = O(\varepsilon^{-1})$. Due to the detailed balance assumption and by $w^0 > 0$, the distinction between fast and slow reactions is indeed well-defined.

In the remainder of the section, we briefly explain how to generalize the proof of the EDP-convergence result also for this situation. Major differences occur at two stages, namely in 1) deriving compactness for slow reaction fluxes, 2) proving the limsup-estimate. The reaction fluxes of the fast reactions are not seen in the limit and have to be reconstructed in an analogous way as in the 2-species situation. Firstly, we explain the compactness result and the liminf-estimate. Secondly, we comment on the limsup-estimate.

6.1 Compactness for slow reaction fluxes and liminf-estimate

Here, we comment on proving compactness and the liminf-estimate for the multi species case. In comparison to the previous situation, compactness for the concentrations, by using strong compactness for coarse-grained variables and convergence towards the slow manifold, can be derived (cf. Lemmas 5.6, 5.10). Moreover, compactness of diffusion fluxes and spatial regularity follows, too (cf. Lemma 5.19).

In contrast to the situation of two species connected with one fast reaction, where no slow reaction fluxes exists, compactness for slow reaction fluxes b_{ij}^ε has to be derived in the multi species case. This follows immediately from Lemma 5.2, once compactness of $\sqrt{c_i^\varepsilon c_j^\varepsilon}$ is obtained. At this point it is clear that weak convergence of $c^\varepsilon \rightharpoonup c^0$ is not sufficient. Instead the previously derived strong convergence of $c^\varepsilon \to c^0$ implies by dominated convergence also strong convergence of $\sqrt{c_i^\varepsilon c_j^\varepsilon} \to \sqrt{c_i^0 c_j^0}$ in $\mathrm{L}^1([0,T]\times\Omega)$, and hence, compactness for the slow fluxes b_{ij}^ε. Compactness for fast reaction fluxes can not be obtained as already mentioned in Remark 5.5. Having proved compactness, the proof of the liminf-estimate is exactly the same as for Theorem 5.12, since the functional $\mathcal{D}_\varepsilon$ is jointly convex in all variables (c, J, b).

6.2 Equilibration and reconstruction of reaction fluxes und recovery sequence

A crucial observation throughout the proof of the Γ-convergence was Lemma 4.4, which provides an equilibration of fluxes assuming microscopic equilibria for the concentrations. In Lemma 4.5, we derived equilibration for the diffusion fluxes. Similarly, also an equilibration of the slow reaction fluxes can be derived. In [MiS20] a general operator-theoretic coarse-graining and reconstruction procedure has been developed. This method can also be applied to derive coarse-grained fluxes and a coarse-grained continuity equation, see [Ste21]. Importantly for us, as in (5.3) the reconstructed slow reaction fluxes depend linearly on the coarse-grained reaction fluxes. The fast reaction fluxes are then of the form

$$b_{ij} = a_1 \mathrm{div} \hat{J}_i + a_2 \hat{J}_i + \sum_{j=3}^{k(i)} a_{ij} \hat{b}_{ij},$$

where all functions a_j are $\mathrm{C}^0(\Omega, \mathbb{R}^{k_j})$, where $k_1 = 1$, $k_2 = d$ and $k_{ij} = 1$.

In order to prove that the constant sequence for smooth and positive concentrations is indeed a recovery sequence, we follow the same reasoning as in the Lemmas 5.14 and 5.21. The only difference comes from the explicit depends on the coarse-grained reaction flux $\hat{b}_{ij}$, Using the bound on the limit dissipation functional (which provides bounds on $\int_0^T \int_\Omega \widetilde{\mathsf{C}}(\sqrt{\hat{c}_i \hat{c}_j}, \hat{b}_{ij}) \mathrm{d}x\mathrm{d}t$) and the next Lemma 6.1, we obtain that $\hat{b}_{ij} \in \mathrm{L}^{\mathsf{C}}([0,T] \times \Omega)$ (we refer to [FrM21] for a proof). Since L^{C} is an Orlicz-space, we conclude that the reconstructed fluxes b_i are in L^{C}. This allows to proceed as in Lemma 5.21 and proves the existence of a recovery sequence.

Lemma 6.1 ([FrM21]). *Let $p > 1$. Then, for all $a \geq 0$ and $B \in \mathbb{R}$ we have*

$$\widetilde{\mathsf{C}}(a, B) \geq \left(1 - \frac{1}{p}\right) \widetilde{\mathsf{C}}(B) - \frac{2}{p} a^p.$$

In particular, setting $a = \sqrt{c_i c_j}$ and $B = b_{ij}$ we have

$$\int_0^T \int_\Omega \widetilde{\mathsf{C}}(\sqrt{c_i c_j}, b_{ij}) \mathrm{d}x\mathrm{d}t + \|\sqrt{c_i c_j}\|^p_{\mathrm{L}^p([0,T]\times\Omega)} \gtrsim \int_0^T \int_\Omega \widetilde{\mathsf{C}}(b_{ij}) \mathrm{d}x\mathrm{d}t,$$

which proves that $b_{ij} \in \mathrm{L}^{\mathsf{C}}([0,T] \times \Omega)$ if $c_i, c_j \in \mathrm{L}^p([0,T] \times \Omega)$ for some $p > 1$.

Acknowledgement: The research was supported by Deutsche Forschungsgemeinschaft (DFG) through the Collaborative Research Center SFB 1114 "*Scaling Cascades in Complex Systems*" (Project no. 235221301), subproject C05 "Effective models for materials and interfaces with multiple scales". The author is grateful to Alexander Mielke for many helpful discussions and for having proposed the problem.

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Part 4

Memory equations as reduced Markov processes

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This is a pre-copy-editing, author-produced PDF of an article accepted for publication in *Discrete and Continuous Systems* following peer review.
The definitive publisher-authenticated version "Discrete and Continuous Systems, Volume 39, Number 4, April 2019, pp. 2133-2155, DOI:10.3934/dcds.2019089" is available online at: http://aimsciences.org/journal/1078-0947/2019/39/4.

Memory equations as reduced Markov processes*

Artur Stephan† and Holger Stephan‡

Abstract

A large class of linear memory differential equations in one dimension, where the evolution depends on the whole history, can be equivalently described as a projection of a Markov process living in a higher dimensional space. Starting with such a memory equation, we propose an explicit construction of the corresponding Markov process. From a physical point of view the Markov process can be understood as a change of the type of some quasiparticles along one-way loops. Typically, the arising Markov process does not have the detailed balance property. The method leads to a more realistic modeling of memory equations. Moreover, it carries over the large number of investigation tools for Markov processes to memory equations like the calculation of the equilibrium state. The method can be used for an approximative solution of some degenerate memory equations like delay differential equations.

1 Introduction

Memory equations describe the time evolution of some quantity, considering the whole prehistory of the evolution: The past influences the future.

Markov processes, or more generally time evolutions with the Markov property, describe the problem under the assumption that the evolution can be predicted, knowing only the current state: The present influences the future.

At first glance, by means of memory equations, it is possible to investigate a wider class of problems, since evolution equations with the Markov property can be regarded as degenerate memory problems, where the dependence of the past is concentrated in one moment.

But from a philosophical point of view, it seems to be natural that a complete description of a problem has to be a Markov one for the following reason: The Markov property means that the solution operator is a semigroup, i.e. it is time shift invariant. Due to Noether's theorem, this invariant corresponds to the conservation of some energy, the dual variable of time. Thus, the Markov property is the typical property of a model, where some energy is conserved.

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Conversely, if the evolution is governed by a non-Markovian equation, it is not complete, some energy is lost. This requires finding more degrees of freedom unless the model is Markovian. In other words, it is to be expected that a non-Markovian description can be regarded as some part or restriction of a more-dimensional Markov process.

This theoretical thought can be confirmed in various practical situations:

- An arbitrary (nonlinear) dynamical system on a compact space $\mathcal{Z}$ can be equivalently formulated as a linear deterministic Markov process on the space of Radon measures on $\mathcal{Z}$ (see, e.g. [Ste05b]) via its Liouville equation.
- A general linear evolution equation that is nonlocal in space and time, including jumps and memory on some domain in $\mathbb{R}^n$, can be understood as a limit of a diffusion process (a special Markov process) on a complicated Riemannian manifold (see [KhS08]).
- The projection of a general Brownian motion (a special Markov process in phase space) on the coordinate space is a diffusion process if the initial velocity is Maxwellian (see [Ste05a]).

Hence, the idea that a memory equation can be regarded as part of a higher dimensional Markov process, does not seem to be very surprising. Indeed, the main result in this paper is that we provide the construction of an easily analyzable Markov process for a linear memory integral equation of convolution type with special non-negative kernel. Mathematically, the kernel is a linear combination of decaying exponentials with coefficients arising from Lagrange polynomials. Physically, such kernel arises in a natural way from modeling memory equations.

Let us briefly revise the basic facts in modeling and analyzing memory equations and Markov processes.

1.1 Memory equations

Memory equations (ME) are differential equations where the evolution depends not only on the current state but also on the past. MEs are a special case of functional differential equations - an equation of unknown functions and their derivatives with different argument values. The mathematical theory of functional differential equations (or integro-differential equations) is treated in [HaV93, KoM99].

From the viewpoint of modeling and analysis, MEs have attracted a lot of attention during the last decades. For example, they arise in modeling flows trough fissured media, [HoS90, Pes95] or in modeling heat conduction with finite wave speeds [GuP68]. We consider MEs of convolution type. Such equations arise also as effective limits of homogenization problems, starting with the pioneering work of L. Tartar [Tar90].

The object of interest is a linear memory equation of the form

$$\dot{u}(t) = -au + K * u = -au + \int_0^t K(t-s)u(s)\mathrm{d}s,\ u(0) = u_0, \tag{1}$$

where $u : [0, \infty[\to \mathbb{R}$ is a scalar state variable, $u_0 \in \mathbb{R}_{\geq 0}$ and $K : \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0}$ is a positive real kernel. Please note, we focus on a scalar variable, but our considerations can be generalized to systems as well as to non-autonomous linear PDEs (like diffusion equations with time-dependent diffusion coefficients).

Let us briefly explain the ME (1). In contrast to $\dot{u} = -au$, where the decay is quite fast, in this equation the decay is damped due to the influence of former states. The ME can be interpreted as a reduction of the mass into unknown depots. Phenomenologically, this can be modeled by $a = a(t)$, which yields a non-autonomous equation. Another way to think about (1) is the following. Introducing the function A defined by $A' = -K$ and $A(0) = a$, we get

$$\dot{u}(t) = -A(0)u - \int_0^t A'(t-s)u(s)\mathrm{d}s = -\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t A(t-s)u(s)\mathrm{d}s.$$

Integrating the above equation, we get

$$u(t) = u(0) - \int_0^t A(t-s)u(s)\mathrm{d}s$$

that can be regarded as a continuous analogue of the time-discrete scheme

$$u_n = u_0 - a_1 u_{n-1} - a_2 u_{n-2} - \dots. \tag{2}$$

Equivalently, using integration by parts we get

$$\dot{u}(t) = -A(t)u_0 - \int_0^t A(t-s)\dot{u}(s)\mathrm{d}s.$$

This form is often considered (e.g. in [Pes95]). Subsequently, we use the form (1).

For solving a ME, the memory described by $K(t)$ or $A(t)$ has to be known for any time $t \geq 0$. This is often postulated, i.e. $K(t)$ is given by heuristic arguments.

A typical and simple example is $K_\alpha(t) = \alpha \mathrm{e}^{-\alpha t}$ for $\alpha > 0$. Then $K_\alpha(t) \geq 0$ and $\int_0^\infty K_\alpha(t)\mathrm{d}t = 1$.

In this case, for $\alpha \longrightarrow +\infty$, the integral on the right-hand side of (1) tends to $u(t)$ – the ME becomes an ordinary differential equation.

In the same sense, a sequence of some other integrals of convolution type can tend to a delay differential equation (DDE), that means $K(t) = \sum_j \alpha_j \delta(t - t_j)$ for large enough $t \geq 0$. So, the kernel K can be interpreted as a measure on the time line that can be approximated by the "simplest" measures: convex combinations of δ-measures. Note that DDEs with the above kernel of the form

$$\dot{u} = -au + \sum_j \alpha_j u(t - t_j),$$

are solved with respect to an initial condition $\phi \in \mathrm{C}([-\max\{t_j\}, 0])$. That means the solution space is infinite dimensional. On the other hand regarding the modeling viewpoint, it is difficult to derive an initial value $\phi \in \mathrm{C}([0, T])$ for a DDE. Often the initial value ϕ is assumed to be constant or a simple given function. See e.g. [Smi11] for more details, where the analysis and applications especially for modeling aftereffect phenomena are presented.

The ME needs the initial value only for one fixed value, say $t = 0$. But, if $t \geq \max\{t_j\}$, the DDE becomes a ME. This means, that the beginning of the evolution is also modeled in the ME. In this sense, MEs include many types of differential equations like ODEs and DDEs. We remark that also from the modeling viewpoint it is more natural to treat kernels that are not located at precise time values but are smeared.

Another important property is the asymptotic behavior. The ME is a non-autonomous differential equation. The equilibrium cannot be calculated setting $\dot{u} = 0$. Assuming $\int_0^\infty K(t)\mathrm{d}t = a$, any constant solution $u(t) = u_0$ satisfies

$$\lim_{t\to\infty}\left(-au(t) + \int_0^t K(s)u(t-s)\mathrm{d}s\right) = 0.$$

Assuming $\int_0^\infty K(t)\mathrm{d}t \neq a$, there is no non-trivial solution that makes the right-hand side zero, so that there is no equilibrium of the ME.

1.2 Markov processes

There is a huge amount of literature on Markov Processes (MP) – see, e.g. [Bob05, Dur10, Dyn65]. Here we introduce our notation.

Let $\mathcal{Z}$ be a given state space, a compact topological space, $\mathcal{C} := \mathrm{C}(\mathcal{Z})$ the Banach space of continuous functions on $\mathcal{Z}$ and $\mathcal{P} := \mathcal{P}(\mathcal{Z})$ the set of probability measures, i.e. the subset of Radon measures p on $\mathcal{Z}$ with $p \geq 0$ and $p(\mathcal{Z}) = 1$.

A family $\mathbf{T}(t)$, $t \geq 0$ of linear bounded operators in $\mathcal{C}$ is called a *Markov semigroup* if it is a semigroup, i.e. if it satisfies

$$\mathbf{T}(t_1 + t_2) = \mathbf{T}(t_1)\mathbf{T}(t_2),\ \mathbf{T}(0) = \mathbf{I},\ t_1, t_2 \geq 0\ ,$$

it is positive $\mathbf{T}(t) \geq 0$ in the cone sense of $\mathcal{C}$ and $\mathbb{1}$, the constant function is a fix-point of $\mathbf{T}(t)$ for all $t \geq 0$, $\mathbf{T}(t)\mathbb{1} = \mathbb{1}$. We refer to [Are86, EnN00]. The semigroup property is often called *Markov property* and it is equivalent to the assumption that the trajectory depends only on the present time point and not on the past.

A linear operator $\mathbf{A}$ on $\mathcal{C}$ is called *Markov generator* if it is the generator of a Markov semigroup, i.e. if $g(t) = \mathbf{T}(t)g_0$, where $\mathbf{T}(t)$ is a Markov semigroup. Then $g(t) = \mathbf{T}(t)g_0$ is the solution of the equation

$$\dot{g}(t) = \mathbf{A}g(t),\ g(0) = g_0 \tag{3}$$

for an initial value g_0 from the domain of $\mathbf{A}$. This equation is called *backward Chapman-Kolmogorov equation*. A MP is the result of the action of the adjoint semigroup $\mathbf{T}^*(t)$ at a probability measure p_0, i.e. $p(t) = \mathbf{T}^*(t)p_0$. Any MP has at least one stationary probability measure $\mu \in \mathcal{P}$. It satisfies $\mathbf{T}^*(t)\mu = \mu$ for all $t \geq 0$. This is a consequence of the Markov-Kakutani Theorem. The stationary probability measure μ is an element of the null-space of $\mathbf{A}^*$.

In this paper we consider continuous-time MPs on discrete state spaces. $\mathcal{Z} = \{z_0, ..., z_N\}$ is a finite set of $N+1$ states. In this case, we have $\mathcal{C} = \mathbb{R}^{N+1}$ and $\mathcal{P}$ is the simplex of probability vectors $\mathcal{P} := \mathrm{Prob}(\{z_0, \ldots, z_N\}) := \{p \in \mathbb{R}^{N+1} : p_i \geq 0, \sum_{i=0}^{N+1} p_i = 1\}$ and a subset of $\mathbb{R}^{N+1}$, too. A Markov semigroup is a real matrix family $\mathbf{T}(t)$ on $\mathbb{R}^{N+1}$ with positive entries and row sum 1. Its adjoint is the transposed matrix family $\mathbf{T}^*(t)$.

A MP is $p(t) = \mathbf{T}^*(t)p_0$, where p_0 is some given probability vector. It satisfies the set of equations

$$\dot{p}(t) = \mathbf{A}^*p(t),\ p(0) = p_0, \tag{4}$$

where $\mathbf{A}^*$ is the adjoint of the corresponding Markov generator. This equation is called *forward Chapman-Kolmogorov equation*. In contrast to equation (3) describing the evolution of moment functions, equation (4) describes the evolution of probability vectors.

This means that one component of the vector $p(t)$ can be understood as the probability of the corresponding state, regardless of the probability of the other states.

It is well known that equation (4) has a unique solution $p(t) \in \mathcal{P}$ if and only if the off-diagonal elements are non-negative and the columns of $\mathbf{A}^*$ sum up to zero. Thus, for $\mathbf{A} = (A_{ij})$ we have $A_{ij} \geq 0$ for $i \neq j$ and $A_{ii} = -\sum_{i \neq j=1}^{n} A_{ij}$.

For a generic Markov matrix the stationary probability μ is unique and all trajectories $\mathbf{T}^*(t)p_0$ for any initial state p_0 converge to μ. We only consider MPs with a unique stationary probability.

The eigenvalues of a Markov generator have always strongly negative real part, except one eigenvalue 0. The corresponding eigenvector is $\mathbb{1}$ for $\mathbf{A}$ and μ for $\mathbf{A}^*$. If the eigenvalues λ_i of $\mathbf{A}^*$ are all different, every component of the solution to (4), i.e. every component of $\mathbf{T}^*(t)p_0$ is a linear combination of $\mathbb{1}$ and exponential decaying functions $\mathrm{e}^{-\lambda_i t}$.

A MP in $\mathbb{R}^{N+1}$ allows for different physical interpretations. Apart from the canonical interpretations as a probability vector, it can be understood as some concentration or amount of $N+1$ different materials. We will follow this interpretation and will assume that this amount of materials is represented by particles of different types. These particles can transform into each other, changing their type, which can be understood as a linear reaction. The entries of the Markov matrix A_{ij} describe the rates of transforming particles of type z_j into particles of type z_i. Therefore, if we are only interested in the amount of material of one type, it is enough to consider the corresponding component of the vector $p(t)$ only. The initial amount of material is p_0. Since $\mathbf{A}$ is a Markov generator, positivity of the concentration and the whole mass is conserved.

If a Markov generator $\mathbf{A} = (A_{ij})$ and its stationary state $\mu = (\mu_i)$ satisfy $A_{ij}\mu_j = A_{ji}\mu_i$ for any $i, j \in \{1, \ldots, n\}$, it is said that the corresponding MP has the detailed balance property. It is equivalent to the case that the matrix (A_{ij}) is symmetric in the L^2-Hilbert space over μ. Such a matrix has to have real eigenvalues. We remark that the opposite is not true in general: A Markov process without the detailed balance can have real eigenvalues, too. Moreover, there can be no Hilbert space at all, where it is symmetric. From a physical point of view, the condition $A_{ij}\mu_j = A_{ji}\mu_i$ means that any transition $z_i \Leftrightarrow z_j$ is in a local equilibrium. Thus, the detailed balance case is easier to analyze but it rarely appears in general. The systems that we consider do not have the detailed balance property in principle.

1.3 What our paper deals with

In this paper, we connect the concepts of Markovian dynamics and non-Markovian dynamics, which seem to be different at first glance. Starting with a MP of a special form, we conclude a ME for the first coordinate. The ME is a scalar differential equation, but our considerations can also be applied to PDEs. The resulting MP can be physically understood; the ME is governed by a kernel which is the sum of exponential functions. Then another path is taken: Starting with a ME with an exponential kernel, we find a MP where its first component again yields the ME. The other components can be understood as hidden degrees of freedom that have to be included in a complete description of the problem. This procedure is not unique and thus, it cannot be said that the hidden degrees of freedom are real physical variables. On the other hand, the construction of the MP out of the kernel is intuitive since the kernel is approximated by its moments. This method can be used to approximate a general positive kernel taking the enlargement of

the MP into account. The simple case of two and three states is presented in chapter 2. In this case, all solutions and kernels can be calculated by hand. In chapter 3 we consider the general case. The main theorems are stated here.

The method has many physical and mathematical advantages – both for the theory of MPs and MEs. We want to highlight only two of them. Firstly, the modeling of a kernel for ME is usually done by heuristic arguments. The method presented here can be used to model kernels in a more convenient manner, since the MP has an underlying physical meaning. Moreover, the modeling of the beginning of the process is also done. Secondly, the asymptotic behavior of a non-autonomous differential equation can immediately be calculated from the Markovian dynamics.

The paper concludes with chapter 4. Here we note the connection to delay differential equations, where the kernel is highly degenerate. This is also reflected in the setting of MP: The underlying Markov generator has a very special form. We observe that the solution of the ME converges to the equilibrium of the MP. The spectral functions of ME and MP also converge.

Summarizing, we have the following connection of modeling levels:

$$\text{MP} \subset \text{DDE} \subset \text{ME} \subset \text{MP'}.$$

Here MP' is a Markov process with a larger number of degrees of freedom.

It is well known that a linear delay equation with delay T in a state space X can be regarded as an autonomous equation in a much larger space $\mathrm{C}([-T,0],X)$, see e.g. [EnN00]. There, the evolution of the delay equation is described by a semigroup of linear operators. This approach is not our aim in this paper. In our setting, the space of the MP' is not so large, typically.

Notion. In this paper, the Laplace transform is frequently used. Some properties are summarized in the appendix. MEs of convolution type have the important property that the Laplace transform maps them into multiplication operators. The Laplace transform $\mathcal{L}(u)$ of a real valued function $t \mapsto u(t)$ is defined by $\mathcal{L}(u)(\lambda) = \hat{u}(\lambda) = \int_0^\infty \mathrm{e}^{-\lambda t} u(t)\mathrm{d}t$. If there is no confusion, we omit the 'hat' on $\hat{u}$ and just write u or $u(\lambda)$.

Some analytical tools concerning Lagrange polynomials and simplex integrals are presented in the appendix, too.

2 Some simple Markov processes and memory equations

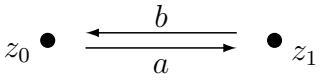
Before starting the general theory, we firstly present the basic ideas focusing on simple low dimensional examples – MPs with two and three states. Apart from the sake of simplicity nearly all phenomena of the general theory are eminent.

2.1 Two states

We consider a MP on a state space of two abstract states $\{z_0, z_1\}$, generated by the Markov generator

$$\mathbf{A} = \begin{pmatrix} -a & a \\ b & -b \end{pmatrix}, \quad \text{and its transpose} \quad \mathbf{A}^* = \begin{pmatrix} -a & b \\ a & -b \end{pmatrix}. \tag{5}$$

The matrix $\mathbf{A}^*$ describes the switching between the two states with given rates $a \geq 0$, $b \geq 0$. We can think of an amount of matter, represented by particles, which can occur in two types. For some reason we are interested only in particles of the first type.



The equation describing the evolution of the vector $p = (u, v)$ reads $\dot{p} = \mathbf{A}^* p$ with $p(0) = p_0$. We assume that in the beginning the total mass is concentrated in the first variable, i.e. $p_0 = (u_0, 0)$. In other words, all particles have type z_0.

The eigenvalues of $\mathbf{A}^*$ are $\{0, -(a+b)\}$. The stationary solution is given by $\mu = \left(\frac{b}{a+b}u_0, \frac{a}{a+b}u_0\right)$. It is unique unless the non interesting case $a = b = 0$. Any MP with two states has the detailed balance property.

For (u, v) the system reads as

$$\begin{cases} \dot{u} = -au + bv \\ \dot{v} = au - bv. \end{cases} \tag{6}$$

Using the Laplace transform and writing $u(\lambda) = \mathcal{L}(u(t))(\lambda)$ and $v(\lambda) = \mathcal{L}(v(t))(\lambda)$, we obtain a system of equations for (u, v) in the form

$$\begin{cases} (\lambda + a)u - u_0 = bv \\ (\lambda + b)v = au. \end{cases}$$

This yields an equation for u in the form

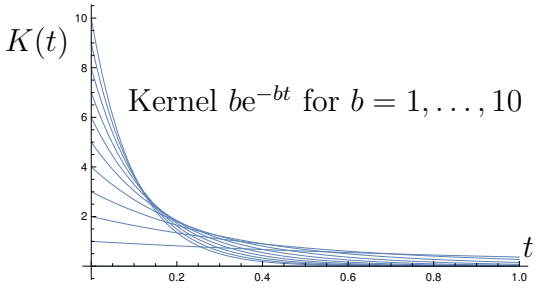
$$(\lambda + a)u - u_0 = \frac{ba}{\lambda + b}u \Rightarrow \lambda u - u_0 = -au + \frac{ba}{\lambda + b}u.$$

Using the inverse Laplace transform, we obtain a memory Equation for u

$$\dot{u} = -au + ab\int_0^t \mathrm{e}^{-b(t-s)}u(s)\mathrm{d}s = -a\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \mathrm{e}^{-b(t-s)}u(s)\mathrm{d}s. \tag{7}$$

The kernel $K(t) = b\mathrm{e}^{-bt}$ describes a dependence of the current state from previous time moments. For $b \longrightarrow \infty$, $K(t)$ tends to $\delta(t)$ and the equation becomes $\dot{u} = 0$.

Thus, the right hand side of equation (7) consists of two terms, the first one, $-au$ describes an exponential decay, whereas the second one, the memory term describes an opposite effect: Particles that disappear, occur after a while.



The time that passes between disappearing and reappearing, decreases with $1/b$. In the end, not all matter disappears like in a pure equation $\dot{u} = -au$ but an equilibrium between disappearance and reappearance arises.

The same effect is caused by the MP, changing the type of the particles. The particle changes the type from z_0 to z_1 with rate $a \geq 0$, it seems to disappear, if we look only at type z_0. After a while it re-changes to type z_1 (it occurs) with rate $b \geq 0$. This give

the exponential time behavior e^{-bt} (corresponding to the memory kernel $K(t) = b\mathrm{e}^{-bt}$), characteristic for MPs.

The equation (7) – or equivalently the system (6) – can be solved explicitly. We obtain for the Laplace transform

$$u(\lambda) = \frac{\lambda + b}{\lambda(\lambda + a + b)} u_0 = \left(\frac{b}{a+b} \frac{1}{\lambda} + \frac{a}{a+b} \frac{1}{\lambda + a + b} \right) u_0$$

and for the solution itself

$$u(t) = \frac{b}{a+b} u_0 + \frac{a}{a+b} e^{-(a+b)t} u_0$$

The solution tends to an equilibrium state $u_\infty = \frac{b}{a+b} u_0$, the first component of the stationary solution μ.

It is not possible to calculate it from the memory equation (7), directly. Setting $\dot{u} = 0$, the equation

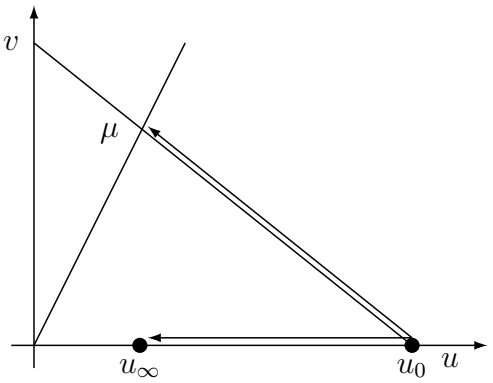
$$\dot{u} = -au + ab \int_0^t \mathrm{e}^{-b(t-s)} u(s) \mathrm{d}s = -a \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t \mathrm{e}^{-b(t-s)} u(s) \mathrm{d}s.$$

does not have any solution at all. Passing to the limit $t \longrightarrow \infty$ (and rewriting at first $\int_0^t \mathrm{e}^{-b(t-s)} u(s) \mathrm{d}s = \int_0^t \mathrm{e}^{-bs} u(t-s) \mathrm{d}s$) we obtain

$$0 = -au_\infty + ab \int_0^\infty \mathrm{e}^{-bs} u_\infty \mathrm{d}s \ .$$

Any constant u_∞ solves this equation. This strange behavior of the solution of memory equations is typical and can be illustrated in a picture, showing the time behavior of both, the solution of the MP and their first component – the solution of the memory equation.

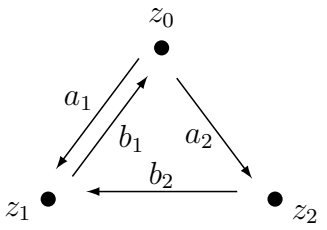
Investigating only the solution of the memory equation, it is not clear why the trajectory $u(t)$ stops in u_∞. Whereas looking from above, the trajectory $(u(t), v(t))$ has to stop at the stationary state μ, the intersection of the subspace $u + v = 1$ with the null space of $\mathbf{A}^*$.



2.2 Three states

A general memory kernel has not to be concentrated in $t = 0$. It can describe a transfer of mass from a very earlier time. It seems that this situation can be modeled by transitions between many quasiparticles before it appears at its starting type again. To understand the action of such a transition loop, we investigate in detail a special case of three states, namely the transformation of a fixed particle (type z_0) in two different quasiparticles.

One of them (type z_1) can be transformed back into type z_0 immediately, whereas the other (type z_2) can be transformed back into type z_0 only by two steps, changing at first to type z_1. This process is illustrated in the picture.



