

Convergence to self-similar profiles in reaction-diffusion systems

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Abstract

We study a reaction-diffusion system on the real line, where the reactions of the species are given by one reversible reaction pair $\alpha X_1 \rightleftharpoons \beta X_2$ satisfying the mass-action law. We describe different positive limits at $x \rightarrow -\infty$ and $x \rightarrow +\infty$ and investigate the long-time behavior. Rescaling space and time according to the parabolic scaling with $\tau = \log(1+t)$ and $y = x/\sqrt{1+t}$, we show that solutions converge exponentially for $\tau \rightarrow \infty$ to a similarity profile. In the original variables, these profiles correspond to asymptotically self-similar behavior describing the phenomenon of diffusive mixing of the different states at infinity.

Our method provides global exponential convergence for all initial states with finite relative entropy. For the case $\alpha = \beta \geq 1$ we can allow for self-similar profiles with arbitrary equilibrated states, while for $\alpha > \beta \geq 1$ we need to assume that the two states at infinity are sufficiently close such that the self-similar profile is relative flat.

1 Introduction

For a nonlinear coupled reaction-diffusion systems with mass-action kinetics satisfying a detailed balance condition, the long-time behavior of its solutions is investigated. While there already exists a wide variety of literature for these systems posed on bounded domains [Ali79, Smo94, DeF06, DeF07, BJ*14, MHM15], much less is known if the underlying domain is chosen to be the whole space $\Omega = \mathbb{R}^d$, see e.g. [HH*18] for the case with finite mass. We will see that in the case of unbounded domains and infinite mass, similarity profiles can be a crucial tool to describe their asymptotic behavior qualitatively. Here we follow the ideas on *diffusive mixing* as developed in [BrK92, CoE92, GaM98]; however, our approach is completely different. Instead of doing a local analysis of the relevant similarity profile, whose existence is established in [MiS23a], we use the relative Boltzmann entropy and derive exponential convergence globally, i.e. for all initial conditions with finite relative entropy. Thus, our work is closer to [BJ*14] which derives global energy-dissipation estimates for suitable relative entropies to study exponential convergence to (non-equilibrium) steady states on bounded domains but with nontrivial prescribed Dirichlet boundary data. To the best of the authors' knowledge, the present work is the first relative-entropy approach to systems with infinite mass.

Asymptotic self-similar behavior for scalar, nonlinear diffusion equations is a classical theory in the case of finite mass, see e.g. [CaT00, Váz07] and the references therein. The case of infinite mass was initiated in [Pel71] and extended in [vaP77, Ber82], where the theory was based on comparison principles. Systems of partial differential equations with different limits at $x \rightarrow -\infty$ and $x \rightarrow \infty$ are studied in [MaP01] in the context of adiabatic gas flow through a porous medium. The Convergence to asymptotic profiles is established using local estimates with weighted Sobolev norms.

For our model, we consider two species X_1 and X_2 on $\Omega = \mathbb{R}^d$ and denote their concentrations at time $t > 0$ and at position $x \in \mathbb{R}^d$ by $\tilde{\mathbf{u}}(t, x) = (\tilde{u}(t, x), \tilde{v}(t, x))^\top$. The species diffuse with diffusion

coefficients $d_1, d_2 > 0$ and interact through the single reversible chemical reaction pair $\alpha X_1 \xrightleftharpoons{k} \beta X_2$ with each other. Here $\alpha, \beta \geq 1$ are the stoichiometric coefficients and $k > 0$ denotes the reaction strength. The change of the concentrations can be described by the corresponding reaction-diffusion system

$$\tilde{\mathbf{u}}_t = \mathbf{D} \Delta \tilde{\mathbf{u}} + \mathbf{R}(\tilde{\mathbf{u}}) \quad \text{for } t > 0, x \in \mathbb{R}^d, \quad (1.1)$$

with diffusion matrix $\mathbf{D} = \text{diag}(d_1, d_2)$ and, by using the law of mass action, reaction term

$$\mathbf{R}(\tilde{\mathbf{u}}) = k(\tilde{v}^\beta - \tilde{u}^\alpha) \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}.$$

Additionally, we require that the solutions are prescribed at infinity by states that are in reactive equilibrium. In the case $d = 1$ this simply means that we require that the solutions are in equilibria at both sides of infinity, thus we have $\tilde{\mathbf{u}}(t, \pm\infty) = (A_\pm^\beta, A_\pm^\alpha)^\top$ for two given constants $A_-, A_+ \geq 0$. Here we use that our system (1.1) has the special property that it possesses a continuum of constant solutions. In contrast to reaction-diffusion systems with a finite number of constant steady states, where the typical long-time behavior is given by traveling waves or pulses (see for example [Smo94, VVV94, Vol14]), we show that the solutions converge to so-called self-similar profiles when time goes to infinity. This *asymptotically self-similar behavior* is called *diffusive mixing* in [CoE92, GaM98, MSU01], where it was studied for the special system of the real Ginzburg-Landau equation.

The existence of relevant self-similar profiles is established in [MiS23a, Sec. 5]. In the present paper, we focus on proving the convergence towards these profiles. Our analysis is based on two crucial steps:

- instead of the physical variables (t, x) we use the parabolic scaling variables (τ, y) defined via $\tau = \log(t+1)$ and $y = x/\sqrt{t+1}$ and
- we derive energy-dissipation estimates for a relative entropy (of Boltzmann type).

Doing the transformation $\mathbf{u}(\tau, y) = \tilde{\mathbf{u}}(t, x)$, the scaled system reads

$$\mathbf{u}_\tau = \mathbf{D} \mathbf{u}_{yy} + \frac{y}{2} \mathbf{u}_y + e^\tau \mathbf{R}(\mathbf{u}) \quad \text{with } \mathbf{u}(\tau, \pm\infty) = (A_\pm^\beta, A_\pm^\alpha)^\top. \quad (1.2)$$

Note that we cannot scale the size of the variables u and v because of the fixed boundary conditions. Clearly, the parabolic scaling is good for the diffusion term, but we see that an additional time dependent factor appears in front of the reaction term. As the prefactor is exponentially growing in time, it forces the reaction to decay fast in order to equilibrate the whole system. This is indeed established in [GaS22] for the case $\alpha = 2$ and $\beta = 1$.

The equation for the asymptotic profile $\mathbf{U} = (U, V) : \mathbb{R} \rightarrow \mathbb{R}^2$ can be motivated as follows. We consider (1.2) with the constraint $\mathbf{R}(\mathbf{u}) = 0$ and replace the limit $e^\tau \mathbf{R}(\mathbf{u}) \rightarrow \infty \mathbf{0}$ by a vector-valued Lagrange multiplier $\boldsymbol{\lambda} = \Lambda(y) \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}$. This leads to the profile equation for \mathbf{U} in the form

$$0 = \mathbf{D} \mathbf{U}''(y) + \frac{y}{2} \mathbf{U}'(y) + \Lambda(y) \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}, \quad 0 = \mathbf{R}(\mathbf{U}(y)), \quad \mathbf{U}(\pm\infty) = \begin{pmatrix} A_\pm^\beta \\ A_\pm^\alpha \end{pmatrix}. \quad (1.3)$$

We refer to [MiS23a] for the treatment of this and more general profile equations, where the approach from [GaM98] relying on the theory of monotone operators is generalized to the vector-valued case.

The idea is to use entropy estimates to study the asymptotic behavior of solutions of reaction-diffusion systems with mass-action kinetic (and detailed balance). It traces back to the works of [Grö83, Grö92,

GGH96] and has been refined by many authors in recent years, see for example [DeF06, DeF07, MHM15, FeT17, PSZ17]. The usual strategy is to take a relative entropy given by

$$\mathcal{E}_\phi(\mathbf{u}(\tau) | \mathbf{U}) = \int_{\Omega} \sum_{j=1}^{j_*} \phi(u_j(\tau, y)/U_j(y)) U_j(y) dy$$

for a convex entropy function ϕ satisfying $\phi(\rho) > \phi(1) = 0$ for all $\rho \neq 1$, and to show that \mathcal{E}_ϕ is a Lyapunov function, i.e. along solutions a so-called entropy-dissipation relation

$$\frac{d}{d\tau} \mathcal{E}_\phi(\mathbf{u}(\tau) | \mathbf{U}) = -\mathcal{D}_\phi(\mathbf{u}(\tau)) \leq 0$$

holds with a non-negative dissipation functional \mathcal{D}_ϕ . If one can establish a lower bound $\mathcal{D}_\phi \geq \mu \mathcal{E}_\phi$ with $\mu > 0$, then Grönwall's lemma gives $\mathcal{E}_\phi(\mathbf{u}(\tau) | \mathbf{U}) \leq e^{-\mu\tau} \mathcal{E}_\phi(\mathbf{u}(0) | \mathbf{U})$ which implies convergence of $\mathbf{u}(\tau)$ to \mathbf{U} because $\mathcal{E}_\phi(\mathbf{u} | \mathbf{U}) = 0$ if and only if $\mathbf{u} = \mathbf{U}$.

Due to the mass-action kinetics, the relative Boltzmann entropy \mathcal{E}_B with Boltzmann function $\phi = \lambda_B : z \mapsto z \log z - z + 1$ is the only choice in order to obtain the right sign for the dissipation term coming from the reaction with $\alpha \neq \beta$. This can be seen in more detail in Proposition 3.1 and will be important in Section 5. We will see in Section 4.2 that for $\alpha = \beta$ other entropies are useful.

The classical studies on the long-time behavior of solutions for the unscaled system (1.1) in a bounded domain Ω (see. e.g. [Grö83, DeF06, Mie17] and the references therein) rely exactly on this approach. However, in our case we will not obtain a true Lyapunov function on the unbounded domain $\Omega = \mathbb{R}^1$, because of the fact that $\mathbf{U} = (U, V)^\top$ is not a true steady state of our scaled system (1.2), see the Lagrange multiplier Λ in the profile equation (1.3). Only in the very special case $\alpha = \beta$ and $d_1 = d_2$ one has $\Lambda \equiv 0$, and we easily will obtain $\mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U}) \leq e^{-\frac{1}{2}\tau} \mathcal{E}_B(\mathbf{u}(0) | \mathbf{U})$.

