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On uniform decay of the entropy for reaction-diffusion systems

Dedicated to the memory of Klaus Kirchgässner

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Abstract

In this work we derive entropy decay estimates for a class of nonlinear reaction-diffusion systems modeling reversible chemical reactions under the assumption of detailed balance. In particular, we provide explicit bounds for the exponential decay of the relative logarithmic entropy, being based essentially on the application of the log-Sobolev inequality and a convexification argument only, making it quite robust to model variations. An important feature of our analysis is the interaction of the two different dissipative mechanisms: pure diffusion, forcing the system asymptotically to the homogeneous state, and pure reaction, forcing the solution to the (possibly inhomogeneous) chemical equilibrium. Only the interaction of both mechanisms provides the convergence to the homogeneous equilibrium. Moreover, we introduce two generalizations of the main result: we allow for vanishing diffusion constants in some chemical components, and we consider different entropy functionals. We provide a few examples to highlight the usability of our approach and shortly discuss possible further applications and open questions.

1 Introduction

Reaction and diffusion processes are the driving forces of many physical, chemical and biological phenomena. In diffusion, a random particle motion is microscopically described by a Brownian stochastic process, and on the other hand, reactions represent instantaneous interactions between particles. Typical examples where both mechanisms take place simultaneously are chemical kinetics, charge carrier transport in semiconductors, flame propagation and combustion, population dynamics, or movement of biological cells in plants and animals. These systems are described by the vector of concentrations $\boldsymbol{c}(t,x) \in [0,\infty[^I$, where $I \in \mathbb{N}$ is the number of components (chemicals, species etc.), $x \in \Omega$ denotes the position variable, and $t \geq 0$ is time. In most parts of this work, the domain $\Omega \subset \mathbb{R}^N$ is assumed to be bounded with Lipschitz boundary and, without loss of generality, we normalize its volume to 1, i.e. $|\Omega| = \int_\Omega 1 \,\mathrm{d}x = 1$. Later, in Section 5.1, we consider a more general case allowing also for unbounded Ω. Then, the reaction-diffusion process is modeled by the semilinear parabolic PDE system

$$\frac{\partial}{\partial t}\boldsymbol{c} = \mathrm{div}\,\big(\mathbb{D}\nabla \boldsymbol{c}\big) - \boldsymbol{R}(\boldsymbol{c}) \quad \text{in } \Omega, \qquad (\nabla \boldsymbol{c})\nu = 0 \quad \text{on } \partial\Omega, \tag{1.1}$$

where we assumed vanishing flow of $\boldsymbol{c}$ through the boundary $\partial\Omega$. The diffusion matrix is diagonal $\mathbb{D}(x) = \mathrm{diag}(\delta_i(x))_{i=1,..,I}$ and positive definite. The species $X_1,\dots,X_I$ are reacting according to the mass-action law,

$$\alpha_1^r X_1 + \cdots + \alpha_I^r X_I \underset{k_\mathrm{b}^r}{\overset{k_\mathrm{f}^r}{\rightleftharpoons}} \beta_1^r X_1 + \cdots + \beta_I^r X_I, \tag{1.2}$$

for $r = 1, \ldots, R$, where $R \in \mathbb{N}$ is the number of reactions, $\boldsymbol{\alpha}^r = (\alpha_1^r, \ldots, \alpha_I^r) \in \mathbb{R}^I$ and $\boldsymbol{\beta}^r = (\beta_1^r, \ldots, \beta_I^r) \in \mathbb{R}^I$ are the vectors of nonnegative stoichiometric coefficients, and $k_\mathrm{b}^r > 0$ and $k_\mathrm{f}^r > 0$ are the forward and backward reaction rate coefficients. The analysis in this paper uses $k_\mathrm{b}^r = k_\mathrm{f}^r = k^r(\boldsymbol{c})$ for $r = 1, \ldots, R$, that is we assume that the *condition of detailed balance* holds for the normalized density vector $\boldsymbol{w}^{\mathrm{eq}} = (1, \ldots, 1)$, see e.g. [Grö92, GGH96, GlH97, Mie13]. We refer to Section 2 for more details on the modeling and to Section 5.1 for the situation where $\boldsymbol{w}^{\mathrm{eq}}$ may depend on $x \in \Omega$. Then, the reaction term in (1.1) takes the form

$$\boldsymbol{R}(\boldsymbol{c}) = \sum_{r=1}^{R} k_r(\boldsymbol{c}) \left(\boldsymbol{c}^{\boldsymbol{\alpha}^r} - \boldsymbol{c}^{\boldsymbol{\beta}^r} \right) (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \quad \text{with } \boldsymbol{c}^{\boldsymbol{\alpha}^r} = \prod_{i=1}^{I} c_i^{\alpha_i^r}. \tag{1.3}$$

Typically, the stoichiometric vectors $\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r$, $r = 1, \ldots, R$, do not span the full space $\mathbb{R}^I$. If $m = \operatorname{codim}(\operatorname{span}\{\, \boldsymbol{\alpha}^r - \boldsymbol{\beta}^r \mid r = 1, \ldots, R\}) > 0$ we can choose a matrix $\mathbb{Q} \in \mathbb{R}^{I \times m}$ of rank m such that $\mathbb{Q}\boldsymbol{R}(\boldsymbol{c}) \equiv 0$. Defining

$$\mathcal{Q}(\boldsymbol{c}) := \int_\Omega \mathbb{Q}\boldsymbol{c}(x)\,\mathrm{d}x, \tag{1.4}$$

we see that all solutions of (1.1) conserve $\mathcal{Q}$, i.e. $\mathcal{Q}(\boldsymbol{c}(t)) = \mathcal{Q}(\boldsymbol{c}(0))$ for all $t > 0$.

Reaction-diffusion systems are nowadays considered a classical topic, going back at least to the works of Fisher [Fis37] and Kolmogorov et al. [KGP37]. The mathematical literature on reaction-diffusion equations is vast, including several classical textbooks such as [Smo83, Rot84, Mur03]. One of the key mathematical issues is the question of stability of linear and nonlinear reaction-diffusion systems. In particular, in 1952 A. M. Turing [Tur52] first pointed out the diffusion-induced instability of stable homogeneous reaction systems in chemistry. In general, the classical mathematical analysis of the long-time asymptotic behavior involves linearized stability techniques, spectral theory, perturbation and invariant regions arguments, or Liapunov stability (see e.g. [CHS78, FHM97]). In this paper we are interested in the so-called entropy approach to study the long-time asymptotics of (1.1). This approach is per se a nonlinear method, avoiding any kind of linearization and capable of providing explicitly computable convergence rates. The condition of *detailed balance* introduced above in fact excludes the Turing instability and is crucial for our analysis.

The particular aim of our paper is to provide explicit bounds for the exponential decay of the relative entropy $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}})$ given as follows. Using the logarithmic entropy function $F_1(z) = z\log z - z + 1$, we set

$$\mathbb{F}(\boldsymbol{a}) = \sum_{i=1}^{I} F_1(a_i) \quad \text{and} \quad \mathbb{H}(\boldsymbol{a}|\boldsymbol{w}) = \sum_{i=1}^{I} w_i F_1(a_i/w_i).$$

For concentration fields $\boldsymbol{c} : \Omega \to [0, \infty[^I$ we then define the functionals

$$\mathcal{F}(\boldsymbol{c}) := \int_\Omega \mathbb{F}(\boldsymbol{c}(x))\,\mathrm{d}x \quad \text{and} \quad \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}) := \int_\Omega \mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}_{\boldsymbol{q}})\,\mathrm{d}x,$$

where $\boldsymbol{w}_{\boldsymbol{q}}$ is the unique constant equilibrium state, corresponding to the vector of conserved quantities $\boldsymbol{q}$, viz. $\mathbb{Q}\boldsymbol{w}_{\boldsymbol{q}} = \boldsymbol{q}$ and $\boldsymbol{R}(\boldsymbol{w}_{\boldsymbol{q}}) = 0$. For all $\boldsymbol{c}$ with $\mathcal{Q}(\boldsymbol{c}) = \boldsymbol{q}$ one then has $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}) = \mathcal{F}(\boldsymbol{c}) - \mathcal{F}(\boldsymbol{w}_{\boldsymbol{q}})$, see Lemma 2.3.

The methods developed originally in [Grö83, Grö92, GGH96] and further refined in [GlH97, Gli04] show that under quite general conditions there exists a $\lambda(\boldsymbol{q}) > 0$, depending *only* on the conserved quantities $\boldsymbol{q}$, such that

$$\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}}) \leq \mathrm{e}^{-\lambda(\boldsymbol{q})t}\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_{\boldsymbol{q}}) \qquad \text{for all } t > 0. \tag{1.5}$$

This entropy estimate can be turned to a standard L^1-norm estimate by the Csiszár-Kullback inequality to obtain

$$\|\boldsymbol{c}(t) - \boldsymbol{w}_{\boldsymbol{q}}\|^2_{\mathrm{L}^1(\Omega;\mathbb{R}^I)} \leq C\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}}) \leq C\mathrm{e}^{-\lambda(\boldsymbol{q})t}\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_{\boldsymbol{q}}) \qquad \text{for all } t > 0,$$

The literature on these inequalities is huge, e.g. we refer to [UA*00], where the classical Csiszár-Kullback inequalities are generalized to not necessarily normalized and possibly non-positive L^1-functions. Also, it is shown there that these new inequalities are in many important cases significantly sharper than the classical ones.

In this paper, however, we will concentrate exclusively on studying the decay of $\mathcal{H}(\,\cdot\,|\boldsymbol{w}_{\boldsymbol{q}})$. The decay rate $\lambda(\boldsymbol{q})$ is obtained via the energy-dissipation relation

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\boldsymbol{c}(t)) = \mathcal{D}(\boldsymbol{c}(t)) := \int_\Omega \sum_{i=1}^I \delta_i \frac{|\nabla c_i|^2}{c_i} + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x, \tag{1.6}$$

with $\mathbb{G}(\boldsymbol{c}) := \sum_{i=1}^I R_i(\boldsymbol{c})\log c_i$, where $R_i(\boldsymbol{c})$ denotes the i-th component of the reaction term $\boldsymbol{R}(c)$. An important consequence of the detailed-balance condition is that the reactive dissipation $\mathbb{G}$ has the form

$$\mathbb{G}(\boldsymbol{c}) := \sum_{r=1}^R k_r(\boldsymbol{c})\Gamma\big(\boldsymbol{c}^{\boldsymbol{\alpha}^r}, \boldsymbol{c}^{\boldsymbol{\beta}^r}\big) \geq 0, \quad \text{where } \Gamma(a,b) = (a-b)(\log a - \log b) \geq 0. \tag{1.7}$$

Here we used the fundamental fact that the mass-action law, involving the monomials $\boldsymbol{c}^{\boldsymbol{\gamma}}$, and the Boltzmann statistics, leading to the logarithmic entropy, are intrinsically linked by the classical logarithm rule $\sum_{i=1}^I \gamma_i \log c_i = \log\big(\boldsymbol{c}^{\boldsymbol{\gamma}}\big)$.

Now we can define the optimal decay rate via

$$\lambda(\boldsymbol{q}) := \inf \frac{\mathcal{D}(\boldsymbol{c})}{\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}})}, \tag{1.8}$$

where the infimum is taken over all sufficiently smooth concentration fields $\boldsymbol{c} : \Omega \to \,]0,\infty[^I$ satisfying the constraint $\mathcal{Q}(\boldsymbol{c}) = \boldsymbol{q}$ and $\boldsymbol{c} \not\equiv \boldsymbol{w}_{\boldsymbol{q}}$. Explicit bounds for special reaction systems were given in [DeF06, DeF07, DeF08], however, their bounds need further specifications for the initial conditions. General reactions systems were considered in [Grö92, GGH96, GlH97], the latter also including electrostatic interactions. Because of the coupling to the electrostatic interaction, their analysis is restricted to two-dimensional domains Ω, but it is clear that without this coupling the result of [GlH97, Thm. 5.2] or [Gli04, Thm. 4.16] transfers to our general setting. Their contradiction and compactness arguments show that $\lambda(\boldsymbol{q}) > 0$ for each $\boldsymbol{q}$.

In this work we start from the characterization of $\lambda(\boldsymbol{q})$ in (1.8) and use the log-Sobolev estimate to derive explicit lower bounds for $\lambda(\boldsymbol{q})$ in terms of the latter and the decay rate in the pure reaction system. As such, our approach is inspired by the recently developed gradient flow structure for general reaction-diffusion systems satisfying the condition of detailed balance, which shows that (1.1) has the form

$$\dot{\boldsymbol{c}} = -\mathcal{K}(\boldsymbol{c})\mathrm{D}\mathcal{F}(\boldsymbol{c}) = -\Big(\mathcal{K}_\mathrm{D}(\boldsymbol{c})+\mathcal{K}_\mathrm{R}(\boldsymbol{c})\Big)\mathrm{D}\mathcal{F}(\boldsymbol{c}),$$

see e.g. [Mie11, GlM12, Mie13, LiM12]. The importance of the result is the interaction of the two different dissipative mechanisms:

pure diffusion forcing the solution to converge to the homogeneous state $\int_\Omega \boldsymbol{c}(0,x)\,\mathrm{d}x$ with rate $\lambda_\mathbb{D}$ given in terms of the log-Sobolev inequality; and

pure reaction forcing the solution at each point $x\in\Omega$ to converge to the x-dependent equilibrium $\boldsymbol{w}_{\boldsymbol{q}(x)}$ where $\boldsymbol{q}(x)=\mathbb{Q}\boldsymbol{c}(0,x)$ with the rate $\lambda_{\boldsymbol{R}}(\boldsymbol{q}(x))$.

Only the interaction of both mechanisms provide the convergence to the homogeneous equilibrium $\boldsymbol{w}_{\boldsymbol{q}}$ with $\boldsymbol{q}=\mathcal{Q}(\boldsymbol{c}(0))$.

The main result of our paper, obtained in Section 3, provides lower bounds on $\lambda(\boldsymbol{q})$, essentially in terms of the rates $\lambda_\mathbb{D}$ and $\lambda_{\boldsymbol{R}}(\boldsymbol{q})$. Our analysis is essentially based on the application of the log-Sobolev inequality and a convexification argument only, making it quite robust to model variations. One main result (cf. Corollary 3.2) reads as follows. Define the log-Sobolev constants r_i as optimal constants in

$$\int_\Omega \delta_i(x)\frac{|\nabla u|^2}{u}\,\mathrm{d}x \geq r_i\overline{u}\int_\Omega F_1\Big(\frac{u(x)}{\overline{u}}\Big)\,\mathrm{d}x \quad \text{where } \overline{u}=\int_\Omega u\,\mathrm{d}x,$$

and set $\lambda_\mathbb{D}:=\min\{\, r_i \mid i=1,\dots,I\,\}$. If for some $\mu_*\geq 0$ the function

$$\Phi_{\mu_*} : [0,\infty[^I \to \mathbb{R};\quad \Phi_{\mu_*}(\boldsymbol{a}) = \mu_*\mathbb{F}(\boldsymbol{a})+\mathbb{G}(\boldsymbol{a})$$

is convex, then we have the explicit lower bound

$$\lambda(\boldsymbol{q}) \geq \min\Big\{\lambda_{\boldsymbol{R}}(\boldsymbol{q})\,,\ \lambda_\mathbb{D}\,\frac{\lambda_{\boldsymbol{R}}(\boldsymbol{q})}{\mu_*+\lambda_{\boldsymbol{R}}(\boldsymbol{q})}\Big\}. \tag{1.9}$$

The assumption that $\mathbb{G}$ is convex privides the lower bound $\lambda(\boldsymbol{q})\geq\min\{\lambda_{\boldsymbol{R}}(\boldsymbol{q}),\lambda_\mathbb{D}\}$.

In Section 3.5 we introduce generalizations of the main result for vanishing diffusion constants in some components or for other entropy functionals. In Section 4 we discuss a few examples to highlight the usability of the approach. The main application involves the system

$$\dot{u} = \mathrm{div}\,\big(\delta_1\nabla u\big)+k(v^2-u), \qquad \dot{v} = \mathrm{div}\,\big(\delta_2\nabla v\big)+2k(u-v^2), \tag{1.10}$$

for which we derive the explicit q-independent lower bound $\lambda(q)\geq\frac{1}{5}\min\{r_1,5r_2,2k\}$. Moreover, Theorem 4.5 covers the case $\delta_2=0$ and provides the q-dependent lower bound $\lambda(q)\geq\frac{1}{100}\min\{r_1,2k\}\min\{10q,7\}$. Such systems with a degenerate diffusion tensor $\mathbb{D}$ were also considered in [Gli04, DeF08].

The final Section 5 discusses possible further applications and addresses open questions as well. In particular, we show that under certain assumptions it is possible to generalize our theory to the case that the thermodynamic equilibrium density $\boldsymbol{w}^{\mathrm{eq}}$, which is $(1, ..., 1)$ in the above case, also depends on $x \in \Omega$. This allows also to deal with cases where Ω has infinite measure but $\int_\Omega \boldsymbol{w}^{\mathrm{eq}}(x)\,\mathrm{d}x$ is finite.

For a relatively recent survey on global existence theory for reaction-diffusion systems, we refer to [Pie10]. Our work is independent of the existence theory, however, let us mention that the reaction-diffusion system (1.1) is perfectly compatible with the condition (P), requiring quasi-positivity of the nonlinearity $\boldsymbol{R}(\boldsymbol{c})$, and the "mass-control structure" condition (M) of [Pie10]. This implies the global existence of (possibly nonunique) weak solutions. All the estimates in our paper hold for these weak solutions.

There is a vast literature on the connection of the long time behavior of convection-diffusion equations and the log-Sobolev inequalities. Here we refer to [AM*01] (and the references therein) for the linear case. The trend to equilibrium for the classical Fokker-Planck equation has been also studied in [MaV00]. Poincaré inequalities for linearizations of very fast diffusion equations have been developed in [CL*02]. For applications of the entropy-entropy dissipation approach to nonlinear convection-diffusion equations, we refer to [MaL01], where certain fast diffusion equations with uniformly convex confinement potential and finite-mass but infinite-entropy equilibrium solutions are treated, or to [CJ*01] for the case of quasilinear (possibly) degenerate parabolic systems in three cases: scalar problems with confinement by a uniformly convex potential, unconfined scalar equations, and unconfined systems. The considered class of problems includes porous media, fast diffusion, p-Laplacian and energy transport systems. We hope that our approach can be extended to vector-valued generalizations of these models.

Finite-volume discretizations (using Voronoi cells) of energy-reaction-diffusion systems coupled to coupled to the Poisson equation have been considered in [Gli08, Gli11], and monotone and exponential decay of the discrete free energy to its equilibrium value has been shown. The fundamental idea here is to estimate the free energy by the dissipation rate indirectly by taking into account sequences of Voronoi meshes. Essential ingredient is a discrete Sobolev-Poincaré inequality, which allows to obtain an exponential decay rate independent of the mesh size.

In [DFFM08], the entropy approach is developed for general linear systems of reaction-diffusion equations, and a nonlinear example of reaction-diffusion-convection system arising in semiconductor or plasma physics as a paradigm for general nonlinear systems. The large time behavior of the drift-diffusion-Poisson system (without recombination-generation terms) as a model for charge transport in bi-polar semiconductor devices has been studied in [AMT00]. The same system with nonlinear recombination-generation terms has been treated in [WMZ08]. In [DiW08], asymptotic stability for the spatially one-dimensional setting of the nonlinear system is approached with the methods of optimal transport (convergence in the Wasserstein topology). See also [MRS86], [MaR87] or the surveys [Mar86], [MRS90] on mathematical modeling of semiconductor devices.