2.2.1 From Markov to memory

The simple MP on a state space of three abstract states $\{z_0, z_1, z_2\}$ is described by the Markov generator

$$\mathbf{A} = \begin{pmatrix} -a_1 - a_2 & a_1 & a_2 \\ b_1 & -b_1 & 0 \\ 0 & b_2 & -b_2 \end{pmatrix}, \quad \mathbf{A}^* = \begin{pmatrix} -a_1 - a_2 & b_1 & 0 \\ a_1 & -b_1 & b_2 \\ a_2 & 0 & -b_2 \end{pmatrix} \tag{8}$$

with $a_1, a_2, b_1, b_2 \geq 0$. The equation, generating the MP is

$$\dot{p}(t) = \mathbf{A}^* p(t), \quad p(0) = p_0. \tag{9}$$

Note, this is a Markov generator depending on four rates. A general Markov generator on $\mathbb{R}^3$ depends on six rates.

The stationary state μ is the solution to $\mathbf{A}^*\mu = 0$ and can be calculated easily as

$$\mu = \left(1 + \frac{a_1 + a_2}{b_1} + \frac{a_2}{b_2}\right)^{-1} \left(1, \frac{a_1 + a_2}{b_1}, \frac{a_2}{b_2}\right) u_0 = \frac{(b_1 b_2, a_1 b_2 + a_2 b_2, a_2 b_1)}{b_1 b_2 + a_1 b_2 + a_2 b_2 + a_2 b_1} u_0.$$

The eigenvalues (they have always non-positive real part) of the matrix are $\lambda_0 = 0$ and

$$\lambda_{1,2} = -\tfrac{1}{2}\left(a_1 + a_2 + b_1 + b_2 \pm \sqrt{(a_1 + a_2 + b_1 + b_2)^2 - 4(a_1 b_2 + a_2 b_1 + a_2 b_2 + b_1 b_2)}\right).$$

Depending on a_1, a_2, b_1, b_2 the eigenvalues can be real (e.g. $\lambda_1 = -5$, $\lambda_2 = -11$ for $a_1 = 2, a_2 = 5, b_1 = 8, b_2 = 1$) or complex (e.g. for $\lambda_{1,2} = -9 \pm 2i$ for $a_1 = 2, a_2 = 5, b_1 = 8, b_2 = 3$). (By the way, these are suitable values for an explicit solution with rational terms, only.)

This MP has the detailed balance property, if $b_1 b_2 a_2 = 0$, which is not interesting, since the coupling chain is broken. Roughly speaking, the detailed balance property means that for any loop in one direction there is a loop backwards with the same product of the rates. But this is not the case in our model. Thus, the MP under consideration violate the detailed balance property, generically.

The stationary state is unique if and only if the real parts of $\lambda_{1,2}$ are strongly negative. Or, equivalently, $b_1 b_2 + a_1 b_2 + a_2 b_2 + a_2 b_1 = 0$. Since the a_i, b_i are non negative, this is a non interesting case that we exclude. Then, the stationary state is the equilibrium state for any initial value. Note, that nevertheless some of the a_i, b_i might be zero.

As in the case of two states, we are interested only in the state z_0 of the system and ask for an evolution equation of this state. To do this, we introduce the notion $p = (u, v_1, v_2)$ and look for the evolution of u with an initial state $p_0 = (u_0, 0, 0)$. This is

naturally, since the states z_1 and z_2 are unknown, and there is no reason to assume that particles with z_1, z_2 exist in the beginning.

Equation (9) is now equivalent to the system

$$\left\{\begin{array}{rcrrrr} \dot{u}(t) &=& -(a_1+a_2)u(t) & +b_1v_1(t) & & \\ \dot{v}_1(t) &=& a_1u(t) & -b_1v_1(t) & +b_2v_2(t) & . \\ \dot{v}_2(t) &=& a_2u(t) & & -b_2v_2(t) & \end{array}\right.$$

Passing to the Laplace transform, we obtain with $u = \mathcal{L}u$, $v_i = \mathcal{L}v_i$ the system

$$\left\{\begin{array}{rcrrrr} \lambda u &=& -(a_1+a_2)u & +b_1v_1 & & +u_0 \\ \lambda v_1 &=& a_1u & -b_1v_1 & +b_2v_2 & . \\ \lambda v_2 &=& a_2u & & -b_2v_2 & \end{array}\right.$$

or equivalently, introducing $a = a_1 + a_2$, we get

$$\left\{\begin{array}{rrr} (\lambda+a)u - u_0 = & & b_1v_1 \\ (\lambda+b_1)v_1 = & a_1u + b_2v_2 & . \\ (\lambda+b_2)v_2 = & & a_2u \end{array}\right.$$

Here, v_1 and v_2 can be eliminated as

$$v_2 = \frac{a_2}{\lambda+b_2}u\ , \quad v_1 = \frac{a_1}{\lambda+b_1}u + \frac{b_2}{\lambda+b_1}v_2 = \frac{a_1}{\lambda+b_1}u + \frac{a_2b_2}{(\lambda+b_1)(\lambda+b_2)}u.$$

We conclude the following equation for u

$$\lambda u - u_0 = \left(-a + a_1\frac{b_1}{\lambda+b_1} + a_2\frac{b_1}{\lambda+b_1}\frac{b_2}{\lambda+b_2}\right)u. \tag{10}$$

This is an equation for the first state, only. It can be solved explicitly with respect to u. But, at this moment, this is not our aim. We are looking for an equation for u. We write

$$\frac{b_1}{\lambda+b_1}\frac{b_2}{\lambda+b_2} = \frac{b_1b_2}{b_2-b_1}\left(\frac{1}{\lambda+b_1} - \frac{1}{\lambda+b_2}\right),$$

and, after transforming inverse, we get an equation for the function $u(t)$, namely

$$\begin{aligned} \dot{u} &= -au + a_1b_1\int_0^t \mathrm{e}^{-b_1s}u(t-s)\mathrm{d}s + a_2\frac{b_1b_2}{b_2-b_1}\int_0^t(\mathrm{e}^{-b_1s} - \mathrm{e}^{-b_2s})u(t-s)\mathrm{d}s \qquad (11)\\ &= -au + (K*u)(t), \end{aligned}$$

where

$$K(t) = b_1a_1\mathrm{e}^{-b_1t} + a_2\frac{b_1b_2}{b_2-b_1}\left(\mathrm{e}^{-b_1t} - \mathrm{e}^{-b_2t}\right) = \tag{12}$$

$$= \left(b_1a_1 + \frac{b_1b_2a_2}{b_2-b_1}\right)\mathrm{e}^{-b_1t} - \frac{b_1b_2a_2}{b_2-b_1}\mathrm{e}^{-b_2t}. \tag{13}$$

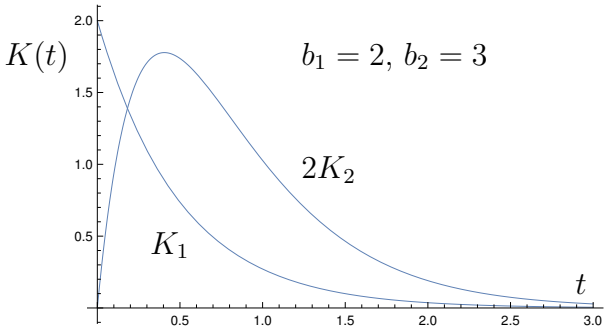
So, we obtain a memory equation with the kernel K. This equation describes the evolution of the first state of our physical system, depending on the whole past from 0 to

time t. Obviously, this dependence is a result of the projection, since nothing else had be done. Thus, $u(t)$ is the solution of two equivalent equations, a memory equation and a component of a Markov system. The kernel $K(t) = a_1K_1(t) + a_2K_2(t)$ is the sum of two parts

$$\begin{aligned} K_1(t) &= b_1 \mathrm{e}^{-b_1 t} \\ K_2(t) &= \frac{b_1 b_2}{b_2 - b_1} \left(\mathrm{e}^{-b_1 t} - \mathrm{e}^{-b_2 t} \right) \end{aligned}$$

each of them is obviously positive. If we denote $m_i = \int_0^\infty t K_i(t) \mathrm{d}t$ the mean time of a kernel, we have

$$m_1 = \frac{1}{b_1}, \; m_2 = \frac{1}{b_1} + \frac{1}{b_2}.$$



The first kernel K_1 describes a memory effect with small mean time and correspond to a small loop $z_0 \xrightarrow{a_1} z_1 \xrightarrow{b_1} z_0$ in the MP. The other kernel K_1 describes a memory effect with longer mean time and correspond to a longer loop $z_0 \xrightarrow{a_2} z_2 \xrightarrow{b_2} z_1 \xrightarrow{b_1} z_0$. The relative coefficients a_i/a form a convex combination. The transitions $z_0 \xrightarrow{a_i} z_i$ split the whole number of particles in parts according to the loops. Let us summarize some properties of the kernel $K(t)$.

- $K(t)$ is the sum of exponential decaying functions, where the exponents are diagonal elements of $\mathbf{A}$.
- The arising memory equation is (11) with $a = \sum_i^N a_i$ or, equivalently, $k(\lambda = 0) = a$
- $K(t) \geq 0$ iff $k(\lambda) \geq 0$, since $a_i, b_i \geq 0$.

Equation (10) can be solved explicitly:

$$\begin{aligned} u \left(\lambda + a - \frac{a_1 b_1}{\lambda + b_1} - \frac{a_2 b_1 b_2}{(\lambda + b_1)(\lambda + b_2)} \right) &= u_0 \\ \Rightarrow \lambda u \left(\frac{\lambda^2 + \lambda(a + b_1 + b_2) + a_2 b_1 + a_1 b_2 + a_2 b_2 + b_1 b_2}{(\lambda + b_1)(\lambda + b_2)} \right) &= u_0 \\ \Rightarrow u = \frac{1}{\lambda} \frac{(\lambda + b_1)(\lambda + b_2)}{\lambda^2 + \lambda(a + b_1 + b_2) + a_2 b_1 + a_1 b_2 + a_2 b_2 + b_1 b_2} & \quad u_0. \end{aligned}$$

To get an explicit term for $u(t)$ we have to factorize the denominator what leads – of course – to the same time behavior as determined by the eigenvalues for the MP.

We compute the asymptotic behavior of the solution $u(t)$, using the asymptotic properties of the Laplace transform. We obtain for the equilibrium state

$$u_\infty = \lim_{\lambda\to 0} \lambda u = \frac{b_1 b_2}{a_2 b_1 + a_1 b_2 + a_2 b_2 + b_1 b_2} u_0.$$

For the other components we get in the same manner

$$\begin{aligned} v_1(t=\infty) &= \frac{a_1 b_2 + a_2 b_2}{a_2 b_1 + a_1 b_2 + a_2 b_2 + b_1 b_2} u_0, \\ v_2(t=\infty) &= \frac{a_2 b_1}{a_2 b_1 + a_1 b_2 + a_2 b_2 + b_1 b_2} u_0. \end{aligned}$$

These are the parts of the initial mass that remain in the states z_1 and z_2.

2.2.2 From memory to Markov

Now, we go the opposite direction and start with a kernel that is the sum of two exponential decaying terms, i.e.

$$K(t) = c_1 \mathrm{e}^{-\alpha_1 t} + c_2 \mathrm{e}^{-\alpha_2 t} \tag{14}$$

with some real coefficients c_1, c_2. We assume $c_i \neq 0$, otherwise we are in the case of 2 states. For definiteness, we assume $\alpha_1 > \alpha_2 > 0$. The α_i has to be strongly positive, otherwise we have no decreasing of the time dependence of the past.

This kernel has to be written in the form (12) with positive coefficients. We have

$$\begin{aligned} K(t) &= c_1 \mathrm{e}^{-\alpha_1 t} + c_2 \mathrm{e}^{-\alpha_2 t} = \\ &= (c_1 + c_2)\mathrm{e}^{-\alpha_1 t} + c_2(\alpha_1 - \alpha_2)\frac{\mathrm{e}^{-\alpha_2 t} - \mathrm{e}^{-\alpha_1 t}}{\alpha_1 - \alpha_2}. \end{aligned}$$

Thus, we have to demand $c_1 + c_2 \geq 0$ and $c_2 \geq 0$. Both are consequences of the positivity of $K(t)$, setting $t = 0$ and $t \longrightarrow \infty$.

Now, the MP is easily constructed. We set

$$\begin{aligned} b_1 &= \alpha_1 \\ b_2 &= \alpha_2 \\ a_2 &= \frac{c_2(\alpha_1 - \alpha_2)}{\alpha_1 \alpha_2} \\ a_1 &= \frac{c_1 + c_2}{\alpha_1}\,. \end{aligned}$$

The entries of the matrix b_1, b_2, a_2 are strongly positive, a_1 is non negative. This guarantees the uniqueness of the stationary solution. Moreover, it violates the detailed balance property.

The existence of a positive equilibrium is fulfilled, we have the equation

$$\dot{u} = -au + \int_0^t K(t-s)u(s)\mathrm{d}s,\ u(0) = u_0,$$

with the property of consistency $k(0) = a = a_1 + a_2 = \frac{\alpha_1 c_2 + \alpha_2 c_1}{\alpha_1 \alpha_2}$. Summarizing, we get the following result:

Proposition 2.1. *The first component of the MP generated by $\boldsymbol{A}^*$ given by (8) is the solution to the ME (11).*

For a ME $\dot{u} = -au + (K * u)$ with a kernel (14) with parameters $c_1, c_2, \alpha_1, \alpha_2$ satisfying $\alpha_1 > \alpha_2 > 0$, $c_1 + c_2 \geq 0$ and $c_2 \geq 0$, it can be constructed a three dimensional MP, where the first component coincides with the solution to the ME.

3 General memory equations as Markov processes

In this chapter, we generalize the ideas from the last chapter to an arbitrary finite dimensional MP. Firstly, we show that the first coordinate of a special MP, consisting of different transformation loops, satisfies a suitable memory equation with a more or less general kernel. Then, we go the opposite direction: We show that a ME with a kernel of a special form yields the MP we started with. The construction of the MP is explicitly.

3.1 From Markov to memory

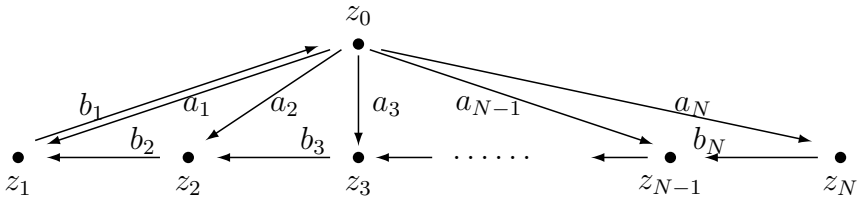
We consider a MP of $N+1$ abstract states $\{z_0, z_1, \ldots, z_N\}$ of the following form

$$\mathbf{A}^* = \begin{pmatrix} -a & b_1 & 0 & 0 & \ldots & 0 \\ a_1 & -b_1 & b_2 & 0 & \ldots & 0 \\ a_2 & 0 & -b_2 & b_3 & \ldots & 0 \\ a_3 & 0 & 0 & -b_3 & \ldots & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ a_{N-1} & 0 & 0 & 0 & -b_{N-1} & b_N \\ a_N & 0 & 0 & 0 & 0 & -b_N \end{pmatrix}, \tag{15}$$

where $a_j \geq 0$ and $b_j > 0$ for $j = 1, \ldots, N$ are non negative rates and we set $a := \sum_{j=1}^{N} a_j$. The condition $b_j > 0$ is reasonable, since otherwise the loop is broken somewhere.

The process $p(t)$ is generated by the equation $\dot{p} = \mathbf{A}^* p$. We set $p = (u, v_1, \ldots, v_N)$ and understand this quantity as the concentration of some particles. We assume that for $t = 0$ the total mass is concentrated in the first coordinate, i.e $p_0 = (u_0, 0, \ldots, 0)$. The equation conserves positivity of p and the whole mass $u + v_1 + \ldots + v_N = u_0$. Thus, p is a vector on the positive simplex in $\mathbb{R}^{N+1}$, intersected by the hyperplane $u + v_1 + \ldots + v_N = u_0$. Of our interest is the first component, i.e. the amount of matter of particles of type z_0.

$\mathbf{A}^*$ is the generator of a special type of MPs. It describes the change of type in the following way: Particles of type z_0 can changes their type to type z_i with rates a_i. The change of a particle of type z_i back to type z_0 does not go in a direct way, but in i steps. Thus, we have an interaction between the $N+1$ types in N loops (see the picture).



Easy calculations show that the stationary solution μ satisfying $A^*\mu = 0$ has the form

$$\mu = \frac{1}{Z}\left(1, \frac{a_1 + \cdots + a_N}{b_1}, \frac{a_2 + \cdots + a_N}{b_2}, \frac{a_3 + \cdots + a_N}{b_3}, \ldots, \frac{a_N}{b_N}\right) u_0,$$

where Z is the suitable normalization such that $\sum_{j=0}^{N} \mu_j = u_0$. Obviously,

$$Z = 1 + \sum_{i=1}^{N} \frac{1}{b_i} \sum_{j=i}^{N} a_j \ . \tag{16}$$

For the zeroth coordinate we have

$$u_\infty = \frac{1}{Z} u_0.$$

Since any $b_j > 0$, this stationary solution is unique and it is the equilibrium state for any initial condition.

Let us check, whether detailed balance with respect to μ is satisfied. We have to check, that $A_{ij}\mu_j = A_{ji}\mu_i$. Since $A_{1j}\mu_j = A_{j1}\mu_1 = 0$ for $j \geq 2$, we obtain that $a_2 = a_3 = \cdots = a_N = 0$. Hence, the evolution of the states $z_2, \ldots, z_N$ is not coupled to the evolution of z_0 and z_1. In this case, we get $N = 1$, the two dimensional case, where every MP has the detailed-balance property. That means, apart from trivial situations, the MP under consideration does not have the detailed balance property.

The equation $\dot{p} = \mathbf{A}^* p$ is equivalent to the following system for $p = (u, v_1, \ldots, v_N)$

$$\begin{cases} \dot{u} = -au + b_1 v_1 \\ \dot{v}_1 = a_1 u - b_1 u + b_2 v_2 \\ \dot{v}_2 = a_2 u - b_2 v_2 + b_3 v_3 \\ \dot{v}_3 = a_3 u - b_3 v_3 + b_4 v_4 \\ \cdots\cdots \\ \dot{v}_{N-1} = a_{N-1} u - b_{N-1} v_{N-1} + b_N v_N \\ \dot{v}_N = a_N u - b_N v_N. \end{cases}$$

Using the Laplace transform, we get the following equation for $(u, v_1, \ldots, v_N)$

$$\begin{cases} (\lambda + a)u - u_0 = b_1 v_1 \\ (\lambda + b_1)v_1 = a_1 u + b_2 v_2 \\ (\lambda + b_2)v_2 = a_2 u + b_3 v_3 \\ (\lambda + b_3)v_3 = a_3 u + b_4 v_4 \\ \cdots\cdots \\ (\lambda + b_{N-1})v_{N-1} = a_{N-1} u + b_N v_N \\ (\lambda + b_1)v_N = a_N u. \end{cases}$$

This yields for u

$$(\lambda + a)u - u_0 = \left(\frac{a_1 b_1}{\lambda + b_1} + \frac{a_2 b_1 b_2}{(\lambda + b_1)(\lambda + b_2)} + \frac{a_3 b_1 b_2 b_3}{(\lambda + b_1)(\lambda + b_2)(\lambda + b_3)} + \ldots + \frac{a_N b_1 b_2 \cdots b_N}{(\lambda + b_1)(\lambda + b_2)\cdots(\lambda + b_N)}\right) u. \tag{17}$$

We define the kernel

$$k(\lambda) = \sum_{j=1}^{N} a_j k_j(\lambda), \quad k_j(\lambda) = \prod_{i=1}^{j} \frac{b_i}{\lambda + b_i}$$

and hence the equation for the Laplace transformed variable u reads

$$\lambda u - u_0 = -au + k(\lambda)u. \tag{18}$$

Now, we formulate the memory equation in terms of $t \geq 0$ and some properties of the kernel. For this purpose, we introduce some quantities, connected with Lagrange polynomials (see the appendix for details) with different support points $b_1, ..., b_N$. Let

$$\psi_i^j = \prod_{k=1, k\neq i}^{j} \frac{b_k}{b_k - b_i} \ ,$$

assuming $b_i \neq b_k$ for $i \neq k$. From the theory of Lagrange polynomials it is well known that

$$k_j(\lambda) = \prod_{i=1}^{j} \frac{b_i}{\lambda + b_i} = \sum_{i=1}^{j} \frac{b_i}{\lambda + b_i} \psi_i^j.$$

Using this, we can transform $k_j(\lambda)$ back and obtain

$$K(t) = \sum_{j=1}^{N} a_j K_j(t), \tag{19}$$

$$K_j(t) = \sum_{i=1}^{j} b_i \psi_i^j \mathrm{e}^{-b_i t}. \tag{20}$$

The assumption $b_i \neq b_j$ for $i \neq j$ is not principal. If some or all b_i coincide, all formulas of the following can be obtained by some suitable limits. This is obviously done for the Laplace transform $k(\lambda)$. For $K(t)$ we get more complicated terms, involving not only exponential but also polynomials with degree, depending on the frequency of the b_i. We do not bore the reader with this technical complexity, since this is well known in the theory of Lagrange polynomials. Moreover, from a practical point of view, in a generic Markov matrix all entries can be chosen differently.

Surely, a different situation is, if the modeling requires equal b_i. This is the case for instance for DDEs. The case is considered in detail in chapter 4.

Now, we are ready for the following

Theorem 3.1. *Let $p = (u, v_1, \ldots, v_N)$ be the solution of $\dot{p} = \boldsymbol{A}^* p$ with $p_0 = (u_0, 0, \ldots, 0)$ where $\boldsymbol{A}^*$ is given via (15). Then $t \mapsto u(t)$ solves the memory equation*

$$\dot{u} = -au + \int_0^t K(t-s)u(s)\mathrm{d}s, \ u(0) = u_0, \tag{21}$$

where $K(t) = \sum_{j=1}^{N} a_j K_j(t)$ with $K_j(t) = \sum_{i=1}^{j} b_i \psi_i^j \mathrm{e}^{-b_i t}$ and $a = \sum_j a_j = k(0)$. Moreover, $K(t) \geq 0$ and $u_\infty = 1/Z u_0$ with Z given by (16).

Proof. From the definition of $k(\lambda)$ it is clear that $u(\lambda)$ defined by the MP is the solution to (18). If the inverse transformed function $t \mapsto u(t)$ is regular enough, it is solution to (21).

Rewriting (17) as

$$\lambda u(\lambda) = \frac{\lambda}{\lambda + a - \sum_{j=1}^{N} a_j k_j(\lambda)}\ u_0 \tag{22}$$

Since the $k_j(\lambda)$ are analytical functions and bounded on the right plane, so is $\lambda u(\lambda)$. Hence from the properties of the Laplace transform it follows that $u(t)$ is continuously differentiable. Thus, it solves (21).

To calculate u_∞ we use the representation (22) and investigate the behavior of $k_j(\lambda)$ for $\lambda \to \infty$. We have

$$\begin{aligned} k_j(\lambda) &= k_j(0) + \lambda k_j'(0) + o(\lambda) = \\ &= 1 + \lambda \left(\frac{b_1 b_2 \cdots b_j}{(\lambda + b_1)(\lambda + b_2) \cdots (\lambda + b_j)} \right)' \Big|_{\lambda=0} + o(\lambda) = \\ &= 1 - \lambda \left. \frac{b_1 b_2 \cdots b_j \cdot \Big(b_1 b_2 \cdots b_j \sum_{i=1}^{j} \frac{1}{b_i} + o(\lambda) \Big)}{\big[(\lambda + b_1)(\lambda + b_2) \cdots (\lambda + b_j)\big]^2} \right|_{\lambda=0} + o(\lambda) = \\ &= 1 - \lambda \sum_{i=1}^{j} \frac{1}{b_i} + o(\lambda). \end{aligned}$$

By definition $a = \sum_{j=1}^{N} a_j$, and hence, it follows from (22)

$$\begin{aligned} u_\infty &= \lim_{\lambda\to\infty} \lambda u(\lambda) = \lim_{\lambda\to\infty} \frac{\lambda}{\lambda + a - \sum_{j=1}^{N} a_j \left[1 - \lambda \sum_{i=1}^{j} \frac{1}{b_i} + o(\lambda)\right]}\ u_0 = \\ &= \frac{1}{1 + \sum_{j=1}^{N} a_j \sum_{i=1}^{j} \frac{1}{b_i}}\ u_0 = \frac{1}{1 + \sum_{j=1}^{N} \frac{1}{b_j} \sum_{i=j}^{N} a_j}\ u_0\ , \end{aligned}$$

what is exactly the zeroth coordinate of μ, i.e. $u_\infty = 1/Z u_0$.

The positivity of the $K_j(t)$, $t \geq 0$ follows from their representation with simplex integrals (see the appendix). We have

$$K_j(t) = \sum_{i=1}^{j} b_i \psi_i^j \mathrm{e}^{-b_i t} = \int_{S_j} (-1)^{j-1} f^{(j-1)}\big(\langle \alpha, s\rangle t\big) \Big|_{s_j = 1 - s_1 - s_2 - s_{j-1}} \mathrm{d}s_{j-1} \cdots \mathrm{d}s_1$$

with $f(x) = \mathrm{e}^{-xt}$ and $\langle \alpha, s\rangle = \alpha_1 s_1 + \alpha_2 s_2 + \ldots + \alpha_j s_j$. Since $(-1)^{j-1} f^{(j-1)}\big(\langle \alpha, s\rangle t\big) = t^{j-1} \mathrm{e}^{-\langle \alpha, s\rangle t} \geq 0$ and any $a_j \geq 0$, we conclude the positivity of $K_j(t)$ and therefore also $K(t) \geq 0$. This completes the proof of the theorem. □

3.2 From memory to Markov

We consider memory equations of the form

$$\dot{u}(t) = -au + K * u = -au + \int_0^t K(t-s)u(s)\mathrm{d}s,$$

where $a > 0$ is a real parameter and K is a positive kernel. The aim is to embed the evolution of u into a MP introducing new variables.

Our main assumptions are $K(t) \geq 0$ and $\int_0^\infty K(t)\mathrm{d}t = a$. Clearly, starting with some given $K(t)$ we want to end up with a kernel of the shape (19-20). Then going forward to a kernel like in (17), the entries of the Markov generator matrix can be taken immediately.

The kernels (20) are positive although they are linear combinations of exponential with – maybe – negative coefficients.

It may seem that any non-negative kernel $K(t)$ can be presented in such a form. But this is not the case. We show this in a

Counterexample: Let

$$K(t) = 3\mathrm{e}^{-t} - 8\mathrm{e}^{-2t} + 6\mathrm{e}^{-3t}$$

and

$$f(t) = \mathrm{e}^{4t}K(t) = 3\mathrm{e}^{3t} - 8\mathrm{e}^{2t} + 6\mathrm{e}^{t}$$

$f(t)$ has a unique minimum $f(0.215315...) = 0.8590718....$ Thus $K(t) \geq 0$.

Seeking for coefficients A, B, C, D, E, F, G (this is the representation (20)) with

$$\begin{aligned} K(t) &= A\mathrm{e}^{-3t} + B\mathrm{e}^{-2t} + C\mathrm{e}^{-t} + D\frac{\mathrm{e}^{-t} - \mathrm{e}^{-2t}}{1} + E\frac{\mathrm{e}^{-t} - \mathrm{e}^{-3t}}{2} + F\frac{\mathrm{e}^{-2t} - \mathrm{e}^{-3t}}{1} + \\ &+ G\left(\frac{\mathrm{e}^{-t}}{1\cdot 2} + \frac{\mathrm{e}^{-2t}}{(-1)\cdot 1} + \frac{\mathrm{e}^{-3t}}{1\cdot 2}\right) \end{aligned}$$

the resulting system for the coefficients leads to

$$0 = 2 + D + E + F + B + C$$

that does not have non-negative solutions.

We think, there is no hope to find a corresponding MP for an arbitrary non-negative kernel. Therefore we go another way and try to derive a class of sensible kernels starting from physical considerations. Furthermore, the following reasoning shows how the time interval of the memory effect is connected with rates of the loops of the MP.

First of all we have to ask: How one can model a meaningful kernel for a ME. We can assume that the dependence on the past is concentrated at some time point before the present, say $t-t_1$, ... $t-t_N$ where t_j are ordered time values, i.e. $0 < t_1 < t_2 < \cdots < t_N$, with some coefficients $\gamma_1, ..., \gamma_N$ with $\gamma_i \geq 0$ and $\sum \gamma_i = 1$ that gives the relative proportion of each time point. The corresponding memory kernel of such an ansatz is

$$\tilde{K}(t) = \sum_{j=1}^{N} \gamma_j \delta(t - t_j)$$

(here δ means the "δ-function", the "density" of the Dirac measure). The kernel $\tilde{K}$ occurs when starting from a discrete time model, like equation (2). Clearly, it is a first guess. A real memory kernel seems to be more smeared. Therefore, we can try to find kernels $\tilde{K}_j(t)$ with mean time at t_j, i.e

$$\int_0^\infty \tilde{K}_j(t)\mathrm{d}t = a, \quad \int_0^\infty t\tilde{K}_j(t)\mathrm{d}t = \int_0^\infty t\delta(t - t_j)\mathrm{d}t = t_j.$$

We will show that such kernels $\tilde{K}_j(t)$ can be found and it is possible to find a suitable MP for them. Note, that this does not determine the kernels $\tilde{K}_j$ uniquely, of course.

We show that our kernels of shape (19) are suitable for this.