In Section 2 we explain our method by applying it to the scaled linear diffusion equation $u_\tau = Du_{yy} + \frac{y}{2}u_y$ with boundary conditions $u(\tau, \pm\infty) = A_\pm > 0$. This leads to the energy-dissipation estimate

$$\frac{d}{d\tau} \mathcal{E}_\phi(u | U) = -\mathcal{I}_{\text{Fisher}}(u) - \frac{1}{2} \mathcal{E}_\phi(u | U) \quad \text{with } \mathcal{I}_{\text{Fisher}}(u) = D \int_{\mathbb{R}} \phi''(u/U) ((u/U)_y)^2 U dy.$$

The new and very helpful term $-\frac{1}{2} \mathcal{E}_\phi(u | U)$ arises from the drift term $\frac{y}{2}u_y$ which stems from the parabolic scaling. Using $\mathcal{I}_{\text{Fisher}} \geq 0$, we obtain $\mathcal{E}_\phi(u(\tau) | U) \leq e^{-\frac{1}{2}\tau} \mathcal{E}_\phi(u(0) | U)$ without using any Poincaré or log-Sobolev estimate on \mathbb{R} . For that reason, the factor 1/2 will be called the *bonus factor*, subsequently.

In Section 3 we show that in our case we have $\frac{d}{d\tau} \mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U}) = -\mathcal{D}_B(\mathbf{u})$ with a dissipation functional that can be written as

$$\mathcal{D}_B = \mathcal{I}_{\text{Fisher}} + e^\tau \mathcal{D}_{\text{react}} + \frac{1}{2} \mathcal{E}_B - \mathcal{I}_\Lambda \quad \text{with } \mathcal{D}_{\text{react}} = \int_{\mathbb{R}} kU^\alpha \Gamma\left(\left(\frac{u(y)}{U(y)}\right)^\alpha, \left(\frac{v(y)}{V(y)}\right)^\beta\right) dy,$$

where $\Gamma(a, b) \geq 0$ is defined by

$$\Gamma(a, b) := \begin{cases} (a-b)(\log a - \log b) \geq 0 & \text{for } a, b > 0, \\ 0 & \text{for } a = b = 0, \\ \infty & \text{for } (0, c) \text{ and } (c, 0) \text{ for } c > 0. \end{cases} \quad (1.4)$$

Here $\mathcal{I}_{\text{Fisher}}$ consists of two non-negative terms, one for u and one for v . The special form of $\mathcal{D}_{\text{react}}$ and its positivity arise from the special interaction of the mass-action law and the Boltzmann entropy, namely with $D\mathcal{E}_B(\mathbf{u} | \mathbf{U}) = \binom{\log u}{\log v}$ and the logarithm rules one finds $(u^\alpha - v^\beta) \binom{\alpha}{-\beta} \cdot \binom{\log u}{\log v} =$

$\Gamma(u^\alpha, v^\beta) \geq 0$. Again we have the bonus factor $1/2$ arising from the drift term $\frac{y}{2}\mathbf{u}_y$. The new and difficult term is the mixed term

$$\mathcal{I}_\Lambda(\mathbf{u}) = \int_{\mathbb{R}} \left(\left(1 - \frac{u}{U}\right)\alpha - \left(1 - \frac{v}{V}\right)\beta \right) \Lambda \, dy,$$

which arises from the fact that \mathbf{U} is not a steady state, but needs the Lagrange multiplier Λ , see the profile equation (1.3). In particular, \mathcal{I}_Λ does not have a specific sign.

The derivation of the useful splitting of \mathcal{D}_B is part of Section 3.2 and the precise statement can be found in Proposition 3.1. Because of the unboundedness of $\Omega = \mathbb{R}^1$ we will not be able to take advantage of the Fisher information $\mathcal{I}_{\text{Fisher}}$, but we can rely on the bonus factor $1/2$. Moreover, the reactive dissipation $\mathcal{D}_{\text{react}}$ has the factor e^τ in front, from which we will benefit in Sections 4 and 5 to control \mathcal{I}_Λ . Since the mixed term \mathcal{I}_Λ has no fixed sign, it is possible that the relative Boltzmann entropy \mathcal{E}_B may grow, i.e. it is not a true Lyapunov function. So our aim will be to show that

$$\frac{1}{2} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) + e^\tau \mathcal{D}_{\text{react}}(\mathbf{u}) - \mathcal{I}_\Lambda(\mathbf{u}) \geq (\eta - \mu e^{-\tau}) \mathcal{E}_B(\mathbf{u} | \mathbf{U}) - K e^{-\sigma\tau} \quad \text{for } \tau \geq 0 \quad (1.5)$$

for some $\eta, \sigma > 0$ and $\mu, K \geq 0$. From this, our convergence results in Theorems 4.1 and 5.2 will follow.

The control of the problematic term \mathcal{I}_Λ is different in the simpler case $\alpha = \beta \geq 1$ (see Section 4) and in the more difficult case $\alpha > \beta \geq 1$ (see Section 5). For $\alpha = \beta \geq 1$, the integrand of \mathcal{I}_Λ only depends on $\frac{u}{U} - \frac{v}{V}$ and thus can be controlled by $\mathcal{D}_{\text{react}}$ alone. Hence, we obtain (1.5) with $\eta = 1/2$ and $\sigma = 1$ if $\alpha = \beta \in [1, 2)$ or $\sigma = 1/(\alpha-1)$ for $\alpha = \beta \geq 2$, without any restriction on the self-similarity profile \mathbf{U} . Using a version of Grönwall's inequality (see Lemma 3.3), we find for $\alpha = \beta \in [1, 3)$ the decay $\mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U}) \leq C e^{-\min\{\eta, \sigma\}\tau} = C e^{-\tau/2}$, whereas for $\alpha = \beta > 3$ we have a slower decay like $e^{-\tau/(\alpha-1)}$.

For $\alpha > \beta \geq 1$ it is more difficult to control \mathcal{I}_Λ and we need to exploit the term $\frac{1}{2} \mathcal{E}_B$ with the bonus factor. From [MiS23a] we know that for small $|A_+ - A_-|$ also $\|\Lambda\|_\infty$ is small. Thus, for sufficiently small $|A_+ - A_-|$, we have

$$\theta := (\alpha - \beta) \sup \left\{ \Lambda(y)/V(y) \mid y \in \mathbb{R} \right\} < 1/2,$$

and Theorem 5.2 shows that (1.5) holds for $\eta = 1/2 - \theta > 0$ and suitable K and σ . It remains open whether in the case $\alpha > \beta$ the asymptotic profiles with large difference $|A_+ - A_-|$ are stable or not. We remark that a flatness condition for the profile \mathbf{U} (which is encoded in $\|\Lambda\|_\infty \leq C|A_+ - A_-|$) appears also in [MaP01, Thm. 1.1].

We expect that our approach based on energy-dissipation estimates is flexible enough to allow for several generalizations. Based on the vector-valued existence results for similarity profiles in [MiS23a], it should be possible to treat general reaction systems for i_* species interacting via r_* reaction pairs with mass-action kinetics, where $m_* := i_* - r_* \geq 1$ provides the dimension of the equilibrium manifold which will then include the similarity profile \mathbf{U} . Of course, the problem of controlling the mixed term \mathcal{I}_Λ will be more involved, because \mathcal{I}_Λ now involves m_* Lagrange multipliers. Moreover, our convergence theory works equally well for space dimension $d \geq 2$: as soon as the existence of similarity profiles is established, the energy-dissipation estimates can be done with a bonus factor $d/2$.

2 Convergence to self-similarity for the linear diffusion equation on the whole space

In this section, we demonstrate our proceeding to the well-studied linear diffusion equation

$$\tilde{u}_t = D \tilde{\Delta} \tilde{u} \text{ on } \mathbb{R}^d, \quad (2.1)$$

with diffusion constant $D > 0$. For initial data $\tilde{u}^0 \in L^1(\mathbb{R}^d)$, it is already known that the solutions behave asymptotically like a Gaussian, see e.g. [Jün16, Sec.2.4]. In this paper, we are interested in the long-time behavior of solutions which have nontrivial boundary conditions for $|x| \rightarrow \infty$, such that the solutions have infinite mass.

In the one-dimensional case, we consider the diffusion equation (2.1) together with the boundary conditions

$$\tilde{u}(t, \pm\infty) := \lim_{x \rightarrow \pm\infty} \tilde{u}(t, x) = A_{\pm}$$

and ask how the solution mixes these two steady states A_{\pm} when time t goes to ∞ . Because of the linearity, it is not difficult to prove that for every given pair $(A_-, A_+) \in \mathbb{R}^2$ of asymptotic boundary conditions, the solution converges uniformly in $x \in \mathbb{R}$ to the following self-similar solution

$$U(x/\sqrt{t}) := \frac{1}{2}(A_+ - A_-) \operatorname{erf}(x/\sqrt{4Dt}) + \frac{1}{2}(A_+ + A_-), \quad (2.2)$$

where $\operatorname{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \exp(-z^2) dz$ is the error function. However, we do not want to use the linearity to verify this convergence, neither the exact representation of the profile given by the error function, with the idea in mind to generalize the following strategy to the given nonlinear reaction-diffusion system. Hence, we will use entropy estimates to prove this convergence.

Before doing so, we look at the profile function (2.2) from a different perspective. We see that U depends on the quotient x/\sqrt{t} instead of the variables t and x separately. This motivates to do a transformation into the so-called parabolic scaling variables given by $y = (1+t)^{-1/2}x \in \mathbb{R}^d$ and $\tau = \log(1+t)$. Returning to the multi-dimensional case, we define

$$u(\tau, y) := \tilde{u}(t, x) = \tilde{u}(e^{\tau} - 1, e^{\tau/2}y)$$

and find the scaled diffusion equation with the same asymptotic boundary conditions:

$$u_{\tau} = D \Delta u + \frac{1}{2}y \cdot \nabla u \quad \text{and} \quad u(\tau, y) - U(y) \rightarrow 0 \text{ for } |y| \rightarrow \infty, \quad (2.3)$$

where Δ and ∇ are now taken with respect to $y \in \mathbb{R}^d$. The asymptotic boundary conditions are given by a fixed function $U : \mathbb{R}^d \rightarrow \mathbb{R}$, which we take as a self-similar profile, i.e. it satisfies the profile equation

$$D \Delta U + \frac{1}{2}y \cdot \nabla U = 0 \text{ on } \mathbb{R}^d. \quad (2.4)$$

Clearly, the solutions in (2.2) provide all possible solutions for the case $d = 1$. For $d \geq 2$ the set of solutions is much richer, even when restricting to the case $U \in C^2(\mathbb{R}^d)$ with $\inf U \geq \underline{U} > 0$. Of course, we again see that $\tilde{u}(t, x) = U((1+t)^{-1/2}x)$ is an exact self-similar solution of the unscaled equation (2.1).