Construction of entropies and entropy productions for a large class of nonlinear evolutionary PDEs of even order in one space dimension is presented in [JüM06], where the task of proving entropy dissipation is reformulated as a decision problem for polynomial systems. The method is successfully applied to the porous-medium equation, the thin film equation and the quantum drift-diffusion model.

2 Set-up of the model

We consider the reaction-diffusion system (1.1) and discuss first the reaction part alone, where we especially emphasize the set of equilibria. Then, we characterize the equilibria of the full reaction-diffusion system (1.1).

2.1 The reaction rate equations and its equilibria

We first discuss the structure of general reaction-rate equations

$$\dot{\boldsymbol{c}} = -\boldsymbol{R}(\boldsymbol{c}), \tag{2.1}$$

which is an ordinary differential equation for $\boldsymbol{c}(t) \in [0,\infty[^I$. Here the reaction kinetics in $\boldsymbol{R}$ is given by the reactions (1.2) according to the mass-action law. Arranging the stoichiometric coefficients in (1.3), $\boldsymbol{\alpha}^r = (\alpha_1^r, \dots, \alpha_I^r) \in [0,\infty[^I$ and $\boldsymbol{\beta}^r = (\beta_1^r, \dots, \beta_I^r) \in [0,\infty[^I$, as column vectors and defining the stoichiometric matrix (called Wegscheider matrix in [GIM12] because of its origin in [Weg02])

$$W = \Big((\boldsymbol{\beta}^r - \boldsymbol{\alpha}^r)_{r=1,\dots,R} \Big)^{\mathsf{T}} \in \mathbb{R}^{R\times I},$$

we can write $\boldsymbol{R}$ in (2.1) in the form of the matrix-vector product

$$\boldsymbol{R}(\boldsymbol{c}) = -W^{\mathsf{T}} \boldsymbol{K}(\boldsymbol{c}), \tag{2.2}$$

where $\boldsymbol{K}(\boldsymbol{c}) \in \mathbb{R}^R$ is the column vector with components

$$K_r(\boldsymbol{c}) = k_{\mathrm{f}}^r(\boldsymbol{c})\boldsymbol{c}^{\boldsymbol{\alpha}^r} - k_{\mathrm{b}}^r(\boldsymbol{c})\boldsymbol{c}^{\boldsymbol{\beta}^r}, \qquad \text{where } \boldsymbol{c}^{\boldsymbol{\alpha}^r} = \prod_{i=1}^{I} c_i^{\alpha_i^r},$$

and $k_{\mathrm{f}}^r \geq 0$ and $k_{\mathrm{b}}^r \geq 0$ are the forward and backward intensities of the rth reaction. In general, these coefficients may depend on the concentrations itself.

We call range$(W^{\mathsf{T}}) \subset \mathbb{R}^I$ the *stoichiometric subspace*, and due to (2.2) we have $\boldsymbol{R}(\boldsymbol{c}) \in$ range(W^{T}). Its orthogonal complement, ker$(W) \subset \mathbb{R}^I$, determines the conserved quantities as follows: For $m = \dim \ker(W)$, choose any matrix $\mathbb{Q} \in \mathbb{R}^{I\times m}$ such that rank $\mathbb{Q} = m$ and $\mathbb{Q}W^{\mathsf{T}} = 0$, i.e., the rows of $\mathbb{Q}$ form a basis of ker(W). Since $\boldsymbol{R}(\boldsymbol{c}) \in$ range(W^{T}), we have

$$\mathbb{Q}\boldsymbol{R}(\boldsymbol{c}) = \boldsymbol{0} \qquad \text{for all } \boldsymbol{c} \in \mathbb{R}^I, \tag{2.3}$$

which implies that all solutions $\boldsymbol{c} : [0,T] \to [0,\infty[^I$ of the reaction-rate equation (2.1) satisfy the conservation rule $\mathbb{Q}\boldsymbol{c}(t) = \mathbb{Q}\boldsymbol{c}(0)$ for all $t \geq 0$.

Following [Grö83, GGH96, GIM12] we now additionally impose the crucial structural assumption that the reaction system given by $\boldsymbol{\alpha}^r,\ \boldsymbol{\beta}^r,\ k_{\mathrm{f}}^r,\ k_{\mathrm{b}}^r$ satisfies the *condition of detailed balance*, which means that there exists a strictly positive equilibrium concentration $\boldsymbol{w}^{\mathrm{eq}} \in\,]0,\infty[^I$ such that all R reactions are in equilibrium similtaneously, i.e.,

condition of detailed balance:

$$\exists\, \boldsymbol{w}^{\mathrm{eq}} \in\,]0,\infty[^I\ \forall\, \boldsymbol{c} \in [0,\infty[^I\ \forall\, r=1,...,R:\ k_{\mathrm{f}}^r(\boldsymbol{c})\boldsymbol{w}_{\mathrm{eq}}^{\boldsymbol{\alpha}^r} = k_{\mathrm{b}}^r(\boldsymbol{c})\boldsymbol{w}_{\mathrm{eq}}^{\boldsymbol{\beta}^r} =: k_r(\boldsymbol{c}). \tag{2.4}$$

In fact, by considering the relative densities $c_i/w_i^{\rm eq}$, we can assume $\boldsymbol{w}^{\rm eq} = (1,...,1)^\mathsf{T} \in \mathbb{R}^I$ without loss of generality and obtain the simplification $k_{\rm f}^r = k_{\rm b}^r =: k^r$ assumed in the introduction and used in the sequel.

The crucial observation of [Mie11] (see also [Mie13, GIM12]) is that (2.1) can be written as a gradient system, namely

$$\dot{\boldsymbol{c}} = -\boldsymbol{R}(\boldsymbol{c}) = -\mathcal{K}_{\rm R}(\boldsymbol{c})\mathrm{D}\mathbb{F}(\boldsymbol{c}), \quad \text{where } \mathbb{F}(\boldsymbol{c}) = \mathbb{H}(\boldsymbol{c}|(1,...,1))$$

and the Onsager matrix $\mathcal{K}_{\rm R}(\boldsymbol{c}) = \mathcal{K}_{\rm R}(\boldsymbol{c})^\mathsf{T} \geq 0$ is given by

$$\mathcal{K}_{\rm R}(\boldsymbol{c}) := \sum_{r=1}^{R} k_r(\boldsymbol{c})\Lambda(\boldsymbol{c}^{\boldsymbol{\alpha}^r}, \boldsymbol{c}^{\boldsymbol{\beta}^r})\big(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r\big)\otimes\big(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r\big) \quad \text{with } \Lambda(a,b) = \frac{a - b}{\log a - \log b}.$$

The following proposition gives the characterization of the relevant steady states of the reaction-rate equation (2.1). The proof is an elementary application of the Lagrange multiplier theorem for minimization under constraints. We first introduce some notation. By

$$\mathrm{im}^+\mathbb{Q} := \{\, \mathbb{Q}\boldsymbol{c} \in \mathbb{R}^m \mid \boldsymbol{c} \in [0,\infty[^I,\ \boldsymbol{c} \neq \boldsymbol{0}\,\} \tag{2.5}$$

we denote the set of all possible conservation vectors $\boldsymbol{q}$. For $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$ the set

$$\mathfrak{C}_{\boldsymbol{q}} := \{\, \boldsymbol{a} \in [0,\infty[^I \mid \mathbb{Q}\boldsymbol{a} = \boldsymbol{q}\,\} \subset \mathbb{R}^I$$

contains all the possible concentration vectors for the given $\boldsymbol{q}$. Moreover, throughout the paper we will use the following notational convention: For a function function $f : \mathbb{R} \to \mathbb{R}$ we define a mapping $\boldsymbol{f} : \mathbb{R}^I \to \mathbb{R}^I$ by applying the function componentwise, viz.

$$\boldsymbol{f}(\boldsymbol{c}) := (f(c_1), \ldots, f(c_I)) \quad \text{and} \quad \frac{\boldsymbol{c}}{\boldsymbol{w}} := \big(\frac{c_i}{w_i}\big)_{i=1,..,I}. \tag{2.6}$$

Proposition 2.1 (Steady states for (2.1)**)** *Assume that $\boldsymbol{R}$ and $\mathbb{Q}$ are given as above, including the detailed balance condition* (2.4)*. Then, for each $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$ there is a unique solution $\boldsymbol{w} = \boldsymbol{w}_{\boldsymbol{q}}$ of $\boldsymbol{R}(\boldsymbol{w}) = 0$ in the set $\mathfrak{C}_{\boldsymbol{q}} \cap\,]0,\infty[^I$. This steady state $\boldsymbol{w}_{\boldsymbol{q}}$ is characterized as the unique global minimizer of $\mathbb{F}$ subject to the constraint $\boldsymbol{c} \in \mathfrak{C}_{\boldsymbol{q}}$. In particular,*

$$\mathbb{Q}\boldsymbol{w}_{\boldsymbol{q}} = \boldsymbol{q}, \qquad \forall\, \boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}} :\ \mathbb{F}(\boldsymbol{a}) \geq \mathbb{F}(\boldsymbol{w}_{\boldsymbol{q}}), \qquad \exists\, \lambda \in \mathbb{R}^m :\ \boldsymbol{\log}\, \boldsymbol{w}_{\boldsymbol{q}} = \mathbb{Q}^\mathsf{T}\lambda. \tag{2.7}$$

Proof: For $\boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}} \cap\,]0,\infty[^I$ the logarithm $\boldsymbol{\log}\,\boldsymbol{a} = \mathrm{D}\mathbb{F}(\boldsymbol{a})$ is well-defined and we have $\boldsymbol{R}(\boldsymbol{a}) = \mathcal{K}_{\rm R}(\boldsymbol{a})\mathrm{D}\mathbb{F}(\boldsymbol{a}) \subset \mathrm{range}(W^\mathsf{T})$. Since $\mathcal{K}_{\rm R}(\boldsymbol{a})$ is invertible on $\mathrm{range}(W^\mathsf{T})$, the relations $\mathbb{Q}\boldsymbol{w} = \boldsymbol{q}$ and $\boldsymbol{R}(\boldsymbol{w}) = 0$ imply $\boldsymbol{\log}\,\boldsymbol{a} = \mathrm{D}\mathbb{F}(\boldsymbol{a}) = \mathbb{Q}^\mathsf{T}\lambda$ for some $\lambda \in \mathbb{R}^m$.

The Lagrange multiplier rule shows that all such points are critical points of the functional $\mathbb{F}$ under the constraint $\mathbb{Q}\boldsymbol{a} = \boldsymbol{q}$. However, since $\mathbb{F}$ is strictly convex, there is only one critical point, namely the global minimizer. ∎

We emphasize that there may be additional steady states on the boundary of $[0,\infty[^I$, such that $\boldsymbol{w_q}$ is *not* the unique steady state in $\mathfrak{C}_{\boldsymbol{q}}$, but only in the interior of $\mathfrak{C}_{\boldsymbol{q}}$. For instance, consider

$$\dot{u} = 2(uv^2 - u^3), \qquad \dot{v} = 2(u^3 - uv^2).$$

We have $\mathbb{Q}(u,v) = u + v = q$ as conserved quantity and find for $q > 0$ the two steady states $\boldsymbol{w_q} = (q/2, q/2)$ and $\overline{\boldsymbol{w_q}} = (0, q)$. In such cases the discussion in [GGH96, Sect. 4] can be used.

Our theory will only be useful in the case that such boundary equilibria do not exist. However, we do not need to exclude such equilibria explicitly. If they occur, we are simply lead to the conclusion that $\lambda_{\mathrm{R}}(\boldsymbol{q}) = 0$ as $\mathbb{G}(\boldsymbol{w}) = 0$ for some $\boldsymbol{w} \in \mathfrak{C}_{\boldsymbol{q}}$. Then, our method does not provide any exponential decay.

2.2 The reaction-diffusion system and its steady states

We consider the reaction-diffusion system (1.1) in a bounded domain $\Omega \subset \mathbb{R}^N$ with Lipschitz boundary. We prescribe homogeneous Neumann boundary datum for $\boldsymbol{c}$. The reaction term $\boldsymbol{R}$ is as in the previous section, and the diffusion matrix $\mathbb{D}$ in (1.1) is diagonal with diagonal elements $\delta_i(x) \geq 0$, $i = 1, \ldots, I$. Recalling $|\Omega| = \int_\Omega 1 \, \mathrm{d}x = 1$ and

$$\mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} \qquad \text{with } \overline{\boldsymbol{c}} = \int_\Omega \boldsymbol{c}(x) \, \mathrm{d}x,$$

the no-flux boundary condition for $\boldsymbol{c}$ on $\partial\Omega$ yields the conservation rule

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}(\boldsymbol{c}(t)) = \mathbb{Q}\mathbb{D}\int_{\partial\Omega} (\nabla \boldsymbol{c})\nu \, \mathrm{d}S - \int_\Omega \mathbb{Q}\boldsymbol{R}(\boldsymbol{c}) \, \mathrm{d}x = 0.$$

Hence, even without assuming the detailed balance condition, all (weak) solutions of (1.1) satisfy $\mathcal{Q}(\boldsymbol{c}(t)) = \mathbb{Q}\overline{\boldsymbol{c}}(t) = \mathcal{Q}(\boldsymbol{c}(0))$ for all $t > 0$.

We now impose the condition of detailed balance (2.4) where the reaction intensities k_r may depend on $x \in \Omega$ and $\boldsymbol{c}$, but it will be crucial that

$$\text{the equilibrium concentration } \boldsymbol{w}^{\mathrm{eq}} \text{ does not depend on } x \in \Omega. \tag{2.8}$$

The problems arising for x-dependent $\boldsymbol{w}^{\mathrm{eq}}$ are discussed in Section 5.1. For our theory we could allow for intensities k_r depending on $(x, \boldsymbol{c})$ as long as $\underline{k}_r(\boldsymbol{c}) := \inf\{\, k_r(x, \boldsymbol{c}) \mid x \in \Omega \,\}$ is positive for all $\boldsymbol{c}$. Since all the following estimates are monotone in each k_r, we can replace $k_r(x, \boldsymbol{c})$ by $\underline{k}_r(\boldsymbol{c})$. Hence, without loss of generality, we will assume that k_r is independent of x.

For $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$ we define the set of the corresponding concentration fields as

$$\mathcal{C}_{\boldsymbol{q}} := \{\, \boldsymbol{c} \in \mathrm{L}^1(\Omega; \mathbb{R}^I) \mid \boldsymbol{c} \geq 0, \ \mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} = \boldsymbol{q} \,\} \subset \mathrm{L}^1(\Omega; \mathbb{R}^I)$$

and show that the equilibria $\boldsymbol{w_q}$ for the reaction-rate equation (2.1) found in Proposition 2.1 represent the equilibrium states for the reaction-diffusion system (1.1).

Proposition 2.2 (Steady states for (1.1)**)** *All steady states $\boldsymbol{w}$ of* (1.1) *are spatially constant and satisfy $\boldsymbol{R}(\boldsymbol{w})=0$. In particular, if $\boldsymbol{w_q}$ is the only steady state of the reaction-rate equation* (2.1) *in $\mathfrak{C}_{\boldsymbol{q}}$ (i.e. with $\mathbb{Q}\boldsymbol{w_q}=\boldsymbol{q}$), then also the reaction-diffusion system* (1.1) *has only the steady state $\boldsymbol{c}\equiv\boldsymbol{w_q}$ in the set $\mathcal{C}_{\boldsymbol{q}}$.*

Moreover, for all conservation vectors $\boldsymbol{q}\in\mathrm{im}^{+}\mathbb{Q}$ the constant state $\boldsymbol{w_q}$ is the unique global minimizer of $\mathcal{F}$ on $\mathcal{C}_{\boldsymbol{q}}$ (i.e. subject to the constraint $\mathcal{Q}(\boldsymbol{c})=\boldsymbol{q}$). Moreover, $\boldsymbol{w_q}$ is the global minimizer of $\mathcal{H}(\,\cdot\,|\boldsymbol{w_q})$ for all $\boldsymbol{c}:\Omega\to[0,\infty[^I$.

Proof: By the gradient structure of the reaction-diffusion system (1.1) a concentration field $\boldsymbol{w}$ is a steady state if and only if the dissipation vanishes, viz. $\mathcal{D}(\boldsymbol{w})=0$, where $\mathcal{D}$ is defined in (1.6). Using $\mathbb{G}(\boldsymbol{w})\geq 0$ from (1.7) we see that $\mathcal{D}$ is the sum of two nonnegative terms, which both have to vanish. This immediately implies that the steady state $\boldsymbol{w}$ is a constant vector such that $\boldsymbol{R}(\boldsymbol{w})=0$, which proves the first part of the proposition. Due to the conservation $\boldsymbol{q}=\mathcal{Q}(\boldsymbol{c}(0)=\mathbb{Q}\overline{\boldsymbol{c}}(0)$, we have $\boldsymbol{w}=\boldsymbol{w_q}$.

When minimizing $\mathcal{F}$ on $\mathcal{C}_{\boldsymbol{q}}$, the strict convexity gives a unique global minimizer. Since the integral functionals $\mathcal{F}$ and $\mathcal{Q}$ are defined via x-independent integrands, the minimizer must be constant. Thus, it coincides with the minimizer of $\mathbb{F}$ on $\mathfrak{C}_{\boldsymbol{q}}$, which proves the second assertion by employing Proposition 2.1.

The last statement follows because $\boldsymbol{c}\mapsto\mathbb{H}(\boldsymbol{c}|\boldsymbol{w_q})\geq 0$ has the unique global minimizer $\boldsymbol{c}=\boldsymbol{w_q}$. By the definition $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q})=\int_\Omega\mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w_q})\,\mathrm{d}x$, we conclude that the global minimizer of $\mathcal{H}(\,\cdot\,|\boldsymbol{w_q})$ is $\boldsymbol{c}=\boldsymbol{w_q}$. ■

The following relations will be useful in the subsequent derivations of energy-dissipation inequalities. They reflect the special structure of the logarithmic entropy and the properties of the steady states $\boldsymbol{w_q}$.

Lemma 2.3 *For all vectors $\boldsymbol{a}$,$\boldsymbol{b}\in\mathbb{R}^I$ and all vector-valued functions $\boldsymbol{c}(x)\in\mathbb{R}^I$, the following relations hold:*

$$
\begin{aligned}
&\mathbb{H}(\boldsymbol{a}|\boldsymbol{b})=\mathbb{F}(\boldsymbol{a})-\mathbb{F}(\boldsymbol{b})+(\boldsymbol{b}-\boldsymbol{a})\cdot\log\boldsymbol{b}, && \text{(2.9a)}\\
&\mathbb{Q}\boldsymbol{a}=\boldsymbol{q}\quad\Longrightarrow\quad\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})=\mathbb{F}(\boldsymbol{a})-\mathbb{F}(\boldsymbol{w_q}), && \text{(2.9b)}\\
&\mathcal{Q}(\boldsymbol{c})=\boldsymbol{q}\quad\Longrightarrow\quad\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q})=\mathcal{F}(\boldsymbol{c})-\mathbb{F}(\boldsymbol{w_q}), && \text{(2.9c)}\\
&\mathcal{H}(\boldsymbol{c}|\overline{\boldsymbol{c}})=\mathcal{F}(\boldsymbol{c})-\mathbb{F}(\overline{\boldsymbol{c}}). && \text{(2.9d)}
\end{aligned}
$$

Proof: (a) Relation (2.9a) follows from an explicit expansion.