Proposition 3.2. *Let a sequence $0 < t_1 < t_2 < \cdots < t_N < \infty$ be given where $(t_j - t_{j-1})$ are pairwise distinct. There are kernels $K(t) = \sum_{j=1}^N a_j K_j(t)$ such that $K \geq 0$ and $\int_0^\infty K(t)\mathrm{d}t = a$ and $\int_0^\infty tK_j(t)\mathrm{d}t = t_j$.*

Proof. We define $b_j \in \mathbb{R}$ via $t_i = \sum_{j=1}^i \frac{1}{b_j}$. Since the t_i are ordered, we get $b_j > 0$. Since $(t_j - t_{j-1})$, the b_j are pairwise distinct. We define

$$K(t) = \sum_{j=1}^N a_j K_j(t), \quad \text{where} \quad K_j(t) = \sum_{i=1}^j b_i \psi_i^j \mathrm{e}^{-b_i t}.$$

We prove that K satisfies the desired properties. Using the Laplace transform, we get

$$\mathcal{L}(K_j(t))(\lambda) = \sum_{i=1}^j b_i \psi_i^j \frac{1}{\lambda + b_i} = \prod_{i=1}^j \frac{b_i}{\lambda + b_i} =: k_j(\lambda).$$

This yields $\int_0^\infty K_j(t)\mathrm{d}t = k_j(\lambda = 0) = 1$. Moreover, $\int_0^\infty tK_j(t)\mathrm{d}t = -k_j'(\lambda = 0)$. We have

$$k_j'(\lambda) = \sum_{i=1}^j \frac{b_1}{\lambda + b_1} \cdot \frac{b_2}{\lambda + b_2} \cdots \frac{-b_i}{(\lambda + b_i)^2} \cdots \frac{b_{j-1}}{\lambda + b_{j-1}} \cdot \frac{b_j}{\lambda + b_j}$$

This yields $-k_j'(\lambda = 0) = \sum_{i=1}^j \frac{1}{b_i} = t_j$, i.e. $\int_0^\infty tK_j(t)\mathrm{d}t = t_j$. □

Theorem 3.3. *Let $K(t)$ be a memory kernel of the form*

$$K(t) = \sum_{j=1}^N \alpha_j K_j(t), \quad \text{where} \quad K_j(t) = \sum_{i=1}^j b_i \psi_i^j \mathrm{e}^{-b_i t}.$$

and $\alpha = \sum_j \alpha_j$. Let u be the solution to the equation $\dot{u}(t) = -\alpha u + K * u$ with $u(0) = u_0$. Then, there is a MP $\dot{p} = \boldsymbol{A}^* p$ in $\mathbb{R}^{N+1}$ generated by a Markov matrix $\boldsymbol{A}$ and an initial condition $p(0)$ such that $u(t) = p_0(t)$.

Proof. Define the Markov generator matrix via $a = \alpha$, $a_i = \alpha_i$, $b_i = \beta_i$. The initial condition for the MP is $p_0 = (u_0, 0, \ldots, 0)$. The claim follows. □

For the asymptotic behavior of the ME, we immediately get the following statement.

Corollary 3.4. *Let $K(t) = \sum_{j=1}^N a_i K_i(t)$, where $K_i(t) = \sum_{j=1}^i b_j \psi_j \mathrm{e}^{-b_j t}$ and $a = \sum_j a_j$. Let u be the solution to the equation $\dot{u}(t) = -au + K * u$ with $u(0) = u_0$. Then $u(t) \to u_\infty$ as $t \to \infty$, where $u_\infty = \frac{1}{Z} u_0$ and Z is given by (16).*

3.3 Remarks

1. Kernels like $k_j(\lambda) = \prod_{i=1}^{j} \left(\frac{b_i}{\lambda+b_i}\right)^{m_i}$ with suitable chosen $m_i \in \mathbb{N}$ may approximates a δ-kernel better. Especially it allows to take into account more moments then only the first one, or equivalently to allow the b_i to be equal. This is possible without any principal problems (see the note above Theorem 3.1). A special case is treated in the next chapter, where one delay is approximated arbitrary precise. To prove positivity of the corresponding functions Lemma 5.1 from the appendix can be used.

   Kernels like in (17) are rational functions of degree N, having poles on the left plane. They approximate meromorphic functions. This makes one able to consider more general kernels then linear combinations of exponents – at least approximately.

2. There are other (similar) MP that lead to a ME and vice versa. For example the MP with the generator

$$\mathbf{A}^* = \begin{pmatrix} -a & c_1 & c_2 & c_3 & \dots & c_N \\ a & -c_1 - b_1 & 0 & 0 & \dots & 0 \\ 0 & b_1 & -c_2 - b_2 & 0 & \dots & 0 \\ 0 & 0 & b_2 & -c_3 - b_3 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & b_{N-1} & -c_N \end{pmatrix},$$

   can also be used for embedding the presented exponential kernels. Such MP can be understood in the same manner like at the picture on page 147 but with reversed arrows. Although this approach is more difficulty from a technical point of view.

3. The presented results can be applied in various manner. We focus on ordinary differential equations to present the general idea. Linear MEs in infinite dimensional space like diffusion equations with time depending diffusion coefficients are also possible.

   Moreover, the well known tools for investigating MP, like inequalities for Lyapunov functions (see [Ste05b]) can now be carried over to explore ME.

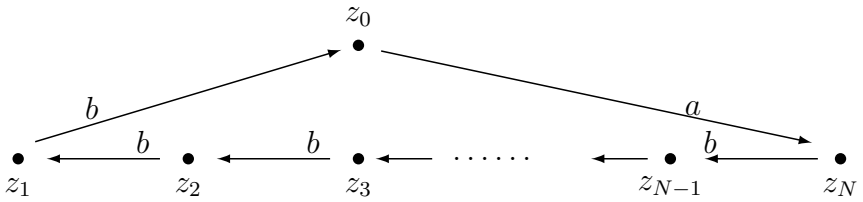
4 Special Markov process leads to a delay differential equation

In this section we consider a special form of the MP. We define $a_j = 0$ for $j = 1, 2, \dots, N-1$ and put $a_N = a$ and $b_j = b \in \mathbb{R}$. Using the observation from the last section we consider a general cyclic MP with one single but long loop. The MP in

$\mathbb{R}^{N+1}$ is generated by the matrix

$$\mathbf{A}^* = \begin{pmatrix} -a & b & 0 & \cdots & 0 \\ 0 & -b & b & \cdots & 0 \\ 0 & 0 & -b & \cdots & 0 \\ \vdots & & & \ddots & b \\ a & \cdots & 0 & \cdots & -b \end{pmatrix}.$$

We assume the initial mass is concentrated in the first reservoir. Then, the equation reads $\dot{p}(t) = \mathbf{A}^* p(t)$ with $p(0) = p_0$, where $p = (u, v_1, v_2, \ldots, v_n)^T$ and $p_0 = (u_0, 0, \ldots, 0)^T$.



The stationary solution is

$$\mu = \frac{1}{Z}\left(\frac{1}{a}, \frac{1}{b}, \frac{1}{b}, ..., \frac{1}{b}\right)^T u_0 \in \mathbb{R}^{N+1},$$

where $Z = \frac{1}{a} + \frac{N}{b} = \frac{b+aN}{ab}$. Note, the system does not have the detailed balance property.

We get

$$(\lambda + a)\hat{u} - u_0 = a\left(\frac{b}{\lambda + b}\right)^N u.$$

It holds

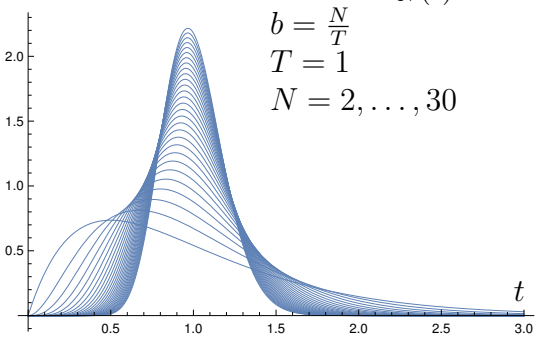
$$\left(\frac{b}{\lambda + b}\right)^N = \mathcal{L}\left(\frac{b^N}{(N-1)!} t^{N-1} \mathrm{e}^{-bt}\right)(\lambda).$$

Hence, we get

$$\begin{aligned} \dot{u}(t) &= -au(t) + \frac{ab^N}{(N-1)!} \int_0^t s^{N-1} \mathrm{e}^{-bs} u(t-s) \mathrm{d}s \\ &= -a\left(u(t) - \int_0^t K_N(s) u(t-s) \mathrm{d}s\right), \end{aligned}$$

where we introduced the kernel

$$K_N(t) := \frac{b^N}{(N-1)!} t^{N-1} \mathrm{e}^{-bt}.$$



Kernel $K_N(t)$ for:
$b = \frac{N}{T}$
$T = 1$
$N = 2, \ldots, 30$

A delay equation can be understood as a memory equation with a δ-kernel. To do this, we fix $T > 0$ and introduce $\delta_T(t) = \delta(t - T)$. We get

$$\int_0^\infty \delta_T(t)\mathrm{e}^{-\lambda t}\mathrm{d}t = \int_0^\infty \delta(t-T)\mathrm{e}^{-\lambda t}\mathrm{d}t = \mathrm{e}^{-\lambda T}.$$

Moreover, for $t > T$ we have

$$u(t-T) = \int_0^\infty u(s)\delta(t-T-s)\mathrm{d}s = \int_0^\infty u(s)\delta_T(t-s)\mathrm{d}s =$$
$$= \int_0^t u(s)\delta_T(t-s)\mathrm{d}s = u(t) * \delta_T(t).$$

Hence,

$$\mathcal{L}(u(t-T))(\lambda) = \hat{u}(\lambda)\mathrm{e}^{-\lambda T}.$$

Putting $b = \frac{N}{T}$, we approximate the Laplace transform of the kernel δ_T, i.e.

$$\mathcal{L}(\delta_T)(\lambda) = e^{-\lambda T} \approx \left(1 + \frac{\lambda T}{N}\right)^{-N} = \left(\frac{\frac{N}{T}}{\frac{N}{T} + \lambda}\right)^N = \mathcal{L}(K_N(t))(\lambda).$$

Hence, we conclude

$$\mathcal{L}(K_N(t))(\lambda) \xrightarrow{N\to\infty} e^{-\lambda T} = \mathcal{L}(\delta(t-T))(\lambda),$$

and the limiting (DDE) reads as

$$\dot{u} = \begin{cases} -au(t), & \text{if } \ 0 \le t \le T \\ -au(t) + au(t-T), & \text{if } \ t \ge T, \end{cases}$$

or equivalently

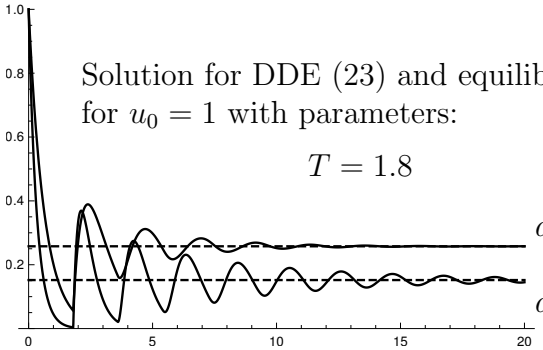
$$\dot{u} = -au(t) + au(t-T), \quad \text{for } \ t \ge T, \quad \text{and} \quad u|_{[0,T]}(t) = \mathrm{e}^{-at}u_0. \tag{23}$$

Let us note that the initial condition $u|_{[0,T]}(t) = \mathrm{e}^{-at}u_0$ results from the modeling ansatz. No other initial condition is possible.

Let us compute the limiting stationary solution for $N \to \infty$ of the first coordinate of the MP. This means the MP has long loops, but mass is transferred with a high rate. We have $Z = \frac{Na+b}{ab}$. Putting $b = \frac{N}{T}$, we conclude for the zeroth coordinate of the stationary solution

$$\mu_0 = \frac{1}{Za}u_0 = \frac{b}{Na+b}u_0 = \frac{\frac{N}{T}}{Na + \frac{N}{T}}u_0 = \frac{1}{1+aT}u_0.$$

The solution of the DDE and the stationary solution μ_0 of the MP can be seen in the picture. The solution of the DDE converges nicely to μ_0.



Solution for DDE (23) and equilibrium $\frac{1}{1+aT}$ for $u_0 = 1$ with parameters:

$$T = 1.8$$

Finally, we remark some properties of the spectrum. The spectrum of the DDE is given by inserting $e^{\lambda t}$ for $\lambda \in \mathbb{C}$ into the equation (see e.g. [Smi11]). This yields for given $a, T \geq 0$ the equation

$$\lambda = -a + ae^{-\lambda T}. \tag{24}$$

This transcendental equation (in $\lambda \in \mathbb{C}$) has in general an infinite discrete amount of solutions.

The eigenvalues of $\mathbf{A}^*$ for fixed $N \in \mathbb{N}$ are given by the characteristic equation

$$\phi(\lambda) = -ab^{N-1} + (\lambda + b)^{N-1}(\lambda + a) = 0,$$

that can be computed easily. Hence, setting $b = \frac{N}{T}$ we get $\phi(\lambda) = 0$ if and only if

$$\frac{a}{a+\lambda} = \left(\frac{\lambda + b}{b}\right)^{N-1} = \left(1 + \frac{\lambda T}{N}\right)^{N-1}.$$

For $N \to \infty$, right hand side converges to $e^{\lambda T}$. So, in the limit $\lambda \in \mathbb{C}$ satisfies the equation

$$\frac{a}{a+\lambda} = e^{\lambda T},$$

i.e. the same equation as (24). Hence, one can say that not only the solution converges but also the spectrum of the MP and of the ME converges to each other. Note, that the convergence of the spectrum is very slow, as the convergence of the exponential function is.

5 Appendix

5.1 Laplace transform

Here, we summarize some facts of the Laplace transform. More details can be found, e.g. in [StS96]. For a given function $u : [0, \infty) \in t \mapsto u(t) \in \mathbb{R}$ that does not grow faster than an exponential function in time, the Laplace transform is defined by

$$\hat{u}(\lambda) = (\mathcal{L}u)(\lambda) = \int_0^\infty e^{-\lambda t} u(t) \mathrm{d}t.$$

We use the following formulas that can be checked easily:

$$\begin{aligned}
\mathcal{L}(\dot{u})(\lambda) &= \lambda \hat{u}(\lambda) - u_0 \\
\mathcal{L}(K * u) &= (\mathcal{L}K) \cdot (\mathcal{L}u) \\
\mathcal{L}(e^{-a\cdot})(\lambda) &= \frac{1}{\lambda + a} \\
\mathcal{L}\left(\frac{1}{(n-1)!} t^{n-1} e^{-at}\right)(\lambda) &= \frac{1}{(\lambda + a)^n}.
\end{aligned}$$

The Laplace transform has an interesting asymptotic behavior. The limit for large times $u(t) \overset{t\to\infty}{\longrightarrow} u_\infty$ can be calculated with the Laplace transform. It holds $\lambda \hat{u}(\lambda) \overset{\lambda\to 0}{\longrightarrow} u_\infty$.

Thus, there is no need to know the whole solution $u(t)$ if one is interested only in the equilibrium case. This is important, since, in general for non-autonomous equations, the equilibrium cannot be calculated by setting $\dot{u} = 0$.

Let us note that the uniform convergence on compact sets of $t \in \mathbb{R}_+$ carries over to uniform convergence on compact sets of λ in the domain of analyticity.

To carry over positivity properties between the original and the transformation the following lemma is useful:

Lemma 5.1. *Let* $K(t) = \sum_{j=1}^N \gamma_j \mathrm{e}^{-\alpha_j t}$ *with its Laplace transform* $k(\lambda) = \sum_{j=1}^N \gamma_j \frac{1}{\lambda+\alpha_j}$. *Then* $K(t) \geq 0$ *if and only if* $\sum_{j=1}^N \frac{\gamma_j}{(\lambda+\alpha_j)^m} \geq 0$ *for any* $m \in \mathbb{N}$.

Proof. Let $K(t) \geq 0$. Since $K(0) \geq 0$, we get $\sum_{j=1}^N \gamma_j \geq 0$, i.e. the claim holds for $m = 0$. For $m \geq 0$, we get $0 \leq \int_0^\infty t^m K(t)\mathrm{e}^{-\lambda t}\mathrm{d}t = (-1)^m k^{(m)}(\lambda) = \sum_{j=1}^N \frac{\gamma_j}{(\lambda+\alpha_j)^{m+1}}$ what proves the claim in one direction.

For the other direction, we put $\lambda = \frac{n}{t}$ and $m + 1 = n$. Then

$$0 \leq \sum_{j=1}^N \frac{\gamma_j (\frac{n}{t})^n}{(\frac{n}{t}+\alpha_j)^n} = \sum_{j=1}^N \frac{\gamma_j}{(1+\frac{\alpha_j n}{t})^n} = \sum_{j=1}^N \gamma_j \left(1 + \frac{\alpha_j t}{n}\right)^{-n} \to$$

$$\to \sum_{j=1}^N \gamma_j \mathrm{e}^{-\alpha_j t}, \quad \text{as} \quad n \to \infty,$$

which proves the claim of the lemma. □

5.2 Simplex integrals

In Theorem 3.1, we proved the positivity of the kernel $K(t)$ using an integral over a simplex. This is based on the following observation.

Let $S_{n-1} \subset \mathbb{R}^n$ be the simplex, defined as

$$S_{n-1} = \{s \in \mathbb{R}^n \mid s_i \geq 0,\ s_1 + ... + s_n = 1\}.$$

We consider functions $g : \mathbb{R}^n \longrightarrow \mathbb{R}$ and their integrals over S_{n-1}. We have

$$\int\limits_{\mathcal{S}_{n-1}} g(s)\mathrm{d}\sigma(s) = \frac{1}{\sqrt{n}} \int\limits_{S_{n-1}} g(s_1, s_2, ..., s_{n-1}, 1-s_1-\ldots-s_{n-1})\mathrm{d}s_1 \cdots \mathrm{d}s_{n-1} =$$

$$= (n-1)! \int_0^1 \mathrm{d}s_1 \int_0^{1-s_1} \mathrm{d}s_2 \int_0^{1-s_1-s_2} \mathrm{d}s_3 \quad \cdots \quad \int_0^{1-s_n-\ldots-s_{n-2}} \mathrm{d}s_{n-1}\ g(s_1, s_2, ..., s_n)\Big|_{s_n=1-s_1-\ldots-s_{n-1}},$$

where $\sigma(\mathrm{d}s)$ is the Lebesgue measure on S_{n-1} and $\sqrt{n}$ is the volume of S_{n-1}.

Let $f : \mathbb{R} \longrightarrow \mathbb{R}$ be a smooth enough function, $f^{(k)}$ its k- derivative and $x_1, ..., x_n$ be given different real values. Set $g(s) = f(\langle x, s\rangle)$, where $\langle x, s\rangle = x_1 s_1 + x_2 s_2 + \ldots + x_n s_n$ is the scalar product in $\mathbb{R}^n$.

Now, using induction one can prove that

$$\sum_{i=1}^n f(x_i) \prod_{j\neq i}^n \frac{1}{x_i - x_j} = \int\limits_{S_{n-1}} f^{(n-1)}(\langle x, s\rangle)\sigma(\mathrm{d}s)\ .$$

This formula gives a powerful tool to switch between expressions connected with Lagrange polynomials and expressions connected with simplex integrals. In Theorem 3.1, we used this formula with $f(x) = \mathrm{e}^{-xt}$.

5.3 Lagrange polynomials

Here we summarize basic facts from the theory of Lagrange polynomials. Let

$$L_i^j(x) = \prod_{k=1,k\neq i}^{j} \frac{x - x_k}{x_i - x_k} \ ,$$

assuming $x_i \neq x_k$ for $i \neq k$. Obviously $L_i^j(x)$ is a polynomial of degree $j-1$ and we have $L_i^j(x_k) = \delta_{ik}$ with δ_{ik} the Kronecker symbol. Hence, the polynomial

$$P(x) = \sum_{i=1}^{j} p_i L_i^j(x)$$

of degree $j-1$ satisfies $P(x_i) = p_i$.

Now, let us fix $z \in \mathbb{R}$. Seeking for a polynomial $P(x) = q_0 + q_1 x + ... + q_{j-1}x^{j-1}$ with the condition $P(x_i) = p_i = \frac{x_i}{z+x_i}$, we get coefficients q_i with $q_0 = \prod_{i=1}^{j} \frac{x_i}{z+x_i}$ among them. Hence, we have on the one hand

$$P(0) = q_0 = \prod_{i=1}^{j} \frac{x_i}{z + x_i}$$

and on the other hand

$$P(0) = \sum_{i=1}^{j} p_i L_i^j(0) = \sum_{i=1}^{j} \frac{x_i}{z + x_i} \prod_{k=1,k\neq i}^{j} \frac{(-x_k)}{x_i - x_k} = \sum_{i=1}^{j} \frac{x_i}{z + x_i} \prod_{k=1,k\neq i}^{j} \frac{x_k}{x_k - x_i} \ .$$

It follows

$$\prod_{i=1}^{j} \frac{x_i}{z + x_i} = \sum_{i=1}^{j} \frac{x_i}{z + x_i} \prod_{k=1,k\neq i}^{j} \frac{x_k}{x_k - x_i} \ .$$

Note, in our explanation we use $\psi_i^j = (-1)^{j-1} L_i^j(0)$ and put $z = \lambda$.

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Part 5

Consistency and convergence for a family of finite volume discretizations of the Fokker–Planck operator

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This preprint has been submitted for publication and was still in the process of reviewing when this thesis was published. A published preprint version is available at the WIAS-preprint server at DOI:10.20347/WIAS.PREPRINT.2684.

Consistency and convergence for a family of finite volume discretizations of the Fokker–Planck operator*

Martin Heida†, Markus Kantner‡, and Artur Stephan§

Abstract

We introduce a family of various finite volume discretization schemes for the Fokker–Planck operator, which are characterized by different Stolarsky weight functions on the edges. This family particularly includes the well-established Scharfetter–Gummel discretization as well as the recently developed square-root approximation (SQRA) scheme. We motivate this family of discretizations both from the numerical and the modeling point of view and provide a uniform consistency and error analysis. Our main results state that the convergence order primarily depends on the quality of the mesh and in second place on the choice of the Stolarsky weights. We show that the Scharfetter–Gummel scheme has the analytically best convergence properties but also that there exists a whole branch of Stolarsky means with the same convergence quality. We show by numerical experiments that for small convection the choice of the optimal representative of the discretization family is highly non-trivial while for large gradients the Scharfetter–Gummel scheme stands out compared to the others.

1 Introduction

The Fokker–Planck equation (FPE), also known as *Smoluchowski equation* or *Kolmogorov forward equation*, is one of the most important equations in theoretical physics and applied mathematics. It describes the time evolution of the probability density function of a particle in an external force field (e.g., fluctuating forces as in Brownian motion). The equation can be generalized to other contexts and observables and has been employed in a broad range of applications, including physical chemistry, protein synthesis, plasma

*M. H. and A. S. are financed by Deutsche Forschungsgemeinschaft (DFG) through Grant CRC 1114 "Scaling Cascades in Complex Systems", Project C05 *Effective models for materials and interfaces with multiple scales.* The work of M. K. received funding from the DFG under Germany's Excellence Strategy – EXC2046: MATH+ (Berlin Mathematics Research Center).

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physics and semiconductor device simulation. Thus, there is a huge interest in the development of efficient and robust numerical methods. In the context of finite volume (FV) methods, the central objective is a robust and accurate discretization of the (particle or probability) flux implied by the FPE.

A particularly important discretization scheme for the flux was derived by Scharfetter and Gummel [ScG69] in the context of the drift-diffusion model for electronic charge carrier transport in bipolar semiconductor devices [vRo50]. The typically exponentially varying carrier densities at p-n junctions lead to unphysical results (spurious oscillations), if the flux is discretized in a naive way using standard finite difference schemes [MiW94]. The problem was overcome by considering the flux expression as a one-dimensional boundary value problem along each edge between adjacent mesh nodes. The resulting Scharfetter–Gummel (SG) scheme provides a robust discretization of the flux as it asymptotically approaches the numerically stable discretizations in the drift- (upwind scheme) and diffusion-dominated (central finite difference scheme) limits. The SG-scheme and its several generalizations to more complex physical problem settings are nowadays widely used in semiconductor device simulation [Mar86, FR*17] and have been extensively studied in the literature [BMP89, EFG06, FKF17, Kan20]. The SG-scheme is also known as *exponential fitting scheme* and was independently discovered by Allan and Southwell [AlS55] and Il'in [Il'69] in different contexts.

Recently, an alternative flux discretization method, called *square-root approximation* (SQRA) scheme, has been derived explicitly for high dimensional problems. The original derivation in [LFW13] aims at applications in molecular dynamics and is based on Markov state models. However, it can also be obtained from a maximum entropy path principle [DJ*15] and from discretizing the Jordan–Kinderlehrer–Otto variational formulation of the FPE [Mie13a]. In Section 3.2, we provide a derivation of SQRA scheme, which is motivated from the theory of gradient flows. In contrast to the SG-scheme, the SQRA is very recent and only sparsely investigated.

The SG and the SQRA schemes both turn out to be special cases of a family of discretization schemes based on weighted Stolarsky means [Sto75], see Section 3.1. This family is very rich and allows for a general convergence and consistency analysis, which we carry out in Sections 4–5. There are also other discretization schemes available in literature. The Chang–Cooper scheme [ChG70] has been derived for computing ion-electron collisions and uses another Stolarsky mean, namely the logarithmic mean. General discretization schemes using different weights are called B-schemes and have been introduced in [ChD11]. We will recall the corresponding results in Section 1.2 below.

1.1 The FPE and the SG and SQRA discretization schemes

In this work, we consider the stationary Fokker–Planck equation

$$-\nabla\cdot(\kappa\nabla u)-\nabla\cdot(\kappa u\nabla V)=f, \tag{1.1}$$

which can be equivalently written as

$$\operatorname{div}\mathbf{J}(u,V)=f$$

using the flux $\mathbf{J}(u,V)=-\kappa(\nabla u+u\nabla V)$, where $\kappa>0$ is a (possibly space-dependent) diffusion coefficient and $V:\Omega\to\mathbb{R}$ is a given potential. The flux $\mathbf{J}$ consists of a diffusive part $\kappa\nabla u$ and a drift part $\kappa u\nabla V$, which compensate for the stationary density $\pi=\mathrm{e}^{-V}$

(Boltzmann distribution) as $\mathbf{J}(\mathrm{e}^{-V}, V) = 0$. This reflects the principle of detailed balance in the thermodynamic equilibrium. The right-hand side f describes possible sink or source terms.

Assumption 1.1. *Unless stated otherwise we assume $V \in C^2(\overline{\Omega})$, $\kappa \in C^1(\overline{\Omega})$, $f \in C(\overline{\Omega})$ real valued functions with $\kappa > 0$. The standard boundary conditions are the homogeneous Dirichlet boundary conditions.*

Remark 1.2. Some results also hold for lower regularity and for κ a symmetric strictly positive definite matrix.

In Section 3.1 we derive the following discretization of (1.1)

$$-\sum_{j:j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(\frac{u_j}{\pi_j} - \frac{u_i}{\pi_i} \right) = f_i, \tag{1.2}$$

where $\pi_i = \mathrm{e}^{-V_i}$, $f_i = \int_{\Omega_i} f$ is the integral of f over the i-th cell, $S_{ij} = S_{\alpha,\beta}(\pi_i, \pi_j)$ is a Stolarsky mean of π_i and π_j and $\sum_{j:j\sim i}$ denotes the sum over all neighbors of cell i. We sometimes refer to the general form (1.2) as *discrete FPE*.

Assumption 1.3. *Under the Assumption 1.1 we additionally assume that for some $\infty > K > \kappa_0 > 0$ it holds $K > \kappa_{ij} \geq \kappa_0$.*

The weighted Stolarsky means [Sto75]

$$S_{\alpha,\beta}(x,y) = \left(\frac{\beta(x^\alpha - y^\alpha)}{\alpha(x^\beta - y^\beta)} \right)^{\frac{1}{\alpha-\beta}}, \qquad \alpha \neq 0,\ \beta \neq 0,\ \alpha \neq \beta,\ x \neq y \tag{1.3}$$

generalize the logarithmic mean and other means and can be extended to the critical points $\alpha = 0$, $\beta = 0$, $\alpha = \beta$, $x = y$ in a continuous way, see Tab. 2. An interesting aspect of the above representation is that all these schemes preserve positivity with the discrete linear operator being an M-matrix. This can be seen introducing the relative density $U = u/\pi$ for which Eq. (1.2) yields

$$-\sum_{j:j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} (U_j - U_i) = f_i, \tag{1.4}$$

which is a discretization of the elliptic equation

$$-\nabla \cdot (\kappa \pi \nabla U) = f, \tag{1.5}$$

where the discrete Fokker–Planck operator becomes a purely diffusive second order operator in U. Furthermore, if κ is a symmetric strictly positive definite uniformly elliptic matrix, the operator in Eq. (1.4) is also symmetric strictly positive definite and uniformly elliptic. In the latter setting, we can thus rule out the occurrence of spurious oscillations in our discretization.

The above formulation underpins the diffusive character both of the discrete and the continuous FPE. Using the relation $S_{\alpha,\beta}(x,y) = x\, S_{\alpha,\beta}(1, y/x)$ and introducing the weight function

$$B_{\alpha,\beta}(x) = S_{\alpha,\beta}(1, \mathrm{e}^{-x}) \quad \text{with} \quad B_{\alpha,\beta}(-x) = \mathrm{e}^x B_{\alpha,\beta}(x), \tag{1.6}$$

Eq. (1.2) can equally be reformulated as

$$-\sum_{j:i\sim j}\frac{m_{ij}}{h_{ij}}\kappa_{ij}\left(B_{\alpha,\beta}\left(V_i-V_j\right)u_j-B_{\alpha,\beta}\left(V_j-V_i\right)u_i\right)=f_i.$$

Two special cases of particular interest are

$$B_{0,-1}\left(V_i-V_j\right)=\frac{V_i-V_j}{\mathrm{e}^{V_i-V_j}-1}=S_{0,-1}\left(\pi_i,\pi_j\right)\pi_j^{-1}, \tag{1.7}$$

$$B_{1,-1}\left(V_i-V_j\right)=\mathrm{e}^{-\frac{1}{2}(V_i-V_j)}=S_{1,-1}\left(\pi_i,\pi_j\right)\pi_j^{-1}. \tag{1.8}$$

With regard to Tab. 2 below, these coefficients are known as the Bernoulli function $B_{0,-1}$ (for SG) and the SQRA-coefficient $B_{1,-1}$. FV schemes with general weight functions B have been investigated in [ChD11, LuL20] (B-schemes).

In the purely diffusive regime, i.e., for $V_i-V_j\to 0$, it holds $B_{\alpha,\beta}\left(V_i-V_j\right)\to 1$ for all α, β, such that the Stolarsky scheme approaches a discrete analogue of the diffusive part of the continuous flux $J_{ij}=\kappa_{ij}\left(B_{\alpha,\beta}\left(V_j-V_i\right)u_i-B_{\alpha,\beta}\left(V_i-V_j\right)u_j\right)/h_{ij}$.