To prepare for the subsequent analysis for reaction-diffusion system, we now show convergence of all solutions of the scaled linear diffusion equation in the sense that the relative entropy

$$\mathcal{E}_{\phi}(u|U) := \int_{\mathbb{R}} \phi(u/U) U dy = \int_{\mathbb{R}} \phi(\rho) U dy, \quad \text{where } \rho = u/U,$$

converges exponentially to 0. Here ϕ is an arbitrary convex entropy function fulfilling $\phi(\rho) \geq \phi(1) = 0$ for all $\rho \geq 0$. We call the arising exponential decay rate $d/2$ the bonus factor, because it solely comes from the scaling, i.e. from the drift term $\frac{1}{2}y \cdot \nabla u$.

Proposition 2.1 (Decay in the linear diffusion equation) *Consider the scaled linear diffusion equation and let $U \in C_b^2(\mathbb{R}^d)$ be the similarity profile satisfying (2.4) and $U(y) \geq \underline{U} > 0$. Then, all solutions u of the Cauchy problem (2.3) fulfilling $\mathcal{E}_\phi(u^0|U) = \int_{\mathbb{R}^d} \phi(u^0/U)U \, dy < \infty$ converge to U in the sense that*

$$\mathcal{E}_\phi(u(\tau)|U) \leq e^{-d\tau/2} \mathcal{E}_\phi(u^0|U) \text{ for all } \tau > 0.$$

Proof. To simplify the calculation we use the relative density $\rho(\tau, y) := u(\tau, y)/U(y)$ and observe that the scaled diffusion equation (2.3) takes the form

$$\begin{aligned} U\rho_\tau &= D(U\Delta\rho + 2\nabla U \cdot \nabla\rho + \rho\Delta U) + \frac{1}{2}y \cdot (U\nabla\rho + \rho\nabla U) \\ &= D(U\Delta\rho + 2\nabla U \cdot \nabla\rho) + \frac{1}{2}Uy \cdot \nabla\rho, \end{aligned}$$

where the last identity follows by inserting the profile equation (2.4) for U .

We compute the time derivative of the relative entropy. It holds

$$\begin{aligned} \frac{d}{d\tau} \mathcal{E}_\phi(u(\tau)|U) &= \int_{\mathbb{R}^d} \phi'(\rho)\rho_\tau U \, dy = \int_{\mathbb{R}^d} \phi'(\rho) \{ D(U\Delta\rho + 2\nabla U \cdot \nabla\rho) + \frac{1}{2}Uy \cdot \nabla\rho \} \, dy \\ &\stackrel{*}{=} \int_{\mathbb{R}^d} \{ -D\phi''(\rho)|\nabla\rho|^2 U + (D\nabla U + \frac{1}{2}Uy) \cdot (\phi'(\rho)\nabla\rho) \} \, dy \\ &\stackrel{*}{=} \int_{\mathbb{R}^d} \{ -D\phi''(\rho)|\nabla\rho|^2 U - (D\Delta U + \frac{1}{2}y \cdot \nabla U + \frac{1}{2}(\operatorname{div} y)U)\phi(\rho) \} \, dy \\ &= -\mathcal{I}_{\text{Fisher}}(\rho) - 0 - \frac{d}{2} \int_{\mathbb{R}^d} \phi(\rho)U \, dy =: -\mathcal{D}_\phi(\rho). \end{aligned}$$

Here $*$ indicates an integration by parts where we use $\rho(y) \rightarrow 1$ and $\phi'(1) = 0$. For the second last identity we used the Fisher information

$$\mathcal{I}_{\text{Fisher}}(\rho) := D \int_{\mathbb{R}^d} \phi''(\rho)|\nabla\rho|^2 U \, dy \geq 0$$

and the profile equation $D\Delta U + \frac{1}{2}y \cdot \nabla U = 0$ once again. The bonus factor arises from $\frac{1}{2} \operatorname{div} y = d/2$.

Thus, the dissipation \mathcal{D}_ϕ is non-negative and satisfies $\mathcal{D}_\phi(\rho) \geq \frac{d}{2} \mathcal{E}_\phi(u|U)$ yielding

$$\frac{d}{d\tau} \mathcal{E}_\phi(u(\tau)|U) = -\mathcal{D}_\phi(\rho) \leq -\frac{d}{2} \mathcal{E}_\phi(u(\tau)|U).$$

By Grönwall's Lemma, we obtain exponential convergence in τ . More precisely, we have

$$\mathcal{E}_\phi(u(\tau)|U) \leq e^{-d\tau/2} \mathcal{E}_\phi(u(0)|U) \text{ for } \tau > 0,$$

as it was claimed. ■

In the above proof, we see the essential benefit of the parabolic scaling. The extra term $\frac{1}{2}y \cdot \nabla u$ featuring in the scaled diffusion equation (2.3) leads to the so-called bonus factor $d/2$ in the differential inequality for the relative entropy, which in turn provides convergence and an explicit decay rate.

3 The reaction-diffusion system

The first part of this section is dedicated to introduce the coupled reaction-diffusion system (1.1) and the scaled one (1.2) together with its important properties in more detail. Then in Section 3.2, we derive the dissipation functional for the scaled system and prove an appropriate splitting of it.

3.1 The system and its similarity profile

Consider a coupled system of two nonlinear reaction-diffusion equations on the unbounded domain $\Omega = \mathbb{R}^1$ which present the concentration change of the diffusing species X_1 and X_2 interacting through the single reversible reaction $\alpha X_1 \rightleftharpoons \beta X_2$ with each other. When we denote their densities with $\tilde{u}, \tilde{v} \geq 0$, respectively, the mass-action law leads to the system

$$\begin{aligned}\tilde{u}_t &= d_1 \tilde{u}_{xx} + \alpha k (\tilde{v}^\beta - \tilde{u}^\alpha), \\ \tilde{v}_t &= d_2 \tilde{v}_{xx} - \beta k (\tilde{v}^\beta - \tilde{u}^\alpha),\end{aligned}\tag{3.1}$$

for $t > 0$ and $x \in \mathbb{R}^1$, where the diffusion constants d_1, d_2 and the reaction rate k are assumed to be positive. The set of constant steady states is a one-parameter family given by

$$\{ (A^\beta, A^\alpha) \mid A > 0 \}.$$

We are interested in the behavior of solutions where the initial data (u^0, v^0) is in equilibria at infinity, i.e. where for two given constants $A_-, A_+ > 0$ the continuous initial data satisfies the asymptotic boundary conditions

$$(\tilde{u}^0(\pm\infty), \tilde{v}^0(\pm\infty)) := \lim_{x \rightarrow \pm\infty} (\tilde{u}^0(\pm x), \tilde{v}^0(\pm x)) = (A_\pm^\beta, A_\pm^\alpha).$$

Motivated by Section 2, we transform the system (3.1) into parabolic scaling coordinates

$$y = x/\sqrt{t+1} \quad \text{and} \quad \tau = \log(t+1).$$

Then the transformed system reads

$$\begin{aligned}u_\tau &= d_1 u_{yy} + \frac{y}{2} u_y + e^\tau \alpha k (v^\beta - u^\alpha), \\ v_\tau &= d_2 v_{yy} + \frac{y}{2} v_y - e^\tau \beta k (v^\beta - u^\alpha).\end{aligned}\tag{3.2}$$

Accordingly, the continuous initial data (u^0, v^0) satisfies the asymptotic boundary conditions

$$(u^0(\pm\infty), v^0(\pm\infty)) = (A_\pm^\beta, A_\pm^\alpha).\tag{3.3}$$

Note the exponential factor that appears in front of the reaction terms in (3.2) as the reaction does not transform like the parabolic terms. At a first glance, one might say that the transformed system looks much more complicated than the original one since it is now non-autonomous. On top of that, the factor is exponentially growing in time, which could impair convergence. On further consideration, however, we will see that the prefactor e^τ is beneficial from a technical point of view and makes things work in the end. Luckily, the reaction term comes with a difference; thus, the prefactor indicates how the solutions probably behave for large times. To prove rigorously that this is true is the aim of Sections 4 and 5.

But already now we can imagine that the exponentially growing factor forces the reaction to equilibrate for $\tau \rightarrow \infty$. However, there might still be nontrivial reaction fluxes $q = ke^\tau(v^\beta - u^\alpha)$ for $\tau \rightarrow \infty$, which can be seen as the limit of the type “ $\infty \cdot 0$ ”. As discussed in [MiS23a, MiS23b], the similarity profile $y \mapsto \mathbf{U}(y) = (U(y), V(y))^\top$ has to satisfy the following differential-algebraic system

$$\begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} d_1 U''(y) + \frac{y}{2} U'(y) \\ d_2 V''(y) + \frac{y}{2} V'(y) \end{pmatrix} + \Lambda(y) \begin{pmatrix} \alpha \\ -\beta \end{pmatrix}, \quad U(y)^\alpha = V(y)^\beta, \quad \begin{pmatrix} U(\pm\infty) \\ V(\pm\infty) \end{pmatrix} = \begin{pmatrix} A_\pm^\beta \\ A_\pm^\alpha \end{pmatrix}. \quad (3.4)$$

It is possible to eliminate Λ and $V = U^{\alpha/\beta}$ algebraically to obtain a nonlinear ODE for U alone, namely

$$(\beta d_1 U + \alpha d_2 U^{\alpha/\beta})'' + \frac{y}{2} (\beta U + \alpha U^{\alpha/\beta})' = 0, \quad \text{with } U(\pm\infty) = A_\pm^\beta.$$

In [MiS23a] it is shown that for all (A_-, A_+) there exists a unique solution \mathbf{U} of (3.4).

We call the functions $\mathbf{U} = (U, V)^\top$ *similarity profiles* and aim to prove that solutions $\mathbf{u} = (u, v)^\top$ to (3.2)–(3.3) converge towards the profiles in the sense that the relative Boltzmann entropy \mathcal{E}_B satisfies the qualitative estimate

$$\mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U}) \leq \tilde{C} e^{-\eta\tau} \mathcal{E}_B(\mathbf{u}(0) | \mathbf{U}) + \tilde{K} e^{-\sigma\tau}, \quad (3.5)$$

where the rates $\eta, \sigma > 0$ and the constants \tilde{C}, \tilde{K} depend only on the given problem data, but not on the initial condition $\mathbf{u}(0)$. This then implies exponential convergence of $\mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U})$ with exponential rate $\min\{\eta, \sigma\} > 0$.