(b) Proposition 2.1 gives $\mathbb{Q}\boldsymbol{w_q}=\boldsymbol{q}$ and $\log\boldsymbol{w_q}\in$ range $\mathbb{Q}^\mathsf{T}$. Inserting this into (2.9a) gives (2.9b).

(c) Employing (2.9a) with $\boldsymbol{a}=\boldsymbol{c}(x)$ and $\boldsymbol{b}=\boldsymbol{w_q}$ we obtain (2.9c) after integration, because $\log\boldsymbol{w_q}\in$ range $\mathbb{Q}^\mathsf{T}$ is constant and $\mathbb{Q}(\boldsymbol{w_q}-\overline{\boldsymbol{c}})=0$.

(d) Finally, (2.9d) also follows from (2.9a) with $\boldsymbol{b}=\overline{\boldsymbol{c}}$. ■

3 Entropy-dissipation estimates

Throughout this section we assume that Ω is a bounded domain in $\mathbb{R}^d$ with Lipschitz boundary $\partial\Omega$. Again we use the normalization $|\Omega| = 1$. The aim is to derive lower estimates of the dissipation $\mathcal{D}(\boldsymbol{c})$ in terms of the relative entropy $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q})$ that depend only on $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$ but not on $\boldsymbol{c} \in \mathcal{C}_{\boldsymbol{q}}$.

3.1 Entropy functionals and functional inequalities

For $\gamma \geq 0$ we consider the entropy functions

$$F_\gamma(z) = \begin{cases} \frac{1}{\gamma(\gamma-1)}\big(z^\gamma - \gamma z + \gamma - 1\big) & \text{for } \gamma \in \mathbb{R} \setminus \{0,1\}, \\ z\log z - z + 1 & \text{for } \gamma = 1, \\ z - \log z - 1 & \text{for } \gamma = 0. \end{cases} \tag{3.1}$$

Note that $F_2(z) = \frac{1}{2}(z{-}1)^2$. We see that all F_γ are convex and satisfy $F_\gamma(1) = F_\gamma'(1) = 0 \leq F_\gamma(z)$. In particular, we have $F_\gamma''(z) = z^{\gamma-2} > 0$. Moreover,

$$\forall\, z > 0 : \quad [0,\infty[\, \ni \gamma \mapsto \gamma F_\gamma(z) \text{ is increasing} \tag{3.2}$$

due to $\partial_\gamma(\gamma F_\gamma(z)) = \frac{z}{(\gamma-1)^2}F_1(z^{\gamma-1}) \geq 0$. Moreover, we have the following identities

$$F_1(uv) = vF_1(u) + uF_1(v) + (u{-}1)(v{-}1), \tag{3.3}$$

$$a^\gamma F_\gamma(u/a) = F_\gamma(u) + \frac{a^\gamma - 1}{\gamma} - u\frac{a^{\gamma-1} - 1}{\gamma - 1}. \tag{3.4}$$

Using $\overline{u} = \int_\Omega u(x)\,\mathrm{d}x$ and $|\Omega| = 1$, an integration of (3.4) gives

$$\overline{u}^\gamma\, \overline{F_\gamma\big(u/\overline{u}\big)} = \overline{F_\gamma(u)} - F_\gamma(\overline{u}). \tag{3.5}$$

Crucial for the forthcoming analysis will be the following estimate, which can be seen as a generalization of the Poincaré and Log-Sobolev inequalities:

$$\forall\, u > 0 : \quad \int_\Omega \frac{|\nabla u|^2}{u^{2-\sigma}}\,\mathrm{d}x \geq \rho(\Omega,\sigma,\gamma)\,\overline{u}^\sigma \int_\Omega F_\gamma(u/\overline{u})\,\mathrm{d}x. \tag{3.6}$$

Using the monotonicity (3.2), we have

$$0 < \gamma_1 < \gamma_2 \quad \Longrightarrow \quad \rho(\Omega,\sigma,\gamma_1) \geq \frac{\gamma_1}{\gamma_2}\rho(\Omega,\sigma,\gamma_2).$$

The case $\sigma = 2$ and $\gamma = 2$ is the *Poincaré inequality*, we then write $\rho_{\mathrm{P}} = \rho(\Omega,2,2)$. The case $\sigma =$ and $\gamma = 1$ is the *logarithmic Sobolev inequality*, we then write $\rho_{\mathrm{LSi}} = \rho(\Omega,1,1)$. Using Trudinger's inequality one can show that $\rho(\Omega,0,0) > 0$ if the dimension satisfies $d \leq 2$.

For further usage we define for $\delta \in \mathrm{L}^\infty(\Omega)$ with $\delta(x) > 0$ a.e. the Log-Sobolev constant $\rho_{\mathrm{LSi}}(\delta)$ as

$$\rho_{\mathrm{LSi}}(\delta) := \inf\left\{ \int_\Omega \delta(x)\frac{|\nabla u(x)|^2}{u(x)}\,\mathrm{d}x \;\middle|\; u > 0,\ \overline{u}\int_\Omega F_1(u/\overline{u})\,\mathrm{d}x = 1 \right\}. \tag{3.7}$$

Clearly, $\delta(x) \geq \delta_0 > 0$ implies $\rho_{\mathrm{LSi}}(\delta) \geq \delta_0\rho_{\mathrm{LSi}}(1) = \delta_0\rho(\Omega,1,1)$.

3.2 The energy-dissipation balance

For a given initial condition $\boldsymbol{c}(0)$ we expect that the solution $\boldsymbol{c}$ of (1.1) converges to the corresponding steady state, namely $\boldsymbol{w}_{\boldsymbol{q}}$ with $\boldsymbol{q} = \mathcal{Q}(\boldsymbol{c}(0)) = \mathbb{Q}\overline{\boldsymbol{c}}(0)$. From now on, we fix $\boldsymbol{w}_{\boldsymbol{q}}$ and consider only initial conditions having the conservation vector $\boldsymbol{q}$. Using (2.9c), the relative entropy $\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}})$ satisfies the energy-dissipation relation

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}}) = -\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\boldsymbol{c}(t)) = \mathcal{D}(\boldsymbol{c}) := \int_\Omega \sum_{i=1}^{I} \delta_i \frac{|\nabla c_i|^2}{c_i} + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x. \tag{3.8}$$

As a first step towards our decay estimates we consider the reaction-rate equation $\dot{\boldsymbol{a}} = -\boldsymbol{R}(\boldsymbol{a})$ and define

$$\lambda_{\boldsymbol{R}}(\boldsymbol{q}) := \inf\Big\{ \frac{\mathbb{G}(\boldsymbol{a})}{\mathbb{H}(\boldsymbol{a}|\boldsymbol{w}_{\boldsymbol{q}})} \,\Big|\, \boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}},\ \boldsymbol{a} \neq \boldsymbol{w}_{\boldsymbol{q}} \Big\}. \tag{3.9}$$

Obviously, we have the decay estimate $\mathbb{H}(\boldsymbol{a}(t)|\boldsymbol{w}_{\boldsymbol{q}}) \leq \mathrm{e}^{-\lambda_{\boldsymbol{R}}(\boldsymbol{q})t}\mathbb{H}(\boldsymbol{a}(0)|\boldsymbol{w}_{\boldsymbol{q}})$ for all $t > 0$ and all $\boldsymbol{a}(0)$. For this we simply note $-\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{H}(\boldsymbol{a}(t)|\boldsymbol{w}_{\boldsymbol{q}}) = \mathbb{G}(\boldsymbol{a}(t)) \geq \lambda_{\boldsymbol{R}}(\boldsymbol{q})\mathbb{H}(\boldsymbol{a}(t)|\boldsymbol{w}_{\boldsymbol{q}})$ and apply Gronwall's inequality.

To find a corresponding exponential decay estimate for the reaction-diffusion system (1.1) it is necessary to estimate $\mathcal{D}$ from below, namely

$$\forall\, \boldsymbol{q} = \mathrm{im}^{+}\mathbb{Q}\ \exists\, \lambda(\boldsymbol{q}) \geq 0\ \forall\, \boldsymbol{c} \in \mathcal{C}_{\boldsymbol{q}}: \quad \mathcal{D}(\boldsymbol{c}) \geq \lambda(\boldsymbol{q})\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}). \tag{3.10}$$

Combining (3.8) and (3.10) we obtain $\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{c}(t|\boldsymbol{w}_{\boldsymbol{q}})) \leq -\lambda(\boldsymbol{q})\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}})$ and conclude the desired decay estimate

$$\mathcal{Q}(\boldsymbol{c}(0)) = \boldsymbol{q} \quad \Longrightarrow \quad \mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}}) \leq \mathrm{e}^{-\lambda(\boldsymbol{q})t}\,\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_{\boldsymbol{q}}) \text{ for } t \geq 0.$$

3.3 The basic estimate

The basic strategy to obtain our decay estimate relies on the entropy estimates for the diffusive dissipation through the gradient terms $|\nabla c_i|^2/c_i$. Using the log-Sobolev estimate (3.7) we obtain

$$\int_\Omega \delta_i(x)\frac{|\nabla c_i|^2}{c_i}\,\mathrm{d}x \;\geq\; \rho_{\mathrm{LSi}}(\delta_i)\,\mathcal{H}(c_i|\overline{c}_i) \;=\; \mathcal{F}(c_i) - F_1(\overline{c}_i), \tag{3.11}$$

where the last identity follows from (2.9a). Thus, the total dissipation can be bounded from below by integrals over the functions $\mathbb{F}(\boldsymbol{c}(x))$ and $\mathbb{G}(\boldsymbol{c}(x))$ and an extra function of the average $\overline{\boldsymbol{c}}$. The idea is now to use convexity arguments on the affine subspace $\mathcal{C}_{\boldsymbol{q}}$. For this we use the convexification Φ^{**} of a function $\Phi : [0,\infty[^I \to \mathbb{R}$, which is the supremum over all affine functions lying below of Φ.

The following general result is derived for the case that all diffusion constants δ_i are positive; however, we will see later that also cases can be handled where some δ_i are 0.

Theorem 3.1 *Assume* $r := \min\{\, \rho_{\mathrm{LSi}}(\delta_i) \mid i=1,..,I\,\} > 0$ *and choose* $\mu \in \mathbb{R}$ *such that*

$$\Phi_\mu(\boldsymbol{a}) := \mu\mathbb{F}(\boldsymbol{a}) + \mathbb{G}(\boldsymbol{a}) \text{ with } \mathbb{G}(\boldsymbol{a}) = \boldsymbol{R}(\boldsymbol{a})\cdot \log \boldsymbol{a}$$

is nonnegative. Denote by Φ_μ^{**} *the convexification of* Φ_μ *and set*

$$s_\mu(\boldsymbol{q}) := \inf\Big\{ \frac{\Phi_\mu^{**}(\boldsymbol{a}) - \mu\mathbb{F}(\boldsymbol{a})}{\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})} \,\Big|\, \boldsymbol{a}\in\mathfrak{C}_{\boldsymbol{q}},\ \boldsymbol{a}\neq \boldsymbol{w_q}\Big\} \tag{3.12a}$$

$$\widehat{\lambda}(\boldsymbol{q}) := \begin{cases} \min\{s_\mu(\boldsymbol{q}), \frac{r s_\mu(\boldsymbol{q})}{\mu+s_\mu(\boldsymbol{q})}\} & \text{for } \mu\geq 0,\\ \min\{r{-}\mu, s_\mu(\boldsymbol{q})\} & \text{for } \mu \leq 0.\end{cases} \tag{3.12b}$$

Then we have the estimate

$$\forall\, \boldsymbol{q}\in \mathrm{im}^+\mathbb{Q}\ \forall\, \boldsymbol{c}\in\mathcal{C}_{\boldsymbol{q}}: \quad \mathcal{D}(\boldsymbol{c}) \geq \widehat{\lambda}(\boldsymbol{q})\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}). \tag{3.13}$$

Proof: We employ (3.7) to obtain for $\theta\in\,]0,1]$ the estimate

$$\begin{aligned}\mathcal{D}(\boldsymbol{c}) &\geq r\mathcal{H}(\boldsymbol{c}|\overline{\boldsymbol{c}}) + \int_\Omega \theta\mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \\ &= (r{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + (r{-}\theta\mu)\mathbb{F}(\boldsymbol{w_q}) - r\mathbb{F}(\overline{\boldsymbol{c}}) + \theta\int_\Omega \mu\mathbb{F}(\boldsymbol{c}) + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x,\end{aligned}$$

where we used $\mathcal{Q}(\boldsymbol{c}) = \boldsymbol{q}$ and Lemma 2.3. With $\Phi_\mu \geq \Phi_\mu^{**}$ and Jensen's inequality we find

$$\begin{aligned}\mathcal{D}(\boldsymbol{c}) &\geq (r{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + (r{-}\theta\mu)\mathbb{F}(\boldsymbol{w_q}) - r\mathbb{F}(\overline{\boldsymbol{c}}) + \theta\Phi_\mu^{**}(\overline{\boldsymbol{c}}) \\ &= (r{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) - (r{-}\theta\mu)\mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w_q}) + \theta\big(\Phi_\mu^{**}(\overline{\boldsymbol{c}}) - \mu\mathbb{F}(\overline{c})\big) \\ &\geq (r{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + \big(\theta s_\mu(\boldsymbol{q}) - (r{-}\theta\mu)\big)\mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w_q}) \\ &\geq (\varrho{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + \big(\theta s_\mu(\boldsymbol{q}) - (\varrho{-}\theta\mu)\big)\mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w_q}) \ \geq\ (\varrho{-}\theta\mu)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}),\end{aligned}$$

if $0<\varrho\leq r$ and $\theta s_\mu(\boldsymbol{q}) \geq \varrho{-}\theta\mu$. To optimize the decay rate $\varrho{-}\theta\mu$ given the above constraint we choose $\varrho\in[0,r]$ and $\theta\in[0,1]$ as follows:

For $\mu=0$ we choose $\varrho=\min\{s_0,r\}$ and $\theta=1$, giving $\widehat{\lambda}=\min\{r,s_0\}$.

For $\mu>0$ let we take $\varrho=\min\{r,\mu{+}s_\mu\}$ and $\theta=\frac{\varrho}{\mu+s_\mu}$, finding $\widehat{\lambda}=\min\{\frac{rs_\mu}{\mu+s_\mu}, s_\mu\}$.

For $\mu<0$ we still have $\mu+s_\mu\geq 0$ and hence take $\theta=1$ and $\varrho=\min\{\mu{+}s_\mu, r\}$. This gives $\widehat{\lambda}=\min\{r{-}\mu, s_\mu\}$, and the result is established. ∎

To obtain a feeling for the role of μ in the definition of $\widehat{\lambda}(\boldsymbol{q})$ we define the function

$$\mathbb{G}_\mu(\boldsymbol{a}) = \Phi_\mu^{**}(\boldsymbol{a}) - \mu\mathbb{F}(\boldsymbol{a}).$$

Using the convexity of $\mathbb{F}$ and the classical estimate $(\Phi{+}\Psi)^{**}\geq \Phi^{**}+\Psi^{**}$ we see that $\mu\mapsto \mathbb{G}_\mu(\boldsymbol{a})$ is monotone, and thus for $\mu_1<\mu_2$ we have $0\leq \mathbb{G}_{\mu_1}\leq\mathbb{G}_{\mu_2}\leq\mathbb{G}$. In particular, this implies that $\mu\mapsto s_\mu(\boldsymbol{q})$ is monotone and bounded from above by $\lambda_{\boldsymbol{R}}(\boldsymbol{q})$. Hence, maximizing the decay rate $\widehat{\lambda}$ in terms of μ means to find a good intermediate value such that $s_\mu(\boldsymbol{q})$ is already big enough, but $\frac{s_\mu}{\mu+s_\mu}$ is not yet too small.

The following result shows that a simple comparison of $\widehat{\lambda}(\boldsymbol{q})$ with $r = \lambda_{\mathbb{D}}$ and $\lambda_{\boldsymbol{R}}(\boldsymbol{q})$ is possible if $\mu\mathbb{F} + \mathbb{G}$ is convex for some μ_*. The result follows simply by observing $\mathbb{G}_\mu = \mathbb{G}$ for all $\mu \geq \mu_*$ and hence $s_\mu(\boldsymbol{q}) = \lambda_{\boldsymbol{R}}(\boldsymbol{q})$ for $\mu \geq \mu_*$.

Corollary 3.2 *With the assumptions of Theorem 3.1, let $\mu_*\mathbb{F} + \mathbb{G}$ be convex. Then* (3.13) *takes the form*

$$\mathcal{D}(\boldsymbol{c}) \geq \widehat{\lambda}(\boldsymbol{q})\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) \quad \textit{with } \widehat{\lambda}(\boldsymbol{q}) = \min\left\{ \lambda_{\boldsymbol{R}}(\boldsymbol{q}) \,,\ \lambda_{\mathbb{D}} \frac{\lambda_{\boldsymbol{R}}(\boldsymbol{q})}{\mu_* + \lambda_{\boldsymbol{R}}(\boldsymbol{q})} \right\}.$$

Even in this general setting we can give arguments showing that $s_\mu(\boldsymbol{q})$ is finite. This is the much simpler, finite-dimensional analog of the results in [GlH97, Gli04]. We need the additional assumption that there are no steady states of $\dot{\boldsymbol{a}} = -\boldsymbol{R}(\boldsymbol{a})$ on the boundary of $\mathfrak{C}_{\boldsymbol{q}}$. Then, the function $\mathbb{G}$ and hence the function $\mathbb{G}_\mu$ converge to $+\infty$ near the boundary. Moreover, in many chemical systems (not for semiconductors) the set $\mathfrak{C}_{\boldsymbol{q}} = \{\, \boldsymbol{a} \in [0,\infty[^I \,|\, \mathbb{Q}\boldsymbol{a} = \boldsymbol{q} \,\}$ is compact. Thus, the function $\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})$ is bounded from above on $\mathfrak{C}_{\boldsymbol{q}}$, while $\mathbb{G}_\mu$ is continuous in the interior of $\mathfrak{C}_{\boldsymbol{q}}$ and $+\infty$ on the boundary. Hence, the fraction $\mathbb{G}_\mu(\boldsymbol{a})/\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})$ can only approach 0 on $\mathfrak{C}_{\boldsymbol{q}} \setminus \{\boldsymbol{w_q}\}$ when converging to the point $\boldsymbol{w_q}$. The following general result establishes a positive lower bound near this point by using the fact that we consider *all* the conserved quantities via $\mathbb{Q}$, i.e. the rows of $\mathbb{Q}$ forming a basis of ker(W).

Proposition 3.3 *For each $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$ and $\mu > 0$ we have*

$$\begin{aligned}\Lambda(\boldsymbol{q}) &:= \liminf_{\mathfrak{C}_{\boldsymbol{q}}\ni\boldsymbol{a}\to\boldsymbol{w_q}} \frac{\Phi_\mu^{**}(\boldsymbol{a}) - \mu\mathbb{F}(\boldsymbol{a})}{\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})} = \liminf_{\mathfrak{C}_{\boldsymbol{q}}\ni\boldsymbol{a}\to\boldsymbol{w_q}} \frac{\mathbb{G}(\boldsymbol{a})}{\mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q})} \\ &= \inf\left\{ \frac{\sum_{r=1}^R k_r(\boldsymbol{w_q})\big(\sum_{i=1}^I \frac{\alpha_i^r - \beta_i^r}{w_i^{\boldsymbol{q}}}\xi_i\big)^2}{\sum_{i=1}^I \frac{1}{w_i^{\boldsymbol{q}}}\xi_i^2} \,\middle|\, \mathbb{Q}\boldsymbol{\xi} = \boldsymbol{0} \right\} > 0.\end{aligned}$$

Proof: The result follows by expanding the nominator and the denominator for $\boldsymbol{a} = \boldsymbol{w_q} + \boldsymbol{\xi}$ with small $\boldsymbol{\xi}$ satisfying $\mathbb{Q}\boldsymbol{\xi} = \boldsymbol{0}$. For the nominator we use the result of Lemma 3.4 below, stating that $\Phi_\mu^{**} = \Phi$ in a neighborhood of $\boldsymbol{w_q}$. This implies $\Phi_\mu^{**}(\boldsymbol{a}) - \mu\mathbb{F}(\boldsymbol{a}) = \mathbb{G}(\boldsymbol{a})$.