In the drift-dominated regime, i.e., for $V_j-V_i\to\pm\infty$, the various $B_{\alpha,\beta}$ behave differently. While $B_{1,-1}\left(V_i-V_j\right)$ cannot be controlled in a reasonable way, asymptotics of $B_{0,-1}$ recover the upwind scheme

$$J_{i,j}\to-\kappa_{i,j}\frac{V_j-V_i}{h_{i,j}}\begin{cases}u_j & \text{if } V_j>V_i\\ u_i & \text{if } V_j<V_i\end{cases}, \tag{1.9}$$

which is a robust discretization of the drift part of the flux, where the density u is evaluated in the donor cell of the flux. Hence, the Bernoulli function $B_{0,-1}$ interpolates between the appropriate discretizations for the drift- and diffusion-dominated limits, which is why the SG scheme is the preferred FV scheme for Fokker–Planck type operators. Mathematically, this is formulated in Section 5.2.

1.2 Major contributions of this work

As main contribution, we investigate the order of convergence for the general Stolarsky scheme. Furthermore, we provide a derivation of the general Stolarsky mean FV discretization in Section 3.1 and discuss the gradient structure of the discretization schemes in view of the natural gradient structure of the FPE in Section 3.2.

In recent years, convergence order has been derived for many different schemes. In [LMV96], quantitative convergence of order $O(h^2)$ for several upwind schemes on rectangular grids has been shown. In [BCC98] the finite volume Scharfetter–Gummel discretization (of steady convection diffusion equations) is connected to a finite element method and convergence of order $O(h)$ is obtained by using results from [XuZ99]. Investigating general B-schemes, [ChD11] proved strong convergence in L^2 for the solutions of the FV scheme to the continuous solution. Recently, convergence of order $O(h)$ for general B-schemes including SG, SQRA as well as Stolarsky means has been proved in 1D [LuL20]. Independently, convergence for the SQRA discretization has been investigated in [Mie13a] in 1D, [DH*] (formally, rectangular meshes) and [Hei18] using G-convergence on grids with random weights.

Here, we are going to derive estimates for the order of convergence in the energy norm for general Stolarsky schemes. We benefit from analytical properties of Stolarsky

means and uses the general theory of consistent meshes in the sense of the recent work [DiD18]. We will see that the error naturally splits into the consistency error for the discretization of the Laplace operator (the consistency of the elliptic operator) plus an error which is due to the convective part. Here we have the possibility to study the error in terms of U and of u, in both cases in the energy norm. While the error in terms of U can be directly inferred from the diffusive estimate in Lemma 2.12, one can also apply a splitting into diffusion- and convection-part of the error, both in terms of U and u. The order of convergence is in general limited by the consistency of the mesh but can be improved up to order $O(h)$ in u (on all Voronoï grids), resp. $O(h^2)$ in U (on cubic grids). It is interesting to observe that the optimal Stolarsky mean can be different in the variables u and U for the same problem on the same mesh. This is indicated by the numerical experiment of Example 7.1.

Despite the latter discrepancy for u and U, the Stolarsky scheme $S_{0,-1}$ (SG scheme) turns out to be special among all schemes as it yields order $O(h^2)$ in u on cubic grids (Theorem 6.3). Due to a perturbation result (Corollary 4.4), the good convergence properties of the SG scheme carry over to every Stolarsky scheme where $\alpha + \beta = -1$.

Using the notations of Section 2, we formulate the above in the following theorems, where $\mathcal{R}_{\mathcal{T}_h} u$ is the pointwise evaluation of u in the centers of the Voronoï cells. Hence the constraint $d \leq 4$ in this work stems from the condition $H^2(\Omega) \hookrightarrow C(\overline{\Omega})$.

Theorem 1.4. *Let $d \leq 4$ and $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ and κ, V satisfying Assumptions 1.1 and 1.3 such that $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ is a family of φ-consistent meshes (Def. 2.14) with* $\mathrm{diam}\mathcal{T}_h \to 0$ *as $h \to 0$ and let the assumptions of Lemma 5.1 hold. If $u \in H^2(\Omega)$ is the solution of* (1.1) *and $u_{\mathcal{T}_h}$ the solution of* (1.2) *then*

$$\|u_{\mathcal{T}_h} - \mathcal{R}_{\mathcal{T}_h} u\|^2_{H_{\mathcal{T},\kappa}} \leq C_1 \left(\|u\|_{H^2} + \|u\|_\infty \|V\|_{H^2}\right) \varphi(h)^2 + C_2 h^2 \,,$$

where C_1 depends on $\mathcal{T}_h$ and κ and C_2 additionally depends on $\|V\|_{C^2}$ and $\|u\|_{H^2}$. In case $S_* = S_{0,-1}$ or $S_* = S_{\alpha,\beta}$ with $\alpha + \beta = -1$ and $u \in C^1(\overline{\Omega})$ the above can be improved to

$$\|u_{\mathcal{T}_h} - \mathcal{R}_{\mathcal{T}_h} u\|^2_{H_{\mathcal{T},\kappa}} \leq C_1 \left(\|u\|_{H^2} + \|u\|_\infty \|V\|_{H^2}\right) \varphi(h)^2 + C_2 h^4 \,.$$

Proof. This is a consequence of Definition 2.14 together with Lemma 2.12, Theorem 5.6 and Corollary 5.7. □

Remark 1.5. As a consequence of former works (see Propositions 2.15 and 2.16) it holds $\varphi(h) = O(h)$ on Voronoï grids and $\varphi(h) = O(h^2)$ on cubic grids. This explains the next result.

Theorem 1.6. *Let $d \leq 4$ and $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ and κ, V satisfying Assumptions 1.1 and 1.3 such that $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ is a family of* cubic *φ-consistent meshes (Def. 2.14) with* $\mathrm{diam}\mathcal{T}_h \to 0$ *as $h \to 0$ and let the assumptions of Lemma 5.1 hold. If $u \in H^2(\Omega)$ is the solution of* (1.1) *and $u_{\mathcal{T}_h}$ the solution of* (1.2) *then*

$$\|u_{\mathcal{T}_h} - \mathcal{R}_{\mathcal{T}_h} u\|^2_{H_{\mathcal{T},\kappa}} \leq C h^2 \,,$$

where C depends on $\mathcal{T}_h$, κ, $\|V\|_{C^2}$ and $\|u\|_{H^2}$. In case $S_* = S_{0,-1}$ or $S_* = S_{\alpha,\beta}$ with $\alpha + \beta = -1$ the above can be improved to

$$\|u_{\mathcal{T}_h} - \mathcal{R}_{\mathcal{T}_h} u\|^2_{H_{\mathcal{T},\kappa}} \leq C h^4 \,.$$

Proof. This is a consequence of Lemma 2.12, Propositions 2.16 (resp. Theorem 6.2) and Theorem 6.3. □

We note at this point, that these estimates are only "worst case" estimates, while the true rate of convergence could also be better. In Section 4 we will see that the rate of convergence is close for different Stolarsky means which share the same value of $\alpha+\beta$. I.e. the difference in the error due to switching $S_{\alpha,\beta}$ with $S_{\tilde{\alpha},\tilde{\beta}}$ is of order h^3 if $\tilde{\alpha}+\tilde{\beta}=\alpha+\beta$, see Corollary 4.3. This explains the shape of the error graphs in Figs. 2 (a, c) and 3 (a, c).

Although we treat the Stolarsky means as an explicit example, note that some of the main results also hold for other smooth means.

1.3 Outlook

The results of this work suggest to search for "optimal" parameters α and β in the choice of the Stolarsky mean in order to reduce the error of the approximation as much as possible. However, from an analytical point of view, the quest for such optimal α and β is quite challenging. Moreover, since the optimal choice might vary locally, depending on the local properties of the potential V, we suggest to implement a learning algorithm that provides suitable parameters α and β depending on the local structure of V and the mesh.

1.4 Outline of this work

After some preliminaries regarding notation and a priori estimates in Section 2, we present a mathematical derivation of the SG scheme in Section 3.1 and discuss its formal relation to SQRA. We will then provide a derivation of SQRA from physical principles in Section 3.2, based on the Jordan–Kinderlehrer–Otto [JKO98] formulation of the FPE. In Section 3.1, we show that SG and SQRA are elements of a huge family of discretization schemes (1.2).

Section 5 provides the error analysis and estimates for the consistency and the order of convergence. We distinguish the cases of small and large gradients and have a particular look at cubic meshes. Section 6 specifies the results to cubic grids.

Finally, we show hat the optimal choice of S_* depends on V and f, but is not unique. If $S_{\alpha,\beta}$ denotes one of the Stolarsky means, we will prove in Section 4 that the Stolarsky means satisfying $\alpha+\beta=\text{const.}$ show similar quantitative convergence behavior as suggested in Corollary 4.3. Finally, this result is illustrated in Section 7 by numerical simulations.

2 Preliminaries and notation

We collect some concepts and notation, which will frequently be used in this work.

2.1 The Mesh

For a subset $A\subset\mathbb{R}^d$, $\overline{A}$ is the topological closure of A.

Definition 2.1. Let $\Omega \subset \mathbb{R}^d$ be a polygonal domain. A finite volume mesh of Ω is a triangulation $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ consisting of a family of control volumes $\mathcal{V} := \{\Omega_i, i = 1, \dots, N\}$ which are convex polytope cells, a family of $(d-1)$-dimensional interfaces

$$\begin{aligned}\mathcal{E} &:= \mathcal{E}_\Omega \cup \mathcal{E}_\partial \\ \mathcal{E}_\Omega &:= \left\{\sigma_{ij} \subset \mathbb{R}^d \,:\, \sigma_{ij} = \partial\Omega_i \cap \partial\Omega_j\right\} \\ \mathcal{E}_\partial &:= \left\{\sigma \subset \mathbb{R}^d \,:\, \sigma = \partial\Omega_i \cap \partial\Omega \text{ is flat}\right\}\end{aligned}$$

and points $\mathcal{P} = \{x_i, i = 1, \dots, N\}$ with $x_i \in \overline{\Omega_i}$ satisfying

(i) $\bigcup_i \overline{\Omega}_i = \overline{\Omega}$

(ii) For every i there exists $\mathcal{E}_i \subset \mathcal{E}$ such that $\overline{\Omega}_i \backslash \Omega_i = \bigcup_{\sigma\in\mathcal{E}_i} \sigma$. Furthermore, $\mathcal{E} = \bigcup_i \mathcal{E}_i$.

(iii) For every i, j either $\overline{\Omega}_i \cap \overline{\Omega}_j = \varnothing$ or $\overline{\Omega}_i \cap \overline{\Omega}_j = \overline{\sigma}$ for $\sigma \in \mathcal{E}_i \cap \mathcal{E}_j$ which will be denoted σ_{ij}.

The mesh is called h-consistent if

(iv) The Family $(x_i)_{i=1\dots N}$ is such that $x_i \neq x_j$ if $i \neq j$ and the straight line D_{ij} going through x_i and x_j is orthogonal to σ_{ij}.

and admissible if

(v) For any boundary interface $\sigma \in \mathcal{E}_\partial \cap \mathcal{E}_i$ it holds $x_i \notin \sigma$ and for $D_{i,\sigma}$ the line through x_i orthogonal to σ it holds that $D_{i,\sigma} \cap \sigma \neq \varnothing$ and let $y_\sigma := D_{i,\sigma} \cap \sigma$.

Property (iv) is assumed in [GHV00] in order to prove a strong form of consistency in the sense of Definition 2.14 below. It is satisfied for example for Voronoï discretizations.

We write m_i for the volume of Ω_i and for $\sigma \in \mathcal{E}$ we denote m_σ its $(d-1)$-dimensional mass. In case $\sigma_{ij} \in \mathcal{E}_i \cap \mathcal{E}_j$ we write $m_{ij} := m_{\sigma_{ij}}$. For the sake of simplicity, we consider $\tilde{\mathcal{P}} := (x_i)_{i=1,\dots,N}$ and $\mathcal{P} := \tilde{\mathcal{P}} \cup \{y_\sigma \,:\, \sigma \in \mathcal{E}_\partial$, according to (v)$\}$. We extend the enumeration of $\tilde{\mathcal{P}}$ to $\mathcal{P} = (x_j)_{j=1,\dots,\tilde{N}}$ and write $i \sim j$ if $x_i, x_j \in \tilde{\mathcal{P}}$ with $\mathcal{E}_i \cap \mathcal{E}_j \neq \varnothing$. Similarly, if $x_i \in \tilde{\mathcal{P}}$ and $x_j = y_\sigma$ for $\sigma \in \mathcal{E}_i$ we write $\sigma_{ij} := \sigma$ and $i \sim j$. Finally, we write $h_{ij} = |x_i - x_j|$.

We further call

$$\mathcal{P}^* := \{u : \mathcal{P} \to \mathbb{R}\}\,, \quad \tilde{\mathcal{P}}^* := \left\{u : \tilde{\mathcal{P}} \to \mathbb{R}\right\}, \quad \text{and} \quad \mathcal{E}^* := \{w : \mathcal{E} \to \mathbb{R}\}$$

the discrete functions from $\mathcal{P}$ resp. $\tilde{\mathcal{P}}$ resp. $\mathcal{E}$ to $\mathbb{R}$.

In this work, we consider function with

$$\text{discrete homogeneous Dirichlet boundary conditions:} \qquad \forall \sigma \in \mathcal{E}_\partial : \quad u(y_\sigma) = 0\,. \tag{2.1}$$

We write the latter also as $u_i = 0$ if $x_i \in \mathcal{P}\backslash\tilde{\mathcal{P}}$. Hence, in what follows we write

$$\forall x_i \in \tilde{\mathcal{P}} : a_i := a(x_i)\,, \qquad \text{with} \quad \sum_i a_i := \sum_{x_i\in\tilde{\mathcal{P}}} a(x_i)\,.$$

For $w \in \mathcal{E}^*$ we write $w_{ij} := w(\sigma)$ if $\sigma_{ij} = \sigma$. Then for fixed i the expression

$$\sum_{j:i\sim j} w_{ij} := \sum_{\sigma_{ij}\in\mathcal{E}_i} w_{ij}$$

symbol	meaning	symbol	meaning
κ	diffusion coefficient	U	u/π
κ_{ij}	$\frac{\bar\kappa_i\bar\kappa_j}{\bar\kappa_i\frac{d_{i,ij}}{h_{ij}}+\bar\kappa_j\frac{d_{j,ij}}{h_{ij}}}$	u	density
κ^*,κ_*	$0<\kappa_*\le\kappa\le\kappa^*<\infty$	m_i	$\mathrm{vol}(\Omega_i)$
V	real potential on $\Omega\subset\mathbb{R}^d$	h_i	$\mathrm{diam}(\Omega_i)$
V^*,V_*	$-\infty<V_*\le V\le V^*<\infty$	σ_{ij}	$\partial\Omega_i\cap\partial\Omega_j$
π	stat. measure $\mathrm{e}^{-V(x)}$ on Ω	m_{ij}	area of σ_{ij}
π_i	stat. measure $\mathrm{e}^{-V(x_i)}$ on Ω_i	$\mathbf{h}_{ij}$	x_i-x_j
u_i	$u(x_i)$	h_{ij}	$\lvert\mathbf{h}_{ij}\rvert$
$\bar f_i$	$\frac{1}{\lvert\Omega_i\rvert}\int_{\Omega_i}f\mathrm{d}x$	$d_{i,ij}$	$\mathrm{dist}\,(x_i,\sigma_{ij})$
f_i	$m_i\bar f_i$	$\mathrm{diam}\mathcal{T}$	diameter, i.e. $\sup_{i\sim j}\lvert x_i-x_j\rvert$
$\mathbf{J}$	$-\kappa\left(\nabla u+u\nabla V\right)$	$J_{ij}^S U$	$-\frac{\kappa_{ij}}{h_{ij}}S_{ij}\left(U_j-U_i\right)$

Tab. 1: Commonly used notations.

is the sum over all w_{ij} such that $\mathcal{E}_i\cap\mathcal{E}_j\neq\varnothing$ and

$$\sum_i\sum_{j:i\sim j}w_{ij}=\sum_{j\sim i}w_{ij}:=\sum_{\sigma_{ij}\in\mathcal{E}}w_{ij}:=\sum_{\sigma\in\mathcal{E}}w(\sigma)$$

is the sum over all edges.

Moreover, we define the diameter of a triangulation $\mathcal{T}$ as

$$\mathrm{diam}\mathcal{T}=\sup_{i\sim j}\lvert x_i-x_j\rvert.$$

The identity

$$\sum_i\sum_{j:j\sim i}A_{ij}=\sum_{j\sim i}\left(A_{ij}+A_{ji}\right)\tag{2.2}$$

will frequently be used throughout this paper, where we often encounter the case $A_{ij}=\alpha_{ij}U_i$ with $\alpha_{ij}=-\alpha_{ji}$:

$$\sum_i\sum_{j:j\sim i}\alpha_{ij}U_i=\sum_{j\sim i}\left(\alpha_{ij}U_i+\alpha_{ji}U_j\right)=\sum_{j\sim i}\alpha_{ij}\left(U_i-U_j\right).\tag{2.3}$$

Formula (2.2) in particular allows for a discrete integration by parts for functions satisfying (2.1):

$$\sum_i\sum_{j:j\sim i}\left(U_j-U_i\right)U_i=\sum_{j\sim i}\left(\left(U_j-U_i\right)U_i+\left(U_i-U_j\right)U_j\right)=-\sum_{j\sim i}\left(U_j-U_i\right)^2.\tag{2.4}$$

On a given mesh $\mathcal{T}=(\mathcal{V},\mathcal{E},\mathcal{P})$, we consider the linear discrete operator $\mathcal{L}_\kappa^\mathcal{T}:\mathcal{P}^*\to\mathcal{P}^*$, which is defined by a family of non-negative weights $\kappa:\mathcal{E}\to\mathbb{R}$ and acts on functions $u\in\mathcal{P}^*$ via

$$\forall x_i\in\mathcal{P}:\ \left(\mathcal{L}_\kappa^\mathcal{T}u\right)_i:=\sum_{i\sim j}\kappa_{ij}\frac{m_{ij}}{h_{ij}}\left(u_j-u_i\right).\tag{2.5}$$

While (2.5) is very general, it is shown in [GHV00], Lemma 3.3, that the property (iv) of Definition 2.1 comes up with some special consistency properties for the choice of

$$\kappa_{ij} := \frac{\bar{\kappa}_i \bar{\kappa}_j}{\bar{\kappa}_i \frac{d_{i,ij}}{h_{ij}} + \bar{\kappa}_j \frac{d_{j,ij}}{h_{ij}}}, \tag{2.6}$$

where $d_{i,ij}$ and $d_{j,ij}$ are the distances between σ_{ij} and x_i and x_j respectively and averaged diffusion coefficient is defined by $\overline{\kappa}_i = m_i^{-1} \int_{\Omega_i} \kappa(x) \mathrm{d}x$.

Lemma 2.2 (A consistency lemma, [GHV00]). *Let the $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ satisfy Definition 2.1 (i)–(v) and let $d \in \{2, 3\}$ and let h_{ij} be uniformly bounded from above and from below. Then for every $u \in H^2(\Omega)$ it holds*

$$\left| \int_{\sigma_{ij}} \kappa \nabla u \cdot \boldsymbol{\nu}_{ij} - \kappa_{ij} \frac{m_{ij}}{h_{ij}} \left(u(x_j) - u(x_i) \right) \right| \leq C m_{ij}^{\frac{1}{2}} h_{ij}^{\frac{1}{2}} \left\| u \right\|_{H^2(\Omega_i \cup \Omega_j)}.$$

Lemma 2.2 was one of the motivations to provide a more general and powerful concept of consistency in [DiD18], as we will discuss in Section 2.5

2.2 Poincaré inequalities

In order to derive the a priori estimates in Section 2.3 we need to exploit (discrete) Poincaré inequalities to estimate $\|u\|_{L^2(\Omega)}$ by $\|\nabla u\|_{L^2(\Omega)}$ or $\|u^{\mathcal{T}}\|_{L^2(\mathcal{P})}$ by $\|Du^{\mathcal{T}}\|_{L^2(\mathcal{E})}$, where $(Du^{\mathcal{T}})_{ij} = u_j - u$. In particular, we use the following theorem which can be found e.g. in [EGH00] or can be proved using Lemma A.1 applied to piecewise constant functions on the cells with $C_{\#} \leq \frac{\mathrm{diam}\Omega}{h_0}$ and the choice $|\boldsymbol{\eta}| > \mathrm{diam}\Omega$.

Theorem 2.3. *Given a mesh $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ let $h_{\inf} := \inf \{|x - y| : (x, y) \in \mathcal{P}^2\} > 0$ and $h_{\sup} := \sup \{|x - y| : (x, y) \in \mathcal{P}^2\} > 0$ correspondingly. Then for every $u \in L^2(\mathcal{P})$ satisfying (2.1) and for every $\boldsymbol{\eta} \in \mathbb{R}^d$ it holds*

$$\int_\Omega \left| \sum_i u_i \chi_{\Omega_i}(x) - \sum_i u_i \chi_{\Omega_i}(x + \boldsymbol{\eta}) \right|^2 dx \leq |\boldsymbol{\eta}| \left(\mathrm{diam}\Omega \frac{h_{\sup}}{h_{\inf}} \sum_{i \sim j} \frac{m_{ij}}{h_{ij}} (u_j - u_i)^2 \right), \tag{2.7}$$

and particularly

$$\|u\|^2_{L^2(\mathcal{P})} \leq (\mathrm{diam}\Omega)^2 \frac{h_{\sup}}{h_{\inf}} \sum_{i \sim j} m_{ij} (u_j - u_i)^2. \tag{2.8}$$

2.3 Existence and a priori estimates

In what follows, we study the properties of (1.4)–(1.5). Putting $U \equiv 1$ in both of these equations, we immediately see that the Boltzmann distribution $u_i := \pi_i = \exp(-V(x_i)) = \exp(-V_i)$, resp. the continuous version $u = \pi$ is the stationary solution for $f = 0$. Hence, from the standard theory of elliptic systems ([Eva98] Chapter 6), we have the following theorem.

Theorem 2.4. *Let Ω be as above and $f \in \mathrm{L}^2(\Omega)$, $\kappa \in C^1\left(\overline{\Omega} : \mathbb{R}^{d \times d}\right)$ such that κ is uniformly bounded, symmetric and elliptic and $V \in \mathrm{C}^2(\overline{\Omega})$. Then there is a unique $u \in \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$ solving $-\nabla \cdot (\kappa \nabla u) - \nabla \cdot (\kappa u \nabla V) = f$ in the weak sense.*

Furthermore, we find the following.

Theorem 2.5. *Let $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ be an admissible mesh in the sense of Definition 2.1 and let $c > 0$ such that $\kappa_{ij} > c$ for every i, j. Furthermore, let $\pi > 0$. Then there exists a unique solution $U^{\mathcal{T}} \in L^2(\tilde{\mathcal{P}})$ to (1.4) satisfying discrete homogeneous Dirichlet boundary conditions (2.1).*

Proof. Multiplying (1.4) with $\phi \in L^2(\tilde{\mathcal{P}})$ and applying (2.4) we find

$$\begin{aligned}\sum_i f_i \phi_i &= \sum_i -\phi_i \sum_{j:j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right) \\ &= \sum_{i\sim j} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right)(\phi_j - \phi_i)\,.\end{aligned}$$

The right hand side is a strictly positive symmetric bilinear form in $L^2(\tilde{\mathcal{P}})$ due to the Poincaré inequality (2.8). Hence there exists a unique solution $U^{\mathcal{T}}$ by the Lax–Milgram theorem. □

Having shown the existence of solutions to (1.5) and (1.4), we recall the derivation of some natural a priori estimates for both the continuous Fokker–Planck equation and the discretization.

Continuous FPE Let u, resp. $U = u/\pi$, be a solution of the stationary Fokker–Planck equation (1.5) with homogeneous Dirichlet boundary conditions. Testing with U, we get from a standard calculation that

$$\int_\Omega \tfrac{1}{\kappa\pi} |\kappa\pi \nabla U|^2 \le C \int_\Omega f^2\,. \tag{2.9}$$

Furthermore, the standard theory of elliptic equations (e.g., [Eva98]) yields $\|U\|_{H^2(\Omega)} \le C \|f\|_{L^2}$, where C depends on the C^1-norm of $\kappa\pi$ and the Poincaré-constant.

Discrete FPE Let $U_i^{\mathcal{T}}$ be a solution of (1.4) with $f_i = m_i \bar{f}_i = \int_{\Omega_i} f \mathrm{d}x$ (as specified in the Tab. 1), i.e.,

$$\forall i: \qquad -\sum_{j:j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right) = m_i \bar{f}_i\,.$$

Then, multiplying with $U_i^{\mathcal{T}}$, summing over all $x_i \in \mathcal{P}$ and using (2.4), we conclude with help of the discrete Poincaré inequality (see Theorem 2.3 below)

$$\begin{aligned}\sum_{j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right)^2 &= \sum_i m_i \bar{f}_i U_i^{\mathcal{T}} \le \sum_i \left((U_i^{\mathcal{T}})^2 m_i + \tfrac{1}{\pi_i} \bar{f}_i^2 m_i\right) \\ \Rightarrow \sum_{j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right)^2 &\le C \sum_i m_i \bar{f}_i^2.\end{aligned}$$

The last estimate can be rewritten as

$$\sum_{j\sim i} \frac{m_{ij}}{h_{ij}} \kappa_{ij} \frac{1}{S_{ij}\kappa_{ij}^2} \left(\kappa_{ij} S_{ij} (U_j^{\mathcal{T}} - U_i^{\mathcal{T}})\right)^2 \le C \sum_i \bar{f}_i^2 m_i. \tag{2.10}$$

2.4 Gradients, Fluxes and L^2-spaces

In order to derive and formulate variational consistence errors for the discrete FPE (1.4), we introduce the discrete fluxes

$$\begin{aligned} J_{ij}^S U^{\mathcal{T}} &:= -\frac{\kappa_{ij}}{h_{ij}} S_{ij} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}} \right) , \\ \overline{J}_{ij} U &:= -\frac{1}{m_{ij}} \int_{\sigma_{ij}} \kappa \pi \nabla U \cdot \boldsymbol{\nu}_{ij} \, . \end{aligned} \tag{2.11}$$

In particular, if $S_{ij} = \sqrt{\pi_i \pi_j}$ we get $J_{ij}^{\mathrm{SQRA}} U^{\mathcal{T}} := -\kappa_{ij} \sqrt{\pi_i \pi_j} \left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}} \right) / h_{ij}$ for the flux of the SQRA scheme. The quantity $J_{ij}^S U^{\mathcal{T}}$ can indeed be considered as a flux in the sense that it will be shown to approximate $\overline{J}_{ij}$, S_{ij} is a discrete approximation of $\pi|_{\sigma_{ij}}$, κ_{ij} is a discrete approximation of $\kappa|_{\sigma_{ij}}$. The differences $\left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}} \right) / h_{ij}$ take the role of gradients ∇U in the continuous problem and hence we refer to them as *discrete gradients* even though they are 1-dimensional objects.

While former approaches focus on the rate of convergence of $\left(u_j^{\mathcal{T}} - u_i^{\mathcal{T}} \right) / h_{ij} \to \nabla u$, we additionally follow the approach of [DiD18] applied to U and are interested in the rate of convergence of $J_{ij}^S U^{\mathcal{T}} \to \mathbf{J}(U)$, which is an indirect approach to the original problem as this rate of convergence is directly related to $\left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}} \right) / h_{ij} \to \nabla U$.

In view of the natural norms for the variational consistency (see (2.16) f.f.), we introduce the following

$$\begin{aligned} \forall U \in L^2(\Omega): \qquad & \|U\|_{L^2(\Omega)}^2 := \int_\Omega U^2 \mathrm{d}x && \|U\|_{L^2_\pi(\Omega)}^2 := \int_\Omega \tfrac{1}{\pi} U^2 \mathrm{d}x \\ \forall U \in \mathcal{P}^*: \qquad & \|U\|_{L^2(\mathcal{P})}^2 := \sum_{i \in \mathcal{P}} m_i U_i^2 && \|U\|_{L^2_\pi(\mathcal{P})}^2 := \sum_{i \in \mathcal{P}} m_i \tfrac{1}{\pi_i} U_i^2 \\ \forall J \in \mathcal{E}^*: \qquad & \|J\|_{L^2(\mathcal{E})}^2 := \sum_{i \sim j} m_{ij} h_{ij} J_{ij}^2 && \|J\|_{L^2_S(\mathcal{E})}^2 := \sum_{i \sim j} m_{ij} h_{ij} \frac{1}{S_{ij}} J_{ij}^2 \end{aligned} \tag{2.12}$$

Let us introduce the discrete flux $J^S U^{\mathcal{T}} \in \mathcal{E}^*$ via $J^S U^{\mathcal{T}}(\sigma_{ij}) := J_{ij}^S U^{\mathcal{T}}$ and similarly also $\frac{1}{\kappa} J^S U^{\mathcal{T}} \in \mathcal{E}^*$ via $J^S U^{\mathcal{T}}(\sigma_{ij}) := \frac{1}{\kappa_{ij}} J_{ij}^S U^{\mathcal{T}}$. With all the above notations, our a priori estimates (2.9) and (2.10) now read

$$\begin{aligned} \| \frac{1}{\sqrt{\kappa}} \mathbf{J}(U) \|_{L^2_\pi(\Omega)}^2 &\le C \|f\|_{L^2_\pi(\Omega)}^2 \\ \left\| \frac{1}{\sqrt{\kappa}} J^S U^{\mathcal{T}} \right\|_{L^2_S(\mathcal{E})}^2 &\le C \|\bar{f}\|_{L^2_\pi(\mathcal{P})}^2 \, . \end{aligned}$$

Assuming that the diffusion coefficient is bounded, i.e. $\kappa^* \ge \kappa \ge \kappa_*$, we further get

$$\begin{aligned} \tfrac{1}{\kappa_*} \|\mathbf{J}(U)\|_{L^2_\pi(\Omega)}^2 &\le C \|f\|_{L^2_\pi(\Omega)}^2 \\ \frac{1}{\kappa^*} \|J^S U^{\mathcal{T}}\|_{L^2_S(\mathcal{E})}^2 &\le C \|\bar{f}\|_{L^2_\pi(\mathcal{P})}^2 \, . \end{aligned}$$

Remark 2.6 (Naturalness of norms)**.** Let us discuss why these norms are natural to consider. The left norms in (2.12) can be interpreted as the Euclidean L^2-norms on Ω, $\mathcal{P}$ and $\mathcal{E}$, while the right norms are the natural norms for the study of the Fokker–Planck equation as they are weighted with the inverse of the Boltzmann distribution π, resp.