In [MiS23a, Lem. 3.2] it is additionally shown that the profiles $\mathbf{U} = (U, V)^\top$ solving (3.4) are monotone, i.e. for $A_- < A_+$ one has $U'(y), V'(y) > 0$ for all $y \in \mathbb{R}$. As a consequence, we have $U(y) > A_-^\beta > 0$ and $V(y) > A_-^\alpha > 0$ for all $y \in \mathbb{R}$ so that the relative entropy, where we have the relative densities $\rho = u/U$ and $\zeta = v/V$ in the argument of the Boltzmann function, is well-defined.

3.2 Suitable split of dissipation

Let us recall that the usual procedure is to take a relative entropy \mathcal{E}_ϕ and to show that it fulfills for all times the so-called entropy-dissipation relation

$$\frac{d}{d\tau} \mathcal{E}_\phi(\mathbf{u} | \mathbf{U}) = -\mathcal{D}_\phi(\mathbf{u}) \leq 0$$

for a *non-negative* dissipation functional \mathcal{D}_ϕ . In our case, we cannot expect the monotonicity of the mapping $\tau \mapsto \mathcal{E}_\phi(\mathbf{u}(\tau) | \mathbf{U})$ as it is posed on the whole space and \mathbf{U} is not a true steady state. This is in contrast to [DeF06, DeF07, BJ*14, Mie17], where the unscaled system (3.1) is studied on bounded domains and where exact steady states exist. However, in Sections 4 and 5 we will prove that the entropy-dissipation relation is correct up to exponentially decaying terms, see (1.5) or Lemma 3.3.

Let us take the relative Boltzmann entropy

$$\mathcal{E}_B(\mathbf{u} | \mathbf{U}) = \int_{\mathbb{R}} (\lambda_B(\rho)U + \lambda_B(\zeta)V) dy \quad \text{where } \rho := \frac{u}{U} \text{ and } \zeta := \frac{v}{V},$$

as it goes hand in hand with the mass-action kinetics.

The aim of this section is first to derive the dissipation functional \mathcal{D}_B that fulfills

$$\frac{d}{d\tau} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) =: -\mathcal{D}_B(\rho, \zeta), \quad (3.6)$$

and second to find a suitable partition of it in good and problematic terms, which is useful since \mathcal{D}_B has – as we already suspect – no fixed sign in our setting. Thus, we will examine the terms of which it consists in an appropriate way. Note that we will write the dissipation terms as functions of the relative densities $\rho = u/U$ and $\zeta = v/V$, whereas we keep the relative entropy in standard form in terms of $\mathbf{u} = (u, v)^\top$.

Proposition 3.1 *The dissipation \mathcal{D}_B fulfilling (3.6) can be decomposed as*

$$\mathcal{D}_B(\rho, \zeta) = \mathcal{I}_{\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) - \mathcal{I}_\Lambda(\rho, \zeta) + e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta),$$

where $\mathcal{D}_{\text{react}}(\rho, \zeta) := \int_{\mathbb{R}} kU^\alpha \Gamma(\rho^\alpha, \zeta^\beta) dy \geq 0$ is the reactive dissipation and $\mathcal{I}_{\text{Fisher}}(\rho, \zeta) := \int_{\mathbb{R}} d_1 U \lambda_B''(\rho) \rho_y^2 + d_2 V \lambda_B''(\zeta) \zeta_y^2 dy \geq 0$ is known as the Fisher information. The bonus term $\frac{1}{2} \mathcal{E}_B$ stems from the transport term $\frac{y}{2} \partial_y \mathbf{u}$, and the remaining term

$$\mathcal{I}_\Lambda(\rho, \zeta) := \int_{\mathbb{R}} ((1-\rho)\alpha - (1-\zeta)\beta) \Lambda dy, \quad (3.7)$$

arises because of the Lagrange multiplier Λ which features in the profile equation (3.4). This term is called the mixed term, because it is the only addend without sign.

Proof. Take the relative Boltzmann entropy \mathcal{E}_B given by the functional

$$\mathcal{E}_B(\mathbf{u} | \mathbf{U}) = \int_{\mathbb{R}} U \lambda_B(\rho) + V \lambda_B(\zeta) dy.$$

The relative densities $\rho(\tau, y) := u(\tau, y)/U(y)$ and $\zeta(\tau, y) := v(\tau, y)/V(y)$ satisfy

$$\begin{aligned} U \rho_\tau &= d_1 (U \rho_{yy} + 2U' \rho_y + U'' \rho) + \frac{y}{2} (U \rho_y + U' \rho) + \alpha k e^\tau U^\alpha (\zeta^\beta - \rho^\alpha), \\ V \zeta_\tau &= d_2 (V \zeta_{yy} + 2V' \zeta_y + V'' \zeta) + \frac{y}{2} (V \zeta_y + V' \zeta) - \beta k e^\tau V^\beta (\zeta^\beta - \rho^\alpha). \end{aligned}$$

Thus, computing the time derivative of the relative entropy yields

$$\begin{aligned} \frac{d}{d\tau} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) &= \int_{\mathbb{R}} U \lambda_B'(\rho) \rho_\tau + V \lambda_B'(\zeta) \zeta_\tau dy \\ &= \int_{\mathbb{R}} \lambda_B'(\rho) \left\{ d_1 (U \rho_{yy} + 2U' \rho_y + U'' \rho) + \frac{y}{2} (U \rho_y + U' \rho) \right\} dy \\ &\quad + \int_{\mathbb{R}} \lambda_B'(\zeta) \left\{ d_2 (V \zeta_{yy} + 2V' \zeta_y + V'' \zeta) + \frac{y}{2} (V \zeta_y + V' \zeta) \right\} dy \\ &\quad - e^\tau \int_{\mathbb{R}} kU^\alpha (\beta \lambda_B'(\zeta) - \alpha \lambda_B'(\rho)) (\zeta^\beta - \rho^\alpha) dy \\ &=: -\mathcal{D}_{\text{diff}}(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta), \end{aligned}$$

where we used the relation $U^\alpha = V^\beta$ to simplify the reaction terms. Let us consider the reactive dissipation first. We can use the logarithmic identities to obtain a sign for $\mathcal{D}_{\text{react}}$. It holds

$$\mathcal{D}_{\text{react}}(\rho, \zeta) := \int_{\mathbb{R}} kU^\alpha (\beta \lambda_B'(\zeta) - \alpha \lambda_B'(\rho)) (\zeta^\beta - \rho^\alpha) dy = \int_{\mathbb{R}} kU^\alpha \Gamma(\rho^\alpha, \zeta^\beta) dy \geq 0,$$

where Γ is defined in (1.4). Next, we explore the remaining diffusive dissipation $\mathcal{D}_{\text{diff}}$. We re-sort and obtain

$$\begin{aligned} \mathcal{D}_{\text{diff}}(\rho, \zeta) &= - \int_{\mathbb{R}} d_1 U \lambda'_B(\rho) \rho_{yy} + d_2 V \lambda'_B(\zeta) \zeta_{yy} dy \\ &\quad - \int_{\mathbb{R}} \lambda'_B(\rho) \rho (d_1 U'' + \frac{y}{2} U') + \lambda'_B(\zeta) \zeta (d_2 V'' + \frac{y}{2} V') dy \\ &\quad - \int_{\mathbb{R}} \lambda'_B(\rho) \rho_y (2d_1 U' + \frac{y}{2} U) + \lambda'_B(\zeta) \zeta_y (2d_2 V' + \frac{y}{2} V) dy. \end{aligned}$$

In the same manner as for the scaled diffusion equation, the idea is to integrate by parts twice. For the boundary terms, we use the limits $\rho(y) \rightarrow 1$ and $\zeta(y) \rightarrow 1$ for $y \rightarrow \pm\infty$ and the property $\lambda'_B(1) = 0$. The first integral addend leads to the Fisher information

$$\mathcal{I}_{\text{Fisher}}(\rho, \zeta) := \int_{\mathbb{R}} d_1 U \lambda''_B(\rho) \rho_y^2 + d_2 V \lambda''_B(\zeta) \zeta_y^2 dy \geq 0.$$

Hence, we obtain

$$\begin{aligned} \mathcal{D}_{\text{diff}}(\rho, \zeta) &= \mathcal{I}_{\text{Fisher}}(\rho, \zeta) - \int_{\mathbb{R}} \lambda'_B(\rho) \rho (d_1 U'' + \frac{y}{2} U') + \lambda'_B(\zeta) \zeta (d_2 V'' + \frac{y}{2} V') dy \\ &\quad - \int_{\mathbb{R}} \lambda'_B(\rho) \rho_y ((2d_1 - d_1) U' + \frac{y}{2} U) + \lambda'_B(\zeta) \zeta_y ((2d_2 - d_2) V' + \frac{y}{2} V) dy. \end{aligned}$$

In the last line, we see the total derivatives of $\lambda_B(\rho)$ and $\lambda_B(\zeta)$, respectively. Thus, integration by parts of these integral terms yields the factors $d_1 U'' + \frac{y}{2} U' + \frac{1}{2} U = -\alpha\Lambda + \frac{1}{2} U$ and $d_2 V'' + \frac{y}{2} V' + \frac{1}{2} V = \beta\Lambda + \frac{1}{2} V$, respectively, where we used the profile equation (3.4). Using additionally $\lambda'_B(\rho) \rho - \lambda_B(\rho) = \rho - 1$ we arrive at

$$\begin{aligned} \mathcal{D}_{\text{diff}}(\rho, \zeta) &= \mathcal{I}_{\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) - \int_{\mathbb{R}} ((1-\rho)\alpha\Lambda - (1-\zeta)\beta\Lambda) dy \\ &= \mathcal{I}_{\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) - \mathcal{I}_\Lambda(\rho, \zeta), \end{aligned}$$

which verifies the desired decomposition. ■

In the proof of Proposition 3.1, we saw that due to the mass-action kinetics, the relative Boltzmann function $\phi = \lambda_B$ is the only choice for the given reaction-diffusion system if $\alpha \neq \beta$ in order to obtain a sign for the reactive dissipation $\mathcal{D}_{\text{react}}$. However, if $\alpha = \beta$, also other entropy functions can be chosen. A common family of entropy functions is given by

$$F_p(z) := \begin{cases} \frac{1}{p(p-1)} (z^p - pz + p - 1) & \text{for } p \in \mathbb{R} \setminus \{0, 1\}, \\ z \log z - z + 1 & \text{for } p = 1, \\ z - \log z - 1 & \text{for } p = 0, \end{cases} \quad (3.8)$$

which is determined by the conditions $F_p''(z) = z^{p-2}$ and $F_p(1) = F_p'(1) = 0$. Further, it satisfies the following lower bounds:

$$\text{For all } p \in (0, 1) \text{ and } z > 0 : \quad F_p(z) \geq \frac{1}{p} F_1(z) = \frac{1}{p} \lambda_B(z), \quad (3.9a)$$

$$\text{for all } p > 0 \text{ and } z > 0 : \quad F_p(z) \geq \frac{1/2}{\max\{p, 1-p\}} F_{1/2}(z), \quad (3.9b)$$

see [MiM18, Eqn. (3.2)]. In fact, using this family of entropies in the case $\alpha = \beta$ leads to improved estimates as we will see in Section 4.2. But also in Section 5, where for $\alpha \neq \beta$ the convergence of the relative Boltzmann entropy is studied, the family of entropy functions (3.8) is used, but in this case only for technical reasons during the estimates.