To see that the infimum on the right-hand side is positive we first observe that it is sufficient to restrict to the sphere $|\boldsymbol{\xi}| = 1$. Using the transformation $\boldsymbol{\xi} = \mathrm{diag}(\boldsymbol{w_q})\boldsymbol{\eta}$, the nominator takes the form $\sum_1^R k_r\big((\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r)\cdot\boldsymbol{\eta}\big)^2$ and, using $k_r > 0$, it can only vanish for $\boldsymbol{\eta} \in$ ker(W). By the definition of $\mathbb{Q}$ there exists $\boldsymbol{y} \in \mathbb{R}^m$ such that $\boldsymbol{\eta} = \mathbb{Q}^\mathsf{T}\boldsymbol{y}$. Thus, we have $0 = \mathbb{Q}\boldsymbol{\xi} = \mathbb{Q}\,\mathrm{diag}(\boldsymbol{w_q})\mathbb{Q}^\mathsf{T}\boldsymbol{y}$. Since $\mathbb{Q}\,\mathrm{diag}(\boldsymbol{w_q})\mathbb{Q}^\mathsf{T}$ is positive definite (as $\boldsymbol{w_q} > 0$ and $\mathrm{rank}(\mathbb{Q}) = m$) we conclude $\boldsymbol{y} = 0$ and hence $\boldsymbol{\xi} = \mathrm{diag}(\boldsymbol{w_q})\mathbb{Q}^\mathsf{T}\boldsymbol{y} = \boldsymbol{0}$, which contradicts $|\boldsymbol{\xi}| = 1$. Hence, the nominator is bounded from below by a positive constant on $\{\, \boldsymbol{\xi} \mid \mathbb{Q}\boldsymbol{\xi} = 0,\ |\boldsymbol{\xi}| = 1 \,\}$, and we conclude $\Lambda_{\boldsymbol{q}} > 0$. ∎

Proposition 3.3 and the definition of $\lambda_{\boldsymbol{R}}(\boldsymbol{q})$ immediately give the estimates

$$\Lambda(\boldsymbol{q}) \geq \lambda_{\boldsymbol{R}}(\boldsymbol{q}) \geq s_\mu(\boldsymbol{q}).$$

The next result shows that in principle every positive μ can be used to derive a bound, since the quotient $\mathbb{G}_\mu(\boldsymbol{a})/\mathbb{H}(\boldsymbol{a}|\boldsymbol{w}_{\boldsymbol{q}})$ is controlled in a neighborhood of the critical point $\boldsymbol{w}_{\boldsymbol{q}}$. Then, for compact sets $\mathfrak{C}_{\boldsymbol{q}}$ it is usually easy to establish $\mathbb{G}_\mu \geq \gamma > 0$ outside of this neighborhood, which then implies $s_\mu(\boldsymbol{q}) > 0$.

Lemma 3.4 *Let $\mathbb{F}$, $\mathbb{G}$, and Φ_μ be defined as above with $\mu > 0$. Take any $\boldsymbol{w} \in \,]0,\infty[^I$ such that $\mathbb{G}(\boldsymbol{w}) = 0$. Then there exists $\delta > 0$ such that for all $\boldsymbol{a}$ with $|\boldsymbol{a}{-}\boldsymbol{w}| \leq \delta$ we have $\Phi_\mu^{**}(\boldsymbol{a}) = \Phi_\mu(\boldsymbol{a})$.*

Proof: We denote by $T^1_{\boldsymbol{a}}f$ the linear approximation of f in the point $\boldsymbol{a}$. We use the abbreviations $\rho = |\boldsymbol{c}{-}\boldsymbol{a}|$ and $\varepsilon = |\boldsymbol{a}{-}\boldsymbol{w}|$, where we assume $\varepsilon \leq \varepsilon_* := \frac{1}{2}\min\{1, w_1, .., w_I\}$.

Since $\mathbb{F}$ satisfies $\mathrm{D}^2\mathbb{F} > 0$, we have

$$\forall\, \boldsymbol{a} \in B_{\varepsilon_*}(\boldsymbol{w})\, \forall\, \boldsymbol{c}: \quad \mathbb{F}(\boldsymbol{c}) - T^1_{\boldsymbol{a}}\mathbb{F}(\boldsymbol{c}) \geq \nu\rho^2/(1{+}\rho).$$

For $\mathbb{G}$ we use $\boldsymbol{G}(\boldsymbol{w}) = \mathrm{D}\boldsymbol{G}(\boldsymbol{w}) = 0$, $\mathrm{D}^2\boldsymbol{G}(\boldsymbol{w}) \geq 0$, and smoothness. Hence for $\boldsymbol{a} \in B_{\varepsilon_*}(\boldsymbol{w})$ we have

$$|\mathbb{G}(\boldsymbol{a})| \leq M\varepsilon^2, \ |\mathrm{D}\mathbb{G}(\boldsymbol{a})| \leq M\varepsilon, \ \mathrm{D}^2\mathbb{G}(\boldsymbol{a}) \leq -M\varepsilon, \ |\mathrm{D}^3\mathbb{G}(\boldsymbol{a})| \leq M.$$

Thus $\mathbb{G} - T^1_{\boldsymbol{a}}\mathbb{G}$ can be estimated locally via

$$\mathbb{G}(\boldsymbol{c}) - T^1_{\boldsymbol{a}}\mathbb{G}(\boldsymbol{c}) \geq -M\varepsilon\rho^2 - M\rho^3.$$

For general $\boldsymbol{c}$ we use $\mathbb{G}(\boldsymbol{c}) \geq 0$ and estimate $|\mathrm{T}^1_{\boldsymbol{a}}\mathbb{G}(\boldsymbol{c})|$ to obtain

$$\mathbb{G}(\boldsymbol{c}) - T^1_{\boldsymbol{a}}\mathbb{G}(\boldsymbol{c}) \geq 0 - M\varepsilon^2 - M\varepsilon\rho.$$

Together we arrive at the lower estimate

$$\mathbb{G}(\boldsymbol{c}) - T^1_{\boldsymbol{a}}\mathbb{G}(\boldsymbol{c}) \geq -M(\varepsilon{+}\rho)\min\{\varepsilon, \rho^2\} \geq -4M\sqrt{\varepsilon}\rho^2/(1{+}\rho).$$

Thus, choosing $\delta = \min\{\varepsilon_*, \mu\nu^2/(4M)^2\} > 0$ we obtain $\Phi_\mu(\boldsymbol{c}) \geq T^1_{\boldsymbol{a}}\Phi_\mu(\boldsymbol{c})$ which implies the desired relation $\Phi_\mu^{**}(\boldsymbol{a}) = \Phi_\mu(\boldsymbol{a})$. ∎

3.4 Exploiting higher entropies

The above result can be generalized by using the stronger entropy estimates involving F_γ for $\gamma > 1$. Thus, exploiting the better growth and stronger convexity of F_γ, one gains more flexibility in handling the reaction terms. However, the convexification will become more troublesome.

We again employ (3.6) but now once with $\gamma=1$ and once with a suitable $\gamma>1$:

$$\begin{aligned}
&\mathcal{D}(\boldsymbol{c}) \geq \theta r_0 \mathcal{D}_1(\boldsymbol{c}) + (1-\theta)\mathcal{D}_2(\boldsymbol{c}) \text{ with}\\
&\mathcal{D}_1(\boldsymbol{c}) = \int_\Omega \sum_{i=1}^I \overline{c}_i F_1(c_i/\overline{c}_i)\,\mathrm{d}x = \mathcal{F}(\boldsymbol{c}) - \mathbb{F}(\overline{\boldsymbol{c}}),\\
&\mathcal{D}_2(\boldsymbol{c}) = \int_\Omega r_1 \sum_{i=1}^I \overline{c}_i F_\gamma(c_i/\overline{c}_i) + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x,
\end{aligned}$$

where $r_0 = \delta\rho(\Omega,1,1)$, $r_1 = \delta\rho(\Omega,1,\gamma)$, and $\theta \in\,]0,1[$ is free to be optimized later. Unfortunately, the expression for $\mathcal{D}_2$ cannot be decomposed into a simple integral (depending on $\boldsymbol{c}$ but not on $\overline{\boldsymbol{c}}$) and a function of $\overline{\boldsymbol{c}}$, since relation (3.5) would need the terms $\overline{c}_i^\gamma$ in front of $F_\gamma(c_i/\overline{c}_i)$. Nevertheless we can define the function

$$\Psi_{\boldsymbol{a}}(\boldsymbol{c}) := r_1 \sum_{i=1}^I a_i F_\gamma(c_i/a_i) + \mathbb{G}(\boldsymbol{c}),$$

denote by $\Psi_{\boldsymbol{a}}^{**}$ its convexification (where $\boldsymbol{a}$ is a fixed vector), and obtain the lower bound $\mathcal{D}_2(\boldsymbol{c}) = \int_\Omega \Psi_{\overline{\boldsymbol{c}}}(\boldsymbol{c}(x))\,\mathrm{d}x \geq \Psi_{\overline{\boldsymbol{c}}}^{**}(\overline{\boldsymbol{c}})$. As in Section 3.3 we arrive at the lower bound

$$\mathcal{D}(\boldsymbol{c}) \geq \theta r_0 \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}) + (1-\theta)\Psi_{\overline{\boldsymbol{c}}}^{**}(\overline{\boldsymbol{c}}) - \theta r_0\big(\mathbb{F}(\overline{\boldsymbol{c}}) - \mathbb{F}(\boldsymbol{w}_{\boldsymbol{q}})\big).$$

Thus, if we define the quantity

$$\widehat{s}(\boldsymbol{q}) := \inf\Big\{ \frac{\Psi_{\boldsymbol{a}}^{**}(\boldsymbol{a})}{\mathbb{H}(\boldsymbol{a}|\boldsymbol{w}_{\boldsymbol{q}})} \,\Big|\, \boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}},\ \boldsymbol{a} \neq \boldsymbol{w}_{\boldsymbol{q}} \Big\} \in [0,\infty] \tag{3.14}$$

and choose $\theta = \widehat{s}(\boldsymbol{q})/(r_0+\widehat{s}(\boldsymbol{q}))$, we obtain the lower bound

$$\mathcal{Q}(\boldsymbol{c}) = \boldsymbol{q} \quad\Longrightarrow\quad \mathcal{D}(\boldsymbol{c}) \geq \lambda(\boldsymbol{q})\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}), \quad \text{where } \lambda(\boldsymbol{q}) = \frac{r_0\,\widehat{s}(\boldsymbol{q})}{r_0 + \widehat{s}(\boldsymbol{q})}.$$

3.5 Allowing for vanishing diffusion constants

It was observed in [Gli04, DeF08] that under certain structural assumption (see [Gli04, Assumption (I,iv)] for a general sufficient condition) the exponential decay to equilibrium persists even in the case when some diffusion constants δ_i vanish. Our method can also be used in such cases. In this section we give the rough idea how the above approach can be modified to obtain explicit bounds for such cases. It is clear that conditions as given in [Gli04] are needed to carry the method through. Again the aim is to obtain explicit bounds by involving a log-Sobolev inequality and convexification.

We now assume that the components c_i are arranged in such a way that the first $J<I$ components have a strictly positive diffusion constant while for $i>J$ the diffusion constants may be zero, viz.

$$r_0 := \min\{\,\rho_{\mathrm{LSi}}(\delta_j) \mid j=1,...,J\,\} > 0 \quad\text{and}\quad \delta_i \geq 0 \text{ for } i=J{+}1,...,I.$$

For the dissipation estimate we obtain

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\boldsymbol{c}(t)) = \mathcal{D}(\boldsymbol{c}) \geq \mathcal{D}_{\text{diff}}(\boldsymbol{c}) + \int_\Omega \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \text{ with}$$

$$\mathcal{D}_{\text{diff}}(\boldsymbol{c}) = \int_\Omega \sum_{j=1}^J \delta_j \frac{|\nabla c_j|^2}{c_j}\,\mathrm{d}x \geq r_0\Big(\int_\Omega \sum_{j=1}^J F_1(c_j(x))\,\mathrm{d}x - \sum_{j=1}^J F_1(\overline{c}_j)\Big).$$

To generate a lower bound in terms of $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q})$, we are missing the terms $F_1(c_i)$ for $i > J$ in the integral of $\mathcal{D}_{\text{diff}}$. To obtain these terms we simply add them to the first term and hope that the necessary subtraction at the second term can be compensated:

$$\mathcal{D}_{\text{diff}}(\boldsymbol{c}) + \int_\Omega \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \geq \theta r_0\Big(\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + \mathbb{F}(\boldsymbol{w_q})\Big) + \mathcal{G}_\theta(\boldsymbol{c}) \text{ where}$$

$$\mathcal{G}_\theta(\boldsymbol{c}) := \int_\Omega G_\theta(\boldsymbol{c}(x))\,\mathrm{d}x - r_0\sum_{j=1}^J F_1(\overline{c}_j) \text{ with}$$

$$G_\theta(\boldsymbol{c}) := (1{-}\theta)r_0\sum_{j=1}^J F_1(c_j) - \theta r_0 \sum_{i=J+1}^I F_1(c_i) + \mathbb{G}(\boldsymbol{c}).$$

Note that the second sum in the definition of G_θ (including the minus sign) is concave. However, the hope is that the last term $\mathbb{G}$ has better convexity properties and can compensate for the concavity of the second term at least for small θ.

As above we estimate $\mathcal{G}_\theta$ from below via Jensen's estimate and obtain

$$\mathcal{D}(\boldsymbol{c}) \geq \theta r_0 \mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) + G_\theta^{**}(\overline{\boldsymbol{c}}) - r_0\sum_{j=1}^J F_1(\overline{c}_j) + \theta r_0\mathbb{F}(\boldsymbol{w_q}).$$

Thus, the desired decay estimate (1.5) follows with $\lambda(\boldsymbol{q}) = \widehat{\theta}(\boldsymbol{q})r_0 > 0$ if, for a given $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}$, we are able to find a positive $\theta = \widehat{\theta}(\boldsymbol{q})$ such that

$$\forall\, \boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}}: \quad G_\theta^{**}(\boldsymbol{a}) - r_0\sum_{j=1}^J F_1(a_j) + \theta r_0 \mathbb{F}(\boldsymbol{w_q}) \geq 0. \tag{3.15}$$

This theory will be successfully applied in the second part of Section 4.2 for a linear system with quadratic entropy and in Section 4.4 for a nonlinear system of two equations where one diffusion constant vanishes. We conjecture that it can be done in general cases if the assumption in [Gli04, Ass. (I,iv)] holds.

Remark 3.5 The above condition can be made plausible by introducing the auxiliary function

$$\widetilde{\mathbb{G}}_\theta(\boldsymbol{a}) := G_\theta^{**}(\boldsymbol{a}) - (1{-}\theta)r_0\textstyle\sum_{j=1}^J F_1(a_j) + \theta r_0 \sum_{i=J+1}^I F_1(a_i),$$

which satisfies $\widetilde{\mathbb{G}}_\theta \leq \mathbb{G}$, since $G_\theta^{**} \leq G_\theta$. For convex G_θ condition (3.15) reduces to the same condition as in the previous case, namely

$$\forall\, \boldsymbol{a} \in \mathfrak{C}_{\boldsymbol{q}}: \quad \widetilde{\mathbb{G}}_\theta(\boldsymbol{a}) \geq \theta r_0\big(\mathbb{F}(\boldsymbol{a}) - \mathbb{F}(\boldsymbol{w_q})\big) = \theta r_0 \mathbb{H}(\boldsymbol{a}|\boldsymbol{w_q}).$$

For $\theta \approx 0$ we can expand G_θ^{**} in the form

$$G_\theta^{**}(\boldsymbol{a}) = G_0^{**}(\boldsymbol{a}) + O(\theta) = r_0 \textstyle\sum_{j=1}^J F_1(a_j) + \widehat{\mathbb{G}}(\boldsymbol{a}) + O(\theta),$$

where $\widehat{\mathbb{G}} \geq 0$ with equality only on $\{\, \boldsymbol{w_q} \,|\, \boldsymbol{q} \in \mathrm{im}^+\mathbb{Q}\,\}$. Thus, we find $\widetilde{\mathbb{G}}_\theta(\boldsymbol{a}) = \widehat{\mathbb{G}}(\boldsymbol{a}) + O(\theta)$, and as in Lemma 3.4 it should be possible to show $\widetilde{G}_\theta(\boldsymbol{a}) = \mathbb{G}(\boldsymbol{a})$ for $\theta \in [0, \theta_0]$ and $\boldsymbol{a}$ in a neighborhood of $\boldsymbol{w_q}$.

4 Applications

In this section we present a series of *simple* examples to see the above theory at work. In Section 5 we give an outlook to further applications to be studied in a subsequent work.

4.1 A scalar reaction-diffusion equation

We consider a single species X_1 with density $c > 0$, which can be absorbed into and recreated from the background according to the reaction $\alpha X_1 \rightleftharpoons \emptyset$, i.e. $\boldsymbol{\alpha} = 1$ and $\boldsymbol{\beta} = 0$. Without loss of generality we can assume that the unique steady state equals $w = 1$. Since $W = 1 \in \mathbb{R}^{1\times 1}$, there are no conserved quantities. The reaction-diffusion equation is

$$\dot{c} = \mathrm{div}\,\big(\delta \nabla c\big) - R(c) \quad \text{with } R(c) = k(c)\big(c^\alpha{-}1\big) \tag{4.1}$$

with $\alpha > 0$. For simplicity, we will assume that the reaction coefficient $k(c) > 0$ is independent of c.

For the entropy $\mathcal{H}(c|1) = \int_\Omega \mathbb{H}(c(x)|1)\,\mathrm{d}x = \int_\Omega F_1(c(x))\,\mathrm{d}x$ we find the dissipation

$$-\dot{\mathcal{H}} = \mathcal{D}(\boldsymbol{c}) = \int_\Omega \delta \frac{|\nabla c|^2}{c} + R(c)\log c \,\mathrm{d}x \geq \int_\Omega r_0 F_1(c) {+} \mathbb{G}(c)\,\mathrm{d}x - r_0 F_1(\overline{c}),$$

where $r_0 = \rho_{\mathrm{LSi}}(\delta)$ and $\mathbb{G}(c) = R(c)\log c \geq 0$. Defining $\Phi(a) = \mu F_1(a) + \mathbb{G}(a)$ and denoting by Φ_μ^{**} its convexification we obtain

$$s_\mu := \inf\Big\{\, \frac{\Phi_\mu^{**}(a){-}\mu F_1(a)}{F_1(a)} \,\Big|\, a > 0,\ a \neq 1 \,\Big\}.$$

Returning to the special case $R(u) = k(u^\alpha{-}1)$ with $1 \leq \alpha \leq 22$, the function $\mathbb{G}(c) = k\,R(u)\log u$ is convex, and we obtain $\Phi_\mu^{**}(a) - \mu F_1(a) = \mathbb{G}(a)$. Thus,

$$s_\mu = k\,\widehat{s}(\alpha) \quad \text{with } \widehat{s}(\alpha) = \inf\Big\{\, \frac{(a^\alpha{-}1)\log a}{F_1(a)} \,\Big|\, a > 0,\ a \neq 1 \,\Big\}.$$

It can be shown that $\widehat{s} : [1, \infty[\, \to \mathbb{R}$ increases from $\widehat{s}(1) = 1$ to $\widehat{s}(\infty) \approx 3.356$. Applying Corollary 3.2 with $\mu_* = 0$, we find that the solutions c of the scalar reaction diffusion equation (4.1) with $\alpha \in [1, 22]$ satisfy the decay estimate

$$\mathcal{H}(c(t)|1) \leq \mathrm{e}^{-\lambda t}\mathcal{H}(c(0)|1) \text{ with } \lambda = \min\{k\widehat{s}(\alpha), \rho_{\mathrm{LSi}}(\delta)\}.$$

Note that this result can even be improved by choosing $\mu_* < 0$. This is especially useful in the case that $\rho_{\mathrm{LSi}}(\delta)$ is very small or even 0.