π_i. Note that assuming V is bounded from above and below, the L^2-norms $\|\cdot\|_{L^2_\pi(\Omega)}$ and $\|\cdot\|_{L^2(\Omega)}$ are equivalent and the same holds true for the two norms in the discrete setting.

Given a discretization $\mathcal{T}$, the linear map

$$C_c\left(\mathbb{R}^d\right) \to \mathbb{R}\,, \qquad f \mapsto \sum_{i\in\mathcal{P}} m_i f(x_i)$$

defines an integral on Ω w.r.t. a discrete measure $\mu_\mathcal{T}$ having the property that $\mu_\mathcal{T} \to \mathcal{L}^d$ vaguely, where $\mathcal{L}^d$ is the d-dimensional Lebesgue measure. In particular $\mu_\mathcal{T}(A) \to \mathcal{L}^d(A)$ for every bounded measurable set with $\mathcal{L}^d(\partial A) = 0$. The norm $\|U\|^2_{L^2(\mathcal{P})}$ is simply the L^2-norm based on the measure $\mu_\mathcal{T}$.

Similar considerations work also for the norm on $\mathcal{E}^*$. The norm $\|\cdot\|^2_{L^2(\mathcal{E})}$ is given via a measure $\tilde{\mu}_\mathcal{T}$ having the property

$$\tilde{\mu}_\mathcal{T} : C_c\left(\mathbb{R}^d\right) \to \mathbb{R}\,, \qquad f \mapsto \sum_{i\sim j} m_{ij} h_{ij} f(x_{ij})\,,$$

with the property that $\tilde{\mu}_\mathcal{T} \to d\cdot\mathcal{L}^d$ vaguely: every Voronoï cell Ω_i consists of disjoint cones with mass $\frac{1}{d} m_{ij} h_{ij}$, where one has to account for all cones with $j \sim i$. In particular, we obtain $\tilde{\mu}_\mathcal{T}(A) \approx d\cdot\mathcal{L}(A)$ for Lipschitz domains – an estimate which then becomes precise in the limit. Without going into details, let us mention that heuristically the prefactor d balances the fact that $J_{ij} \approx \frac{(\mathbf{x}_i - \mathbf{x}_j)}{|x_i - x_j|}\cdot\nabla U$ which yields for functions $U \in C^1_c(\mathbb{R}^d)$:

$$\sum_{i\sim j} m_{ij} h_{ij} \left|\frac{(\mathbf{x}_i - \mathbf{x}_j)}{|x_i - x_j|}\cdot\nabla U\right|^2 \to \int_{\mathbb{R}^d} |\nabla U|^2\,.$$

For the particular case of a rectangular mesh, this is straight forward to verify.

2.5 Consistency and inf-sup stability

Results such as Lemma 2.2 motivated the authors of the recent paper [DiD18] to define the concepts of consistency and inf-sup stability as discussed in the following. For readability, we will restrict the general framework of [DiD18] to cell-centered finite volume schemes and refer to general concepts only as far as needed.

Definition 2.7 (inf-sup stability)**.** A bilinear form $a_\mathcal{T}$ on $L^2(\mathcal{P})$ for a given mesh $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ is called *(uniformly) inf-sup stable* with respect to a norm $\|\cdot\|_{H_\mathcal{T}}$ on a subspace $H_\mathcal{T} \subset L^2(\mathcal{P})$ if there exists $\gamma > 0$ (independent from $\mathcal{T}$) such that

$$\forall u \in H_\mathcal{T} : \quad \gamma \|u\|_{H_\mathcal{T}} \le \sup_{v\in H_\mathcal{T}} \frac{a_\mathcal{T}(u,v)}{\|v\|_{L^2(\mathcal{P})}}\,.$$

Usually, and particularly in our setting, $a_\mathcal{T}$ is the discretization of a continuous bilinear form, say e.g. $a(u,v) = \int_\Omega \nabla u\cdot(\kappa\nabla v)$. We are interested in discretizing the problem

$$\forall v \in H^1_0(\Omega) : \quad a(u,v) = l(v)\,, \tag{2.13}$$

where $l : H^1_0(\Omega) \to \mathbb{R}$ is a continuous linear map, and in the convergence of the solutions $u_\mathcal{T}$ of the discrete problems

$$\forall v \in L^2(\mathcal{T}) : \quad a_\mathcal{T}(u_\mathcal{T}, v) = l_\mathcal{T}(v) \tag{2.14}$$

to the solutions u for (2.13).

Definition 2.8 (Consistency)**.** Let $B \subset H_0^1(\Omega)$ be a continuously embedded Banach subspace and for given $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ consider continuous linear operators $\mathcal{R}_\mathcal{T} : B \to L^2(\mathcal{P})$ with uniform bound. Let u be the solution to the linear equation (2.13) and let $l_\mathcal{T} : L^2(\mathcal{P}) \to \mathbb{R}$ be a family of linear functionals. The *variational consistency error* of $u \in B$ is the linear form $\mathfrak{E}_\mathcal{T}(u;\cdot) : L^2(\mathcal{P}) \to \mathbb{R}$ where

$$\mathfrak{E}_\mathcal{T}(u;\cdot) := l_\mathcal{T}(\cdot) - a_\mathcal{T}(\mathcal{R}_\mathcal{T} u, \cdot) .$$

Let now a family $(\mathcal{T}, a_\mathcal{T}, l_\mathcal{T})$ with $\operatorname{diam}\mathcal{T} \to 0$ be given and consider the corresponding family of linear discrete problems (2.14) and let $u \in B$ be a solution of (2.13). We say that

$$\text{consistency holds if} \quad \|\mathfrak{E}_\mathcal{T}(u;\cdot)\|_{H_\mathcal{T}^*} := \sup_{v \in H_\mathcal{T} \setminus \{0\}} \frac{|\mathfrak{E}_\mathcal{T}(u;v)|}{\|v\|_{H_\mathcal{T}}} \to 0 \quad \text{as} \quad \operatorname{diam}\mathcal{T} \to 0 .$$

Remark 2.9. A typical situation is the case $d \le 3$, where $H^2(\Omega) \cap H_0^1(\Omega) \hookrightarrow C_0(\Omega)$ continuously. We then might set $B = H^2(\Omega) \cap H_0^1(\Omega)$ and $(\mathcal{R}_\mathcal{T} u)_i := u(x_i)$.

Consistency measures the rate at which $\mathcal{R}_\mathcal{T} u - u_\mathcal{T} \to 0$ and particularly provides a positive answer to the question whether the numerical scheme converges, at least if the solution of (2.13) lies in B. This is formulated in Theorem 10 of [DiD18].

Theorem 2.10 (Theorem 10, [DiD18])**.** *Using the above notation, it holds*

$$\|u_\mathcal{T} - \mathcal{R}_\mathcal{T} u\|_{H_\mathcal{T}} \le \gamma^{-1} \|\mathfrak{E}_\mathcal{T}(u;\cdot)\|_{H_\mathcal{T}^*} \tag{2.15}$$

In our setting, $\|\cdot\|_{H_\mathcal{T}} = \|\cdot\|_{H_{\mathcal{T},\kappa}}$ (see (2.16)) is a norm on $L^2(\mathcal{P})$ defined in terms of the discrete gradients. By the discrete Poincaré inequality, (2.15) also implies a convergence estimate for the discrete solutions itself. The theorem can be understood as a requirement on the regularity of u, resp. the right hand side of (2.13) for convergence of the scheme.

We introduce

$$H_\mathcal{T} := \left\{ u \in L^2(\mathcal{P}) : u \text{ satisfies hom. Dir. b.c. (2.1)} \right\}$$

with the $H_\mathcal{T}$-norm through

$$\|u\|_{H_{\mathcal{T},\kappa}} := \sum_{i \sim j} \frac{m_{ij}}{h_{ij}} \kappa_{ij} (u_j - u_i)^2 \tag{2.16}$$

and find by the uniform bound $\kappa_{ij} > \kappa_0$ that $\|\cdot\|_{H_{\mathcal{T},\kappa}}$ and the following norms are equivalent:

$$\|u\|_{L^2,H_{\mathcal{T},\kappa}} := \|u\|_{H_{\mathcal{T},\kappa}} + \|u\|_{L^2(\mathcal{P})} , \qquad \|u\|_{L^2,H_\mathcal{T}} := \|u\|_{L^2,H_{\mathcal{T},1}} = \sum_{i \sim j} \frac{m_{ij}}{h_{ij}} (u_j - u_i)^2 + \|u\|_{L^2(\mathcal{P})} .$$

Due to the discrete Poincaré inequality (2.8), this holds uniformly, i.e. for every κ there exist constants $C_1, C_2, C_3, C_4 > 0$ independent from $\mathcal{T}$ such that for all functions $u \in L^2(\mathcal{P})$ with homogeneous Dirichlet boundary values

$$\|u\|_{H_{\mathcal{T},1}} \le C_1 \|u\|_{L^2,H_\mathcal{T}} \le C_2 \|u\|_{L^2,H_{\mathcal{T},\kappa}} \le C_3 \|u\|_{H_{\mathcal{T},\kappa}} \le C_4 \|u\|_{H_{\mathcal{T},1}} . \tag{2.17}$$

Using these relations, we can prove the following theorem for the bilinear discrete and continuous forms

$$a(u,v) = \int_\Omega \nabla u \cdot \kappa \nabla v + u \nabla V \cdot \kappa \nabla v \,,$$
$$a_{\mathcal{T}}(u,v) = \sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j} \kappa_{ij} \left(\frac{u_j}{\pi_j} - \frac{u_i}{\pi_i} \right) (v_j - v_i) \,.$$

We furthermore need the following relation

$$a_1 b_1 - a_2 b_2 = \frac{1}{2}(a_1 - a_2)(b_1 + b_2) + \frac{1}{2}(a_1 + a_2)(b_1 - b_2) \,. \tag{2.18}$$

Lemma 2.11. *Under the Assumption 1.1 the following holds: Let $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ be a family of meshes that satisfy Assumption 1.3 and inequalities* (2.8) *and* (2.17) *uniformly for functions $u \in H_{\mathcal{T}}$. Then $a_{\mathcal{T}}$ is uniformly inf-sup stable for $\|\cdot\|_{H_{\mathcal{T},\omega}}$, where $\omega = \kappa$ or $\omega = 1$ and where γ_ω in both cases depends on Ω, $\frac{h_{\sup}}{h_{\inf}}$, K, κ_0, $\|\pi\|_\infty$ and $\|\nabla\pi\|_\infty$.*

Proof. We first observe that (2.18) yields

$$U_j - U_i = \frac{u_j}{\pi_j} - \frac{u_i}{\pi_i} = \frac{1}{2}\frac{(\pi_i + \pi_j)}{\pi_i \pi_j}(u_j - u_i) + \frac{1}{2}(u_i + u_j)\left(\pi_i^{-1} - \pi_j^{-1}\right) \,.$$

Introducing $\bar{u}_{ij} := \frac{1}{2}(u_i + u_j)$ we obtain with the triangle inequality

$$2\sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} \left((U_j - U_i)(U_j - U_i) + \bar{u}_{ij}^2 \left(\pi_j^{-1} - \pi_i^{-1}\right)^2 \right)$$
$$\geq \sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} \frac{1}{4} \left(\frac{(\pi_i + \pi_j)}{\pi_i \pi_j} \right)^2 (u_j - u_i)^2 \,.$$

Observing that

$$\sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} \bar{u}_{ij}^2 \left(\pi_j^{-1} - \pi_i^{-1}\right)^2 \leq 2 \sum_i U_i^2 \sum_{j:\, j\sim i} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} \pi_i^2 \left(\pi_j^{-1} - \pi_i^{-1}\right)^2$$

and exploiting (2.17) we observe that

$$\sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} (U_j - U_i)(U_j - U_i) \geq C \|u\|_{H_{\mathcal{T},1}} \,,$$

where C depends on Ω, $\frac{h_{\sup}}{h_{\inf}}$, K, κ_0, $\|\pi\|_\infty$ and $\|\nabla\pi\|_\infty$. On the other hand

$$\sum_{i\sim j} \frac{m_{ij}}{h_{ij}} S_{i,j}\kappa_{ij} (U_j - U_i)(U_j - U_i) = a_{\mathcal{T}}(u,U) \leq \sup_{v\in H_{\mathcal{T}}} \frac{a_{\mathcal{T}}(u,v)}{\|v\|_{L^2(\mathcal{P})}} \,,$$

which together implies uniform inf-sup stability. □

Next we derive $\mathfrak{E}_{\mathcal{T}}$ in terms of κ, π and $\mathcal{T}$ and provide an estimate on $\mathfrak{E}_{\mathcal{T}}$. The main message of Lemma 2.12 is that the consistency error can be estimated by two separate expressions, one estimating the error contributed by the diffusive term and one estimating the error contributed by the convective term in the FPE.

Lemma 2.12. *Let $k \geq 1$ such that $H^k(\Omega)$ embeds into $C(\overline{\Omega})$ let $u \in H^k(\Omega) \cap H^1_0(\Omega)$ be a solution to*

$$\forall v \in H^1_0(\Omega): \quad a(u,v) = l(v)\,,$$

where

$$l(v) = \int_\Omega f\, v\,, \qquad l_{\mathcal{T}}(v) = \sum_i f_i v_i\,.$$

Using the notation (2.11) *the consistency of u is given through*

$$\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v) = \sum_{i\sim j}(v_j - v_i)\left(m_{ij}J^S_{ij}U - m_{ij}\overline{J}_{ij}U\right) \tag{2.19}$$

$$= \mathfrak{E}_{\mathcal{T},\kappa}(u;v) + \mathfrak{E}_{\mathcal{T},\kappa,\mathrm{conv}}(u;v)\,, \tag{2.20}$$

where with $u_i = (\mathcal{R}_{\mathcal{T}}u)_i$

$$\mathfrak{E}_{\mathcal{T},\kappa}(u;v) = \sum_{i\sim j}(v_j - v_i)\left(\int_{\sigma_{ij}} \kappa\nabla u\cdot\boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}(u_j - u_i)\right), \tag{2.21}$$

$$\mathfrak{E}_{\mathcal{T},\kappa,\mathrm{conv}}(u;v) = \sum_{i\sim j}(v_j - v_i)\left(\int_{\sigma_{ij}} \kappa u\nabla V\cdot\boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}\left(\frac{S_{ij}-\pi_j}{\pi_j}u_j - \frac{S_{ij}-\pi_i}{\pi_i}u_i\right)\right). \tag{2.22}$$

In particular, for both $\omega = \kappa$ or $\omega = 1$ we obtain

$$\|\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)\|^2_{H^*_{\mathcal{T},\omega}} \leq \sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(m_{ij}J^S_{ij}U - m_{ij}\overline{J}_{ij}U\right)^2 \tag{2.23}$$

$$\leq 2\,\|\mathfrak{E}_{\mathcal{T},\kappa}(u;\cdot)\|^2_{H^*_{\mathcal{T},\omega}} + 2\,\|\mathfrak{E}_{\mathcal{T},\kappa,\mathrm{conv}}(u;\cdot)\|^2_{H^*_{\mathcal{T},\omega}} \tag{2.24}$$

$$\|\mathfrak{E}_{\mathcal{T},\kappa}(u;\cdot)\|^2_{H^*_{\mathcal{T},\omega}} \leq |\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(u)$$

$$:= \sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa\nabla u\cdot\boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}\left((\mathcal{R}_{\mathcal{T}}u)_j - (\mathcal{R}_{\mathcal{T}}u)_i\right)\right)^2, \tag{2.25}$$

$$\|\mathfrak{E}_{\mathcal{T},\kappa,\mathrm{conv}}(u;\cdot)\|^2_{H^*_{\mathcal{T},\omega}} \leq |\mathfrak{E}|_{\mathcal{T},\kappa,\omega,\mathrm{conv}}(u) \tag{2.26}$$

$$:= \sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa u\nabla V\cdot\boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}\left(\frac{S_{ij}-\pi_j}{\pi_j}u_j - \frac{S_{ij}-\pi_i}{\pi_i}u_i\right)\right)^2. \tag{2.27}$$

Remark. The expression for $|\mathfrak{E}|_{\mathcal{T},\kappa}(u)$ was explicitly provided before in [DiD18].

Proof. In what follows, we combine ideas of the proofs of Theorems 27 and 33 in [DiD18]. However, since our grid and our coefficients have a simple structure, our calculations are much shorter. We first observe that the definition of f_i and (1.1) imply

$$f_i = \int_{\Omega_i} f = -\int_{\Omega_i}\nabla\cdot(\kappa\nabla u + \kappa u\nabla V)\,.$$

Hence, Gauß' theorem yields

$$l_{\mathcal{T}}(v) = -\sum_i v_i\int_{\Omega_i}\nabla\cdot(\kappa\nabla u + \kappa u\nabla V) = \sum_{i\sim j}(v_j - v_i)\int_{\sigma_{ij}}(\kappa\nabla u + \kappa u\nabla V)\cdot\boldsymbol{\nu}_{ij}$$

and hence (2.19). By an abuse of notation we write $u_j \coloneqq (\mathcal{R}_\mathcal{T} u)_j$ and $u_i = (\mathcal{R}_\mathcal{T} u)_i$ for simplicity. Then we obtain

$$S_{ij}\left(\frac{u_j}{\pi_j} - \frac{u_i}{\pi_i}\right) = (u_j - u_i) + \left(\frac{S_{ij}-\pi_j}{\pi_j}u_j - \frac{S_{ij}-\pi_i}{\pi_i}u_i\right)$$

and hence

$$\begin{aligned}\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v) &= l_\mathcal{T}(\cdot) - a_\mathcal{T}(\mathcal{R}_\mathcal{T} u, \cdot)\\ &= \sum_{i\sim j}(v_j - v_i)\left(\int_{\sigma_{ij}} \kappa \nabla u \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}(u_j - u_i)\right).\\ &\quad + \sum_{i\sim j}(v_j - v_i)\left(\int_{\sigma_{ij}} \kappa u \nabla V \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}\left(\frac{S_{ij}-\pi_j}{\pi_j}u_j - \frac{S_{ij}-\pi_i}{\pi_i}u_i\right)\right).\end{aligned}$$

From here we conclude by direct calculation and by the definition of the dual norm $\|\cdot\|^2_{H^*_{\mathcal{T},\omega}}$. □

A particular focus of the calculations below will lie on the following structure.

Lemma 2.13. *Let $\mathcal{T} = (\mathcal{V}, \mathcal{E}, \mathcal{P})$ be a mesh and $d \le 4$. Let $g \in C(\overline{\Omega})$ and let $g^\mathcal{T} \in \mathcal{E}^*$ with $g^\mathcal{T}(\sigma_{ij}) = g_{ij}$. Then for every $v \in H^2(\Omega)$ it holds*

$$\begin{aligned}&\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}} \kappa g \nabla v \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}} g_{ij}\kappa_{ij}(v_j - v_i)\right)^2\\ &\qquad \le \left(\sup_{i,j}|g_{ij}|\right)|\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(v;\cdot) + \sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}} \kappa(g - g_{ij})\nabla v \cdot \boldsymbol{\nu}_{ij}\right)^2\end{aligned}$$

Proof. We obtain

$$\begin{aligned}&\frac{1}{2}\left|\int_{\sigma_{ij}} \kappa g \nabla v \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}} g_{ij}\kappa_{ij}(v_j - v_i)\right|^2 \le\\ &\quad \le \left|\int_{\sigma_{ij}} \kappa g \nabla v \cdot \boldsymbol{\nu}_{ij} - \int_{\sigma_{ij}} \kappa g_{ij} \nabla v \cdot \boldsymbol{\nu}_{ij}\right|^2 + \left|\int_{\sigma_{ij}} \kappa g_{ij} \nabla v \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}} g_{ij}\kappa_{ij}(v_j - v_i)\right|^2\\ &\quad \le \left|\int_{\sigma_{ij}} \kappa(g - g_{ij})\nabla v \cdot \boldsymbol{\nu}_{ij}\right|^2 + |g_{ij}|^2\left|\int_{\sigma_{ij}} \kappa \nabla v \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}}\kappa_{ij}(v_j - v_i)\right|^2\end{aligned}$$

This implies the claim. □

With regard to (2.15) and Lemma 2.2, the above considerations motivate the following definition.

Definition 2.14 (φ-consistency)**.** Let $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ be a family of meshes with $\mathrm{diam}\mathcal{T}_h \to 0$ as $h \to 0$. We say that $\mathcal{T}_h$ is φ-consistent (satisfies φ-consistency) on the subspace $B \subset H^1_0(\Omega)$ if for every $u \in B$ there exists $C \ge 0$ such that for every $h > 0$

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(u) \le C\,\|u\|_{H^2}\,\varphi(h)^2\,.$$

Hence, we immediately obtain the following.

Proposition 2.15. *Let $d \leq 3$. Under the assumptions of Lemma 2.2 and assuming $h_{ij} \leq Ch$ for some constant $C > 0$ the mesh is φ-consistent with $\varphi(h) = h$, i.e.*

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\kappa}(u) \leq C \|u\|_{H^2} h^2 .$$

We say that the mesh is h-consistent.

In case the mesh is cubic, we even obtain the following [EGH00].

Proposition 2.16. *Let $d \leq 3$ and let the mesh be cubic with all cubes of equal size and let $\kappa \equiv 1$. Under the assumptions of Lemma 2.2 and assuming $h_{ij} \leq Ch$ for some constant $C > 0$ the mesh is φ-consistent with $\varphi(h) = h^2$, i.e.*

$$|\mathfrak{E}|_{\mathcal{T},1,1}(u) \leq C \|u\|_{H^2} h^4 .$$

We say that the mesh is h^2-consistent.

3 Derivation of the methods and formal comparison

In this section, we repeat the original derivation of the Scharfetter–Gummel scheme in a more general way and show that both the SG and the SQRA scheme are members of a huge family of discretization schemes. Then we provide a physically motivated derivation of the SQRA scheme which assigns the SQRA a special place in the family of Stolarsky discretizations.

As mentioned in the introduction, also the SG scheme takes a special role, which is of mathematical nature and will discussed in Section 5.2.

3.1 A family of discretization schemes

We Repeat the derivation of the SG scheme from a different point of view to reveal some additional structure and to put it into a broader context.

In one dimension, the Scharfetter–Gummel scheme for the discrete flux on the interval $[0, h]$ is derived under the assumption of constant flux J and constant diffusion coefficient κ on $[0, h]$. In particular, we consider the two-point boundary value problem

$$J = -\kappa \left(u'(x) + u(x) V'(x)\right) \qquad \text{on } [0,h], \qquad u(0) = u_0, \qquad u(h) = u_h, \tag{3.1}$$

for a general potential $V : [0, h] \to \mathbb{R}$ not necessarily assumed to be affine. The general solution reads

$$u(x) = -\left(\frac{1}{\kappa} J \int_0^x \mathrm{e}^V + u_0 \mathrm{e}^{V_0}\right) \mathrm{e}^{-V(x)}.$$

The flux can be computed explicitly from the assumption $J = \text{const.}$ and setting $x = h$ in the above formula. This yields

$$J = -\kappa \frac{u_h \mathrm{e}^{V_h} - u_0 \mathrm{e}^{V_0}}{\int_0^h \mathrm{e}^V} = -\kappa \frac{1}{h} \left(\frac{1}{h} \int_0^h \pi^{-1}\right)^{-1} \left(\frac{u_h}{\pi_h} - \frac{u_0}{\pi_0}\right) = -\kappa \pi_{\mathrm{mean}} \frac{1}{h} \left(\frac{u_h}{\pi_h} - \frac{u_0}{\pi_0}\right)$$

for the averaged $\pi_{\mathrm{mean}} = \left(\frac{1}{h} \int_0^h \pi^{-1}\right)^{-1}$, which clearly determines the constant flux along the edge. In particular, assuming that V is affine, i.e. $V(x) = \frac{V_h - V_0}{x_h - x_0} (x - x_0) + V_0$, one

easily checks that $\pi_{\mathrm{mean}} = (V_h - V_0)/(\mathrm{e}^{V_h} - \mathrm{e}^{V_0})$, which yields the Scharfetter–Gummel discretization. However, a potential can also be approximated not by piecewise affine interpolation but in other ways, resulting in different means π_{mean}. We provide an example of such an approximation for the SQRA in the Appendix A.4.

Generalizing the later considerations to higher dimensions, we find for the flux on the edge between two neighboring points in the discretization from the one dimensional considerations of (2.11) the expression

$$J_{ij}^S u^{\mathcal{T}} := -\frac{\kappa_{ij}}{h_{ij}} S_{ij} \left(\frac{u_j^{\mathcal{T}}}{\pi_j} - \frac{u_i^{\mathcal{T}}}{\pi_i} \right),$$

where κ_{ij} relates to κ and S_{ij} relates to π_{mean}.

We aim to express π_{mean} by means of the values π_0 and π_h at the boundaries. The choice of this average is non-trivial and determines the quality of the discretization scheme, as we will see below. In the present work, we focus on the (weighted) Stolarsky mean, putting $\pi_{\mathrm{mean}} = S(\pi_i, \pi_j)$ although there are also other means like general f-means ($M_f(x,y) = f\left([f^{-1}(x) + f^{-1}(y)]/2\right)$ for a strictly increasing function f). The Stolarsky mean has the advantage that it is a closed formula for a broad family of popular means and that its derivatives can be computed explicitly.

The weighted Stolarsky mean $S_{\alpha,\beta}$ [Sto75] is given as (1.3) whenever these expressions are well defined and continuously extended otherwise, i.e. $S_{\alpha,\beta}(x,x) = x$. We note the symmetry properties $S_{\alpha,\beta}(x,y) = S_{\alpha,\beta}(y,x) = S_{\beta,\alpha}(x,y)$. Interesting special limit cases are

$$S_{0,1}(x,y) = (x-y)/\log(x/y) = \Lambda(x,y)$$

(logarithmic mean), $S_{-1,1}(x,y) = \sqrt{xy}$ (geometric mean) and $S_{0,-1}(x,y) = xy/\Lambda(x,y)$ (Scharfetter–Gummel mean). A list of further Stolarsky means is given in Table 2.

An explicit calculation shows that $\partial_x^2 S_{0,-1}(x,x) = -(3x)^{-1}$ and $\partial_x^2 S_{-1,1}(x,x) = -(4x)^{-1}$. For the general Stolarsky mean $S_{\alpha,\beta}$ one obtains (see Appendix A.3)

$$\begin{aligned} \partial_x S_{\alpha,\beta}(x,x) = \partial_y S_{\alpha,\beta}(x,x) &= \frac{1}{2}, \\ \partial_x^2 S_{\alpha,\beta}(x,x) = \partial_y^2 S_*(x,x) = -\partial_{xy}^2 S_*(x,x) = -\partial_{yx}^2 S_*(x,x) &= \frac{1}{12x}(\alpha+\beta-3), \end{aligned} \tag{3.2}$$

particularly reproducing the above findings for $\partial_x^2 S_{0,-1}$ and $\partial_x^2 S_{-1,1}$.

Interestingly, the derivation of the SQRA in Section 2.2 of [LFW13] relies on the assumption that the flux through a FV-interface has to be proportional to $\left(u_j^{\mathcal{T}}/\pi_j - u_i^{\mathcal{T}}/\pi_i\right)$ with the proportionality factor given by a suitable mean of π_i and π_j. The choice of $S_{-1,1}$ in [LFW13] seems arbitrary, yet it yields very good results [WeE17, FK*19, DH*].

3.2 The Wasserstein gradient structure of the Fokker–Planck operator and the SQRA method

The choice of S_* turns out to be crucial for the convergence properties. In this section, we look at physical structures which are desirable to be preserved in the discretization procedure. Our considerations are based on the variational structure of the Fokker–Planck equation. Let us note at this point that a physically reasonable discretization

mean	α	β	$\alpha+\beta$	$S_{\alpha,\beta}(x,y)$	$B_{\alpha,\beta}(x)$
max	$+\infty$	1	$+\infty$	$\max(x,y)$	$\begin{cases}\mathrm{e}^{-x}, & x\le 0\\ 1, & x>0\end{cases}$
quadratic mean	4	2	6	$\sqrt{\frac{1}{2}(x^2+y^2)}$	$\sqrt{\frac{1}{2}(1+\mathrm{e}^{-2x})}$
arithmetic mean	2	1	3	$\frac{1}{2}(x+y)$	$\frac{1}{2}(1+\mathrm{e}^{-x})$
logarithmic mean	1	0	1	$(x-y)/\log(x/y)$	$\frac{1}{x}(1-\mathrm{e}^{-x})$
geometric mean (SQRA)	1	-1	0	$\sqrt{xy}$	$\mathrm{e}^{-x/2}$
Scharfetter–Gummel mean	0	-1	-1	$xy\log(x/y)/(x-y)$	$x/(\mathrm{e}^x-1)$
harmonic Mean	-2	-1	-3	$2xy/(x+y)$	$2/(\mathrm{e}^x+1)$
min	$-\infty$	1	$-\infty$	$\min(x,y)$	$\begin{cases}\mathrm{e}^{x}, & x\le 0\\ 1, & x>0\end{cases}$

Tab. 2: Several mean values expressed as Stolarsky means $S_{\alpha,\beta}$ with corresponding weight functions $B_{\alpha,\beta}$, see Eq. (1.6). The geometric mean corresponds to the SQRA scheme, the $S_{0,-1}$-mean to the Scharfetter–Gummel discretization.

is not necessarily the best from the rate of convergence point of view. Indeed, this last point will be underlined by numerical simulations in Section 7. However, the physical consideration is helpful to understand the family of Stolarsky discretizations from a further, different point of view.