We can define the relative entropy associated to the function F_p by

$$\mathcal{E}_p(\mathbf{u}(\tau) | \mathbf{U}) := \int_{\mathbb{R}} U(y)F_p(\rho(y)) + V(y)F_p(\zeta(y)) dy \quad \text{where } \rho := u/U \text{ and } \zeta := v/V,$$

such that $\mathcal{E}_1 = \mathcal{E}_B$. The entropy $\mathcal{E}_{1/2}$ is special because $F_{1/2}(u/U)U = 2(\sqrt{u} - \sqrt{U})^2$. Hence we have

$$\int_{\mathbb{R}} F_{1/2}(u/U)U dy = 2\|\sqrt{u} - \sqrt{U}\|_{L^2}^2 =: 2\text{He}(u, U)^2,$$

where He denotes the Hellinger distance between two (densities of) non-negative measures. Using (3.9a) we see that the Hellinger distance between $\mathbf{u} = (u, v)^\top$ and $\mathbf{U} = (U, V)^\top$ can be controlled by \mathcal{E}_p for all $p > 0$. Indeed we have

$$\text{He}(u, U)^2 + \text{He}(v, V)^2 = \frac{1}{2}\mathcal{E}_{1/2}(\mathbf{u} | \mathbf{U}) \leq \max\{p, 1-p\}\mathcal{E}_p(\mathbf{u} | \mathbf{U}). \quad (3.10)$$

As last part of this section, we will derive the corresponding dissipation functional \mathcal{D}_p which fulfills

$$\frac{d}{d\tau}\mathcal{E}_p(\mathbf{u}(\tau) | \mathbf{U}) = -\mathcal{D}_p(\rho, \zeta)$$

and clarify the terms of which it consists. Notice that the following is only true if the stoichiometric coefficients coincide.

Proposition 3.2 *Let $\alpha = \beta$ and $p \notin \{0, 1\}$. The dissipation functional \mathcal{D}_p fulfilling the above can be written as*

$$\mathcal{D}_p(\rho, \zeta) = \mathcal{I}_{p, \text{Fisher}}(\rho, \zeta) + \frac{1}{2}\mathcal{E}_p(\mathbf{u} | \mathbf{U}) - \mathcal{I}_{p, \Lambda}(\rho, \zeta) + e^\tau \mathcal{D}_{p, \text{react}}(\rho, \zeta),$$

where $\mathcal{D}_{p, \text{react}}(\rho, \zeta) := \int_{\mathbb{R}} kU^\alpha \frac{\alpha}{p-1} (\zeta^{p-1} - \rho^{p-1})(\zeta^\alpha - \rho^\alpha) dy \geq 0$ is the reactive dissipation, the Fisher information takes the form $\mathcal{I}_{p, \text{Fisher}}(\rho, \zeta) := \int_{\mathbb{R}} d_1 U \rho^{p-2} \rho_y^2 + d_2 V \zeta^{p-2} \zeta_y^2 dy \geq 0$, and the mixed term, given by

$$\mathcal{I}_{p, \Lambda}(\rho, \zeta) := \int_{\mathbb{R}} \frac{1}{p} (\zeta^p - \rho^p) \alpha \Lambda dy$$

is again the only addend without sign.

Proof. Following the steps of the proof of Proposition 3.1 and using $\alpha = \beta$ yields

$$\frac{d}{d\tau}\mathcal{E}_p(\mathbf{u} | \mathbf{U}) = -\mathcal{D}_{p, \text{diff}}(\rho, \zeta) - e^\tau \mathcal{D}_{p, \text{react}}(\rho, \zeta),$$

where the reactive dissipation takes the form

$$\begin{aligned} \mathcal{D}_{p, \text{react}}(\rho, \zeta) &= \int_{\mathbb{R}} kU^\alpha \alpha (F'_p(\zeta) - F'_p(\rho)) (\zeta^\alpha - \rho^\alpha) dy \\ &= \int_{\mathbb{R}} kU^\alpha \frac{\alpha}{p-1} (\zeta^{p-1} - \rho^{p-1})(\zeta^\alpha - \rho^\alpha) dy \geq 0, \end{aligned}$$

and where for the diffusive part a similar integration by parts gives

$$\begin{aligned} \mathcal{D}_{p,\text{diff}}(\rho, \zeta) &= \mathcal{I}_{p,\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_p(\mathbf{u} | \mathbf{U}) \\ &\quad - \int_{\mathbb{R}} (F'_p(\rho)\rho - F_p(\rho))(d_1 U'' + \frac{y}{2} U') + (F'_p(\zeta)\zeta - F_p(\zeta))(d_2 V'' + \frac{y}{2} V') dy \\ &= \mathcal{I}_{p,\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_p(\mathbf{u} | \mathbf{U}) - \int_{\mathbb{R}} \left((F'_p(\zeta)\zeta - F_p(\zeta)) - (F'_p(\rho)\rho - F_p(\rho)) \right) \alpha \Lambda dy, \end{aligned}$$

since $\alpha = \beta$. Further, with $F'_p(\rho)\rho - F_p(\rho) = \frac{1}{p}(\rho^p - 1)$, this leads to

$$\mathcal{D}_{p,\text{diff}}(\rho, \zeta) = \mathcal{I}_{p,\text{Fisher}}(\rho, \zeta) + \frac{1}{2} \mathcal{E}_p(\mathbf{u} | \mathbf{U}) - \int_{\mathbb{R}} \frac{1}{p} (\zeta^p - \rho^p) \alpha \Lambda dy. \quad \blacksquare$$

3.3 Decay estimates

After deriving the entropy-dissipation relation (3.6), the next step requires to find a so-called entropy-dissipation estimate, that is an estimate of the form $\mathcal{D}_\phi(\mathbf{u}) \geq \Psi(\mathcal{E}_\phi(\mathbf{u}))$ for a non-negative function Ψ . Under appropriate assumptions on Ψ , this usually gives exponential convergence to the equilibrium, where for specific Ψ the rate can be estimated explicitly. For instance, if one even obtains the inequality $\mathcal{D}_\phi(\mathbf{u}) \geq \eta \mathcal{E}_\phi(\mathbf{u})$ for a positive constant η , one can easily see that η is exactly the desired rate by using Grönwall's inequality. Since the dissipation functional \mathcal{D}_ϕ from Proposition 3.1 has no fixed sign due to the mixed term, these bounds above can scarcely be expected for the given problem. But in fact, the nonnegativity for *all* times is not a necessary assumption to obtain convergence. If a dissipation functional without sign can be estimated by

$$\mathcal{D}_\phi(\mathbf{u}) \geq \eta \mathcal{E}_\phi(\mathbf{u}) - K e^{-\gamma\tau}, \quad (3.11)$$

for example, with $\gamma > 0$ and $K \geq 0$, then this will still yield convergence with a rate that is the minimum of η and γ (see Lemma 3.3 below for the precise statement). The non-negative function $\tau \mapsto K e^{-\gamma\tau}$ can be interpreted then as an upper bound for the relative entropy for not being a true Lyapunov function. Since the function decays exponentially in time, this error is well-behaved when time is large enough. We will see later that in some cases, namely for the stoichiometric coefficients fulfilling $\alpha, \beta \geq 2$, the inequality (3.11) is exactly what we will prove for the given dissipation \mathcal{D}_B from Proposition 3.1. In the other case for $\alpha, \beta \in [1, 2)$, we need the following more general statement.

Lemma 3.3 *Let $E : [0, \infty) \rightarrow \mathbb{R} \cup \{\infty\}$ be a function satisfying $E(0) < \infty$ and the ordinary differential inequality*

$$\frac{d}{d\tau} E(\tau) \leq -(\eta - \mu e^{-\tau}) E(\tau) + K e^{-\gamma\tau}$$

for $\eta, \gamma > 0$ and $K, \mu \geq 0$. Then we have $E(\tau) < \infty$ for all $\tau > 0$ and

$$E(\tau) \leq e^{-\eta\tau + \mu} (E(0) + R(\tau)) \quad \text{with} \quad R(\tau) := K \int_0^\tau e^{(\eta-\gamma)s} ds.$$

Calculating the function R gives $E(\tau) \leq e^{-\min\{\eta, \gamma\}\tau + \mu} (E(0) + 2K|\eta - \gamma|^{-1})$ if $\eta \neq \gamma$ and $E(\tau) \leq e^{-\eta\tau + \mu} (E(0) + K\tau)$ in the case $\eta = \gamma$.

The proof of this lemma can be found in the appendix. We see that this weaker version of an entropy-dissipation estimate is enough to obtain the desired convergence (3.5). In the following sections this differential inequality is exactly what we want to derive for the relative entropy as a function of time.

4 Convergence for the special case $\alpha = \beta$

Let us begin with considering the special case $\alpha = \beta \geq 1$. That is, we study the solutions $\mathbf{u} = (u, v)^\top$ of the reaction-diffusion system

$$\begin{aligned} u_\tau &= d_1 u_{yy} + \frac{y}{2} u_y + e^\tau \alpha k(v^\alpha - u^\alpha), \\ v_\tau &= d_2 v_{yy} + \frac{y}{2} v_y - e^\tau \alpha k(v^\alpha - u^\alpha) \end{aligned} \quad (4.1)$$

together with continuous initial data $\mathbf{u}^0 = (u(0), v(0))^\top$ fulfilling the asymptotic boundary conditions

$$\mathbf{u}^0(\pm\infty) = (A_\pm^\alpha, A_\pm^\alpha)^\top. \quad (4.2)$$

In this special case, the mixed term \mathcal{I}_Λ from (3.7) simplifies significantly, namely

$$\mathcal{I}_\Lambda(\rho, \zeta) = \int_{\mathbb{R}} (\zeta - \rho) \alpha \Lambda \, dy.$$

The main point is that $\mathcal{D}_{\text{react}}$ is able to control $\zeta - \rho$ through the term $\Gamma(\rho^\alpha, \zeta^\alpha)$, which will be part of Section 4.1, where we focus on the Boltzmann entropy. Afterwards, in Section 4.2, we will allow more general entropy functions and aim to control $\mathcal{I}_{p,\Lambda}$ with $\mathcal{D}_{p,\text{react}}$ from Proposition 3.2 in a similar way.