4.2 Linear exchange reactions

In this subsection we treat linear systems where the reaction terms are given in terms of a time-continuous Markov chain with finite state space $\{1, ..., I\}$, namely

$$\boldsymbol{R}(\boldsymbol{c}) = \sum_{i<j} k_{ij} \big(\tfrac{c_i}{w_i^{\mathrm{eq}}} - \tfrac{c_j}{w_j^{\mathrm{eq}}} \big) \big(\boldsymbol{e}^i - \boldsymbol{e}^j \big)$$

where $\boldsymbol{e}^j \in \mathbb{R}^I$ denotes the jth unit vector. Here $\boldsymbol{w}^{\mathrm{eq}} = (w_1^{\mathrm{eq}}, .., w_I^{\mathrm{eq}}) \in]0,1[^I$ is a nontrivial steady state, which provides the detailed-balance condition (also called reversibility in Markov chains, see [Mie12, Maa11, ErM11]).

The specific nice property is that the dissipation function

$$\mathbb{G}(\boldsymbol{c}) \cdot \big(\log(\tfrac{c_i}{w_i^{\mathrm{eq}}}) \big)_{i=1,..,I} = \sum_{i<j} k_{ij}\, \Gamma(\tfrac{c_i}{w_i^{\mathrm{eq}}}, \tfrac{c_j}{w_j^{\mathrm{eq}}})$$

is convex, since the function $(a,b) \mapsto \Gamma(a,b) = (a-b)\log(a/b)$ is convex. Hence we can apply Corollary 3.2 and obtain the decay estimate

$$\mathcal{D}(\boldsymbol{c}) \geq \lambda(\boldsymbol{q}) \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\mathrm{eq}}) \quad \text{with } \lambda(\boldsymbol{q}) = \min \big\{ \min\{ \rho_{\mathrm{LSi}}(\delta_i) \mid i = 1, .., I \}, \lambda_{\mathsf{Mk}}(\boldsymbol{q}) \big\},$$

where $\lambda_{\mathsf{Mk}}(\boldsymbol{q})$ is the decay rate for the linear Markov chain $\dot{\boldsymbol{a}} = -\boldsymbol{R}(\boldsymbol{a})$ under the constraint $\mathbb{Q}\boldsymbol{a}(t) = \boldsymbol{q}$.

However, the results can be improved, since one does not necessarily need all diffusion constants to be positive. To show the applicability of our method, we look at a simple system with two densities u and v and a degenerate diffusion, namely

$$\dot{u} = \delta \Delta u + \alpha v - \beta u, \quad \dot{v} = \beta u - \alpha v. \tag{4.2}$$

Clearly, for solutions $\boldsymbol{c} = (u, v)$ we have the conserved quantity $\mathcal{Q}(\boldsymbol{c}) = \overline{u} + \overline{v}$, and the unique steady states $\boldsymbol{w}_q$ with $\mathcal{Q}(\boldsymbol{w}_q) = q > 0$ are given via $\boldsymbol{w}_q = \frac{q}{\alpha+\beta}(\alpha, \beta)$. By linearity it is sufficient to study one $q > 0$ and we choose $q = \alpha + \beta$ giving $\boldsymbol{w}_q = (\alpha, \beta)$.

Unfortunately, we are not able to use the approach explained in Section 3.5, since for $\theta > 0$ the function $G_\theta(u,v) = aF_1(u) + (\alpha v - \beta u) \log\big(\frac{\alpha v}{\beta u} \big) - \theta F_1(v)$ is not bounded from below by an affine function, i.e. $G_\theta^{**} \equiv -\infty$. Instead, we show the usability of the theory by looking at the quadratic entropies instead: even there the argument is illuminating. We define

$$\begin{aligned} &\mathcal{B}(\boldsymbol{c}) = \int_\Omega \mathbb{B}(\boldsymbol{c}(x)|\alpha, \beta)\, \mathrm{d}x \quad \text{with} \\ &\mathbb{B}(u, v|\alpha, \beta) = \alpha F_2(\tfrac{u}{\alpha}) + \beta F_2(\tfrac{v}{\beta}) = \tfrac{1}{2\alpha}(u-\alpha)^2 + \tfrac{1}{2\beta}(v-\beta)^2. \end{aligned}$$

With the Poincaré constant $\rho_{\mathrm{P}} = \rho(\Omega, 2, 2)$ for Ω we set $r = \delta \rho_{\mathrm{P}}$ and $\mathbb{G}(\boldsymbol{c}) = \frac{1}{\alpha\beta} \big(\beta u - \alpha v \big)^2$, and the method of Section 3.5 yields the following result.

Proposition 4.1 *The solutions $\boldsymbol{c} = (u, v)$ of (4.2) satisfy $\mathcal{B}(\boldsymbol{c}(t)) \leq \mathrm{e}^{-\lambda t} \mathcal{B}(\boldsymbol{c}(0))$ with $\lambda = r + \alpha + \beta - \big((r+\alpha+\beta)^2 - 4\alpha r \big)^{1/2}$.*

It can be checked by linear spectral theory that this λ is identical to the optimal rate obtained by twice the smallest nontrivial eigenvalue of the linear system.

Proof: As in Section 3.5 we define the auxiliary function $\Phi_\theta(\boldsymbol{c}) = (1-\theta)ru^2/\alpha - \theta rv^2/\beta + \mathbb{G}(\boldsymbol{c})$. Using $\mathcal{Q}(\boldsymbol{c}(t)) = \alpha+\beta$, the dissipation estimate gives

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{B}(\boldsymbol{c}) &= \int_\Omega \frac{\delta}{\alpha}|\nabla u|^2 + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \;\geq\; \int_\Omega \frac{r}{\alpha}(u-\overline{u})^2 + \mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \\ &= 2\theta r\Big(\int_\Omega \mathbb{B}(\boldsymbol{c}|\alpha,\beta)\,\mathrm{d}x + \frac{\alpha+\beta}{2}\Big) + \int_\Omega \Phi_\theta(\boldsymbol{c}(x))\,\mathrm{d}x - r\overline{u}^2/\alpha. \end{aligned}$$

For $0 \leq \theta \leq \Theta := \big(r+\alpha+\beta - \big((r{+}\alpha{+}\beta)^2 - 4\alpha r\big)^{1/2}\big)/(2r)$ the function Φ_θ is convex and we can estimate

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{B}(\boldsymbol{c}) \geq 2\theta r\mathcal{B}(\boldsymbol{c}) + \Phi_\theta(\overline{\boldsymbol{c}}) - r\overline{u}^2/\alpha = 2\theta r\mathcal{B}(\boldsymbol{c}) + \mathbb{G}(\overline{u},\overline{v}) - \theta r\big(\overline{u}^2/\alpha{+}\overline{v}^2/\beta{-}\alpha{-}\beta\big).$$

For $\overline{u}+\overline{v} = \alpha+\beta$ the last two terms are nonnegative if and only if $\theta \leq (\alpha{+}\beta)/r$. Since $\Theta \leq (\alpha{+}\beta)/r$, we obtain the desired result $-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{B}(\boldsymbol{c}) \geq 2r\Theta\mathcal{B}(\boldsymbol{c})$. ■

4.3 A system with quadratic nonlinearity

We consider a system with two species X_u and X_v with densities $u, v \geq 0$ interacting through one reaction of the type $X_u \rightleftharpoons 2\,X_v$. Normalizing the densities suitably, this leads to the following system for $\boldsymbol{c} = (u,v)$:

$$\begin{aligned} \dot{u} &= \delta_u\Delta u + \;k\big(v^2{-}u\big), \\ \dot{v} &= \delta_v\Delta v + 2k\big(u{-}v^2\big), \end{aligned} \tag{4.3}$$

which has the conserved quantity

$$\mathcal{Q}(\boldsymbol{c}) = \int_\Omega 2u(x){+}v(x)\,\mathrm{d}x = 2\overline{u}+\overline{v}, \quad \text{i.e. } \mathbb{Q} = (2\;\;1) \in \mathbb{R}^{1\times 2}.$$

Depending on the given value $q = \mathcal{Q}(\boldsymbol{c}(0))$ we have the unique steady state

$$\boldsymbol{w}_q = (u_q, v_q) \quad \text{with } u_q^2 = v_q \text{ and } 2u_q + v_q = q.$$

We apply the theory of Section 3.3 to the functional $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_q)$, giving a lower dissipation bound $\mathcal{D}(\boldsymbol{c}) \geq \int_\Omega \Phi(\boldsymbol{c}(x))\,\mathrm{d}x - r_uF_1(\overline{u}) - r_vF_1(\overline{v})$ with $(r_u, r_v) = (\rho_{\mathrm{LSi}}(\delta_u), \rho_{\mathrm{LSi}}(\delta_v))$ and

$$\Phi(u,v) = r_uF_1(u) + r_vF_1(v) + k\mathbb{G}(u,v) \;\text{ with } \mathbb{G}(u,v) := (v^2{-}u)\log(v^2/u) \geq 0.$$

The entropy decay for the reaction-rate equation $\dot{\boldsymbol{a}} = -\boldsymbol{R}(\boldsymbol{a})$ with $\mathbb{Q}\boldsymbol{a}(0) = q$ is given by $\mathbb{H}(\boldsymbol{a}(t)|\boldsymbol{w}_q) \leq \mathrm{e}^{-\lambda_{\boldsymbol{R}}(q)t}\mathbb{H}(\boldsymbol{a}(0)|\boldsymbol{w}_q)$ for $t > 0$, where the decay rate is $\lambda_{\boldsymbol{R}}(q) = k\sigma_{\mathbb{G}}(q)$ with

$$\sigma_{\mathbb{G}}(q) := \inf\Big\{ \frac{\mathbb{G}(u,v)}{\mathbb{H}(u,v|\boldsymbol{w}_q)} \;\Big|\; (u,v) \in \mathfrak{C}_q,\; (u,v) \neq \boldsymbol{w}_q \Big\}, \tag{4.4}$$

Proposition 4.4 below gives an explicit estimate of the form $\sigma_{\mathbb{G}}(q) \geq \max\{2/5, \sqrt{8q}{-}2/5\}$. The main result for the reaction-diffusion system (4.3) is the following decay estimate.

Theorem 4.2 *Along the solutions $\boldsymbol{c} = (u, v)$ of* (4.3) *with $\mathcal{Q}(\boldsymbol{c}(t)) = q$ we have the estimate $\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_q) \leq \mathrm{e}^{-\lambda(q)t}\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_q)$, where*

$$\lambda(q) = \min\Big\{\frac{\sigma_{\mathbb{G}}(q)}{\mu_*+\sigma_{\mathbb{G}}(q)}\, r_u\,,\ r_v,\ k\sigma_{\mathbb{G}}(q)\Big\} \geq \frac{1}{5}\min\{r_u, 5r_v, 2k\}, \tag{4.5}$$

where $\mu_* = 1/\kappa_* \approx 1.1675$ with $\kappa_* \approx 0.8565$ specified in Lemma 4.3.

The estimate for $\lambda(q)$ is close to optimal since the three terms in the minimum are clearly identified as the two diffusion terms and the reaction term. However, we will show in Section 4.4 that $\lambda(q)$ stays positive even in the case $\delta_v = 0$.

The proof of the above theorem is a slight modification of the theory in Section 3.3, since we do not construct the convexification of Φ_μ but omit the term $F_1(v)$. Without this term one can use a scaling argument to reduce the convexification to a one-dimensional problem.

Lemma 4.3 *For $\kappa > 0$ consider the function $\phi_\kappa : [0,\infty[^2 \to [0,\infty]$ with*

$$\phi_\kappa(u, v) = F_1(u) + \kappa\mathbb{G}(u, v) \quad \text{with } \mathbb{G}(u, v) = (v^2{-}u)\log(v^2/u).$$

Then, we have the lower bound

$$F_1(u) + \kappa\mathbb{G}(u, v) \geq \frac{4\kappa}{1 + 4\kappa}F_1(v) \quad \text{for all } (u, v). \tag{4.6}$$

Moreover, ϕ_κ is convex for $\kappa \in [0, \kappa_*]$ where $\kappa_* \approx 0.8565$. In particular, we have

$$\phi^{**}_\kappa(u, v) \geq \phi_{\min\{\kappa_*,\kappa\}}(u, v) = F_1(u) + \min\{\kappa_*, \kappa\}\mathbb{G}(u, v). \tag{4.7}$$

For $\kappa \geq 1$ the convexification is given in the form

$$\begin{aligned} &\phi^{**}_\kappa(u, v) = v^2 g_\kappa(u/v^2) + 2u \log v + 1 - v^2 \\ &\text{with } g_\kappa(z) = \begin{cases} F_1(z) + \kappa(z{-}1)\log z & \text{for } z \in [0, Z_\kappa], \\ 2z \log z - B_\kappa z + 1 & \text{for } z \geq Z_\kappa \end{cases} \end{aligned} \tag{4.8}$$

where $B_\kappa = 1 + \kappa\frac{1-Z_\kappa}{Z_\kappa}\log Z_\kappa \in [1, 1{+}1/\mathrm{e}]$ and $Z_\kappa > 1$ is the unique solution z of $\log z + (\kappa{-}1)z/\kappa = 1$. In particular, for $\kappa = 1$ we have $Z_1 = \mathrm{e}$ and $B_1 = 1{+}1/\mathrm{e}$.

The proof of Lemma 4.3 is given in Section A.1.

Remark: Adding $F_1(v)$ to ϕ_κ does not help to increase the threshold κ_*, since the scaling properties of $\phi_\kappa(u, v)$ and $F_1(v)$ are different.

Proof of Theorem 4.2: We now return to the full estimate in the general Section 3.3 but do a slight variation because of the different handling of $F_1(u)$ and $F_1(v)$. The solutions $\boldsymbol{c} = (u, v)$

satisfy the estimate

$$
\begin{aligned}
-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(u,v|\boldsymbol{w}_q) &= \int_\Omega \delta_u\frac{|\nabla u|^2}{u} + \delta_u\frac{|\nabla v|^2}{v} + k\mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \\
&\geq \int_\Omega r_u\overline{v}F_1(u/\overline{u}) + r_v\overline{v}F_1(v/\overline{v}) + k\mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \\
&\geq r_\theta\int_\Omega \mathbb{H}(\boldsymbol{c}(x)|\overline{\boldsymbol{c}})\,\mathrm{d}x + \theta r_u\int_\Omega F_1(u){-}F_1(\overline{u}){+}\tfrac{k}{\theta r_u}\mathbb{G}(\boldsymbol{c})\,\mathrm{d}x \\
&= r_\theta\Big(\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_q) - \mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w}_q)\Big) + \theta r_u\int_\Omega \phi_{k/(\theta r_u)}(\boldsymbol{c})\,\mathrm{d}x - \theta r_u F_1(\overline{u}) \\
&\overset{(4.7)}{\geq} r_\theta\Big(\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_q) - \mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w}_q)\Big) + \min\{\theta r_u\kappa_*, k\}\mathbb{G}(\overline{\boldsymbol{c}}) \\
&\geq r_\theta\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_q) + \big(\min\{\theta r_u\kappa_*, k\}\sigma_\mathbb{G}(m) - r_\theta\big)\mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w}_q),
\end{aligned}
$$

where, for the last step, we used the definition of $\sigma_\mathbb{G}$ and $\mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} = q$. The desired result (4.5) follows by choosing θ as small as possible under the constraint that the prefactor of $\mathbb{H}(\overline{\boldsymbol{c}}|\boldsymbol{w}_q) \geq 0$ remains nonnegative. This leads to the choice

$$
1{-}\theta = \min\{\kappa_*\sigma_\mathbb{G}/(1{+}\kappa_*\sigma_\mathbb{G}), r_v/r_u, k\sigma_\mathbb{G}/r_u\},
$$

and the first estimate in (4.5) is establish. The second estimate follows from $\sigma_\mathbb{G} \geq 2/5$ and the given value of κ_*. ■

Finally we give the explicit estimate for the function $\sigma_\mathbb{G}$ that was used above.

Proposition 4.4 *Define for $q > 0$ the value $\mu_q > 0$ as solution of $2\mu^2 + \mu = q$. Then, we have the estimate*

$$
\sigma_\mathbb{G}(q) \geq \max\Big\{\frac{8\mu(1{+}2\mu)}{1+4\mu}\,,\,\frac{1+2\mu}{1+\big(\mu F_1(1{+}\frac{1}{2\mu})\big)^{-1}}\Big\} \geq \max\{2/5, \sqrt{8q}{-}2/5\}.
$$

Proof: For fixed $q > 0$ every $(u,v) \in \mathfrak{C}_q$ can be written in the form

$$
u = \mu^2\big(1 + \tfrac{1-\beta}{2\mu}\big), \quad v = \beta\mu \quad \text{with } \beta \in [0, 2\mu{+}1].
$$

Step 1: The fraction $\gamma(\beta)$ in the definition of $\sigma_\mathbb{G}$ can be written in the form $U(\beta)/L(\beta)$, and for $\beta \in\,]0, 2\mu{+}1[$ we have

$$
L(\beta) = F_1\big(1{+}\tfrac{1-\beta}{2\mu}\big) + \tfrac{1}{\mu}F_1(\beta) \leq 2F_2\big(1{+}\tfrac{1-\beta}{2\mu}\big) + \tfrac{2}{\mu}F_2(\beta) = \tfrac{1+4\mu}{4\mu^2}(\beta{-}1)^2,
$$

where we used (3.2). For U we use $(v^2{-}u)\log(v^2/u) \geq 4(v{-}\sqrt{u})^2$ and obtain

$$
U(\beta) \geq 4\Big(\beta - \big(1{+}\tfrac{1-\beta}{2\mu}\big)^{1/2}\Big)^2 \geq \tfrac{(1+4\mu)^2}{4\mu^2}(\beta{-}1)^2,
$$

since $\big(1{+}\frac{1-\beta}{2\mu}\big)^{1/2} \geq 1 - \frac{\beta-1}{4\mu}$ for $\beta \in [1, 2\mu{+}1]$. Together we found the estimate $\gamma(\beta) = U(\beta)/L(\beta) \leq 1{+}4\mu$ for $\beta > 1$.

Step 2: Similarly we may obtain an estimate on the interval $\beta \in]0,1[$ by keeping the upper bound for $L(\beta)$. For U we now estimate $\big(1+\frac{1-\beta}{2\mu}\big)^{1/2} \geq 1+\big((1+1/(2\mu))^{1/2}-1\big)(1-\beta)$ and obtain as above $U(\beta) \geq 4(1+\frac{1}{2\mu})(\beta-1)^2$. Thus we arrive at $\gamma(\beta) = U(\beta)/L(\beta) \geq \frac{8\mu(1+2\mu)}{1+4\mu}$ for $\beta \in [0,1]$. Since the bound for $\beta > 1$ gave a lower constant we arrive at the first lower bound, namely $\sigma_{\mathbb{G}}(2\mu^2+\mu) \geq \frac{8\mu(1+2\mu)}{1+4\mu}$.