In [JKO98] it was proved that the Fokker–Planck equation

$$\dot{u} = \nabla\cdot(\kappa\nabla u + \kappa u\nabla V) \tag{3.3}$$

has the gradient flow formulation $\dot{u} = \partial_\xi\Psi^*(u,-\mathrm{D}E(u))$ where

$$E(u) = \int_\Omega u\log u + Vu - u + 1 = \int_\Omega u\log\left(\frac{u}{\pi}\right) - u + 1\,, \qquad \Psi^*(u,\xi) = \frac{1}{2}\int_\Omega \kappa u\,|\nabla\xi|^2\,, \tag{3.4}$$

and $\pi = \mathrm{e}^{-V}$ is the stationary solution of (3.3). Indeed, one easily checks that $\mathrm{D}E(u) = \log u + V = \log(u/\pi)$ and $\partial_\xi\Psi^*(u,\xi) = -\nabla\cdot(\kappa u\nabla\xi)$ such that it formally holds

$$\partial_\xi\Psi^*(u,\xi)|_{\xi=-\mathrm{D}E(u)} = -\nabla\cdot(\kappa u\nabla\xi)|_{\xi=-\mathrm{D}E(u)} = \nabla\cdot\left(\kappa u\left(\frac{\nabla u}{u}+\nabla V\right)\right) = \nabla\cdot(\kappa\nabla u + \kappa u\nabla V) = \dot{u}.$$

Given a particular partial differential equation, the gradient structure might not be unique. For example, the simple parabolic equation $\partial_t u = \Delta u$ can be described by (3.4) with $V = 0$. But at the same time one might choose $E(u) = \int u^2$ with $\Psi^*(\xi) = \int|\nabla\xi|^2$, which plays a role in phase field modeling (see [HMR11] and references therein) or $E(u) = -\int\log u$ with $\Psi^*(\xi) = \int u^2|\nabla\xi|^2$.

In view of this observation, one might pose the question about "natural" gradient structures of the discretization schemes. This is reasonable if one believes that discretization schemes should incorporate the underlying physical principles. The energy functional is clearly prescribed by (3.4) with the natural discrete equivalent

$$E_{\mathcal{T}}(u) = \sum_i m_i\left(u_i\log\left(\frac{u_i}{\pi_i}\right) - u_i + 1\right). \tag{3.5}$$

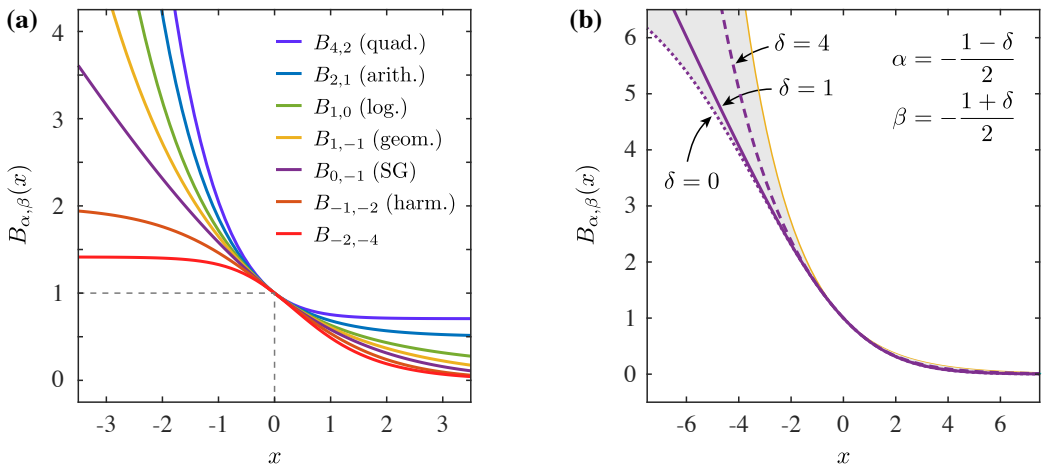

Fig. 1. **(a)** Weight functions $B_{\alpha,\beta}$ of the discrete flux scheme for different Stolarsky means $S_{\alpha,\beta}$ according to Eq. (1.6), cf. Tab. 2. **(b)** Weight functions for $\alpha + \beta = -1$ using the parametrization $\alpha = -(1-\delta)/2$, $\beta = -(1+\delta)/2$ for $\delta \geq 0$. The SG-mean $(\alpha, \beta) = (0, -1)$ is obtained for $\delta = 1$. The grey shaded region indicates the full range $\delta = [0, \infty)$, where the limit $\delta \to \infty$ is given by the weight function $e^{-x/2}$ of the SQRA scheme.

The discrete linear evolution equation can be expected to be linear. Since we identified the continuous flux to be $\mathbf{J} = -\kappa\pi\nabla U$ with $U = u/\pi$, we expect the form

$$\dot{u}_i m_i = \partial_\xi \Psi^*_{\mathcal{T}}(u, -\mathrm{D}E_{\mathcal{T}}(u)) = \sum_{j:i\sim j} \frac{m_{ij}}{h_{ij}} \kappa_{i,j} \pi_{ij} \left(\frac{u_j}{\pi_j} - \frac{u_i}{\pi_i} \right) \tag{3.6}$$

for some suitably averaged π_{ij}. Equation (3.6) can be understood as a time-reversible (or detailed balanced) Markov process on the finite state space $\mathcal{P}$. Recently, various different gradient structures have been suggested for (3.6): [Mie11, Maa11, ErM12, CH*12, Mie13b] for a quadratic dissipation as a generalization of the Jordan–Kinderlehrer–Otto approach; and [MPR14, MP*17], where a dissipation of cosh-type was appeared in the Large deviation rate functional for a hydrodynamic limit of an interacting particle system. All of them can be written in the abstract form

$$\Psi^*_{\mathcal{T}}(u, \xi) = \frac{1}{2} \sum_i \frac{1}{m_i} \sum_{j:i\sim j} \frac{m_{ij}}{h_{ij}} S_{ij} a_{ij}(u, \pi) \psi^*(\xi_i - \xi_j) , \tag{3.7}$$

where

$$a_{ij}(u, \pi) = \left(\frac{u_i}{\pi_i} - \frac{u_j}{\pi_j} \right) \partial_\xi \psi^* \left(\log\left(\frac{u_i}{\pi_i}\right) - \log\left(\frac{u_j}{\pi_j}\right) \right)^{-1} . \tag{3.8}$$

In fact, any positive and convex function ψ^* defines a reasonable dissipation functional Ψ^* by (3.7) and (3.8). A special case is when choosing for ψ^* and exponentially fast growing function $\psi^*(r) := \mathsf{C}^*(r) := 2(\cosh(r/2) - 1)$. Then a_{ij} simplifies to

$$a_{ij}(u, \pi) = \sqrt{\frac{u_i u_j}{\pi_i \pi_j}},$$

and hence, the square root appears. Choosing $S_{ij} = \sqrt{\pi_i \pi_j}$, we end up with a dissipation functional of the form

$$\Psi^*_{\mathcal{T}}(u, \xi) = \sum_i \sum_{j:i\sim j} m_{ij} h_{ij} \sqrt{u_i u_j} \frac{1}{h_{ij}^2} \mathsf{C}^*(\xi_i - \xi_j) . \tag{3.9}$$

There are (at least) three good reasons why choosing this gradient structure, i.e., modeling fluxes in exponential terms: a historical, a mathematical and a physical:

1. Already in Marcelin's PhD thesis from 1915 ([Mar15]) exponential reaction kinetics have been derived, which are still common in chemistry literature.

2. Recently, convergence for families of gradient systems has been derived based on the energy-dissipation principle (the so-called EDP-convergence [Mie16, LM*17, DFM18]). Vice versa, the above cosh-gradient structure appears as an effective gradient structure applying EDP-convergence to Wasserstein gradient flow problems [LM*17, FrL19].

3. Recalling the gradient structure for the continuous Fokker–Planck equation (3.4), we observe that the dissipation mechanism Ψ^* is totally independent of the particular form of the energy $\mathcal{E}$, which is determined by the potential V. This is physically understandable, since a change of the energy resulting, e.g., from external fields should not influence the dissipation structure. The same holds for the discretized version (3.9). In fact it was shown in [MiS19], that the only discrete gradient structure, where the dissipation does not depend on V resp. $\pi = \mathrm{e}^{-V}$, is the cosh-gradient structure with the SQRA discretization $S_{ij} = S_{-1,1}(\pi_i, \pi_j)$. In particular, this characterizes the SQRA. For convenience, we add a proof for that to the Appendix A.2.

We think that these properties distinguish the SQRA, although in the following the convergence proofs do not really rely on the particular discretization weight S_{ij}.

Remark 3.1 (Convergence of energy and dissipation functional)**.** Let us finally make some comments on the convergence of $E_\mathcal{T}$ and $\Psi^*_\mathcal{T}$ given in (3.5) and (3.9) to the continuous analogies E and Ψ^*. Γ-convergence can be shown if the fineness of $\mathcal{T}$ tends to 0. For the energies it is clear, since $u \mapsto u\log(u/\pi) - u$ is convex. For the dissipation potentials $\Psi^*_\mathcal{T}(u,\xi)$ we observe the following: For smooth functions u and ξ, we have $\frac{1}{h_{ij}^2}\mathsf{C}^*(\xi_i - \xi_j) \approx \frac{1}{2}\left(\frac{\mathbf{x}_i - \mathbf{x}_j}{|x_i - x_j|}\cdot\nabla\xi\right)^2 + O(h_{ij}^2)$ and $\sqrt{u_i u_j} \approx u\left(\frac{1}{2}(x_i + x_j)\right)$. The considerations from Section 2.4 then yield $\Psi^*_\mathcal{T}(u,\xi) \approx \frac{1}{2}\int_{\boldsymbol{Q}} u\,|\nabla\xi|^2$.

For quadratic dissipation, qualitative convergence results using the underlying gradient structure and the energy-dissipation principle are obtained in [DiL15] in 1 D, and in [FMP20] for multiple dimensions. In [GK*19] convergence of the associated metric is proved.

4 Comparison of discretization schemes

We mutually compare any two discretization schemes of the form (1.2) in case of Dirichlet boundary conditions. In this case, even though the problem is only defined on $\tilde{\mathcal{P}}$, we can simply sum over all $\mathcal{P}$ once we multiplied with a test function that assumes the value 0 at all $\mathcal{P}\backslash\tilde{\mathcal{P}}$.

Let us recall the formula (2.11) for the fluxes

$$J_{ij}^S U = -\frac{\kappa_{ij}}{h_{ij}} S_{ij}(U_j - U_i).$$

Moreover, let $u_i = U_i\pi_i$ and $\tilde{u}_i = \tilde{U}_i\pi_i$ be the solution of the discrete FPE (1.2) for two different smooth mean coefficients $S_{ij} = S(\pi_i, \pi_j)$ and $\tilde{S}_{ij} = \tilde{S}(\pi_i, \pi_j)$ (e.g. once for Scharfetter–Gummel and once for SQRA) such that

$$\sum_{k:k\sim i} m_{ik}h_{ik}J^S_{ik}U = m_i\bar{f}_i \tag{4.1}$$

$$\sum_{k:k\sim i} m_{ik}h_{ik}J^{\tilde{S}}_{ik}\tilde{U} = m_i\bar{f}_i. \tag{4.2}$$

In order to compare the solutions of (4.1) and (4.2) we take the difference of these two equations and multiply with $E_i = U_i - \tilde{U}_i$. We obtain

$$\begin{aligned} 0 &= \sum_i \sum_{k:k\sim i} m_{ik}h_{ik}\left(J^S_{ik}U - J^{\tilde{S}}_{ik}\tilde{U}\right)E_i \\ &= \sum_i \sum_{k:\,k\sim i} \frac{m_{ik}}{h_{ki}}\kappa_{ij}(S_{ik}(U_i - U_k) - \tilde{S}_{ik}(\tilde{U}_i - \tilde{U}_k))E_i \end{aligned}$$

Introducing the notation $\alpha_{ik} = \kappa_{ik}\frac{m_{ik}}{h_{ik}}$ and using (2.3) we get

$$\begin{aligned} 0 &= \sum_{k\sim i}\alpha_{ik}\left(S_{ik}(U_i - U_k) - S_{ik}(\tilde{U}_i - \tilde{U}_k) + \left(S_{ik} - \tilde{S}_{ik}\right)(\tilde{U}_i - \tilde{U}_k)\right)(E_i - E_k) \\ &= \sum_{k\sim i}\alpha_{ik}\left(S_{ik}\left(E_i - E_k\right) + \left(S_{ik} - \tilde{S}_{ik}\right)\left(\tilde{U}_i - \tilde{U}_k\right)\right)(E_i - E_k)\,. \end{aligned}$$

Using the notation $\mathrm{D}_{ik}A = A_k - A_i$ for discrete gradients

$$(\tilde{S}_{ik} - S_{ik})\left(\tilde{U}_i - \tilde{U}_k\right)(E_i - E_k) \le \frac{1}{2}\left[S_{ik}\left(\mathrm{D}_{ik}E\right)^2 + \frac{(S_{ik} - \tilde{S}_{ik})^2}{S_{ik}}\left(\mathrm{D}_{ik}\tilde{U}\right)^2\right]$$

we get

$$\frac{1}{2}\sum_{k\sim i}\alpha_{ik}S_{ik}\left(\mathrm{D}_{ik}E\right)^2 \le \frac{1}{2}\sum_{k\sim i}\frac{(\tilde{S}_{ik} - S_{ik})^2}{S_{ik}\tilde{S}_{ik}}\alpha_{ik}\tilde{S}_{ik}\left(\mathrm{D}_{ik}\tilde{U}\right)^2\,. \tag{4.3}$$

In the case of Stolarsky means the constants are more explicit. We have the following expansion of S_{ij}: writing $\pi_{ij} = \frac{1}{2}(\pi_i + \pi_j)$, $\pi_+ = \pi_- = \frac{1}{2}(\pi_i - \pi_j)$ and $\pi_i = \pi_0 + \pi_+$ and $\pi_j = \pi_0 - \pi_-$

$$\begin{aligned} S_{ij} &= S_{\alpha,\beta}(\pi_{ij}, \pi_{ij}) + \frac{1}{2}(\pi_+ - \pi_-) + \frac{1}{2}\partial_x^2 S_{\alpha,\beta}(\pi_{ij}, \pi_{ij})(\pi_+ + \pi_-)^2 + O\left(\pi_\pm^3\right) \\ &= \pi_{ij} + \frac{\frac{1}{3}(\alpha+\beta) - 1}{8\,\pi_{ij}}(\pi_i - \pi_j)^2 + O(\pi_i - \pi_j)^3\,. \end{aligned} \tag{4.4}$$

In case $(\alpha + \beta) = \left(\tilde{\alpha} + \tilde{\beta}\right)$, we obtain $S_{ij} - \tilde{S}_{ij} = O(\pi_i - \pi_j)^3$ and hence this yields the following first comparison result:

Proposition 4.1. *Let $\mathcal{T}$ be a mesh with right hand side $f \in L^2(\mathcal{P})$ and let u and $\tilde{u}$ be a two solution of the discrete FPE for different Stolarsky mean coefficients $S_{ij} = S_{\alpha,\beta}(\pi_i, \pi_j)$ and $\tilde{S}_{ij} = S_{\tilde{\alpha},\tilde{\beta}}(\pi_i, \pi_j)$ respectively. Then*

$$\begin{aligned} &\frac{1}{2}\sum_{k\sim i}\kappa_{ik}\frac{m_{ik}}{h_{ik}}S_{ik}\left(U_k - \tilde{U}_k - \left(U_i - \tilde{U}_i\right)\right)^2 \\ &\qquad \le \frac{1}{2}\sum_{k\sim i}\left(\frac{\left((\alpha+\beta) - \left(\tilde{\alpha}+\tilde{\beta}\right)\right)^2}{24^2\,\pi_{ij}^2\tilde{S}_{ik}S_{ik}}(\pi_i - \pi_k)^4 + O(\pi_i - \pi_k)^5\right)\kappa_{ik}\frac{m_{ik}}{h_{ik}}\left(\tilde{U}_k - \tilde{U}_i\right)^2 \end{aligned}$$

In case $(\alpha+\beta)=\left(\tilde{\alpha}+\tilde{\beta}\right)$ *we furthermore find*

$$\frac{1}{2}\sum_{k\sim i}\kappa_{ik}\frac{m_{ik}}{h_{ik}}S_{ik}\left(U_k-\tilde{U}_k-\left(U_i-\tilde{U}_i\right)\right)^2=\frac{1}{2}\sum_{k\sim i}O\left(\pi_i-\pi_k\right)^6\kappa_{ik}\frac{m_{ik}}{h_{ik}}\left(\tilde{U}_k-\tilde{U}_i\right)^2.$$

We aim to refine the above result to an order of convergence result for $J^SU-J^{\tilde{S}}\tilde{U}$.. We introduce a third Stolarsky mean $\hat{S}_{ik}=\hat{S}(\pi_i,\pi_k)$ and find

$$\begin{aligned}\hat{S}_{ik}\left(E_i-E_k\right)&=\hat{S}_{ik}\left(U_i-\tilde{U}_i-\left(U_k-\tilde{U}_k\right)\right)\\&=S_{ik}(U_i-U_k)-S_{ik}(U_i-U_k)+\tilde{S}_{ik}(\tilde{U}_i-\tilde{U}_k)-\tilde{S}_{ik}(\tilde{U}_i-\tilde{U}_k)+\hat{S}_{ik}\left(U_i-\tilde{U}_i-\left(U_k-\tilde{U}_k\right)\right)\\&=m_{ik}\alpha_{ik}^{-1}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)+\left(\hat{S}_{ik}-S_{ik}\right)\left(U_i-U_k\right)-\left(\hat{S}_{ik}-\tilde{S}_{ik}\right)\left(\tilde{U}_i-\tilde{U}_k\right).\end{aligned}$$

Hence, we have

$$\begin{aligned}&\sum_{k\sim i}\alpha_{ik}\left(S_{ik}(U_i-U_k)-\tilde{S}_{ik}\left(\tilde{U}_i-\tilde{U}_k\right)\right)\left(E_i-E_k\right)\\&\quad=\sum_{k\sim i}\frac{h_{ik}}{\kappa_{ik}}m_{ik}\frac{1}{\hat{S}_{ik}}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)^2\\&\qquad+\sum_{k\sim i}m_{ik}\frac{1}{\hat{S}_{ik}}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)\left[\left(\hat{S}_{ik}-S_{ik}\right)\left(U_i-U_k\right)+\left(\hat{S}_{ik}-\tilde{S}_{ik}\right)\left(\tilde{U}_i-\tilde{U}_k\right)\right],\end{aligned}$$

and using Cauchy–Schwartz inequality, we get

$$\begin{aligned}\sum_{k\sim i}\alpha_{ik}\left(S_{ik}(U_i-U_k)-\tilde{S}_{ik}\left(\tilde{U}_i-\tilde{U}_k\right)\right)\left(E_i-E_k\right)&\leq-\frac{1}{2}\sum_{k\sim i}\frac{h_{ik}m_{ik}}{\kappa_{ik}}\frac{1}{\hat{S}_{ik}}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)^2\\&\quad+\sum_{k\sim i}\frac{m_{ik}\kappa_{ik}}{h_{ik}\hat{S}_{ik}}\left(\left(\hat{S}_{ik}-S_{ik}\right)^2\left(U_i-U_k\right)^2+\left(\hat{S}_{ik}-\tilde{S}_{ik}\right)^2\left(\tilde{U}_i-\tilde{U}_k\right)^2\right).\end{aligned}$$

Altogether we obtain

$$\begin{aligned}\frac{1}{2}\sum_{k\sim i}\frac{h_{ik}m_{ik}}{\kappa_{ik}}\frac{1}{\hat{S}_{ik}}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)^2&\leq\sum_{k\sim i}\frac{m_{ik}h_{ik}}{\kappa_{ik}\hat{S}_{ik}S_{ik}^2}\left(\hat{S}_{ik}-S_{ik}\right)^2\left(\frac{\kappa_{ik}}{h_{ik}}S_{ik}\left(U_i-U_k\right)\right)^2\\&\quad+\sum_{k\sim i}\frac{m_{ik}h_{ik}}{\kappa_{ik}\hat{S}_{ik}\tilde{S}_{ik}^2}\left(\hat{S}_{ik}-\tilde{S}_{ik}\right)^2\left(\frac{\kappa_{ik}}{h_{ik}}\tilde{S}_{ik}\left(\tilde{U}_i-\tilde{U}_k\right)\right)^2.\end{aligned}$$

We make once more use of (4.4) writing $C_{\alpha,\beta}:=\frac{1}{24}\left(\alpha+\beta\right)$ and exploiting $\pi_i=\pi_{ij}+\pi_{ij}\left(V_i-V_{ij}\right)+O\left(V_i-V_{ij}\right)^2$ with

$$\begin{aligned}\pi_i-\pi_j&=\pi_{ij}\left(V_i-V_j\right)+O\left(V_i-V_{ij}\right)^2+O\left(V_j-V_{ij}\right)^2\\S_{ij}&=\pi_{ij}+O\left(\pi_i-\pi_j\right).\end{aligned}$$

Hence, we conclude the following result.

Theorem 4.2. *Let* $\mathcal{T}$ *be a mesh with right hand side* $f\in L^2(\mathcal{P})$ *and let* u *and* $\tilde{u}$ *be two solutions of the discrete FPE for different Stolarsky means* S *and* $\tilde{S}$*. Moreover, let* $\hat{S}$ *be any Stolarsky mean and assume that either* $\alpha+\beta\neq\hat{\alpha}+\hat{\beta}$ *or* $\tilde{\alpha}+\tilde{\beta}\neq\hat{\alpha}+\hat{\beta}$*. Then the solutions* u *and* $\tilde{u}$ *of the discretized FPE satisfy the symmetrized error estimate up to higher order*

$$\begin{aligned}\frac{1}{2}\sum_{k\sim i}\frac{h_{ik}m_{ik}}{\kappa_{ik}}\frac{1}{\hat{S}_{ik}}\left(J_{ik}^SU-J_{ik}^{\tilde{S}}\tilde{U}\right)^2&\leq\sum_{k\sim i}\frac{m_{ik}h_{ik}}{\kappa_{ik}S_{ik}}\left(C_{\alpha,\beta}-C_{\hat{\alpha},\hat{\beta}}\right)\left(V_i-V_j\right)^2\left(J_{ik}^SU\right)^2\\&\quad+\sum_{k\sim i}\frac{m_{ik}h_{ik}}{\kappa_{ik}\tilde{S}_{ik}}\left(C_{\tilde{\alpha},\tilde{\beta}}-C_{\hat{\alpha},\hat{\beta}}\right)\left(V_i-V_j\right)^2\left(J_{ik}^{\tilde{S}}\tilde{U}\right)^2.\end{aligned}$$

More general, for any mean we have

$$\frac{1}{2\kappa^*}\|J^S U - J^{\tilde S}\tilde U\|^2_{L^2_{\hat S}(\mathcal{E})} \leq \frac{1}{\kappa_*}\left\{\sup_{i,k}\frac{\left(\hat S_{ik}-S_{ik}\right)^2}{\hat S_{ik}S_{ik}}\left\|J^S U\right\|^2_{L^2_S(\mathcal{E})} + \sup_{i,k}\frac{\left(\hat S_{ik}-\tilde S_{ik}\right)^2}{\hat S_{ik}\tilde S_{ik}}\left\|J^{\tilde S}\tilde U\right\|^2_{L^2_{\tilde S}(\mathcal{E})}\right\}, \quad (4.5)$$

and in particular for Stolarsky means with $\alpha+\beta=\tilde\alpha+\tilde\beta=\hat\alpha+\hat\beta$ we find the following result:

Corollary 4.3. *Let $\mathcal{T}$ be a mesh with right hand side $f\in L^2(\mathcal{P})$ and let u and $\tilde u$ be two solutions of the discrete FPE for different Stolarsky mean coefficients $S_{ij}=S_{\alpha,\beta}(\pi,\pi_j)$ and $\tilde S_{ij}=S_{\tilde\alpha,\tilde\beta}(\pi,\pi_j)$ with $\alpha+\beta=\tilde\alpha+\tilde\beta=\hat\alpha+\hat\beta$. Then estimate (4.5) holds. In particular, we find the refined estimate*

$$\frac{1}{2\kappa^*}\|J^S U - J^{\tilde S}\tilde U\|^2_{L^2_{\hat S}(\mathcal{E})} = O\left(\pi_i-\pi_j\right)^6\left(\left\|J^S U\right\|^2_{L^2_S(\mathcal{E})} + \left\|J^{\tilde S}\tilde U\right\|^2_{L^2_{\tilde S}(\mathcal{E})}\right).$$

In particular, the last result shows that convergence rates are similar up to order 3 for different α,β which satisfy $\alpha+\beta=\text{const}$.

Corollary 4.4. *Let $\mathcal{T}$ be a mesh with right hand side $f\in L^2(\mathcal{P})$ and let u and $\tilde u$ be two solutions of the discrete FPE for different Stolarsky mean coefficients $S_{ij}=S_{\alpha,\beta}(\pi,\pi_j)$ and $\tilde S_{ij}=S_{\tilde\alpha,\tilde\beta}(\pi,\pi_j)$ with $\alpha+\beta=\tilde\alpha+\tilde\beta=\hat\alpha+\hat\beta$. Then estimate (4.5) holds. For both S_{ij} and $\tilde S_{ij}$ let the quantities of Lemma 2.12 which depend on S be denoted by $\mathfrak{E}^S_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)$ and $\mathfrak{E}^{\tilde S}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)$ as well as $\mathfrak{E}^S_{\mathcal{T},\kappa,\mathrm{conv}}(u;v)$ and $\mathfrak{E}^{\tilde S}_{\mathcal{T},\kappa,\mathrm{conv}}(u;v)$. If $\pi>c>0$ is uniformly bounded from below then*

$$\left\|\mathfrak{E}^S_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)\right\|^2_{H^*_{\mathcal{T},\omega}} \leq 2\left\|\mathfrak{E}^{\tilde S}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)\right\|^2_{H^*_{\mathcal{T},\omega}} + O(h^6).$$

Proof. We obtain from Lemma 2.12

$$\left\|\mathfrak{E}^S_{\mathcal{T},\mathrm{FPE},\kappa}(u;v)\right\|^2_{H^*_{\mathcal{T},\omega}} \leq 2\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(m_{ij}J^{\tilde S}_{ij}U - m_{ij}\overline{J}_{ij}U\right)^2 + 2\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(m_{ij}J^{\tilde S}_{ij}U - m_{ij}J^S_{ij}U\right)^2$$

and from Corollary 4.3 we obtain the claim upon uniform boundedness of π. □

5 Convergence of the discrete FPE

In this section, we derive general estimates for the order of convergence of the Stolarsky FV operators. Throughout this section, we assume that the mesh satisfies the consistency property of Definition 2.14 with a suitable consistency function $\varphi:\mathbb{R}_{\geq 0}\to\mathbb{R}_{\geq 0}$ and discretization operator $\mathcal{R}_{\mathcal{T}}: H^1(\Omega)\supset B\to L^2(\mathcal{P})$. The parameters π_i and u_i below are then given in terms of

$$\pi_i = \left(\mathcal{R}_{\mathcal{T}}\pi\right)_i, \qquad u_i = \left(\mathcal{R}_{\mathcal{T}}u\right)_i, \qquad U_i = \left(\mathcal{R}_{\mathcal{T}}U\right)_i.$$

We derive consistency errors for U in Section (5.1) and consistency errors for u in Section (5.2). For both calculations we will need the following result.