Another much less important point is that the profile equation (3.4) simplifies also significantly, such that U , V , and Λ can be solved explicitly. Indeed, by inserting $\alpha = \beta$ one can see that the profile $\mathbf{U} = (U, V)^\top$ is characterized by solving the linear ODE

$$\begin{aligned} \frac{d_1 + d_2}{2} U''(y) + \frac{y}{2} U'(y) &= 0 \quad \text{with } U(\pm\infty) = A_\pm^\alpha, \\ V(y) = U(y) \quad \text{and} \quad \Lambda &= \frac{d_2 - d_1}{2\alpha} U''(y). \end{aligned} \quad (4.3)$$

This means that U is of error-function type like the profile (2.2) for the linear diffusion equation, but with respect to the average of the diffusivities $(d_1 + d_2)/2$. However, we do not need this outcome in the following calculations; thus, we do not close the door for further generalizations as this is not true if $\alpha \neq \beta$. The aim of this section is twofold: in Section 4.1 we show exponential convergence for the case of the relative Boltzmann entropy \mathcal{E}_B , and in Section 4.2 we show that in this case estimates with different relative entropies are possible and even more advantageous. In both cases, the result is obtained by proving a suitable bound for the dissipation functional, like inequality (3.11).

4.1 The case $\alpha = \beta \geq 1$ with Boltzmann entropy

Here we restrict to the case that ϕ is given by the Boltzmann function $\lambda_B(z) = z \log z - z + 1$, which is intrinsically linked to reaction diffusion systems, see e.g. [DeF06, Mie11] and the recent justification via Large Deviation principles in [MPR14, MP*17, Mit18].

Our convergence result reads as follows.

Theorem 4.1 (Convergence for $\alpha = \beta \geq 1$ with Boltzmann entropy) *Consider the relative Boltzmann entropy $E(\tau) := \mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U})$ for the unique similarity profile \mathbf{U} that solves (4.3). Then, for*

all solutions \mathbf{u} of the scaled system (4.1) with $E(0) < \infty$, the following differential inequalities are satisfied:

$$\text{For } \alpha = 1, \text{ it holds} \quad \dot{E}(\tau) \leq -\left(\frac{1}{2} - \mu_0 e^{-\tau}\right) E(\tau) + K_0 e^{-\tau} \quad \text{for all } \tau > 0, \quad (4.4a)$$

$$\text{for } 1 < \alpha < 2, \text{ we have} \quad \dot{E}(\tau) \leq -\left(\frac{1}{2} - \mu_1 e^{-\tau}\right) E(\tau) + K_1 e^{-\tau} \quad \text{for all } \tau > 0, \quad (4.4b)$$

$$\text{and if } \alpha \geq 2, \text{ then} \quad \dot{E}(\tau) \leq -\frac{1}{2} E(\tau) + K_2 e^{-\tau/(\alpha-1)} \quad \text{for all } \tau > 0, \quad (4.4c)$$

where all constants μ_0, μ_1, K_0, K_1 , and K_2 only depend on the problem data and are precisely defined in Lemmas 4.5, 4.7, and 4.8, respectively.

Here we provide estimates for the relative Boltzmann entropy $\mathcal{E}_B = \mathcal{E}_1$ only and refer to Theorem 4.10 and Corollary 4.11 for relative entropies $\mathcal{E}_p(\mathbf{u}|\mathbf{U})$.

Notice that all constants above are explicit and depend only on the given data and not on the solutions. The proof of this result relies on a series of lemmas and will be completed at the end of this section. We will see that the essential step in the case $\alpha = \beta$ is to use that \mathcal{I}_Λ can be written as a function of $\rho - \zeta$ and hence can be controlled by $\mathcal{D}_{\text{react}}$ alone. This simplifies the analysis and gives better convergence results. In particular, we do not need additional assumptions on the similarity profile \mathbf{U} , as will be needed in Section 5. We start by summarizing our results on the mixed term discussed above.

Lemma 4.2 *In the case $\alpha = \beta$, the mixed term from Proposition 3.1 reduces to*

$$\mathcal{I}_\Lambda(\rho, \zeta) = \int_{\mathbb{R}} (\zeta(y) - \rho(y)) \alpha \Lambda(y) dy, \quad \text{where} \quad \Lambda(y) = \frac{d_2 - d_1}{2\alpha} U''(y).$$

Notice that the simplified mixed term \mathcal{I}_Λ vanishes if we have equal diffusivities $d_1 = d_2$ as then $\Lambda \equiv 0$. This means that in the very special case where additionally to $\alpha = \beta$ also the diffusivities coincide, \mathcal{E}_B is a true Lyapunov function, and we have an explicit decay rate through the bonus factor $1/2$.

Corollary 4.3 *In addition to the assumptions of Theorem 4.1, assume $d_1 = d_2$ and $\alpha = \beta \geq 1$. Then, we obtain exponential convergence of all solutions \mathbf{u} to the profile \mathbf{U} :*

$$\mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U}) \leq e^{-\tau/2} \mathcal{E}_B(\mathbf{u}(0) | \mathbf{U}) \quad \text{for } \tau > 0.$$

Let us continue with two diffusivities $d_1, d_2 > 0$ that do not coincide in general. At first, the dissipation functional can naively be estimated by omitting the Fisher information

$$\mathcal{D}_B(\rho, \zeta) \geq \frac{1}{2} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) - \mathcal{I}_\Lambda(\rho, \zeta) + e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta).$$

Since we have the bonus factor, we are not dependent on exploiting the Fisher information in order to obtain a qualitative convergence result. Most often, estimation of the Fisher information, for example by using the Logarithmic Sobolev inequalities, leads to the fact that the dissipation functional can be bounded in terms of the relative entropy. Thanks to the parabolic scaling, the corresponding term is $\frac{1}{2} \mathcal{E}_B(\mathbf{u}|\mathbf{U})$, so we can drop the Fisher information, in contrast to [Grö83, DeF06, Mie17, MiM18], where the unscaled system (3.1) is studied on bounded domains. Even more, the fact that we can consider unbounded domains at all is precisely due to the scaling and the resulting bonus factor.

Nevertheless, it might be possible to improve the estimates if the Fisher information can be used. But in contrast to bounded domains, it seems to be much more complicated on the unbounded domain \mathbb{R} . And to the authors' best knowledge no way is found until now.

The idea is now to control the mixed term with the reactive dissipation and its useful prefactor e^τ . As mentioned earlier, the simple structure of the mixed term in Proposition 4.2 makes it easier to bound the dissipation functional from below. Indeed, Lemma 4.2 implies

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &= \int_{\mathbb{R}} (\zeta - \rho) \alpha \Lambda \, dy - e^\tau \int_{\mathbb{R}} k U^\alpha \Gamma(\rho^\alpha, \zeta^\alpha) \, dy \\ &= \int_{\mathbb{R}} \rho \left(\frac{\zeta}{\rho} - 1 \right) \alpha \Lambda - e^\tau k (\rho U)^\alpha \left(\frac{\zeta^\alpha}{\rho^\alpha} - 1 \right) \log(\zeta^\alpha / \rho^\alpha) \, dy. \end{aligned}$$

Next, we set $z := \frac{\zeta}{\rho} - 1$ as a new auxiliary variable and define, for $\alpha \geq 1$, the following family of functions

$$\Phi_\alpha(z) := \begin{cases} ((z+1)^\alpha - 1) \log((z+1)^\alpha) & \text{for } z > -1, \\ +\infty & \text{for } z \leq -1. \end{cases} \quad (4.5)$$

Note that for all $\tau > 0$ and $y \in \mathbb{R}$, we have $z > -1$. We only need to extend Φ_α for technical reasons. This leads to

$$\mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) = \int_{\mathbb{R}} \alpha \Lambda \rho z - e^\tau k (\rho U)^\alpha \Phi_\alpha(z) \, dy.$$

With respect to the auxiliary variable z , the integrand can be seen as the difference of a linear term and the function Φ_α . Remember that for a (not necessarily convex) function Φ , its Legendre transform Φ^* is defined as $\Phi^*(\xi) := \sup_z \{ \langle \xi, z \rangle - \Phi(z) \}$. Thus, we obtain

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &\leq \int_{\mathbb{R}} e^\tau k (\rho U)^\alpha \Phi_\alpha^* \left(\frac{\alpha \Lambda}{k U^\alpha} \rho^{1-\alpha} e^{-\tau} \right) \, dy \\ &= \int_{\mathbb{R}} e^\tau k (\rho U)^\alpha \Phi_\alpha^* \left(\tilde{\Lambda} \rho^{1-\alpha} e^{-\tau} \right) \, dy \quad \text{with } \tilde{\Lambda}(y) := \frac{\alpha \Lambda(y)}{k U^\alpha(y)} = \frac{(d_2 - d_1) U''(y)}{2k U(y)^\alpha}. \end{aligned} \quad (4.6)$$

Unfortunately, the Legendre transform Φ_α^* cannot be calculated explicitly, but a suitable estimate of Φ_α^* from above is sufficient to continue with (4.6). For this, we have the following auxiliary result, which is proved in Appendix A.

Lemma 4.4 *Consider for $\alpha \geq 1$ the function Φ_α defined in (4.5). Its Legendre transform Φ_α^* satisfies, for all $\xi \in \mathbb{R}$, the following estimates, where $\tilde{c}_\alpha = \left(\frac{2}{\alpha^2} \right)^{1/(\alpha-1)} \frac{\alpha-1}{\alpha}$:*

- 1 For $\alpha = 1$ we have $\Phi_1^*(\xi) \leq e^\xi - \xi - 1$;
- 2 for $\alpha \in (1, 2]$ it holds $\Phi_\alpha^*(\xi) \leq \max \{ \tilde{c}_\alpha |\xi|^{\alpha/(\alpha-1)}, \frac{1}{2\alpha} \xi^2 \}$;
- 3 and if $\alpha \geq 2$ then $\Phi_\alpha^*(\xi) \leq \tilde{c}_\alpha |\xi|^{\alpha/(\alpha-1)}$.