Step 3: Since the lower bound in Step 2 vanishes for $\mu \to 0$, we improve the estimate for $\gamma(\beta)$ for $\beta \in]0,1[$. For this we use the rescaling $z = (1-\beta)/(2\mu)$ and need to consider $z \in]0, 1/(2\mu)[$. Again we write $\gamma(z) = U(z)/L(z)$ with

$$L(z) = F_1(1+z) + \tfrac{1}{\mu}F_1(1-2\mu z) \leq F_1(1+z) + 4\mu z^2 \leq \big(1+c_\mu\big)F_1(1+z)$$

where we used $F_1(u) \leq 2F_2(u) = (u-1)^2$. Moreover, since $z^2/F_1(1+z)$ increases for $z > 0$, we can choose $c_\mu = 1/\big(\mu F_1(1+\frac{1}{2\mu})\big)$ giving $c_\mu \to 0$ for $\mu \to 0_+$ and $c_\mu/\mu \to 8$ for $\mu \to \infty$. For $z \in]0, 1/(2\mu)[$ we have

$$\begin{aligned} U(z) &= \big(z + 4\mu z(1-\mu z)\big) \log \frac{1+z}{(1-2\mu z)^2} \;\geq\; \big(z + 4\mu z\tfrac{1}{2}\big)\big(\log(1+z) - 2\log(1-2\mu z)\big) \\ &\geq\; (1+2\mu)z\big(\log(1+z)+0\big) \geq (1+2\mu)F_1(1+z). \end{aligned}$$

Thus, for $0 < z < 1/(2\mu)$ we obtain $\gamma(z) = U(z)/L(z) \geq \frac{1+2\mu}{1+c_\mu}1+2\mu$, which strictly decreases from 1 at $\mu = 0$ to $1/4$ for $\mu \to \infty$.

Step 4: Combining Steps 2 and 3 gives the first assertion. The final estimate is obtained by a numerical comparison of the two functions. ■

4.4 The quadratic system with $\delta_v = 0$

We consider the same system as in Section 4.3, but now allow for $\delta_v = 0$ and show that it is possible to derive a decay estimate independent of $\delta_v \geq 0$. Thus, the system under consideration is

$$\dot{u} = \operatorname{div}\big(\delta \nabla u\big) + k(v^2-u), \quad \dot{v} = 2k(u-v^2). \tag{4.9}$$

We have the same equilibria $\boldsymbol{w}_q = (u_q, v_q)$ defined via $q = \mathbb{Q}\boldsymbol{w}_q = 2u_q + v_q$ and $u_q = v_q^2$ and the same free energy as above:

$$\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_q) = \int_\Omega \mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}_q)\,\mathrm{d}x \quad \text{with } \mathbb{H}(u,v|u_q,v_q) = u_q F_1(u/u_q) + v_q F_1(v/v_q).$$

Our main result is the following.

Theorem 4.5 *Assume that $r_u := \rho_{\mathrm{LSi}}(\delta) > 0$ and $k > 0$ in* (4.9)*. Then, for all $q > 0$ there exists $\lambda(q) > 0$ such that the solutions $\boldsymbol{c}$ of* (4.9) *with $\mathcal{Q}(\boldsymbol{c}(0)) = \mathbb{Q}\overline{\boldsymbol{c}}(0) = q$ satisfy*

$$\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_q) \leq \mathrm{e}^{-\lambda(q)t}\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_q) \quad \textit{for all } t > 0. \tag{4.10}$$

In particular, we have the explicit lower bound

$$\lambda(q) \geq \min\{r_u,\, 2k\}\min\{\, q/10\,,\, 7/100\,\} > 0.$$

We note that the asymptotic behavior of $\lambda(q)$ in the limits $q \to 0_+$ and $q \to \infty$ is optimal. Linearizing around the steady state $\boldsymbol{w}_q = (u_q, v_q) = (\mu^2, \mu)$ with $2\mu^2 + \mu = q$ gives the smallest nontrivial eigenvalue

$$\lambda_{\text{exact}}(q) = \frac{\widehat{r}}{2}\Big(1 + \widehat{\rho} + 4\mu - \big((1+\widehat{\rho}+4\mu)^2 - 4\widehat{\rho}\mu\big)^{1/2}\Big),$$

where $\widehat{\rho} = k/\widehat{r}$, and $\widehat{r}$ is the Poincaré constant (first nontrivial eigenvalue) of the operator $u \mapsto -\operatorname{div}\big(\delta\nabla u\big)$ with Neumann boundary conditions. Clearly, we have $\lambda_{\text{exact}}(q) = O(q)$ for $q \to 0$ and $\lambda_{\text{exact}}(q) \to \lambda_* > 0$ for $q \to \infty$.

Proof: The energy-dissipation balance leads to the estimate

$$-\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}) = \mathcal{D}(\boldsymbol{c}) = \int_\Omega \delta\tfrac{|\nabla u|^2}{u} + k\mathbb{G}(\boldsymbol{c}(x))\,\mathrm{d}x \;\geq\; \int_\Omega r_u\overline{u}F_1(u(x)/\overline{u}) + k\mathbb{G}(\boldsymbol{c}(x))\,\mathrm{d}x,$$

where $\mathbb{G}(u,v) = (v^2{-}u)\log(v^2/u)$. As in Sections 3.5 and 4.2 we define the auxiliary function

$$\Phi_\theta(u,v) = (1{-}\theta)rF_1(u) + k\mathbb{G}(u,v) - \theta rF_1(v).$$

Then the dissipation can be estimated from below via

$$\mathcal{D}(\boldsymbol{c}) \geq \int_\Omega r_uF_1(u){+}k\mathbb{G}(\boldsymbol{c})\,\mathrm{d}x{-}r_uF_1(\overline{u}) = \theta r_u\mathcal{H}(\boldsymbol{c}|\boldsymbol{w_q}){+}\int_\Omega \Phi_\theta(\boldsymbol{c}(x))\,\mathrm{d}x{+}\theta r_u\mathbb{F}(\boldsymbol{w}_q){-}r_uF_1(\overline{u}).$$

Thus, we have to find suitable lower bounds for Φ_θ^{**}, namely

$$\Phi_\theta^{**}(\boldsymbol{c}) + \theta r_u\mathbb{H}(\boldsymbol{w}_q) \geq r_uF_1(u) \quad \text{for all } \boldsymbol{c} = (u,v) \in \mathfrak{C}_q, \tag{4.11}$$

or the equivalent form (4.13) given below, which is obtained via simple rearrangements. Proposition 4.7, which is given below, guarantees, for each $q > 0$, the existence of a positive $\theta_*(q)$ such that the lower bound for $\Phi^{**}_{\theta_*(q)}$ holds. Hence, we can set $\lambda(q) = r_u\theta_*(q)$ and the existence of a positive decay rate is established.

To obtain the explicit lower bound, we set $\gamma = \min\{r_u, 2k\}$. Then, we can replace r_u and k in the above estimates by γ and $\gamma/2$, respectively. Hence we are in the situation $\rho = 1/\kappa = 2$ and can apply the explicit estimates stated at the end of Proposition 4.7. ∎

The estimate (4.11) (or equivalently (4.13) below) is derived using two different arguments. First, in Lemma 4.6 we show that for all (u,v) with $v > 0$ we have $\Phi_\theta^{**}(u,v) = \Phi_\theta(u,v)$ for sufficiently small θ depending on (u,v). Second we use that $\mathbb{G}(u,v) \to \infty$ for $uv \to 0$ while $u + v \geq c_0 > 0$.

Lemma 4.6 *Let $\rho = r_u/k = 1/\kappa$ and assume $\rho\kappa_* > 1$. Then for all $\boldsymbol{c} \in \,]0,\infty[^2$ there exists $\Theta(\rho,\boldsymbol{c})$ such that*

$$\theta \in [0,1] \text{ and } \rho\theta \leq \Theta((1{-}\theta)\rho, \boldsymbol{c}) \quad\Longrightarrow\quad \Phi_\theta^{**}(\boldsymbol{c}) = \Phi_\theta(\boldsymbol{c}). \tag{4.12}$$

Moreover, $\Theta(\rho,u,v) = v\Xi(\rho,u/v^2)$ with $\partial_\rho\Xi(\rho,z) \geq 0$ and $\xi(\rho) = \inf\{\,\Xi(\rho,z) \mid z > 0\,\} > 0$. Numerically, we find $\xi(3/2) \geq 1.3037$.

The proof of this result is given in Section A.2.

Proposition 4.7 *If $\rho\kappa_* > 1$, then*

$$\forall\, q>0\;\exists\,\theta_*>0\;\forall\,\boldsymbol{c}\in\mathfrak{C}_q:\quad \Phi^{**}_{\theta_*}(\boldsymbol{c})-(1{-}\theta_*)r_uF_1(u)+\theta_*r_uF_1(v)\geq\theta_*r_u\mathbb{H}(\boldsymbol{c}|\boldsymbol{w}_q). \tag{4.13}$$

In particular, if $\rho=1/\kappa=2$, we can choose $\theta_*=\min\{\,q/10\,,\,7/100\,\}$

Proof: Throughout we fix $q>0$, and consider $\boldsymbol{c}\in\mathfrak{C}_q=\{\,((q{-}v)/2,v)\mid v\in[0,q]\,\}$. Recall $(u_q,v_q)=(\mu^2,\mu)$ with $2\mu^2+\mu=q$.

Step 1: We fix a constant $\beta_0\in\,]0,1/2]$ to be optimized later. Restricting our attention to $(u,v)\in\mathfrak{C}_q$ with $v\geq\beta_0v_q$, we can use Lemma 4.6. Choose $\theta_1\in\,]0,1]$ such that

$$\theta_1\leq\beta_0v_q\,\xi\big((1{-}\theta_1)\rho\big)\leq\Theta((1{-}\theta_1)\rho,u,v),$$

then for all $\theta\in[0,\theta_1]$ we have $\Phi^{**}_\theta(\boldsymbol{c})=\Phi_\theta(\boldsymbol{c})$. Thus, condition (4.13) reduces to $k\mathbb{G}(\boldsymbol{c})\geq\theta r\mathbb{H}(\boldsymbol{c}|\boldsymbol{w}_q)$. With $\sigma_{\mathbb{G}}(q)$ defined in (4.4) we obtain

$$\forall\,(u,v)\in\mathfrak{C}_q\text{ with }v\geq\beta_0v_q:\ \text{(4.13) holds for }0\leq\theta\leq\theta_2:=\min\{\theta_1,\kappa\sigma_{\mathbb{G}}(q)\}. \tag{4.14}$$

Step 2: To estimate $\Phi_\theta(u,v)$ from below for small v, we do not use convexity but coercivity, namely $\mathbb{G}(u,v)\to\infty$ for $v\to0+$. With $\eta:=1+\rho/4$ we have

$$\begin{aligned}\frac{1}{r}\Phi_\theta(\boldsymbol{c})&=(1{-}\eta\theta)\big(F_1(u)+\frac{1}{\rho}\mathbb{G}(\boldsymbol{c})\big)+\theta\big(\eta F_1(u)+\frac{\eta}{\rho}\mathbb{G}(\boldsymbol{c})-F_1(v)\big)\\&\geq(1{-}\eta\theta)\phi_{\min\{\kappa_*,1/\rho\}}(\boldsymbol{c})+0\end{aligned}$$

where we used (4.6) and the definition of η to obtain the last 0. Since ϕ_κ is convex for $0\leq\kappa\leq\kappa_*$, we obtain $\frac{1}{r}\Phi^{**}_\theta(\boldsymbol{c})\geq(1{-}\eta\theta)F_1(u)+(1{-}\eta\theta)\min\{\kappa_*,1/\rho\}\mathbb{G}(\boldsymbol{c})$. Thus, using the equivalent form (4.11) we see that (4.13) is a consequence of

$$(1{-}\eta\theta)\mathbb{G}(\boldsymbol{c})\geq\theta(1{+}\eta)\rho F_1(u). \tag{4.15}$$

We establish this estimate for $(u,v)=(\mu^2{+}\mu(1{-}\beta)/2,\beta\mu)\in\mathfrak{C}_q$ where $\mu=v_q$ and $0\leq\beta\leq\beta_0\leq1/2$. For these (u,v) we find the estimates

$$\begin{aligned}&F_1(u)\leq\max\{1,F_1(q/2)\},\\&\mathbb{G}(\boldsymbol{c})=(u{-}v^2)\log(u/v^2)=\big(\mu^2{+}\tfrac{\mu}{2}(-\beta){-}\beta^2\mu^2\big)\log\big((2\mu{+}1{-}\beta)/(2\mu\beta^2)\big)\\&\qquad\geq\frac{3\mu^3{+}\mu}{4}\log(1/\beta^2)\ \geq\ \frac{q}{2}\log(1/\beta).\end{aligned}$$

Hence choosing $\theta_3>0$ such that $(1{-}\eta\theta_3)\frac{q}{2}\log(1/\beta_0)\geq\theta_3(1{+}\eta)\rho\max\{1,F_1(q/2)\}$, condition (4.15), and hence (4.13) for the appropriate $\boldsymbol{c}\in\mathfrak{C}_q$, is satisfied for $\theta\in[0,\theta_3]$.

Step 3: Summarizing Steps 1 to 3 for $\beta_0=1/2$, we have already constructed one desired θ_*, namely $\theta_*=\min\{\theta_1,\theta_2,\theta_3\}$.

Step 4: We finally optimize β_0 for the case $\rho = 2$ and provide a more explicit bound for θ. We assume $\theta \le 1/4$ such that $(1-\theta)\rho \ge 3/2$. With $\xi(3/2) \ge 1.3$ (see the end of Section A.2) and $\sigma_{\mathbb{G}}(q) \ge 2/5$ (cf. Proposition 4.4), Step 1 leads to the bound

$$\theta_2 = \min\{\tfrac{1}{4}\,,\, \beta_0 v_q 1.3\,,\, \tfrac{1}{2}\tfrac{2}{5}\} = \tfrac{1}{10}\min\{2, 13\beta_0 v_q\}.$$

Using $\eta = 3/2$ and $\theta_3 \le 1/5$ the condition of Step 3 gives $\theta \le \theta_3 := \frac{7\,q\log(1/\beta_0)}{100\max\{1,F_1(q/2)\}}$.

Now, we are in the situation where we can optimize with respect to β_0, since θ_3 improves for smaller β_0 while θ_2 deteriorates. For $q \le 3$ we have $F_1(q/2) \le 1$ and $\mu \le 1$, which implies $\mu = v_q \ge m/3$. Thus, choosing $\beta_0 = 0.234$, both bounds involving β_0 can be estimated from below by $q/10$, i.e. we can choose $\theta_* := \min\{1/5, q/10\}$ for $q \le 3$.

For $q \ge 3$ we choose $\beta_0 = 1/(10\sqrt{q})$. Using $v_q = \mu \ge \sqrt{q/3}$ we first obtain $\theta_2 \ge 0.075$. Moreover, we have $\theta_3 = \frac{7\,q\log(10\sqrt{q})}{100\max\{1,F_1(q/2)\}} \ge 7/100$ for all $q \ge 3$. Thus, we found the bound $\theta_* = 7/100$ for all $q \ge 3$, and the result is established. ∎

5 Possible further applications

Finally, we give a outlook to further models which might be attacked by the theory developed in this paper.

5.1 Inhomogeneous reaction-diffusion systems

We now consider reaction-diffusion systems with inhomogeneous coefficients, also called *heterostructures* in [GIH97]. In this case the equilibrium states $\boldsymbol{w_q}$ will be functions on Ω that are strongly related to the local thermodynamic equilibrium density $\boldsymbol{w}^{\mathrm{eq}} : \Omega \to]0,\infty[^I$ which is considered to be given as material datum. We may allow for the situation that Ω is unbounded, but we always assume that

$$\overline{\boldsymbol{w}}^{\mathrm{eq}} = \int_\Omega \boldsymbol{w}^{\mathrm{eq}}(x)\,\mathrm{d}x \in]0,\infty[^I$$

is finite. In particular, we will no longer use the normalization $|\Omega| = 1$, but we will normalize with respect to $\boldsymbol{w}^{\mathrm{eq}}$.

As before, the relative density is defined via $\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\mathrm{eq}}) = \int_\Omega \mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}^{\mathrm{eq}}(x))\,\mathrm{d}x$ and the equilibria $\boldsymbol{w_q}$ are again defined via

$$\boldsymbol{w_q} = \text{argmin}\{\, \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\mathrm{eq}}) \mid \mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} = \boldsymbol{q} \,\} \text{ for } \boldsymbol{q} \in \mathfrak{C}.$$

The strict convexity of $\mathcal{H}(\cdot|\boldsymbol{w}^{\mathrm{eq}})$ shows that $\boldsymbol{w_q}$ is well defined. By the Lagrange multiplier rule for constraint minimizers we find that there is a constant vector $\lambda_{\boldsymbol{q}} \in \mathbb{R}^m$ such that

$$\boldsymbol{w_q}(x) = \mathrm{e}^{\mathbb{Q}^\mathsf{T}\lambda_{\boldsymbol{q}}}\boldsymbol{w}^{\mathrm{eq}}(x), \quad \text{i.e. } \Big(\log\big(w_{\boldsymbol{q},i}(x)/w_i^{\mathrm{eq}}(x)\big)\Big)_{i=1,..,I} = \mathbb{Q}^\mathsf{T}\lambda_{\boldsymbol{q}} = \text{const.} \tag{5.1}$$

As in the previous case, where $\boldsymbol{w}^{\rm eq}$ was constant and normalized to $(1,..,1)$, we have the following identities:

$$\mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} = \boldsymbol{q} \quad \Longrightarrow \quad \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}) = \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\rm eq}) - \mathcal{H}(\boldsymbol{w}_{\boldsymbol{q}}|\boldsymbol{w}^{\rm eq}), \tag{5.2a}$$

$$\mathcal{H}(\boldsymbol{c}|\tfrac{\overline{\boldsymbol{c}}}{\overline{\boldsymbol{w}}^{\rm eq}}\boldsymbol{w}^{\rm eq}) = \mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\rm eq}) - \mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}^{\rm eq}), \tag{5.2b}$$

$$\mathcal{H}(\boldsymbol{w}_{\boldsymbol{q}}|\boldsymbol{w}^{\rm eq}) = \mathbb{H}(\overline{\boldsymbol{w}}_{\boldsymbol{q}}|\overline{\boldsymbol{w}}^{\rm eq}) = \min\{\, \mathbb{H}(\boldsymbol{a}|\overline{\boldsymbol{w}}^{\rm eq}) \mid \boldsymbol{a} \in [0,\infty[^I,\ \mathbb{Q}\boldsymbol{a} = \boldsymbol{q}\,\}. \tag{5.2c}$$

For the last relation we essentially use (5.1). In (5.2b) the concentration vector $\frac{\overline{\boldsymbol{c}}}{\overline{\boldsymbol{w}}^{\rm eq}}\boldsymbol{w}^{\rm eq}$ means $\big(\frac{\overline{c}_i}{\overline{w}_i^{\rm eq}} w_i^{\rm eq}(x)\big)_{i=1,..,I}$.