Lemma 5.1. *Assume there exists a constant $C > 0$ such that for all cells Ω_i, Ω_j with $h_i = \mathrm{diam}\Omega_i$ it holds*

$$\forall f \in H^1(\Omega_i): \qquad \|f\|^2_{L^2(\sigma_{ij})} \leq \frac{1}{h_i} C^2 \|f\|^2_{H^1(\Omega_i)}\,, \tag{5.1}$$

$$\forall f \in H^1(\Omega_i) \cap C(\overline{\Omega}_i): \qquad \|f - f_i\|^2_{L^2(\sigma_{ij})} \leq h_i C^2 \|\nabla f\|^2_{L^2(\Omega_i)}\,. \tag{5.2}$$

Then for C^2-smooth Stolarsky means S_* and for every function $\varpi, U \in H^2(\Omega)$ with $\varpi_i := \varpi(x_i)$ and $S_{ij} := S_*(\varpi_i, \varpi_j)$ it holds

$$\left|\int_{\sigma_{ij}} (\varpi - S_{ij})\, \kappa \nabla U \cdot \boldsymbol{\nu}_{ij}\right| \leq C \begin{cases} \sum_{k=i,j} \|\nabla \varpi\|_{L^2(\Omega_k)} \|\kappa \nabla U\|_{H^1(\Omega_k)} \\ (m_{ij} h_i)^{\frac{1}{2}} \|\kappa \nabla U\|_{H^1(\Omega_i)} \\ \sum_{k=i,j} h_k^{\frac{1}{2}} \|\nabla \varpi\|_{L^2(\Omega_k)} \left(\int_{\sigma_{ij}} |\kappa \nabla U|^2\right)^{\frac{1}{2}} \end{cases} + O(h_{ij}^2)\,. \tag{5.3}$$

Remark. Note that (5.1)–(5.2) can be easily verified for convex sets with uniform bound on the relation $\frac{\mathrm{diam}_{\max}(\Omega_i)}{\mathrm{diam}_{\min}(\Omega_i)}$ between maximal and minimal diameter of a given cell. In particular, given $f \in H^1(\Omega_i)$ with $f_h(x) := f(\frac{x}{h})$ we find the scaled inequality

$$\frac{1}{h^{d-1}} \int_{h\partial\Omega_i} |f_h|^2 \leq C \frac{1}{h^d} \int_{h\Omega_i} \left(|f_h|^2 + h^2 |\nabla f_h|^2\right).$$

Furthermore, for $f \in H^1(\Omega_i) \cap C(\overline{\Omega}_i)$ one finds for a calculation similar to the Poincaré inequality for zero average functions (and for $x_i = 0$)

$$\int_{h\Omega_i} |f_h - f_i|^2 \leq C \int_{h\Omega_i} h^2 |\nabla f_h|^2\,.$$

Proof. Observe that

$$\int_{\sigma_{ij}} |\varpi - S_{ij}|\, |\kappa \nabla U \cdot \boldsymbol{\nu}_{ij}| \leq \left(\int_{\sigma_{ij}} |\varpi - S_{ij}|^2\right)^{\frac{1}{2}} \left(\int_{\sigma_{ij}} |\kappa \nabla U \cdot \boldsymbol{\nu}_{ij}|^2\right)^{\frac{1}{2}} \tag{5.4}$$

It remains to study $\frac{1}{m_{ij}} \int_{\sigma_{ij}} |\varpi - S_{ij}|^2$ in more detail. We have

$$S(\varpi_i, \varpi_j) - S\left(\frac{\varpi_i + \varpi_j}{2}, \frac{\varpi_i + \varpi_j}{2}\right) = \frac{1}{2}(\varpi_i - \varpi_j) \nabla S \cdot (1, -1)^T + O(|\varpi_i - \varpi_j|)^2 = O(|\varpi_i - \varpi_j|)^2$$

and thus

$$\begin{aligned} \varpi - S_{ij} &= \frac{1}{2}(\varpi - \varpi_i) + \frac{1}{2}(\varpi - \varpi_j) + \left(\frac{\varpi_i + \varpi_j}{2} - S_{ij}\right) \\ &= \frac{1}{2}(\varpi - \varpi_i) + \frac{1}{2}(\varpi - \varpi_j) + O(|\varpi_i - \varpi_j|)^2\,. \end{aligned}$$

The first term can be estimated by $|\varpi - \varpi_i| \leq h_i \cdot \nabla \varpi + O(h_i^2)$ and a similar estimate holds for the second term. Using (5.1)–(5.2) we obtain in total

$$\int_{\sigma_{ij}} |\varpi - S_{ij}|\, |\kappa \nabla U \cdot \boldsymbol{\nu}_{ij}| \leq C \sum_{k=i,j} h_k \|\nabla \varpi\|_{L^2(\Omega_k)} \left(\frac{1}{h_k} \|\kappa \nabla U\|^2_{H^1(\Omega_k)}\right)^{\frac{1}{2}}.$$

□

5.1 Error Analysis in U

In what follows, we assume that the discrete and the continuous solution satisfy homogeneous Dirichlet conditions. In view of the continuous and the discrete FPE given in the form (1.5) and (1.4) as well as formula (2.19) we observe that the natural variational consistency error for a given Stolarsky mean S equivalently takes the form

$$\begin{aligned}\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(u;v) &= \tilde{\mathfrak{E}}_{\mathcal{T},\mathrm{FPE},\kappa}(U;v)\\ &:= \sum_{i\sim j}(v_j - v_i)\left(\int_{\sigma_{ij}} \kappa\pi\nabla U\cdot\boldsymbol{\nu}_{ij} - \kappa_{ij}S_{ij}\frac{m_{ij}}{h_{ij}}\left((\mathcal{R}_{\mathcal{T}}U)_j - (\mathcal{R}_{\mathcal{T}}U)_i\right)\right).\end{aligned}$$

We recall that an estimate for $\tilde{\mathfrak{E}}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)$ implies an order of convergence estimate by (2.15). Our main result of this section provides a connection between $\tilde{\mathfrak{E}}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)$ and the variational consistency $\tilde{\mathfrak{E}}_{\mathcal{T},\kappa}(U;\cdot)$ (given by (2.21)) of the second order equation

$$-\nabla\cdot(\kappa\nabla U) = f$$

with the discretization scheme

$$\forall i: \qquad -\sum_{j:\,j\sim i}\kappa_{ij}\frac{m_{ij}}{h_{ij}}\left(U_j^{\mathcal{T}} - U_i^{\mathcal{T}}\right) = f_i\,.$$

Proposition 5.2. *Let $\mathcal{T} = (\mathcal{V},\mathcal{E},\mathcal{P})$ be a mesh. The variational consistency error $\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)$ can be estimated by*

$$\left\|\tilde{\mathfrak{E}}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)\right\|^2_{H^*_{\mathcal{T},\kappa S}} \le \|\pi\|_\infty\,|\mathfrak{E}|_{\mathcal{T}}(U;\cdot) + \sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\kappa_{ij}^{-1}S_{ij}^{-1}\left(\int_{\sigma_{ij}}(\pi - S_{ij})\,\kappa\nabla U\cdot\boldsymbol{\nu}_{ij}\right)^2. \quad (5.5)$$

Proof. This is a direct consequence of Lemma 2.13. □

Using the above estimates, we can now show the main result of the section.

Theorem 5.3 (Localized order of convergence)**.** *Let $d\le 4$ and the mesh $\mathcal{T}$ be admissible in sense of Definition 2.1 and φ-consistent in sense of Definition 2.14. Let $u\in C_0^2(\Omega)$ be the solution to* (1.1)*. Let $f^{\mathcal{T}} := \mathcal{R}^*_{\mathcal{T}}f$ and let $u^{\mathcal{T}}\in\mathcal{S}^{\mathcal{T}}$ be the solution to* (2.4)*. Moreover, let $\kappa\le\kappa^*$, $b>0$ and $S\in C^2(\mathbb{R}_{\ge0}\times\mathbb{R}_{\ge0})$. Then it holds*

$$\begin{aligned}\|\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)\|^2_{H^*_{\mathcal{T},\kappa S}} &\le C(\kappa_*,\pi,d,\|U\|_{C^2})\times\left(\varphi(h)^2+h^2\right).\\ \|u^{\mathcal{T}} - \mathcal{R}_{\mathcal{T}}u\|_{H_{\mathcal{T},\kappa S}} &\le C(\kappa_*,\pi,d,\|U\|_{C^2})\times\left(\varphi(h)^2+h^2\right).\end{aligned}$$

Proof. Inserting estimate (5.3) into (5.5), we get

$$\begin{aligned}\|\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(U;\cdot)\|^2_{H^*_{\mathcal{T},\kappa S}} &\le \|\pi\|_\infty\,|\mathfrak{E}|_{\mathcal{T},\kappa S}(U;\cdot) + C\sum_{i\sim j}h_{ij}\kappa_{ij}^{-1}S_{ij}^{-1}h_i\|\kappa\nabla U\|^2_{H^1(\Omega_i)}\\ &\le \|\pi\|_\infty\,|\mathfrak{E}|_{\mathcal{T},\kappa S}(U;\cdot) + C(\kappa_*,\pi,d)\;h^2\sum_i\|\kappa\nabla U\|^2_{H^1(\Omega_i)}.\end{aligned}$$

Using (2.15) we obtain an estimate for the discretization error in the form

$$\|u^{\mathcal{T}} - \mathcal{R}_{\mathcal{T}}u\|^2_{H_{\mathcal{T},\kappa\mathcal{S}}} \le \|\pi\|_\infty\,|\mathfrak{E}|_{\mathcal{T},\kappa S}(U;\cdot) + C(\kappa_*,\pi,d,\|U\|_{C^2})\;\mathrm{Size}(\mathcal{T})^2.$$

Using the consistency assumption on the discretization of the pure elliptic problem we obtain the desired estimate. □

5.2 Error Analysis in u

We will now derive an alternative estimate for the consistency error which accounts more for the convective aspect of the FPE. In Lemma 2.12 we have split the consistency error $\mathfrak{E}_{\mathcal{T},\mathrm{FPE},\kappa}(u;\cdot)$ into the two parts $\mathfrak{E}_{\mathcal{T},\kappa}(u;\cdot)$ and $\mathfrak{E}_{\mathcal{T},\mathrm{conv},\kappa}(u;\cdot)$. The error $\mathfrak{E}_{\mathcal{T},\kappa}(u;\cdot)$ relates to the elliptic part and is well understood in literature. Therefore, it remains to study the second part.

Proposition 5.4. *Using the notation of Lemma 2.12 it holds in $d \leq 4$*

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\mathrm{conv},\omega}(u) \leq \sum_{i\sim j} \frac{h_{ij}}{m_{ij}} \omega_{ij}^{-1} \left(\int_{\sigma_{ij}} \kappa u \nabla V \cdot \boldsymbol{\nu}_{ij} - \frac{m_{ij}}{h_{ij}} \kappa_{ij} \frac{1}{2} \frac{S_{ij}}{\pi_i \pi_j} (\pi_i - \pi_j)(u_i + u_j) \right)^2 + C\, h^4, \tag{5.6}$$

where C depends on $\|\pi\|_\infty$, $\|\nabla\pi\|_\infty$, $\|u\|_\infty$, $\|\nabla u\|_\infty$.

Proof. We use (2.18) to find

$$\frac{S_{ij} - \pi_j}{\pi_j} u_j - \frac{S_{ij} - \pi_i}{\pi_i} u_i = \frac{1}{2} \frac{S_{ij}}{\pi_i \pi_j} (\pi_i - \pi_j)(u_i + u_j) + \frac{1}{2} \frac{1}{\pi_i \pi_j} (S_{ij}\pi_i + S_{ij}\pi_j - 2\pi_i\pi_j)(u_i - u_j)$$

and in a next step we find on behalf of (3.2)

$$(S_{ij}\pi_i + S_{ij}\pi_j - 2\pi_i\pi_j) = \left(\frac{1}{2} + C_{\alpha,\beta} \left(\frac{\pi_j}{\pi_i} + \frac{\pi_i}{\pi_j} \right) \right) (\pi_i - \pi_j)^2 + O(\pi_i - \pi_j)^3$$

for $C_{\alpha,\beta} = \frac{1}{12}(\alpha + \beta - 3)$ and thus we conclude from

$$\begin{aligned}
&\mathfrak{E}_{\mathcal{T},\mathrm{conv},\kappa}(u;v) = \\
&\quad = \sum_{i\sim j} \left(\frac{m_{ij}}{h_{ij}} \kappa_{ij} \frac{1}{2} \frac{S_{ij}}{\pi_i \pi_j} (\pi_i - \pi_j)(u_i + u_j) - \int_{\sigma_{ij}} \kappa u \nabla V \cdot \boldsymbol{\nu}_{ij} \right) (v_j - v_i) \\
&\quad + \sum_{i\sim j} \left(\frac{m_{ij}}{h_{ij}} \kappa_{ij} \frac{1}{2} \frac{1}{\pi_i \pi_j} \left(\left(\frac{1}{2} + C_{\alpha,\beta} \left(\frac{\pi_j}{\pi_i} + \frac{\pi_i}{\pi_j} \right) \right) (\pi_i - \pi_j)^2 (u_i - u_j) + O(\pi_i - \pi_j)^3 \right) \right) (v_j - v_i)
\end{aligned}$$

that (5.6)holds. □

Note that in general it holds

$$\frac{S_{ij}}{\pi_i \pi_j} (\pi_i - \pi_j) = \frac{1}{2} S_{ij} \left(\frac{1}{\pi_i} + \frac{1}{\pi_j} \right) (V_j - V_i) + O(h). \tag{5.7}$$

The Scharfetter Gummel scheme turns out to be special at this point.

Lemma 5.5 (SG is superior for large convection)**.** *In case of the Stolarsky mean $S_{0,-1}$ (the Scharfetter–Gummel case), it holds*

$$\frac{1}{2} \frac{S_{ij}}{\pi_i \pi_j} (\pi_i - \pi_j)(u_i + u_j) = (V_j - V_i) \frac{1}{2} (u_i + u_j) .$$

Proof. This follows immediately from $S_{0,-1}(x,y) = \frac{xy}{x-y} \log(x/y)$ and $\pi(x) = e^{-V(x)}$. □

The last observation plays an important role in the estimation of the right hand side of (5.6).

Theorem 5.6. *Let $d \le 4$ and $\mathcal{T}_h = (\mathcal{V}_h, \mathcal{E}_h, \mathcal{P}_h)$ be a family of meshes with $\operatorname{diam}\mathcal{T}_h \to 0$ as $h \to 0$ and let the assumptions of Lemma 5.1 hold. Using the notation of Lemma 2.12 let $u_{ij} := \frac{1}{2}(u_i + u_j)$. Then*

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\mathrm{conv},\omega}(u) = 2\|u\|_\infty |\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(V;\cdot) + 2\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa(u-u_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right)^2 + O(h^2).$$

In case $S_* = S_{0,-1}$ or $S_* = S_{\alpha,\beta}$ with $\alpha+\beta=-1$ the above can be improved to

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\mathrm{conv},\omega}(u) = 2\|u\|_\infty |\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(V;\cdot) + 2\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa(u-u_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right)^2 + O(h^4).$$

In all cases, $O(\cdot)$ depends on $\|\nabla V\|_\infty$.

Proof. We start from (5.6) applying (5.7). Defining $g := u$, $g_{ij} := \frac{1}{4}S_{ij}\left(\frac{1}{\pi_i}+\frac{1}{\pi_j}\right)(u_i+u_j)$ applying Lemma 2.13 yields

$$\begin{aligned}&|\mathfrak{E}|_{\mathcal{T},\kappa,\mathrm{conv},\omega}(u)\\ &\le 2\left(\sup_{i,j}|g_{ij}|\right)|\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(V;\cdot) + 2\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa(u-g_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right)^2 + O(h^2).\end{aligned}$$

We observe that $\frac{1}{2}S_{ij}\left(\frac{1}{\pi_i}+\frac{1}{\pi_j}\right) = 1 + O(h)$, where $O(h)$ depends on $\|\nabla V\|_\infty$ such that

$$\left|\int_{\sigma_{ij}}\kappa(u-g_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right| \le \left|\int_{\sigma_{ij}}\kappa(u-u_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right| + O(h).$$

The claim now follows for general S_*. For $S_* = S_{0,-1}$ we apply Lemma 5.5 instead of (5.7). For general $S_* = S_{\alpha,\beta}$ with $\alpha+\beta=-1$ we apply Corollary 4.4. □

Corollary 5.7. *Under the assumptions of Theorem 5.6 it further holds*

$$\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa(u-u_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right)^2 \le Ch^2\|V\|_{C^2}^2\|\nabla u\|_{L^2(\Omega)}^2.$$

In case $u \in C^1(\Omega)$ it even holds

$$\sum_{i\sim j}\frac{h_{ij}}{m_{ij}}\omega_{ij}^{-1}\left(\int_{\sigma_{ij}}\kappa(u-u_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right)^2 \le Ch^5\|V\|_{C^2}^2\|\nabla u\|_\infty^2.$$

Proof. In view of Lemma 5.1 we obtain in total

$$\left|\int_{\sigma_{ij}}\kappa(u-g_{ij})\nabla V\cdot\boldsymbol{\nu}_{ij}\right| \le C\|V\|_{C^2}\sum_{k=i,j}h^{\frac{3}{2}}\|\nabla u\|_{L^2(\Omega_k)} + O(h)$$

and $\|\nabla u\|_{L^2(\Omega_k)} \le h^{\frac{3}{2}}\|\nabla u\|_\infty$. □

6 Cubic Meshes

In view of Section 5 we consider the following specialization of Lemma 5.1 to cubic grids. Throughout this section we consider $d \leq 3$ and a polygonal domain $\Omega \subset \mathbb{R}^d$ with a cubic mesh where $\Omega_i = x_i + [-h/2, h/2]^d$, $x_i \in h\mathbb{Z} \subset \Omega$.

Lemma 6.1. *Let $\Omega \subset \mathbb{R}^d$ be a polygonal domain with $d \leq 4$ and a cubic mesh where $\Omega_i = x_i + [-h/2, h/2]^d$, $x_i \in h\mathbb{Z} \subset \Omega$. Then for every function $\varpi \in C^2$ with $\varpi_i := \varpi(x_i)$ and $S_{ij} := S_*(\varpi_i, \varpi_j)$ it holds*

$$\left| \int_{\sigma_{ij}} (\varpi - S_{ij})\, \kappa \nabla U \cdot \boldsymbol{\nu}_{ij} \right| = O(h^2)\,. \tag{6.1}$$

Proof. The following calculations are quite standard and, therefore, we shorten our considerations. We have for $x \in \sigma_{ij}$

$$\begin{aligned} S_{ij} - \varpi(x) &= S(\varpi_i, \varpi_j) - S(\varpi(x), \varpi(x)) = \\ &= \nabla S(x) \cdot \begin{pmatrix} \varpi_i - \varpi(x) \\ \varpi_j - \varpi(x) \end{pmatrix} + \begin{pmatrix} \varpi_i - \varpi(x) \\ \varpi_j - \varpi(x) \end{pmatrix} \cdot \nabla^2 S(x) \cdot \begin{pmatrix} \varpi_i - \varpi(x) \\ \varpi_j - \varpi(x) \end{pmatrix} + O(h^3). \end{aligned}$$

The gradient of S is given by $(1/2, 1/2)^T$ and hence, we $S_{ij} - \varpi(x) = \frac{\varpi_i + \varpi_j - 2\varpi(x)}{2} + O(h^2)$. We compute the first term in more detail. We have $\varpi_j - \varpi(x) = \nabla\varpi \cdot (x_j - x) + O(h^2)$ and correspondingly for $j \rightsquigarrow i$ and the sum yields

$$\varpi_i + \varpi_j - 2\varpi(x) = \nabla\varpi \cdot (x_i + x_j - 2x) + O(h^2) = \frac{1}{2} \nabla\varpi \cdot \tilde{x} + O(h^2)\,,$$

where $\tilde{x} = x - \frac{x_i + x_j}{2}$ the coordinate on the cell surface with respect to the middle point $\bar{x} = \frac{x_i + x_j}{2}$. Hence, we get

$$\int_{\sigma_{ij}} (\varpi - S_{ij}) \kappa \nabla U \cdot \nu_{ij} = \frac{1}{4} \int_{\sigma_{ij}} \nabla\varpi(x) \cdot \tilde{x} \kappa(x) \nabla U(x) \cdot \nu_{ij} \mathrm{d}\sigma(\tilde{x}) + O(h^2).$$

Now we can fix the function $s(x) = \kappa(x) \nabla U(x) \cdot \nu_{ij} \nabla\varpi(x)$ with respect to $\bar{x}$. We have $s(x) = s(\bar{x}) + (x - \bar{x}) \nabla s(\bar{x}) + O(h^2)$, which implies (assuming that $U, \varpi \in \mathrm{C}^2$ and $\kappa \in \mathrm{C}^1$) that

$$\int_{\sigma_{ij}} (\varpi - S_{ij}) \kappa \nabla U \cdot \nu_{ij} = \frac{1}{4} \int_{\sigma_{ij}} (s(\bar{x}) + (x - \bar{x}) \nabla s(\bar{x})) \cdot \tilde{x} \mathrm{d}\sigma(\tilde{x}) + O(h^2) = \frac{1}{4} \int_{\sigma_{ij}} s(\bar{x}) \cdot \tilde{x} \mathrm{d}\sigma(\tilde{x}) + O(h^2)\,.$$

But the first vanishes, since the interface σ_{ij} is symmetric w.r.t. the mid point $\bar{x}$ and we are integrating along $\tilde{x}$. Hence, we have (6.1). □

6.1 Consistency of purely elliptic operators on cubic meshes

Theorem 6.2 (Consistency on cubic meshes)**.** *Let $\Omega \subset \mathbb{R}^d$ with $d \leq 4$ be a polygonal domain with a cubic mesh where $\Omega_i = x_i + [-h/2, h/2]^d$, $x_i \in h\mathbb{Z} \subset \Omega$. Then*

$$|\mathfrak{E}|_{\mathcal{T},\kappa,\omega}(u) \leq C h^4.$$

Proof. It holds

$$\left| m_{ij}\kappa_{ij}\frac{\hat{U}_j-\hat{U}_i}{h} - \int_{\sigma_{ij}} \kappa\nabla U\cdot\nu_{ij}\right| \le |\kappa_{ij}|\left| m_{ij}\frac{\hat{U}_j-\hat{U}_i}{h} - \int_{\sigma_{ij}} \nabla U\cdot\nu_{ij}\right| + \left|\int_{\sigma_{ij}} (\kappa_{ij}-\kappa)\,\nabla U\cdot\nu_{ij}\right|.$$

We have $\hat{U}_j = U(x)+\nabla U\cdot(x_j-x)+O(h^2)$ and $\hat{U}_i = U(x)+\nabla U\cdot(x_i-x)+O(h^2)$. Moreover, we can write $x_i - x = -\frac{h}{2}\nu_{ij}+\tilde{x}$ where $\tilde{x}\perp\nu_{ij}$ and $x_j - x = \frac{h}{2}\nu_{ij}+\tilde{x}$ (the normal ν_{ij} points outside or inside of Ω_i). Hence, we conclude

$$\hat{U}_j = U(x) + \nabla U\cdot(\frac{h}{2}\nu_{ij}+\tilde{x}) + O(h^2)$$
$$\hat{U}_i = U(x) + \nabla U\cdot(-\frac{h}{2}\nu_{ij}+\tilde{x}) + O(h^2).$$

Subtracting both equations, we end up with $\frac{\hat{U}_j-\hat{U}_i}{h} = \nabla U\cdot\nu_{ij}+O(h^2)$, and hence,

$$\left| m_{ij}\frac{\hat{U}_j-\hat{U}_i}{h} - \int_{\sigma_{ij}} \nabla U\cdot\nu_{ij}\right| \le m_{ij}O(h^2).$$

The Theorem follows from Lemma 6.1, the definition of κ_{ij} and the cubic geometry. □

6.2 Quantitative estimate on cubic meshes in the diffusive representation

In view of Theorem 5.6 combined with Theorem 6.2 and Lemma 6.1 with $\frac{1}{2}(u_i+u_j) = S_{2,1}(u_i,u_j)$ we also obtain the following.

Theorem 6.3. *Let $d\le 4$. On a polygonal domain $\Omega\subset\mathbb{R}^d$ with a cubic mesh where $\Omega_i = x_i+[-h/2,h/2]^d$, $x_i\in h\mathbb{Z}\subset\Omega$, it holds: Using the notation of Lemma 2.12 it holds*

$$|\mathfrak{E}|_{\mathcal{T},\omega,\mathrm{conv}}(u) = O(h^2)\,.$$

In case $S_* = S_{0,-1}$ or $S_* = S_{\alpha,\beta}$ with $\alpha+\beta=-1$ the above can be improved to

$$|\mathfrak{E}|_{\mathcal{T},\omega,\mathrm{conv}}(u) = O(h^4)\,.$$

7 Numerical simulation and convergence analysis

In this section, we provide a numerical convergence analysis of the flux discretization schemes based on Stolarsky means described in the previous sections. For the sake of simplicity, we restrict ourselves to one-dimensional examples with equidistant meshes, for which already non-trivial results can be observed.

Example 7.1. We consider the potential $V(x) = 2\sin(2\pi x)$, the right hand side $f(x) = x(1-x)$ on $x=(0,1)$ with $\kappa=1$ and Dirichlet boundary conditions $u(0)=0$ and $u(1)=1$. The Stolarsky mean discretizations are compared point-wise with a numerically computed reference solution u_{ref} (and J_{ref}) that was obtained using a shooting method (involving a fourth order Runge–Kutta scheme) together with Brent's root finding algorithm [Bre71] on a very fine grid with 136474 nodes.

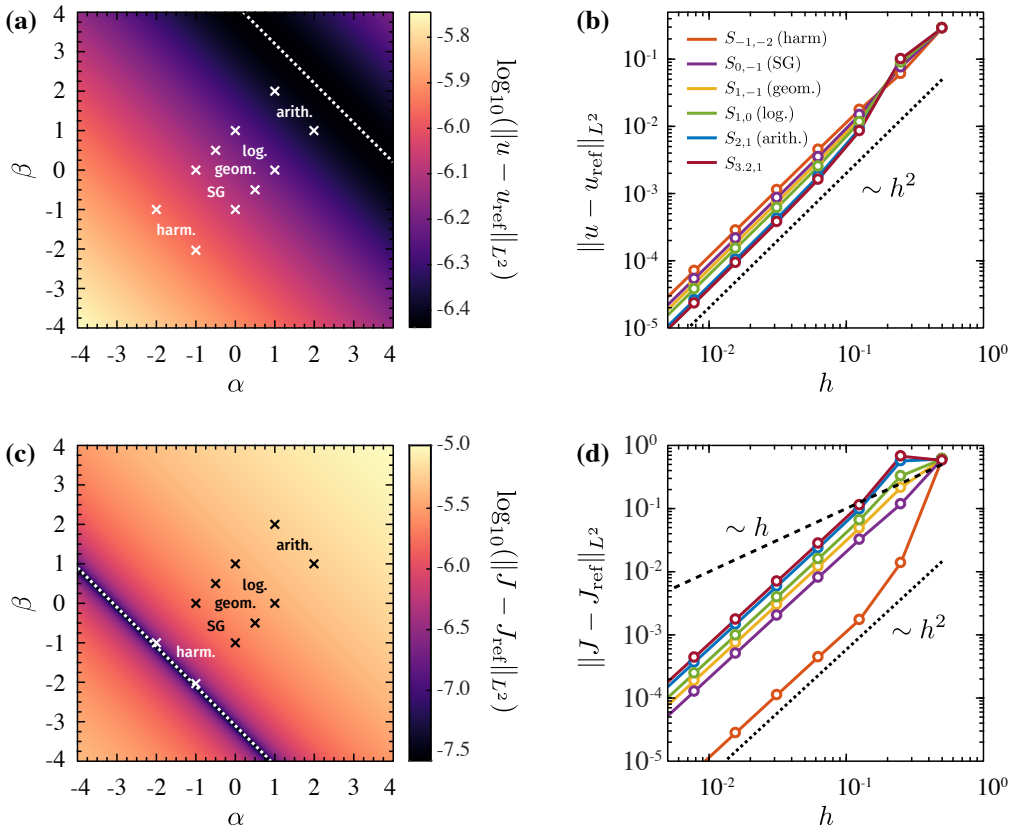

Fig. 2. Numerical results for example 7.1. **(a)** Discretization error $\log_{10}(\|u - u_{\text{ref}}\|_{L_2})$ in the (α, β)-plane on an equidistant mesh with $2^{10} + 1$ nodes. The error is color-coded. Several special means an highlighted by crosses (notice the symmetry $S_{\alpha,\beta}(x, y) = S_{\beta,\alpha}(x, y)$). **(b)** Quadratic convergence of the discrete solution to the exact reference solution u_{exact} under mesh refinement in the L_2-norm. See the inset for a legend and color-coding of the considered means $S_{\alpha,\beta}$. In the present example, the best numerical result for u is achieved by $S_{3.2,1}$. **(c)** Logarithmic error of the numerically computed flux density $\log_{10}(\|j - j_{\text{ref}}\|_{L_2})$ in the (α, β)-plane on the same mesh as in (a). **(d)** Convergence of the numerically computed flux density to j_{exact}. In contrast to the convergence of u shown in (b), here the harmonic average $S_{-1,-2}$ performs best.

The convergence results are summarized in Fig. 2. In Fig. 2 (a), the logarithmic error $\log_{10}(\|u - u_{\text{ref}}\|_{L_2})$ is shown in the (α, β)-plane of the Stolarsky mean parameters for an equidistant mesh with $2^{10} + 1 = 1025$ nodes. First, we note that the accuracy for a mean $S_{\alpha,\beta}$ is indeed practically invariant along $\alpha + \beta = \text{const.}$, which is consistent with our analytical result in Section 4. In this particular example, we observe optimal accuracy at about $\alpha + \beta \approx 4.2$. This coincides with the convergence results under mesh refinement shown in Fig. 2 (b), where the fastest convergence is obtained for the scheme involving the $S_{3.2,1}$-mean. The other considered schemes, however, show as well a quadratic convergence behavior with a slightly larger constant. Interestingly, for the same example, we find that the optimal mean for an accurate approximation of the flux J is on $\alpha + \beta = -3$, see Fig. 2 (c). This is further evidenced in Fig. 2 (d), where the harmonic mean $S_{-1,-2}$ converges significantly faster than the other schemes. Obviously, in the present example, the minimal attainable error for both u and J can not be achieved by the same discretization scheme.

Example 7.2. We consider the potential $V(x) = 5(x + 1)x$ and keep the right hand side function, the diffusion constant and the boundary conditions as in the previous example.

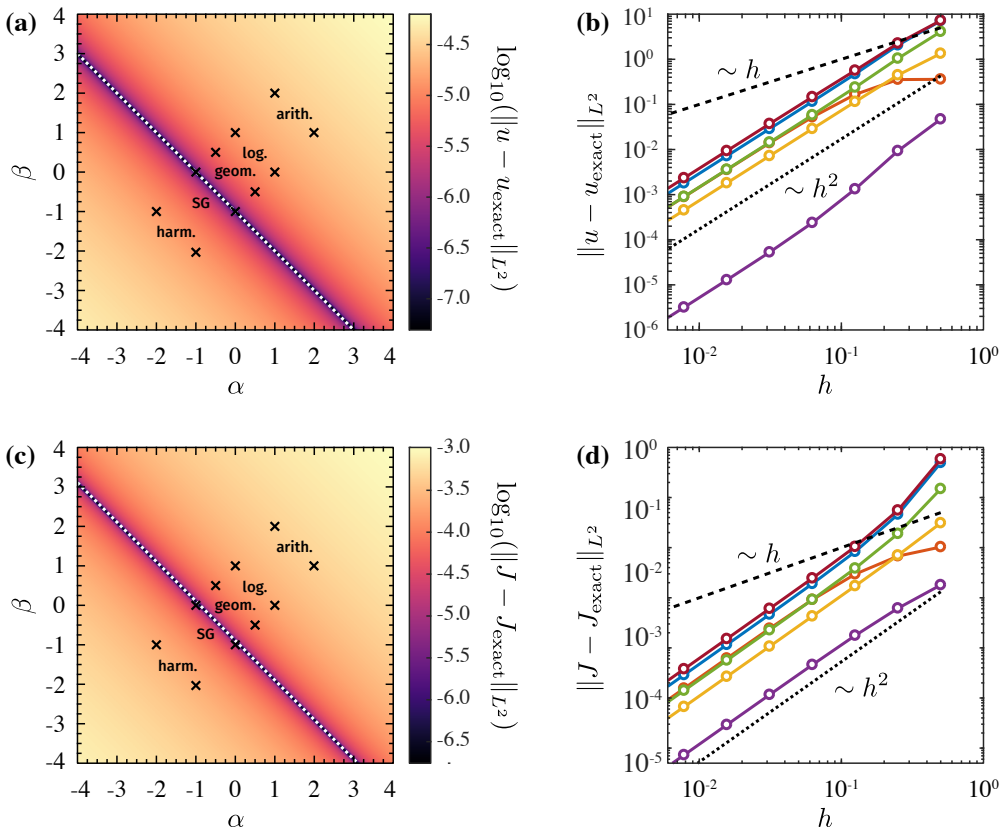

Fig. 3. Discretization errors and convergence behavior of the numerically computed u and J in example 7.2 using the Stolarsky mean schemes. The errors in **(a)** and **(c)** are color-coded. The coloring of the means in **(b)** and **(d)** is the same as in Fig. 2 (b). The plots clearly show a superior performance of the Scharfetter–Gummel scheme (i.e., the Stolarsky mean $S_{0,-1}$) for the approximation of both the density u and the flux J.