Moreover, for all $\alpha \geq 1$ we have $\Phi_\alpha^*(\xi) \leq \frac{1}{2\alpha} \xi^2$ for $|\xi| \leq \alpha$.

The bounds on the Legendre transform Φ_α^* will help us to find a bound for the dissipation functional. We start with the mathematically easier case $\alpha = \beta \geq 2$. In this case the dissipation functional fulfills the estimate (3.11), which is the inequality from Lemma 3.3 with $\mu = 0$. The other case $\alpha \in [1, 2)$ will be treated afterwards.

Lemma 4.5 *Let $\alpha = \beta \geq 2$. The dissipation functional \mathcal{D}_B from Proposition 3.1 can be bounded from below by*

$$\mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) \leq K_2 e^{-\tau/(\alpha-1)} \quad \text{for } K_2 := \frac{\tilde{c}_\alpha}{k^{1/(\alpha-1)}} \int_{\mathbb{R}} \left| \frac{\alpha \Lambda(y)}{U(y)} \right|^{\alpha/(\alpha-1)} dy < \infty$$

with \tilde{c}_α from Lemma 4.4.

Proof. We start from estimate (4.6) and insert the upper estimate for Φ_α^* from Lemma 4.4 (case $\alpha \geq 2$) to arrive at

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &\leq e^\tau k \int_{\Omega} (\rho U)^\alpha \tilde{c}_\alpha \left| \tilde{\Lambda} \rho^{1-\alpha} e^{-\tau} \right|^{\alpha/(\alpha-1)} dy \\ &= e^{-\tau/(\alpha-1)} \frac{\tilde{c}_\alpha}{k^{1/(\alpha-1)}} \int \left| \frac{\alpha \Lambda(y)}{U(y)} \right|^{\alpha/(\alpha-1)} dy = K_2 e^{-\tau/(\alpha-1)}. \end{aligned}$$

The dependence on ρ is exactly canceled out, such that the assertion is established. \blacksquare

Although we certainly lose some optimality in estimating the function Φ_α^* , we see that we get a profitably bound. Estimating by a function with exponent $\alpha/(\alpha-1)$ is the only choice that leads to a uniform bound for all solutions, because only then ρ cancels out. However, we obtain a decay rate $e^{-\tau/(\alpha-1)}$ only, which is not really optimal in terms of decay for $\tau \rightarrow \infty$ as is shown in the following remark. But it has the advantage that it is valid globally, i.e. for all solutions.

Remark 4.6 (Improved decay rate) *Using the exponential convergence of $u = \rho U$ to U (with the smaller decay rate from above) and parabolic regularity theory (involving the term $\mathcal{I}_{\text{Fisher}}$ dropped so far), it is possible to show that $\rho(\tau, y) \in [\underline{c}, \bar{c}]$ for all $y \in \mathbb{R}$ and $\tau \geq \tau_1$, where $0 < \underline{c} < 1 < \bar{c} < \infty$ and τ_1 may depend on ρ . Thus, we can use the better quadratic estimate $\frac{1}{2\alpha} \xi^2$ for $\Phi_\alpha^*(\xi)$ for $|\xi| \leq \alpha$, see the end of Lemma 4.4. Setting $\tau_2 = \log(\|\tilde{\Lambda}\|_\infty / (\alpha \underline{c}^{\alpha-1}))$ we obtain for $\tau \geq \max\{\tau_1, \tau_2\}$ the better decay estimate*

$$\mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) \leq e^\tau k \int_{\Omega} \frac{(\rho U)^\alpha}{2\alpha} \left| \frac{\tilde{\Lambda} e^{-\tau}}{\rho^{\alpha-1}} \right|^2 dy \leq e^{-\tau} \frac{\alpha}{2k} \frac{\bar{c}^\alpha}{\underline{c}^{\alpha 1}} \int \Lambda(y)^2 U(y)^{\alpha-2} dy.$$

Another way of deriving the optimal decay like $e^{-\tau/2}$ is given in Corollary 4.11, where $\mathcal{E}_B = \mathcal{E}_1$ is replaced by the higher order entropies \mathcal{E}_p with $p = \alpha - 1$, see estimate (4.10a).

With Lemma 3.3, we identified a bound for the dissipation functional that still yields the desired convergence although its sign is not necessarily non-negative for all times. In the previous proof, we obtained the estimate (4.4) with $\mu_j = 0$. Next, we study the cases $\alpha = \beta \in (1, 2)$ and $\alpha = \beta = 1$ and will see that the additional term $\mu_j e^{-\tau}$ will appear then. That is because there will be some terms containing ρ that cannot be estimated uniformly, so they need to be estimated by the relative entropy.

Lemma 4.7 *Let $\alpha = \beta \in (1, 2)$. Then for all times $\tau > 0$ the dissipation functional \mathcal{D}_B can be bounded from below by*

$$\mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) \leq \mu_1 e^{-\tau} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) + K_1 e^{-\tau},$$

where the constants μ_1 and K_1 are given by

$$\mu_1 = \frac{1}{k} \left\| \frac{\alpha^2 \Lambda^2}{U^{3-\alpha}} \right\|_{L^\infty} \quad \text{and} \quad K_1 = \int_{\mathbb{R}} \left(\frac{\alpha^2 \Lambda^2}{k U^{2-\alpha}} + \frac{\tilde{c}_\alpha}{k^{1/(\alpha-1)}} \left| \frac{\alpha \Lambda}{U} \right|^{\alpha/(\alpha-1)} \right) dy.$$

Proof. We again start with the estimate (4.6) and insert the upper estimate for Φ_α^* as derived in Lemma 4.4, where we estimate $\max\{a, b\} \leq a + b$:

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &\leq \int_{\mathbb{R}} e^\tau k U^\alpha \rho^\alpha \Phi_\alpha^* \left(\tilde{\Lambda} \rho^{1-\alpha} e^{-\tau} \right) dy \\ &\leq \int_{\mathbb{R}} e^\tau k (\rho U)^\alpha \left(\frac{1}{2\alpha} \tilde{\Lambda}^2 \rho^{2-2\alpha} e^{-\tau} + \tilde{c}_\alpha |\tilde{\Lambda}|^{\alpha/(\alpha-1)} \rho^{-\alpha} e^{-\tau\alpha/(\alpha-1)} \right) dy \\ &\leq e^{-\tau} \int_{\mathbb{R}} \frac{\alpha^2 \Lambda^2}{k U^{2-\alpha}} \frac{\rho^{2-\alpha}}{2\alpha} dy + e^{-\tau/(\alpha-1)} \int_{\mathbb{R}} \frac{\tilde{c}_\alpha}{k^{1/(\alpha-1)}} \left| \frac{\alpha \Lambda}{U} \right|^{\alpha/(\alpha-1)} dy. \end{aligned}$$

In the second term we can estimate $e^{-\tau/(\alpha-1)} \leq e^{-\tau}$ because of $\alpha \in (1, 2)$. In the first term we still need to estimate $\rho^{2-\alpha}$ where the exponent is less than 1. For this we use $\rho^{2-\alpha}/(2\alpha) \leq \lambda_B(\rho) + 1$ for $\rho \geq 0$ and $\alpha \in [1, 2]$ and obtain

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &\leq e^{-\tau} \int_{\mathbb{R}} \left(\frac{\alpha^2 \Lambda^2}{k U^{2-\alpha}} (\lambda_B(\rho) + 1) + \frac{\tilde{c}_\alpha}{k^{1/(\alpha-1)}} \left| \frac{\alpha \Lambda}{U} \right|^{\alpha/(\alpha-1)} \right) dy \\ &\leq e^{-\tau} \frac{1}{k} \|\alpha^2 \Lambda^2 / U^{3-\alpha}\|_\infty \int_{\mathbb{R}} \lambda_B(\rho) U dy + e^{-\tau} K_1, \end{aligned}$$

with K_1 as in the assertion. The desired result follows from $\int_{\mathbb{R}} \lambda_B(\rho) U dy \leq \mathcal{E}_B(\mathbf{u} | \mathbf{U})$. \blacksquare

The remaining case $\alpha = \beta = 1$ is important as this linear case relates to the case of Markov semi-groups. We proceed similarly as above but obtain a rather large bound because Φ_1^* has exponential growth. A better bound for this case is obtained in Section 4.2.

Lemma 4.8 *For $\alpha = \beta = 1$ the dissipation functional \mathcal{D}_B can be bounded from below by*

$$\mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) \leq \mu_0 e^{-\tau} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) + K_0 e^{-\tau},$$

where the constants μ_0 and K_0 are given in terms of $\lambda^* := \|\Lambda/U\|_{L^\infty}$ by

$$\mu_0 = \frac{(\lambda^*)^2 e^{\lambda^*/k}}{2k} \quad \text{and} \quad K_0 = \frac{e^{\lambda^*/k}}{k} \int_{\mathbb{R}} \frac{\alpha^2 \Lambda^2}{U} dy.$$

Proof. As before we start from (4.6) and now need to estimate $\Phi_1^*(\tilde{\Lambda} \rho^0 e^{-\tau})$. The decisive advantage is that $\rho^0 = 1$ provides automatically a bound independently of ρ , and the exponential growth does not harm too much.

Clearly, we have $|\tilde{\Lambda}(y) e^{-\tau}| \leq \lambda^*/k$ for all $\tau \geq 0$ and $y \in \mathbb{R}$. Using $(\Phi_1^*)''(\xi) = e^\xi$ we obtain the quadratic upper estimate

$$\Phi_1^*(\xi) \leq \frac{e^{\lambda^*/k}}{2} \xi^2 \quad \text{for } |\xi| \leq \lambda^*/k.$$

Inserting this into (4.6) first and using $\rho \leq \lambda_B(\rho) + 2$ we find

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &\leq \int_{\mathbb{R}} e^\tau k (\rho U) \frac{e^{\lambda^*/k}}{2} \tilde{\Lambda}^2 e^{-2\tau} dy \\ &\leq e^{-\tau} \frac{e^{\lambda^*/k}}{2k} \int_{\mathbb{R}} (\lambda_B(\rho) + 2) U \frac{\alpha^2 \Lambda^2}{U^2} dy \leq e^{-\tau} \mu_0 \mathcal{E}_B(\mathbf{u} | \mathbf{U}) + K_0 e^{-\tau}, \end{aligned}$$

which is the desired result. \blacksquare

The estimate in Lemma 4.8 has rather large constants because of the term $e^{\lambda^*/k}$. Since the linear case has many applications, in particular as Kolmogorov forward equation for Markov processes, we provide a better bound in Corollary 4.11. There we replace the Boltzmann entropy $\mathcal{E}_B = \mathcal{E}_1$ by the relative entropy \mathcal{E}_p with $p = 1/2$, which gives exactly the Hellinger distance, see (3.10).