Following the analysis and modeling in [GGH96, GlH97, Gli04, Mie11] we consider the RDS given as the gradient system

$$\dot{\boldsymbol{c}} = -\mathcal{K}(\boldsymbol{c})\mathrm{D}_{\boldsymbol{c}}\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\rm eq}) \tag{5.3}$$

where the Onsager operator consists of a diffusion part and a reaction part:

$$\mathcal{K}(\boldsymbol{c})\boldsymbol{\xi} = -\Big(\operatorname{div}\big(a_i c_i \nabla \xi_i\big)\Big)_{i=1,..,I} + \mathbb{K}(x,\boldsymbol{c})\boldsymbol{\xi} \qquad \text{with}$$

$$\mathbb{K}(x,\boldsymbol{c}) = \sum_{r=1}^{R} k_r(x,\boldsymbol{c})\Lambda\big(\tfrac{\boldsymbol{c}^{\boldsymbol{\alpha}^r}}{\boldsymbol{w}^{\rm eq}(x)^{\boldsymbol{\alpha}^r}}, \tfrac{\boldsymbol{c}^{\boldsymbol{\beta}^r}}{\boldsymbol{w}^{\rm eq}(x)^{\boldsymbol{\beta}^r}}\big)(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r)\otimes(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r),$$

where $\Lambda(\mu,\nu) = \frac{\mu-\nu}{\log(\mu/\nu)}$, see [Mie11, GlM12]. We find the RDS

$$\dot{\boldsymbol{c}} = \operatorname{div}\Big(a_i w_i^{\rm eq}\nabla\big(c_i/w_i^{\rm eq}\big)\Big)_{i=1,..,I} - \boldsymbol{R}(x,\boldsymbol{c}) \text{ with } \boldsymbol{R}(x,\boldsymbol{c}) = \mathbb{K}(x,\boldsymbol{c})\big(\log(c_i/w_i^{\rm eq})\big)_{i=1,..,I}.$$

Here the detailed-balance condition is already built into $\boldsymbol{R}$ via the matrix $\mathbb{K}$.

Since $\mathcal{Q}(\boldsymbol{c}(t)) = \mathcal{Q}(\boldsymbol{c}(0)) = \boldsymbol{q}$ we can use (5.2a) and obtain the entropy balance

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}) = -\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}^{\rm eq}) = \mathcal{D}_{\text{diff}}(\boldsymbol{c}) + \mathcal{D}_{\rm R}(\boldsymbol{c}),$$

$$\text{where } \mathcal{D}_{\text{diff}}(\boldsymbol{c}) = \sum_{i=1}^{I}\mathcal{D}_i(c_i) \text{ with } \mathcal{D}_i(c_i) := \int_\Omega \tfrac{a_i (w_i^{\rm eq})^2}{c_i}\big|\nabla\big(\tfrac{c_i}{w_i^{\rm eq}}\big)\big|^2\,\mathrm{d}x$$

$$\text{and } \mathcal{D}_{\rm R}(\boldsymbol{c}) = \int_\Omega \boldsymbol{G}\big(x,\boldsymbol{c}(x)/\boldsymbol{w}^{\rm eq}(x)\big)\,\mathrm{d}x \text{ with } \boldsymbol{G}(x,\boldsymbol{v}) := \mathbf{log}\,\boldsymbol{v}\cdot\mathbb{K}(x,\boldsymbol{c})\,\mathbf{log}\,\boldsymbol{v}.$$

The dissipation obtained from diffusion can again be estimated from below by a suitable version of the log-Sobolev inequality. For this we must assume that all the probability densities $\zeta_i = \frac{1}{\overline{w}_i^{\rm eq}}w_i^{\rm eq} \in \mathrm{L}^1(\Omega)$ satisfy a log-Sobolev estimate, namely

$$\int_\Omega \frac{1}{v(x)}|\nabla v(x)|^2\zeta_i(x)\,\mathrm{d}x \geq \widehat{\rho_{\rm LSi}}(\zeta_i)\int_\Omega \mathbb{H}(v(x)|\langle v\rangle_{\zeta_i})\zeta_i(x)\,\mathrm{d}x \text{ for smooth } v>0, \tag{5.4}$$

where $\langle v\rangle_{\zeta_i} = \int_\Omega v(x)\zeta_i(x)\,\mathrm{d}x$ is the average with respect to the probability measure $\zeta_i\,\mathrm{d}x$. Now, setting $v = c_i/w_i^{\rm eq}$ in the definition of $\mathcal{D}_i$ and using the identity $\langle v\rangle_{\zeta_i} = \overline{c}_i/\overline{w}_i^{\rm eq}$, we obtain the estimate

$$\mathcal{D}_i(c_i) \geq \overline{w}_i^{\rm eq}\inf_{x\in\Omega}a_i(x)\ \int_\Omega \frac{1}{v}|\nabla v|^2\zeta_i\,\mathrm{d}x \geq \widehat{r}_i\int_\Omega \mathbb{H}(v|\langle v\rangle_{\zeta_i})\zeta_i\,\mathrm{d}x = \frac{\widehat{r}_i}{\overline{w}_i^{\rm eq}}\int_\Omega \mathbb{H}\big(c_i|\tfrac{\overline{c}_i}{\overline{w}_i^{\rm eq}}\big)\,\mathrm{d}x,$$

where we used $w_i^{\rm eq} = \overline{w}_i^{\rm eq}\zeta_i$ and the 1-homogeneity $\mathbb{H}(a|b)\zeta = \mathbb{H}(\zeta a|\zeta b)$ for the last identity. Adding up the different components we obtain the vector-valued log-Sobolev inequality

$$\mathcal{D}_{\sf diff}(\boldsymbol{c}) \geq r\mathcal{H}\big(\boldsymbol{c}|\tfrac{\overline{\boldsymbol{c}}}{\overline{\boldsymbol{w}}^{\rm eq}}\boldsymbol{w}^{\rm eq}\big) \quad \text{with } r := \min\{\,\widehat{\rho_{\rm LSi}}(\tfrac{w_i^{\rm eq}}{\overline{w}_i^{\rm eq}}) \inf_{x\in\Omega} a_i(x) \mid i = 1,..,I\,\}.$$

We are now in the position of mimicking the approach in Section 3.3, where we still have to use the final ingredient, namely a suitable generalization of Jensen's inequality allowing us to extract information about $\overline{\boldsymbol{c}}$ from pointwise estimates over the whole domain Ω. Using $\mathcal{Q}(\boldsymbol{c}) = \mathbb{Q}\overline{\boldsymbol{c}} = \boldsymbol{q}$, the relations (5.2) give the identity

$$\begin{aligned} &r\mathcal{H}(\boldsymbol{c}|\tfrac{\overline{\boldsymbol{c}}}{\overline{\boldsymbol{w}}^{\rm eq}}\boldsymbol{w}^{\rm eq}) = r\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\rm eq}) - r\mathbb{H}(\overline{c}|\overline{\boldsymbol{w}}^{\rm eq}) \\ &= (r{-}\mu\theta)\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}_{\boldsymbol{q}}) - (r{-}\mu\theta)\mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}_{\boldsymbol{q}}) + \theta\big(\mu\mathcal{H}(\boldsymbol{c}|\boldsymbol{w}^{\rm eq}) - \mu\mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}^{\rm eq})\big) \end{aligned}$$

for all $\mu \geq 0$ and $\theta \in \,]0,1]$. Thus, after adding the dissipation from the reactions, namely $\mathcal{D}_{\rm R}$, we need to find $s_\mu(\boldsymbol{q})$ such that

$$\mathcal{Q}(\boldsymbol{c}) = \boldsymbol{q} \implies \int_\Omega \mu\mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}^{\rm eq}(x)){+}\boldsymbol{G}\big(x, \tfrac{\boldsymbol{c}(x)}{\boldsymbol{w}^{\rm eq}(x)}\big)\,{\rm d}x{-}\mu\mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}^{\rm eq}) \geq s_\mu(\boldsymbol{q})\mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}_{\boldsymbol{q}}).$$

Then, we obtain the decay rate $\widehat{\lambda}(\boldsymbol{q})$ as in Theorem 3.1.

In the case that $\boldsymbol{w}^{\rm eq}$ is spatially homogeneous, we could use Jensen's inequality for the convexification of the integrand. For nonconstant $\boldsymbol{w}^{\rm eq}$ it is not obvious how convexification can be used in general. However, there is one case where we can still use Jensen's inequality but now for a measure associated to $\boldsymbol{w}^{\rm eq}$. We assume that

$$\boldsymbol{w}^{\rm eq}(x) = \zeta(x)\overline{\boldsymbol{w}}^{\rm eq} \text{ for some } \zeta \in {\rm L}^1(\Omega),\ \zeta \geq 0, \int_\Omega \zeta\,{\rm d}x = 1. \tag{5.5}$$

As in all the previous sections, there is no loss in generality by assuming $\overline{\boldsymbol{w}}^{\rm eq} = (1,..,1)$. For the vector of relative densities $\boldsymbol{v} = \boldsymbol{c}/\boldsymbol{w}^{\rm eq}$, we have

$$\mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}^{\rm eq}(x)) = \mathbb{F}(\boldsymbol{v}(x))\zeta(x), \quad \text{where as before } \mathbb{F}(\boldsymbol{a}) = \mathbb{H}(\boldsymbol{a}|(1,..,1)).$$

Similarly, we can assume that the reaction rates $k_r(x,\boldsymbol{c})$ satisfy a lower bound $k_r(x,\boldsymbol{c}) \geq \underline{k}_r\zeta(x)$ for all $x \in \Omega$ and all $\boldsymbol{c}$, where $\underline{k}_r > 0$. Then, we find the lower estimate

$$\boldsymbol{G}(x,\boldsymbol{v}) \geq \zeta(x)\mathbb{G}(\boldsymbol{v}) \tag{5.6}$$

for a suitable function $\mathbb{G}$ satisfying the properties in Section 3.3. Applying Jensen's inequality to the probability measure $\zeta\,{\rm d}x$ and $\Phi_\mu(\boldsymbol{v}) := \mu\mathbb{F}(\boldsymbol{v}) + \mathbb{G}(\boldsymbol{v})$ yields

$$\int_\Omega \mu\mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}^{\rm eq}(x)) + \boldsymbol{G}\big(x, \tfrac{c_i(x)}{w_i^{\rm eq}(x)}\big)\,{\rm d}x \geq \int_\Omega \Phi_\mu(\boldsymbol{v}(x))\zeta(x)\,{\rm d}x \geq \Phi_\mu^{**}\Big(\textstyle\int_\Omega \boldsymbol{v}\zeta\,{\rm d}x\Big).$$

In particular, assuming that Φ_μ is convex and using $\int_\Omega \boldsymbol{v}\zeta\,{\rm d}x = \overline{\boldsymbol{c}}$, we find

$$\int_\Omega \mu\mathbb{H}(\boldsymbol{c}(x)|\boldsymbol{w}^{\rm eq}(x)) + \boldsymbol{G}\big(x, \tfrac{c_i(x)}{w_i^{\rm eq}(x)}\big)\,{\rm d}x - \mu\mathbb{H}(\overline{\boldsymbol{c}}|\overline{\boldsymbol{w}}^{\rm eq}) \geq \mu\mathbb{F}(\overline{\boldsymbol{c}}) + \mathbb{G}(\overline{\boldsymbol{c}}) - \mu\mathbb{F}(\overline{\boldsymbol{c}}) = \mathbb{G}(\overline{\boldsymbol{c}}).$$

Thus, imposing the three assumptions (5.4), (5.5), and (5.6), we see that the convexification theory of Section 3.3 can be transferred to the case of inhomogeneous thermodynamic equilibrium states $\boldsymbol{w}^{\mathrm{eq}}$, providing explicit decay rates. It would be interesting to generalize the rather restrictive assumption (5.5). By the compactness theory developed in [GGH96, GlH97, Gli04] it is clear that under natural conditions the decay rates $\lambda(\boldsymbol{q})$ are positive even in the general case of inhomogeneous $\boldsymbol{w}^{\mathrm{eq}}$.

5.2 A semiconductor model

We conjecture that the theory may be applied to the semiconductor model without electrostatic potential, namely

$$\begin{aligned} \dot{u} &= \delta_u \Delta u + k(1{-}uv), \\ \dot{v} &= \delta_v \Delta v + k(1{-}uv). \end{aligned} \tag{5.7}$$

The conserved quantity is

$$\mathcal{Q}(\boldsymbol{c}) = \int_\Omega u(x) - v(x)\,\mathrm{d}x = \mathbb{Q}(\overline{u}, \overline{v}) = \overline{u} - \overline{v}.$$

The main difference is now that $\mathfrak{C}_q$ is not compact. The equilibria are defined via

$$\boldsymbol{w}_q = (u_q, v_q) \quad \text{with } u_q - v_q = q \text{ and } u_q v_q = 1.$$

Writing $\mathbb{G}(u,v) = (uv{-}1)\log(uv)$ we have

$$\sigma_{\mathbb{G}}(m) := \inf\Big\{ \frac{\mathbb{G}(u,v)}{\mathbb{H}(u,v|\boldsymbol{w}_q)} \,\Big|\, (u,v) \in \mathfrak{C}_q,\ (u,v) \neq \boldsymbol{w}_q \Big\} > 0.$$

There is hope that the theory can be applied even in this case where $\mathfrak{C}_q$ is not compact. However, the main challenge would be to include the electrostatic interaction as was done in [GGH96, GlH97, Gli04]. However, it is not clear how the log-Sobolev inequality can be used for this situation.

5.3 A system with three concentrations

One may apply the theory to the reaction model currently investigated by Desvillettes & Fellner, namely

$$\begin{aligned} \dot{u} &= \delta_u \Delta u \ + k\alpha(w^\gamma {-} u^\alpha v^\beta), \\ \dot{v} &= \delta_v \Delta v \ + k\beta(w^\gamma {-} u^\alpha v^\beta), \\ \dot{w} &= \delta_w \Delta w - k\gamma(w^\gamma {-} u^\alpha v^\beta). \end{aligned} \tag{5.8}$$

Here α, β, and γ are positive exponents. The conserved quantities for $\boldsymbol{c} = (u,v,w)$ are

$$\mathcal{Q}(\boldsymbol{c}) = \int_\Omega \mathbb{Q}\boldsymbol{c}(c)\,\mathrm{d}x = \mathbb{Q}\overline{\boldsymbol{c}} \quad \text{with } \mathbb{Q} = \begin{pmatrix} \gamma & 0 & \alpha \\ 0 & \gamma & \beta \end{pmatrix}.$$

Now the sets $\mathfrak{C}_{\boldsymbol{q}}$ are compact, viz. $\mathfrak{C}_{\boldsymbol{q}} = \{\, \frac{1}{\gamma}(q_1{-}\alpha w, q_2{-}\beta w, \gamma w) \mid w \in [0, \min\{\frac{q_1}{\alpha}, \frac{q_2}{\beta}\}]\,\}$. Moreover, there are no steady states on the boundary of $[0,\infty[^3$, which implies that $\boldsymbol{w}_{\boldsymbol{q}}$ is the only steady state in $\mathfrak{C}_{\boldsymbol{q}}$. Hence, the theory of Section 3.3 applies.

However, it remains a highly nontrivial task to derive explicit estimates for $\lambda(\boldsymbol{q})$. The major difficulty will be to characterize the convexification Φ_μ^{**} of

$$\Phi_\mu : \boldsymbol{a} \mapsto \mu\mathbb{F}(\boldsymbol{a}) + \mathbb{G}(\boldsymbol{a}) \quad \text{with } \mathbb{G}(u,v,w) = (u^\alpha v^\beta {-} w^\gamma)\big(\log(u^\alpha v^\beta){-}\log w^\gamma\big).$$

Nevertheless the arguments in Section 3.3 imply the following result.

Theorem 5.1 *For each $\boldsymbol{q} \in \mathrm{im}^+\mathbb{Q} =]0,\infty[^2$ there exists $\lambda(\boldsymbol{q}) > 0$ such that the solutions $\boldsymbol{c}(t)$ of* (5.8) *with $\mathcal{Q}(\boldsymbol{c}(0)) = \boldsymbol{q}$ satisfy*

$$\mathcal{H}(\boldsymbol{c}(t)|\boldsymbol{w}_{\boldsymbol{q}}) \leq \mathrm{e}^{-\lambda(\boldsymbol{q})t}\mathcal{H}(\boldsymbol{c}(0)|\boldsymbol{w}_{\boldsymbol{q}}) \quad \textit{for all } t > 0.$$

5.4 A temperature-dependent model

Following [HMM13] it would be interesting to study a simplified system where one species X_c with density c can be absorbed by or released from the background. The equilibrium density w for c depends on the temperature θ. Following the arguments in [AGH02, Mie11, LiM12, Mie13] we formulate the system as a gradient flow driven by minus the physical entropy. We use using the density c (of the non-absorbed species) and the internal energy u as the dependent variables, rather than the temperature θ. The coupled system reads

$$\dot c = \delta\Delta c - k(c,u)(c{-}w(u)), \quad \dot u = \delta\Delta u \quad \text{in } \Omega, \qquad \nabla c\cdot\nu = \nabla u\cdot\nu = 0 \text{ on } \partial\Omega. \quad (5.9)$$

Clearly, the only conserved quantity is the total energy $\mathcal{Q}(c,u) = \overline{u} = q$. Obviously, there is a unique steady state for each q, namely $\boldsymbol{w}_q = (w(q), q)$.

The physical entropy is $\mathcal{S}(c,u) = \int_\Omega S(c(x),u(x))\,\mathrm{d}x$ and the Onsager operator is

$$\mathcal{K}(c,u)\boldsymbol{\xi} = -\,\mathrm{div}\,\Big(\delta(-\mathrm{D}^2S(c,u)^{-1})\nabla\boldsymbol{\xi}\Big) + \begin{pmatrix}\kappa(c,u) & 0\\ 0 & 0\end{pmatrix}\boldsymbol{\xi},$$

where we assume, in accordance with physical requirements, that the entropy density S is a strictly concave function of the extensive variables c and u. Hence, the Einstein relation for the mobility tensor $\mathbb{M}(c,u) = -\delta\mathrm{D}^2S(c,u)^{-1}$ gives a positive definite mobility. Then, (5.9) has the form $\partial_t(c,u) = \mathcal{K}(c,u)\mathrm{D}\mathcal{S}(c,u)$ if S and $\kappa > 0$ are chosen appropriately. In fact, we can choose $S(c,u) = s_0u^\sigma - w(u)F_1(c/w(u))$ with $w(u) = w_0u^\gamma$, and $\kappa(c,u) = k(c,u)(c{-}w(u))/\log(c/w(u))$, where $w_0, s_0 > 0$ and $\sigma,\gamma \in]0,1[$, cf. [HMM13, Mie13].

For this system we define a nonstandard convex relative entropy

$$\widehat{\mathcal{F}}_q(c,u) := \int_\Omega s_1q^\sigma F_\sigma\Big(\frac{u(x)}{q}\Big) + w(u(x))F_1\Big(\frac{c(x)}{w(u(x))}\Big)\,\mathrm{d}x \quad \text{with } s_1 = s_0\sigma(1{-}\sigma)$$

and F_σ from (3.1). Hence, we have $\widehat{\mathcal{F}}_q(c,u) = -\mathcal{S}(c,u) + c_0 + c_1\overline{u}$ and $\widehat{\mathcal{F}}_q(c,u) \geq 0$ with equality if and only if $(c,u) \equiv \boldsymbol{w}_q$.