The problem has an exact solution involving the imaginary error function, that is related to the Dawson function, which has been obtained using Mathematica [Wol17].

The numerical results are shown in Fig. 3. The discretization errors for both the density u and the flux J are depicted in Fig. 3 (a) and (c) show a sharp minimum for $\alpha + \beta = -1$. This involves the Scharfetter–Gummel mean $S_{0,-1}$, which converges fastest to the analytical solutions for u and J, as shown in 3 (b) and (d). The SQRA scheme, with geometric mean $S_{\alpha,-\alpha}$, is found to be second best in the present example.

The numerical results are in line with Theorem 1.6: In the case of strong gradients ∇V, the Scharfetter–Gummel scheme provides the most accurate flux discretization, in particular, the SG mean $S_{0,-1}$ is the only Stolarsky mean that recovers the upwind scheme (1.9). Away from that drift-dominated regime, the situation is less clear and other averages $S_{\alpha,\beta}$ can be superior, see for instance Example 7.1.

A Appendix

A.1 A General Poincaré Inequality

We derive a general Poincaré inequality on meshes. The idea behind the proof seems to go back to Hummel [Hum99] and has been adapted in a series of works e.g. [Hei18, HKP17].

Let $e_0 = 0$ and $(e_i)_{i=1,\dots,n}$ be the canonical basis of $\mathbb{R}^n$. Define:

$$D^{d-1} := \{\nu \in \mathbb{S}^{d-1} \mid \exists m \in \{1,\cdots,d\} : \nu \cdot e_i = 0 \ \forall\ i \in \{0,1,\cdots,m-1\} \text{ and } \nu \cdot e_m > 0\}\,.$$

Every $\nu \in \mathbb{S}^{d-1}$ satisfies $\nu \cdot e_i \neq 0$ for at least one e_i. Thus, for every $\nu \in \mathbb{S}^{d-1}$ it holds $\nu \in D^{d-1}$ if and only if $-\nu \notin D^{d-1}$.

We denote $\Gamma = \bigcup_{\sigma\in\mathcal{E}_\Omega} \sigma$ and say that $x \in \Gamma$ is a Lipschitz point if Γ is a Lipschitz graph in a neighborhood of x. The set of Lipschitz-Points is called $\Gamma_L \subset \Gamma$ and we note that for the $(d-1)$-dimensional Hausdorff-measure of $\Gamma\backslash\Gamma_L$ it holds $\mathcal{H}^{d-1}(\Gamma\backslash\Gamma_L) = 0$.

For $x \in \Gamma_L$, we denote $\nu_x \in D^{d-1}$ the normal vector to Γ in x.. Let

$$\mathcal{C}^1_0(\Omega;\Gamma) := \left\{u \in C(\Omega\backslash\Gamma) \ :\ u|_{\partial\Omega} \equiv 0\,,\ \forall i\, \exists v_i \in C^1\left(\overline{\Omega_i}\right) :\ u|_{\Omega_i} = v_i\right\}$$

and for $u \in \mathcal{C}^1_{K,0}(\Omega)$ define in Lipschitz points $x \in \Gamma_L$

$$u_\pm(x) := \lim_{h\to 0}\left(u\left(x \pm h\nu_x\right)\right)\,, \qquad [\![u]\!](x) := u_+(x) - u_-(x)\,.$$

For two points $x, y \in \mathbb{R}^n$ denote (x,y) the closed straight line segment connecting x and y and for $\xi \in (x,y)\cap\Gamma_L$ denote

$$[\![u]\!]_{x,y}(\xi) := \lim_{h\to 0}\left(u\left(\xi + h(y-x)\right) - u\left(\xi - h(y-x)\right)\right)$$

the jump of the function u at ξ in direction $(y-x)$, i.e. $[\![u]\!]_{x,y}(\xi) \in \pm[\![u]\!](\xi)$. We can extend $[\![u]\!]$ to Γ by $[\![u]\!](x) = 0$ for $x \in \Gamma\backslash\Gamma_L$ and define

$$\|u\|_{H^1(\Omega;\Gamma)} := \left(\int_{\Omega\backslash\Gamma} |\nabla u|^2 + \int_\Gamma [\![u]\!]^2\right)^{\frac{1}{2}}\,,$$
$$H^1_0(\Omega;\Gamma) := \overline{\mathcal{C}^1_0(\Omega;\Gamma)}^{\|\cdot\|_{H^1(\Omega;\Gamma)}}\,.$$

Then we find the following result:

Lemma A.1 (Semi-discrete Poincaré inequality)**.** *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain. The space $H^1_0(\Omega;\Gamma)$ is linear and closed for every $s \in [0,\frac{1}{2})$ and there exists a positive constant $C_s > 0$ such that the following holds: Suppose there exists a constant $C_\# > 0$ such that for almost all $(x,y) \in \Omega^2$ it holds $\#((x,y)\cap\Gamma) \le C_\#$.. Then for every $u \in H^1_0(\Omega;\Gamma)$ it holds*

$$\|u\|^2_{H^s(\Omega)} \le C_s\left(C_\# \int_\Gamma [\![u]\!]^2 + \|\nabla u\|^2_{L^2(\Omega\backslash\Gamma)}\right)\,. \tag{A.1}$$

Furthermore, for every $u \in H^1(\Omega;\Gamma)$ and every $\boldsymbol{\eta} \in \mathbb{R}^d$ it holds

$$\int_\Omega |u(x) - u(x+\boldsymbol{\eta})|^2\,dx \le |\boldsymbol{\eta}|\left(C_\# \int_\Gamma [\![u]\!]^2 + \|\nabla u\|^2_{L^2(\Omega\backslash\Gamma)}\right)\,. \tag{A.2}$$

Proof. In what follows, given $u \in \mathcal{C}^1_0(\Omega;\Gamma)$, we write $\widehat{\nabla u}(x) := \nabla u(x)$ if $x \in \Omega\backslash\Gamma$ and $\widehat{\nabla u}(x) = 0$ else. For $y \in \mathbb{R}^d$ we denote $(x,y) = \{x + s\,(y-x) : s \in [0,1]\}$. Using $2ab < a^2 + b^2$, we infer for $u \in \mathcal{C}^1_0(\Omega;\Gamma)$ and $x, y \in \overline{\Omega}\backslash\Gamma$ such that $(x,y)\cap\Gamma$ is finite the inequality

$$\begin{aligned}|u(x) - u(y)|^2 &\le \left(\sum_{\xi\in(x,y)\cap\Gamma} [\![u]\!]_{x,y}(\xi) + \int_0^1 \widehat{\nabla u}\left(x + s(y-x)\right)\cdot(x-y)\,ds\right)^2\\ &< |x-y|^2 \int_0^1 \left|\widehat{\nabla u}\left(x + s(y-x)\right)\right|^2 ds + \left(\sum_{\xi\in(x,y)\cap\Gamma} [\![u]\!]_{x,y}(\xi)\right)^2\end{aligned}$$

Since $[\![u]\!]_{x,y} = [\![u]\!]$ we compute

$$\left(\sum_{\xi\in(x,y)\cap\Gamma} [\![u]\!]_{x,y}(\xi)\right)^2 \leq \#\left((x,y)\cap\Gamma\right) \sum_{\xi\in(x,y)\cap\Gamma} [\![u]\!]^2(\xi)$$

and obtain

$$\begin{aligned} |u(x)-u(y)|^2 < |x-y|^2 \int_0^1 \left|\widehat{\nabla u}\left(x+s(y-x)\right)\right|^2 ds \\ + \#\left((x,y)\cap\Gamma\right) \sum_{\xi\in(x,y)\cap\Gamma} [\![u]\!]^2(\xi)\,. \end{aligned} \tag{A.3}$$

We fix $\eta > 0$ and consider the orthonormal basis $(e_i)_{i=1,\dots,d}$ of $\mathbb{R}^d$. The determinant of the first fundamental form of Γ is bigger than 1 almost everywhere. Hence we can observe that

$$\begin{aligned} \int_\Omega \sum_{\xi\in(x,x+\eta e_1)\cap\Gamma} [\![u]\!]^2(\xi)\,\mathrm{d}x &= \int_{\mathbb{R}} \left(\int_{\mathbb{R}^{d-1}} \sum_{\xi\in(x,x+\eta e_1)\cap\Gamma} [\![u]\!]^2(\xi)\,\mathrm{d}x_2 \dots \mathrm{d}x_d \right) \mathrm{d}x_1 \\ &\leq \int_{\mathbb{R}} \int_{\Gamma\cap((x_1,x_1+\eta)\times\mathbb{R}^{d-1})} [\![u]\!]^2(x)\,\mathrm{d}\sigma\,\mathrm{d}x_1 \\ &\leq \eta \int_\Gamma [\![u]\!]^2(x)\,\mathrm{d}x\,, \end{aligned}$$

where we used that the surface elements are bigger than 1.. Furthermore, we have

$$\eta^2 \int_0^1 \left|\widehat{\nabla u}\left(x+s\eta e_1\right)\right|^2 ds = \eta \int_0^\eta \left|\widehat{\nabla u}\left(x+se_1\right)\right|^2 ds\,.$$

Replacing e_1 in the above calculations with any unit vector e, we obtain from integration of (A.3) with $y = x+\boldsymbol{\eta}$, $\boldsymbol{\eta} = \eta e$, over Ω that

$$\int_\Omega |u(x)-u(x+\boldsymbol{\eta})|^2\,dx \leq |\boldsymbol{\eta}| \left(C_\# \int_\Gamma [\![u]\!]^2 + \|\nabla u\|^2_{L^2(\Omega\setminus\Gamma)} \right).$$

Dividing by $|\boldsymbol{\eta}|$ and integrating over $\boldsymbol{\eta}\in\mathbb{R}^d$, we obtain that for every $s\in[0,\frac{1}{2})$ there exists a positive constant $C_s > 0$ independent from u and K such that

$$\|u\|^2_{H^s(\Omega)} \leq C_s \left(C_\# \int_\Gamma [\![u]\!]^2 + \|\nabla u\|^2_{L^2(\Omega\setminus\Gamma)} \right). \tag{A.4}$$

Hence, by approximation, the last two estimates hold for all $u\in H^1_0(\Omega;\Gamma)$.. □

A.2 Physical relevance of the geometric mean

Theorem A.2. *Let $S_{ij} = S_*(\pi_i,\pi_j)$ be a Stolarsky mean and let ψ^* be a symmetric strictly convex function with $\psi^*(0) = 0$. If $\partial_\pi(S_{ij}a_{ij}) = 0$ then $S_{ij} = \sqrt{\pi_i\pi_j}$ and ψ^* is proportional to C^*.*

Proof of Theorem A.2. The case $S_{ij} = \sqrt{\pi_i\pi_j}$ and $\psi^*(\xi) = \cosh\xi - 1$ was explained in detail in [Hei18].

In the general case, symmetry of ψ^* in $\xi_i - \xi_j$ implies $\psi^*(\xi_i-\xi_j) = \psi^*(|\xi_i-\xi_j|)$. We make use of the fact that the original $\mathsf{C}^*(\xi) = \cosh\xi - 1$ is a bijection on $[0,\infty)$ and suppose that hence $\psi^*(\xi_i-\xi_j) = \theta(\mathsf{C}^*(\xi_i-\xi_j))$. This implies particularly that

$$0 \leq x\,\partial_x\left(\theta\left(\mathsf{C}^*(x)\right)\right) = x\,\partial_\xi\theta\left(\mathsf{C}^*(x)\right)\partial_x\mathsf{C}^*(x)\,.$$

Furhtermore, the symmetry of ψ^* implies by the last inequality that $\partial_\xi\theta\left(\mathsf{C}^*(x)\right) > 0$. Inserting this information in (3.7) and (3.8) we observe that

$$S_{ij}\left(\frac{u_i}{\pi_i}-\frac{u_j}{\pi_j}\right)\partial_\xi\theta\left(\mathsf{C}^*\left(\ln\left(\frac{u_i}{\pi_i}\right)-\ln\left(\frac{u_j}{\pi_j}\right)\right)\right)^{-1}\sinh\left(\ln\left(\frac{u_i}{\pi_i}\right)-\ln\left(\frac{u_j}{\pi_j}\right)\right)^{-1}$$

has to be independent from π_i and π_j. From the above case $S_{ij} = \sqrt{\pi_i\pi_j}$, we know that

$$\sqrt{\pi_i\pi_j}\left(\frac{u_i}{\pi_i}-\frac{u_j}{\pi_j}\right)\sinh\left(\ln\left(\frac{u_i}{\pi_i}\right)-\ln\left(\frac{u_j}{\pi_j}\right)\right)^{-1}$$

is constant in π_i and π_j. Hence it remains to show that

$$f(\pi_i,\pi_j) := S_{ij}\sqrt{\pi_i\pi_j}^{-1}\partial_\xi\psi\left(\frac{u_i}{u_j}\frac{\pi_j}{\pi_i}+\frac{u_j}{u_i}\frac{\pi_i}{\pi_j}\right)^{-1}$$

is independent from π_i and π_j if and only if $\partial_\xi\psi = const$ and $S_{ij} = \sqrt{\pi_i\pi_j}$.

Assume first that $S_{ij}\sqrt{\pi_i\pi_j}^{-1} = const$. Then for $p = \frac{\pi_i}{\pi_j}$ we obtain that

$$\partial_p\left(\partial_\xi\theta\left(\frac{u_i}{u_j}p^{-1}+\frac{u_j}{u_i}p\right)^{-1}\right) = 0$$

has to hold. This implies that $\partial_\xi\psi = const$.

If $S_{ij}\sqrt{\pi_i\pi_j}^{-1} \neq const$, we use the definition of the weighted Stolarsky means given in (1.3) and note that

$$S_{ij} := S(\pi_i,\pi_j) = \left(\frac{\beta(\pi_i^\alpha-\pi_j^\alpha)}{\alpha(\pi_i^\beta-\pi_j^\beta)}\right)^{\frac{1}{\alpha-\beta}} = \pi_j\left(\frac{\beta(p^\alpha-1)}{\alpha(p^\beta-1)}\right)^{\frac{1}{\alpha-\beta}},$$

where again $p = \frac{\pi_i}{\pi_j}$. Hence we obtain that

$$\begin{aligned} f(\pi_i,\pi_j) = \tilde f(p) &:= \sqrt{\frac{1}{p}}\left(\frac{\beta(p^\alpha-1)}{\alpha(p^\beta-1)}\right)^{\frac{1}{\alpha-\beta}}\partial_\xi\theta\left(\frac{u_i}{u_j}p^{-1}+\frac{u_j}{u_i}p\right)^{-1} \\ &= \left(\frac{\beta\left(p^{\frac{\alpha}{2}}-p^{-\frac{\alpha}{2}}\right)}{\alpha\left(p^{\frac{\beta}{2}}-p^{-\frac{\beta}{2}}\right)}\right)^{\frac{1}{\alpha-\beta}}\partial_\xi\theta\left(\frac{u_i}{u_j}p^{-1}+\frac{u_j}{u_i}p\right)^{-1} \end{aligned}$$

has to be independent of π_i and π_j. But then, $\tilde f$ is independent of p. Now, we define $a = \frac{u_j}{u_i}$ and observe that

$$\tilde f\left(\frac{1}{a^2p}\right) = \left(\frac{\beta\left((a^2p)^{-\frac{\alpha}{2}}-(a^2p)^{\frac{\alpha}{2}}\right)}{\alpha\left((a^2p)^{-\frac{\beta}{2}}-(a^2p)^{\frac{\beta}{2}}\right)}\right)^{\frac{1}{\alpha-\beta}}\partial_\xi\theta\left(\frac{u_i}{u_j}p^{-1}+\frac{u_j}{u_i}p\right)^{-1}.$$

We assume for $\alpha \neq \beta$. The case $\alpha = \beta$ can follows by continuity. For any p it should holds $\tilde f\left(\frac{1}{a^2p}\right) = \tilde f(p)$, which implies

$$\left(\frac{\beta\left(p^{\frac{\alpha}{2}}-p^{-\frac{\alpha}{2}}\right)}{\alpha\left(p^{\frac{\beta}{2}}-p^{-\frac{\beta}{2}}\right)}\right)^{\frac{1}{\alpha-\beta}} = \left(\frac{\beta\left((a^2p)^{-\frac{\alpha}{2}}-(a^2p)^{\frac{\alpha}{2}}\right)}{\alpha\left((a^2p)^{-\frac{\beta}{2}}-(a^2p)^{\frac{\beta}{2}}\right)}\right)^{\frac{1}{\alpha-\beta}},$$

or equivalently, after introducing $q^2 = p$,

$$\left(a^\alpha - a^\beta\right) q^{\alpha+\beta} + \left(a^\beta - a^{-\alpha}\right) q^{\beta-\alpha} + \left(a^{-\beta} - a^\alpha\right) q^{\alpha-\beta} + \left(a^{-\alpha} - a^{-\beta}\right) q^{-\beta-\alpha} = 0.$$

Since $\alpha \neq \beta$, one of the terms $q^{\pm\alpha\pm\beta}$ grows faster than the other. Hence we conclude that $a^\alpha = a^{\pm\beta}$ which means, $a = 1$, a contradiction. □

A.3 Properties of the Stolarsky mean

Lemma A.3. *For every of the above Stolarsky means $S_*(x,y)$ it holds*

$$\partial_x S_*(x,x) = \partial_y S_*(x,x) = \frac{1}{2} \text{ and } \partial_x^2 S_*(x,x) = \partial_y^2 S_*(x,x) = -\partial_{xy}^2 S_*(x,x) = -\partial_{yx}^2 S_*(x,x)\,.$$

Proof. Since $S_*(x,x) = x$ and S_* is symmetric in x and y, we find from differentiating $\partial_x S_* = \partial_y S_* = \frac{1}{2}$. From the last equality, we find $\partial_x S_*(x,x) - \partial_y S_*(x,x) = 0$ as well as $\partial_x S_*(x,x) + \partial_y S_*(x,x) = 1$ and differentiation yields

$$\partial_x^2 S_*(x,x) - \partial_y^2 S_*(x,x) - \partial_{xy}^2 S_*(x,x) + \partial_{yx}^2 S_*(x,x) = 0\,, \tag{A.5}$$
$$\partial_x^2 S_*(x,x) + \partial_y^2 S_*(x,x) + \partial_{xy}^2 S_*(x,x) + \partial_{yx}^2 S_*(x,x) = 0\,. \tag{A.6}$$

Since $-\partial_{xy}^2 S_*(x,x) + \partial_{yx}^2 S_*(x,x) = 0$, equation (A.5) yields $\partial_x^2 S_*(x,x) = \partial_y^2 S_*(x,x)$. Inserting the last two relations into (A.6) yields $\partial_{xy}^2 S_*(x,x) = \partial_{yx}^2 S_*(x,x) = -\partial_x^2 S_*(x,x)$. □

Lemma A.4. *It holds* (3.2)$\partial_x^2 S_{\alpha,\beta}(\pi,\pi) = \frac{1}{12\pi}(\alpha+\beta-3)$.

Proof. We know from Lemma A.3 that $\partial_x S_{\alpha,\beta}(x,x) = \frac{1}{2}$, $\partial_x^2 S_{\alpha,\beta}(x,x) = -\partial_y\partial_x S_{\alpha,\beta}(x,x)$. Hence we find

$$\partial_x S_{\alpha,\beta}(x+h,x-h) - \frac{1}{2} = \begin{pmatrix} h \\ -h \end{pmatrix} \begin{pmatrix} \partial_x^2 S_{\alpha,\beta}(x,x) \\ \partial_y\partial_x S_{\alpha,\beta}(x,x) \end{pmatrix} = 2h\partial_x^2 S_{\alpha,\beta}(x,x)\,.$$

We make use of the explicit form

$$\partial_x S_{\alpha,\beta}(x,y) = \left(\frac{\beta}{\alpha}\right)^{\frac{1}{\alpha-\beta}} \frac{\left(x^\alpha - y^\alpha\right)^{\frac{1}{\alpha-\beta}-1}}{\left(x^\beta - y^\beta\right)^{\frac{1}{\alpha-\beta}-1}} \frac{\alpha\left(x^\beta - y^\beta\right)x^\alpha - \beta\left(x^\alpha - y^\alpha\right)x^\beta}{(\alpha-\beta)\;x\;\left(x^\beta - y^\beta\right)^2}$$

for $x \neq y$. We insert $x = x+h$ and $y = x-h$ and make use of the following expansions

$$\begin{aligned}
\left((x+h)^\alpha - (x-h)^\alpha\right)^c &= \left(\alpha h x^{\alpha-1}\right)^c \left(2^c + O\left(h^2\right)\right) \\
\beta\left((x+h)^\alpha - (x-h)^\alpha\right)(x+h)^\beta &= 2\alpha\beta h x^{\alpha+\beta-1} + 2\alpha\beta^2 h^2 x^{\alpha+\beta-2} \\
&\quad + \frac{1}{3}\alpha\beta h^3\left(\alpha^2 - 3\alpha + 3\beta^2 - 3\beta + 2\right) + O\left(h^4\right) \\
\alpha\left((x+h)^\beta - (x-h)^\beta\right)(x+h)^\alpha &= 2\alpha\beta h x^{\alpha+\beta-1} + 2\alpha^2\beta h^2 x^{\alpha+\beta-2} \\
&\quad + \frac{1}{3}\alpha\beta h^3\left(\beta^2 - 3\beta + 3\alpha^2 - 3\alpha + 2\right) + O\left(h^4\right) \\
(x+h)\left((x+h)^\beta - (x-h)^\beta\right)^2 &= 4\beta^2 h^2 x^{2\beta-1} + 4\beta^2 h^3 x^{2\beta-2} + O\left(h^4\right)
\end{aligned}$$

$$\alpha\left((x+h)^\beta-(x-h)^\beta\right)(x+h)^\alpha-\beta\left((x+h)^\alpha-(x-h)^\alpha\right)(x+h)^\beta$$
$$=2\alpha\beta\left(\alpha-\beta\right)h^2x^{\alpha+\beta-2}+\frac{\alpha\beta}{3}h^3x^{\alpha+\beta-3}\left(2\alpha^2-2\beta^2\right)+O\left(h^4\right)$$

to obtain

$$\frac{\beta\left(x^\alpha-y^\alpha\right)x^\beta-\alpha\left(x^\beta-y^\beta\right)x^\alpha}{\left(\alpha-\beta\right)\ x\ \left(x^\beta-y^\beta\right)^2}=\frac{\alpha\left(x^{\alpha+\beta-2}+h\frac{1}{3}x^{\alpha+\beta-3}\left(\alpha+\beta\right)+O\left(h^2\right)\right)}{2\beta\left(x^{2\beta-1}+hx^{2\beta-2}+O\left(h^2\right)\right)}$$

and

$$\frac{\left(x^\alpha-y^\alpha\right)^{\frac{1}{\alpha-\beta}-1}}{\left(x^\beta-y^\beta\right)^{\frac{1}{\alpha-\beta}-1}}\approx\left(\frac{\alpha}{\beta}\right)^{\frac{1}{\alpha-\beta}-1}\left(\frac{x^{\alpha-1}\left(1+O\left(h^2\right)\right)}{x^{\beta-1}\left(1+O\left(h^2\right)\right)}\right)^{\frac{1}{\alpha-\beta}-1}.$$

Together with

$$\frac{a+bh}{c+dh}=\frac{a}{c}+\frac{bc-ad}{c^2}h+O\left(h^2\right)$$
$$\left(\frac{1+ah^2}{1+bh^2}\right)^c=1+ch^2(a-b)+O\left(h^4\right)$$

we find

$$\partial_xS_{\alpha,\beta}\left(x+h,x-h\right)=\left(\frac{\left(1+O\left(h^2\right)\right)}{\left(1+O\left(h^2\right)\right)}\right)^{\frac{1}{\alpha-\beta}-1}\left(\frac{\left(1+h\frac{1}{3}x^{-1}\left(\alpha+\beta\right)+O\left(h^2\right)\right)}{2\left(1+hx^{-1}+O\left(h^2\right)\right)}\right)$$
$$=\left(\frac{1}{2}+\frac{\frac{2}{3}\left(\alpha+\beta\right)-2}{4\,x}\,h\right)+O\left(h^2\right)$$

and hence (3.2). □

A.4 Approximation of potential to get the SQRA mean

The aim of this section is to provide a class of potentials which are easy to handle and which generate the SQRA-mean $S_{-1,1}(\pi_0,\pi_h)$ by $\pi_{\text{mean}}=\left(\frac{1}{h}\int_0^h\pi^{-1}\right)^{-1}$. Clearly, choosing the constant potential $V(x):=V_c:=-\log S_{-1,1}(\pi_0,\pi_h)$ we obtain right mean. Although this works for any means, this has two drawbacks

1. The potential jumps and hence the gradient is somewhere infinite, which means that at these points the force on the particles is infinitely high which is not physical.
2. Approximating a general function by piecewise constants, on each interval the accuracy is only of order h. However, approximating a function by affine interpolation the accuracy is of order h^2 on each interval (see below for the calculation).

So we want to get a potential which may be used as a good approximation (i.e. approximating of order h^2), is physical (i.e. continuous) and generates the SQRA-mean. Note, that most considerations below also work for other Stolarsky means. For simplicity we focus on the SQRA mean $S_{-1,1}$.

A.4.1 Approximation order for linear approximation

Let us first realize that a linear interpolation provides an approximation of order h^2. Let $V : [0,h] \to \mathbb{R}$ be a general C^2-potential. We define with $V(0) = V_0$ and $V(h) = V_h$

$$\tilde{V}(x) = V_0 + \frac{V_h - V_0}{h} x.$$

Then one easily checks that

$$V(x) = V_0 + \partial_x V(0)x + \frac{1}{2}\partial_x^2 V(0)x^2 + O(h^3)$$

and hence,

$$V(x) - \tilde{V}(x) = \left(\partial_x V(0) - \frac{V_h - V_0}{h}\right) x + \frac{1}{2}\partial_x^2 V(0)x^2 + O(h^3).$$

Clearly, we also have

$$V_h = V_0 + \partial_x V(0)h + \frac{1}{2}\partial_x^2 V(0)h^2 + O(h^3)$$

which yields

$$V(x) - \tilde{V}(x) = -\frac{1}{2}\partial_x^2 V(0)hx + \frac{1}{2}\partial_x^2 V(0)x^2 + O(h^3) = \frac{1}{2}\partial_x^2 V(0)(x-h)x + O(h^3) = O(h^2).$$

A.4.2 Definition of potentials $\hat{V}$ which generate the SQRA mean

We consider a piecewise linear potential of the form

$$\hat{V}(x) = \begin{cases} \frac{V_c - V_0}{x_1} x + V_0 & , x \in [0, x_1] \\ V_c & , x \in [x_1, x_2] \\ \frac{V_h - V_c}{h - x_2}(x - x_2) + V_c & , x \in [x_2, h] \end{cases}.$$

where $x_1, x_2 \in [0,h]$ are firstly arbitrary and $V_c = -\log S_{-1,1}(\pi_0, \pi_h) = \frac{1}{2}(V_h + V_0)$. The potential is clearly continuous. Then

$$\frac{1}{h}\int_0^h \mathrm{e}^{\hat{V}(x)}\mathrm{d}x = \frac{x_1}{h}\frac{\mathrm{e}^{V_c} - \mathrm{e}^{V_0}}{V_c - V_0} + \frac{x_2 - x_1}{h}\mathrm{e}^{V_c} + \frac{h - x_2}{h}\frac{\mathrm{e}^{V_h} - \mathrm{e}^{V_c}}{V_h - V_c}.$$

Introducing the ratios $\alpha = \frac{x_1}{h}$ and $\beta = \frac{h - x_2}{h}$ (which are in $[0, 1/2]$) , we want to solve $\frac{1}{h}\int_0^h \mathrm{e}^{\hat{V}(x)}\mathrm{d}x = \mathrm{e}^{\frac{1}{2}(V_h + V_0)}$. Indeed, introducing the difference of the difference of the potentials $\bar{V} = V_h - V_0$, we obtain

$$\lambda = \frac{\alpha}{\beta} = \frac{\mathrm{e}^{\bar{V}/2} - \bar{V}/2 - 1}{\mathrm{e}^{-\bar{V}/2} + \bar{V}/2 - 1} \approx 1 + \frac{1}{3}\bar{V} + \frac{1}{18}\bar{V}^2.$$

Hence, any value α, β satisfying this ratio generates a potential with the SQRA-mean.

A.4.3 Proof that the potential approximates an arbitrary potential of order h^2

Since the linear potentials approximates a general potential of order h^2 it suffices to approximate the linear potential $\tilde{V}$ by $\hat{V}$. We show that there are α, β satisfying $\frac{\alpha}{\beta} = \lambda$, such that $\|\hat{V} - \tilde{V}\|_{C([x_i, x_{i+1}])} = O(h^2)$. The difference of $\hat{V}$ and $\tilde{V}$ is the largest at $x = x_1$ or $x = x_2$. We estimate both differences. We have

$$\tilde{V}(x_1) = V_0 + \frac{V_h - V_0}{h} x_1 = V_0 + \alpha \bar{V}, \quad \tilde{V}(x_2) = V_0 + \frac{V_h - V_0}{h} x_2 = V_0 + (1 - \beta)\bar{V}.$$

Hence we have to estimate

$$\Delta_1 := |V_0 - V_c + \alpha \bar{V}|, \quad \Delta_2 := |V_0 - V_c + (1 - \beta)\bar{V}|.$$

In the case of SQRA, one possible choice for α, β is $\alpha + \beta = 1$. Then $\Delta_1 = \Delta_2 = |V_0 - V_c + \alpha \bar{V}| = |V_0 - V_c + \frac{\lambda}{1+\lambda}\bar{V}| = \frac{1}{1+\lambda}|(1 + \lambda)(V_0 - V_c) + \lambda \bar{V}|$. We have $V_0 - V_c = -\bar{V}/2$, and hence

$$\Delta_1 = \Delta_2 = \frac{1}{1 + \lambda} \frac{\bar{V}}{2} |\lambda - 1|.$$

One can check that $\lambda \approx 1 + \bar{V}/3$ and hence, $\Delta_1 + \Delta_2 \approx \frac{\bar{V}^2}{6} \approx O(h^2)$.

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