To see the structure of the dissipation estimate we use Hessian of S given via

$$-\mathrm{D}^2 S(c,u) = \begin{pmatrix} \frac{1}{c} & -\frac{\gamma}{u} \\ -\frac{\gamma}{u} & \frac{c\gamma}{u^2} \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \frac{s_2}{u^{2-\sigma}} - \frac{w_2}{u^{2-\gamma}} \end{pmatrix} \text{ with } \begin{array}{l} s_2 = s_0\sigma(1-\sigma), \\ w_2 = w_0\gamma(1-\gamma). \end{array}$$

To proceed further we recall that $w(u) = w_0 u^\gamma$ was considered to be given by the system (5.9). However, we are able to choose $s_0 = 2w_0$ and $\sigma = \gamma$. Then, we can estimate $-\mathrm{D}^2 S(u,c)$ from below by $-\binom{\xi}{\eta} \cdot \mathrm{D}^2 S(c,u)\binom{\xi}{\eta} \geq \frac{1-\gamma}{c}\xi^2 + \frac{w_2}{u^{2-\gamma}}\eta^2$ and the dissipation satisfies

$$\begin{aligned} \mathcal{D}(c,u) &\geq \int_\Omega (1-\gamma)\delta\tfrac{|\nabla c|^2}{c} + w_2\delta\tfrac{|\nabla u|^2}{u^{2-\gamma}} + \mathbb{G}(c,u)\,\mathrm{d}x, \quad \mathbb{G}(c,u) = k(c,u)\Lambda(w(u),c) \\ &\geq \int_\Omega r_c F_1(c) + r_u q^\sigma F_{\widehat{\gamma}}\big(\tfrac{u}{q}\big) + \mathbb{G}(c,u)\,\mathrm{d}x - r_c F_1(\overline{c}), \end{aligned}$$

where $r_c = \rho_{\mathrm{LSi}}(\delta) = \delta\rho(\Omega,1,1)$ and $r_u = \delta\rho(\Omega,\gamma,\widehat{\gamma})$, cf. (3.6). The hope is that there exists some $\widehat{\gamma} \geq \gamma$ such that $r_u > 0$ and that the last integrand provides an upper bound for a small multiple of $\widehat{\mathcal{F}}_q$. This will be considered in subsequent work.

A Appendices

A.1 Proof of Lemma 4.3

Proof: For deriving the lower bound (4.6) we use $F_1(z) \geq \frac{1}{2}F_{1/2}(z) = (\sqrt{z}-1)^2$ and $\mathbb{G}(u,v) \geq 4(v-\sqrt{u})^2$ to obtain

$$F_1(u) + \kappa\mathbb{G}(u,v) \geq (\sqrt{u}-1)^2 + 4\kappa(v-\sqrt{u})^2 \geq \tfrac{4\kappa}{1+4\kappa}(v-1)^2,$$

where we have minimized explicitly with respect to $\sqrt{u}$. The estimate follows using $(z-1)^2 = 2F_2(z) \geq F_1(z)$.

For the analysis of the convexity the basic observation is that ϕ_κ has the scaling property

$$\phi_\kappa(s^2u, sv) = s^2\phi_\kappa(u,v) + 2s^2 u\log s + 1 - s^2,$$

which follows from $\mathbb{G}(s^2u, sv) = s^2\mathbb{G}(u,v)$ and (3.3). Since this scaling is affine in (u,v,ϕ) (for each s), this property is inherited by the convexification ϕ_κ^{**}. Introducing $h_\kappa(z) = \phi_\kappa(z,1)$ and $g_\kappa(z) = \phi_\kappa^{**}(z,1)$, we have the representations

$$\phi_\kappa(u,v) = v^2 h_\kappa(u/v^2) + 2u\log v + 1 - v^2, \tag{A.1}$$

$$\phi_\kappa^{**}(u,v) = v^2 g_\kappa(u/v^2) + 2u\log v + 1 - v^2, \tag{A.2}$$

A direct calculation of $\mathrm{D}^2\phi_\kappa^{**}$ shows that ϕ_κ^{**} defined as in (A.2) is convex if and only if

$$g_\kappa''(z) \geq 0 \text{ and } g_\kappa''(z)\big(g_\kappa(z) - z g_\kappa'(z) + 3z - 1\big) \geq 2. \tag{A.3}$$

Inserting $h_\kappa : z \mapsto F_1(z) + \kappa(z-1)\log z$ into this criterion one obtains convexity of ϕ_κ for $\kappa \in [0,\kappa_*]$ with $\kappa_* \approx 0.8564998142$, where at $z \approx 12.683$ the second criterion in (A.3) holds with equality. In fact, for h_κ the second criterion in (A.3) can be rewritten, after dividing by $\kappa > 0$, in the form

$$z^2 + 3z - z\log z \geq \kappa\big(z^2 - 1 + (1{+}z)\log z\big) \quad \text{for all } z > 0.$$

Using $\log z \leq \log 3 + z/3 - 1$ it is easy to see that the estimate holds for $\kappa = 1/2$, and we conclude $\kappa_* \geq 1/2$. Moreover, since the right-hand side is positive for all $z > 0$ while the left-hand side is negative for $z < 1$, we have the explicit characterization

$$\kappa_* := \inf\{ \tfrac{z^2+3z-z\log z}{z^2-1+(1+z)\log z} \mid z > 1 \}.$$

For $\kappa \geq 1$ we obtain an upper bound on g_κ by estimating $g_\kappa(z) = \phi_\kappa^{**}(z,1)$ with $(1{-}\theta)\phi_\kappa(0,0){+}\theta\phi_\kappa(z/\theta, 1/\theta)$. Using $\phi_\kappa(0,0) = 1$, (A.1), and defining $r = 1/\theta > 1$, yields

$$g_\kappa(z) \leq r h_\kappa(z/r) + 2z\log r + 1 - r = h_\kappa(z) + \beta_\kappa(r,z).$$
$$\text{with } \beta_\kappa(r,z) = (rk{-}kz{+}z)\log r - k(r{-}1)\log z.$$

Analyzing $\beta_\kappa(\cdot, z)$ on the interval $[1,\infty[$, we find the following: Define Z_κ as in the statement of the lemma (where we use $\kappa \geq 1$); then $Z_1 = \mathrm{e}$ and $\kappa \mapsto Z_\kappa$ decreases monotonously with $Z_\infty = 1$. For $z \leq Z_\kappa$ we have $\beta_\kappa(r,z) \geq \beta_\kappa(1,z) = 0$. For $z > Z_\kappa$ the unique minimizer r of $\beta_\kappa(\cdot,z)$ is given as $r = z/Z_\kappa$. Thus, for $z > Z_\kappa$ we have

$$g_\kappa(z) \leq h_\kappa(z) + \beta_\kappa(z/Z_\kappa, z) = 2z\log z - B_\kappa + 1,$$

with B_κ as given in the statement of the lemma. Note that $B_1 = 1 + 1/\mathrm{e}$ and that $\kappa \mapsto B_\kappa$ decays monotonously with $B_\infty = 1$.

It remains to be shown that ϕ_κ^{**} in (A.2) with g_κ defined in (4.8) is convex. For this we check (A.3). For $z \geq Z_\kappa$ this is immediate, since the second estimate holds with equality. For $z \leq Z_\kappa$ we consider h_κ and obtain

$$a_\kappa(z) := h_\kappa''\big(h_\kappa - zh_\kappa'' + 3z - 1\big) - 2 = \frac{\kappa}{z^2}\Big(\kappa - \kappa z^2 + 3z + z^2 - \big(\kappa + z + \kappa z\big)\log z\Big).$$

For $z \leq 1$ we immediately have $a_\kappa(z) > 0$. For $z > 1$ we can rearrange to

$$a_\kappa(z) = \frac{\kappa}{z^2}\,(1{+}z)(z{+}\log z{-}1)\big(f_1(z)f_2(z) - \kappa\big)$$
$$\text{with } f_1(z) = \tfrac{z}{z+\log z-1} \text{ and } f_2(z) = \tfrac{3+z-\log z}{1+z}.$$

We have $f_2(z) \geq \frac{2+\mathrm{e}}{1+\mathrm{e}} > 1.268$ for $z \in [1, \mathrm{e}]$. Moreover $f_1'(z) < 0$ for $z > 1$ which gives, for all $z \in [1, Z_\kappa]$ the estimate $f_1(z) \geq f_1(Z_k) = \kappa$. Using $Z_\kappa \leq \mathrm{e}$ we obtain $f_1(z)f_2(z) - \kappa \geq 0.268\kappa > 0$ and conclude $a_\kappa(z) > 0$. Thus, the convexity of ϕ_κ^{**} given in (4.8) is established, and Lemma 4.3 is proved. ■

A.2 Proof of Lemma 4.6

Proof: We have to show that for each $\boldsymbol{a} = (a,b)$ there exists $\Theta(\boldsymbol{a})$ such that $\Phi_\theta^{**}(\boldsymbol{a}) = \Phi_\theta(\boldsymbol{a})$ for $\theta \in [0, \Theta(\boldsymbol{a})]$. The argument relies on the fact that for $\theta < 1 - k/(r\kappa_*)$ the function

$\boldsymbol{c} \mapsto (1{-}\theta)rF_1(u) + k\mathbb{G}(\boldsymbol{c})$ is strictly convex and coercive. Hence subtracting $\theta F_2(v)$ with sufficiently small θ produces a function that still coincides with its lower convex hull in a large region. To be more precise, we have to show that Φ_θ lies above its Taylor polynomial $\mathrm{T}^1_{\boldsymbol{a}}\Phi_\theta$ of first order expanded in $\boldsymbol{a}$:

$$\big(\mathrm{T}^1_{\boldsymbol{a}}\Phi_\theta\big)(\boldsymbol{c}) := \Phi_\theta(\boldsymbol{a}) + \mathrm{D}\Phi_\theta(\boldsymbol{a})\cdot(\boldsymbol{c}{-}\boldsymbol{a}).$$

For this we use special relations for the entropy functions F_0 and F_1, namely

$$F_1(z) = \big(\mathrm{T}^1_w F_1\big)(z) + wF_1(z/w) \quad \text{and} \quad F_0(z) = \big(\mathrm{T}^1_w\big)F_0(z) + F_0(z/w).$$

For $\mathbb{G}(u,v) = \Gamma(u,v^2) = v^2\Gamma(u/v^2,1)$ we use the relation $\Gamma(z,1) = F_0(z) + F_1(z)$ and obtain

$$\mathbb{G}(u,v) = v^2\Big(F_1\big(\tfrac{a}{b^2}\big){+}F_0\big(\tfrac{a}{b^2}\big)\Big){+}\Big(F_1'\big(\tfrac{a}{b^2}\big){+}F_0'\big(\tfrac{a}{b^2}\big)\Big)\big(u{-}\tfrac{av^2}{b^2}\big){+}v^2\Big(\tfrac{a}{b^2}F_1\big(\tfrac{ub^2}{v^2a}\big){+}F_0\big(\tfrac{ub^2}{v^2a}\big)\Big).$$

Note that F_0, F_1, and $\mathbb{G}(\cdot,v)$ are convex functions, hence the last term in the expansion, which represents the remainder with respect to the first-order Taylor polynomial, is nonnegative and vanishes at $\boldsymbol{c} = \boldsymbol{a}$.

Thus, we obtain the decomposition of the remainder $\mathcal{R}$ for Φ_θ in the form

$$\begin{aligned}
&\mathcal{R}_{\boldsymbol{a}}(\boldsymbol{c}) := \tfrac{1}{k}\Big(\Phi_\theta(\boldsymbol{c}) - \big(\mathrm{T}^1_{\boldsymbol{a}}\Phi_\theta\big)(\boldsymbol{c})\Big) = M(\boldsymbol{a},v) + N_{(1-\theta)\rho}(\boldsymbol{a},u,v) - \theta\rho bF_1\big(\tfrac{v}{b}\big) \quad \text{with}\\
&M(\boldsymbol{a},v) := \big(\tfrac{v^2}{b^2}-1\big)\big(\mathbb{G}(\boldsymbol{a}){-}a\mathrm{D}_a\mathbb{G}(\boldsymbol{a})\big) - \mathrm{D}_b\mathbb{G}(\boldsymbol{a})(v{-}b) = \big(\mathbb{G}(\boldsymbol{a}){-}a\mathrm{D}_a\mathbb{G}(\boldsymbol{a})\big)\big(\tfrac{v}{b}{-}1\big)^2\\
&N_{\widetilde\rho}(\boldsymbol{a},u,v) := \widetilde\rho aF_1\big(\tfrac{u}{a}\big) + v^2\Big(\tfrac{a}{b^2}F_1\big(\tfrac{ub^2}{v^2a}\big){+}F_0\big(\tfrac{ub^2}{v^2a}\big)\Big) \geq 0.
\end{aligned}$$

To show positivity for all $\boldsymbol{c}$ we first minimize $N_\theta(\boldsymbol{a},u,v)$ with respect to u, which occurs in a convex manner. The assumption $\rho = 1/\kappa > 1/\kappa_*$ and the convexity of ϕ_κ (cf. Lemma 4.3) guarantee $M(\boldsymbol{a},v) + N_\theta(\boldsymbol{a},\boldsymbol{c}) \geq 0$. In particular, setting

$$\widehat n(\widetilde\rho,\boldsymbol{a},v) = \min\{\, N_{\widetilde\rho}(\boldsymbol{a},u,v) \mid u>0\,\} \geq 0$$

we obtain $M(\boldsymbol{a},v) + N_{\widetilde\rho}(\boldsymbol{a},\boldsymbol{c}) \geq M(\boldsymbol{a},v) + \widehat n(\widetilde\rho,\boldsymbol{a},v)$. Thus, we have $\mathcal{R}_{\boldsymbol{a}}(\boldsymbol{c}) \geq 0$ if $\rho\theta \in [0,\Theta((1{-}\theta)\rho,\boldsymbol{a})]$ where

$$\Theta(\widetilde\rho,\boldsymbol{a}) := \inf\Big\{\, \frac{M(\boldsymbol{a},v) + \widehat n(\widetilde\rho,\boldsymbol{a},v)}{bF_1(v/b)} \,\Big|\, v\geq 0,\ v\neq b\,\Big\}.$$

Since $\widehat n \geq 0$ and $M(\boldsymbol{a},v)$ grows quadratically with v, the infimum has to be achieved at a finite value of v. Since nominator and denominator are smooth functions and strictly positive for $v\neq b$, it suffices to control the behavior for $v\to b$.

Writing $w = a/b^2$ and $v = b{+}\delta$ we have

$$M(\boldsymbol{a},v) = \mu(w)\delta^2 \text{ with } \mu(w) = 1{-}\log w{-}w \quad \text{and} \quad \widehat n(\boldsymbol{a},v) = \frac{2(1{+}w)(\widetilde\rho w)}{1+w+\widetilde\rho w}\delta^2{+}O(|\delta|^3).$$

We see that $\mu(w) + \frac{2(1+w)(\widetilde{\rho}w)}{1+w+\widetilde{\rho}w} > 0$ for all $w > 0$ if and only if $\widetilde{\rho} > 1/\kappa_*$ with κ_* defined in Lemma 4.3. Thus, we have proved $\Theta(\widetilde{\rho}, \boldsymbol{a}) > 0$, but without an explicit lower bound.

From the definition of $\widehat{n}$ via $N_{\widetilde{\rho}}$ it is clear that $\partial_{\widehat{\rho}}\widehat{n} \geq 0$, which implies the monotonicity of $\Theta(\cdot, \boldsymbol{a})$. Using scaling arguments one finds $M(\boldsymbol{a}, v) + \widehat{n}(\boldsymbol{a}, v) = b^2\big(M(a/b^2, 1, v/b) + \widehat{n}(a/b^2, 1, v/b)\big)$. By scaling the denominator as well we obtain

$$\Theta(\widetilde{\rho}, a, b) = b\Xi(\widetilde{\rho}, a/b^2) \quad \text{with } \Xi(\widetilde{\rho}, w) = \Theta(\widetilde{\rho}, w, 1).$$

From $N_{\widetilde{\rho}} \geq 0$ we easily see

$$\Xi(\widetilde{\rho}, w) \geq \inf\{\, M(w, 1, v)/F_1(v) \,|\, v > 0\,\} = \mu(w) \inf\{\, (v{-}1)^2/F_1(v) \,|\, v > 0\,\} = \mu(w),$$

which gives a positive lower bound for $w < 1$. To see the behavior for $w \geq 1$ we express $\widehat{n}$ in terms of the Legendre transform γ_* of $\gamma(z) = (z{-}1)\log z$:

$$\gamma_*(\zeta) = \sup\{\, z\zeta - \gamma(z) \mid z > 0\,\}$$

Obviously $\gamma_* \in \mathrm{C}^\infty(\mathbb{R}; \mathbb{R})$ with $\gamma_*'(\zeta) > 0$ everywhere. The behavior is

$$\gamma_*(\zeta) \approx -\log|\zeta| \text{ for } \zeta \ll 1, \quad \gamma_*(0) = 0, \quad \gamma_*(\zeta) \approx \mathrm{e}^\zeta \text{ for } \zeta \gg 1.$$

Using the scaling laws for F_1 and F_0, see (3.4), we have

$$\alpha F_1(s) + F_0(s) = F_1(\alpha s) + F_0(\alpha s) - s(\alpha \log a + \alpha - 1) + \alpha + \log \alpha - 1$$

and conclude $\min\{\, \alpha F_1(s){+}F_0(s){-}\beta s | s > 0\,\} = \alpha{+}\log\alpha{-}1{-}\gamma_*\big(\beta/\alpha{+}\log\alpha{+}1{-}1/\alpha\big)$. We use this expression for $N_{\widetilde{\rho}}$ with $b = 1$, $u = asv^2$ and $\alpha = (1{+}\widetilde{\rho})a$ to obtain

$$\widehat{n}(\widetilde{\rho}, a, 1, v) = v^2\Big(\alpha{+}\log\alpha - 1 - \gamma_*\big(1{+}\log\alpha - 1/\alpha - \widehat{\rho}\log v^2\big)\Big) - \alpha\widehat{\rho}(v^2{-}1)$$

with $\widehat{\rho} = \frac{\widetilde{\rho}}{1+\widetilde{\rho}} > \frac{1}{1+\kappa_*}$. Now the infimum $\Xi(\widetilde{\rho}, a)$ can be found numerically by minimizing $\big(\mu(a)(v{-}1)^2 + \widehat{n}(\widetilde{\rho}, a, 1, v)\big)/F_1(v)$ with respect to $v > 0$.

Moreover, the function $\xi(\rho) := \inf\{\, \Xi(\rho, a) \,|\, a > 0\,\}$ can be obtained directly by minimizing $h(a, \rho, v, w) = (1{-}a{-}\log a)(v{-}1)^2 + a\rho F_1(wv) + v^2(aF_1(w/v) + F_0(w/v))$ with respect to $a > 0$ first. Using $(v{-}1)^2 = F_1(wv) - 2vF_1(w) + v^2F_1(w/v)$ we obtain

$$H(\rho, v, w) := \inf_{a>0} h(a, \rho, v, w) = (v{-}1)^2\Big(2 + \log\big(\tfrac{2vF_1(w)+(\rho-1)F_1(wv)}{(v-1)^2}\big)\Big) + v^2F_0(\tfrac{w}{v})$$

and conclude

$$\xi(\rho) = \inf\Big\{\, \frac{H(\rho, v, w)}{F_1(v)} \,\Big|\, 1 \neq v > 0,\ w > 0\,\Big\}.$$

Clearly $\xi(1/\kappa_*) = 0$, and numerically we find $\xi(1/\kappa_*) = 0$, $\xi(1.36976) \approx 1.0$, $\xi(1.5) = 1.3038$, $\xi(2) = 1.99374$, and $\xi(3) = 2.669$. This concludes the proof of Lemma 4.6. ∎

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