As we have covered now all the cases $\alpha = \beta \geq 1$ we are now ready to summarize which completes the proof of our main result.

Proof of Theorem 4.1. Abbreviate the relative Boltzmann entropy by $E(\tau) := \mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U})$. At first, Proposition 3.1 and the nonnegativity of the Fisher information give

$$\frac{d}{d\tau} E = -\mathcal{D}_B \quad \text{with } \mathcal{D}_B \geq \frac{1}{2} E + e^\tau \mathcal{D}_{\text{react}} - \mathcal{I}_\Lambda.$$

Since $\alpha = \beta$, the mixed term reduces to $\mathcal{I}_\Lambda(\rho, \zeta) = \int_{\mathbb{R}} (\zeta - \rho) \alpha \Lambda \, dy$. In all three cases for α we have shown $\mathcal{I}_\Lambda - e^\tau \mathcal{D}_{\text{react}} \leq \mu_j e^{-\tau} E(\tau) + K_j e^{-\sigma_j \tau}$ with $\mu_2 = 0$. Inserting this we arrive exactly at (4.4), and our result is established. \blacksquare

4.2 The case $\alpha = \beta$ with general entropies

While for the case $\alpha \neq \beta$ it is really necessary to take the Boltzmann entropy, we have more flexibility with the choice of entropy functions if $\alpha = \beta$. In this section, we choose general entropies which will improve the results, in particular for the case $\alpha = \beta = 1$.

Recall the family of entropy functions F_p introduced in (3.8) and consider $p \notin \{0, 1\}$ so that all the formulas are well-defined. Of course, it is possible to consider the cases $p = 0$ and $p = 1$ by passing to the limit and use that $\lim_{p \rightarrow 0} \frac{1}{p}(\zeta^p - 1) = \log(\zeta)$.

We can define the relative entropy associated to the function F_p by

$$\mathcal{E}_p(\mathbf{u}(\tau) | \mathbf{U}) := \int_{\mathbb{R}} U(y) F_p(\rho(y)) + V(y) F_p(\zeta(y)) \, dy \quad \text{with } \rho := u/U \text{ and } \zeta := v/V.$$

From Proposition 3.2 we know

$$\frac{d}{d\tau} \mathcal{E}_p(\mathbf{u} | \mathbf{U}) = -\mathcal{D}_p(\rho, \zeta) \leq -\frac{1}{2} \mathcal{E}_p(\mathbf{u} | \mathbf{U}) - e^\tau \mathcal{D}_{p,\text{react}}(\rho, \zeta) + \mathcal{I}_{p,\Lambda}(\rho, \zeta).$$

Thus, the strategy is to estimate the difference $\mathcal{I}_{p,\Lambda} - e^\tau \mathcal{D}_{p,\text{react}}$, like in the previous section. We have

$$\begin{aligned} \mathcal{I}_{p,\Lambda}(\rho, \zeta) - e^\tau \mathcal{D}_{p,\text{react}}(\rho, \zeta) &= \int_{\mathbb{R}} \frac{1}{p} (\zeta^p - \rho^p) \alpha \Lambda - e^\tau k U^\alpha \frac{\alpha}{p-1} (\zeta^{p-1} - \rho^{p-1}) (\zeta^\alpha - \rho^\alpha) \, dy \\ &= \int_{\mathbb{R}} \frac{1}{p} \rho^p \left(\frac{\zeta^p}{\rho^p} - 1 \right) \alpha \Lambda - e^\tau k U^\alpha \frac{\alpha}{p-1} \rho^{\alpha+p-1} \left(\frac{\zeta^{p-1}}{\rho^{p-1}} - 1 \right) \left(\frac{\zeta^\alpha}{\rho^\alpha} - 1 \right) \, dy. \end{aligned}$$

Defining $z := \frac{\zeta^p}{\rho^p} - 1 > -1$ as an auxiliary variable and the following two-parameter family of functions

$$\Phi_{p,\alpha}(z) := \begin{cases} \frac{\alpha}{p-1} \left((z+1)^{\frac{p-1}{p}} - 1 \right) \left((z+1)^{\frac{\alpha}{p}} - 1 \right) & \text{for } z > -1, \\ +\infty & \text{for } z \leq -1. \end{cases} \quad (4.7)$$

as a generalization of (4.5), this yields

$$\begin{aligned} \mathcal{I}_{p,\Lambda}(\rho, \zeta) - e^\tau \mathcal{D}_{p,\text{react}}(\rho, \zeta) &\leq \int_{\mathbb{R}} \frac{1}{p} \rho^p \alpha \Lambda z - e^\tau k U^\alpha \rho^{\alpha+p-1} \Phi_{p,\alpha}(z) \, dy \\ &\leq \int_{\mathbb{R}} e^\tau k U^\alpha \rho^{\alpha+p-1} \Phi_{p,\alpha}^* \left(\frac{1}{p} \tilde{\Lambda} \rho^{1-\alpha} e^{-\tau} \right) \, dy \quad \text{with } \tilde{\Lambda}(y) := \frac{\alpha \Lambda(y)}{k U^\alpha(y)} = \frac{(d_2 - d_1) U''(y)}{2k U(y)^\alpha}. \end{aligned} \quad (4.8)$$

From our theory above, we know that it is advantageous to estimate $\Phi_{p,\alpha}$ from below by a multiple of z^2 , because then $\Phi_{p,\alpha}^*$ has a quadratic upper bound. Hence, we prepare the following result.

Lemma 4.9 (Quadratic bound for $\Phi_{p,\alpha}^*$) For $\alpha > 0$ and $p \in (0, \max\{\alpha/2, \alpha-1\}]$ we have

$$\widehat{M}_{p,\alpha} := \sup \left\{ \frac{\alpha^2}{4p^2} \frac{z^2}{\Phi_{p,\alpha}(z)} \mid z \in \mathbb{R} \setminus \{0\} \right\} < \infty$$

and the quadratic upper bound $\Phi_{p,\alpha}^*(\zeta) \leq \widehat{M}_{p,\alpha} \left(\frac{p}{\alpha} \zeta\right)^2$ for all $\zeta \in \mathbb{R}$.

In the given range we always have $\widehat{M}_{p,\alpha} \geq 1/4$.

For $p = 1/2$ and $\alpha \geq 1$ we have $\widehat{M}_{1/2,\alpha} \leq \alpha/2$ and $\widehat{M}_{1/2,1} = 1/2$.

For $p > 0$ and $\alpha = p+1$ we have $\widehat{M}_{p,p+1} = 1/4$.

Proof. We fix a pair (α, p) in the given range and set $f(z) = z^2/\Phi_{p,\alpha}(z)$ for $z \in (-1, 0) \cup (0, \infty)$.

We first observe that $z \mapsto \Phi_{p,\alpha}(z)$ behaves like z^2 for $z \approx 0$. Hence, f is bounded near $z = 0$. Moreover, $\Phi_{p,\alpha}$ is bounded from below on intervals $(-1, -1+\delta)$ for small δ . Since $\Phi_{p,\alpha}$ is analytic in $(-1, 0)$ and in $(0, \infty)$, the same is true for f . Thus, f is bounded on the interval $(-1, R)$ for all $R > 0$. To obtain boundedness of f it suffices to study its polynomial growth. Indeed, we have $f(z) \sim z^\gamma$ with $\gamma = 2 - \max\{0, (p-1)/p\} - \alpha/p$. However, the range for (α, p) was chosen exactly such that $\gamma \leq 0$, hence $\widehat{M}_{p,\alpha}$ is finite.

From $\Phi_{p,\alpha}(z) \geq \left(\frac{\alpha}{p} z\right)^2 / (4\widehat{M}_{p,\alpha})$ we obtain $\Phi_{p,\alpha}^*(\zeta) \leq \widehat{M}_{p,\alpha} \left(\frac{p}{\alpha} \zeta\right)^2$ by the properties of the Fenchel-Legendre transformation. With $\Phi_{p,\alpha}(z) = \frac{\alpha^2}{p^2} z^2 + \text{h.o.t.}$, we find $\widehat{M}_{p,\alpha} \geq 1/4$.

For the two explicit estimates we argue as follows. For $p = 1/2$ and $\alpha \geq 1$ we have for all $z > -1$ the estimate

$$\Phi_{1/2,\alpha}(z) = 2\alpha \frac{z}{z+1} \left((z+1)^{2\alpha} - 1 \right) \geq 2\alpha \frac{z}{z+1} \left((z+1)^2 - 1 \right) = \frac{2\alpha z^2 (z+2)}{z+1} \geq 2\alpha z^2, \quad (4.9)$$

where we use $(z+1)^{2\alpha} \geq (z+1)^2$ for $z > 0$ and $(z+1)^{2\alpha} \leq (z+1)^2$ for $z < 0$. Thus, we have $\widehat{M}_{1/2,\alpha} \leq \alpha/2$. Using $\Phi_{1/2,\alpha}(z) = 4\alpha^2 z^2 + \text{h.o.t.}$, we obtain $\widehat{M}_{1/2,\alpha} \geq 1/4$. For the case $\alpha = 1$ we observe that the first “ \geq ” in (4.9) is an equality, such that $\Phi_{1/2,1}(z) \geq 2z^2$ is optimal, and $\widehat{M}_{1/2,1} = 1/2$ follows.

For the case $\alpha = p+1 > 1$ we set $\lambda = 1/p > 0$ and $w = z+1$. For $w > 0$ we have

$$\begin{aligned} \Phi_{p,p+1}(z) &= \frac{p+1}{p-1} \left(w^{(p-1)/p} - 1 \right) \left(w^{(p+1)/p} - 1 \right) \\ &= \frac{(p+1)^2}{p^2} G_\lambda(w) \text{ with } G_\lambda(w) = \frac{1}{1-\lambda^2} \left(w^2 - w^{1-\lambda} - w^{1+\lambda} + 1 \right). \end{aligned}$$

Calculating the first three derivatives of G_λ , we find $G_\lambda'''(w) = \lambda(w^{\lambda-2} - w^{-\lambda-2})$ and conclude $G_\lambda''(w) \geq G_\lambda''(1) = 2$. This implies $G_\lambda(w) \geq (w-1)^2$ and hence $\Phi_{p,p+1}(z) \geq \frac{(p+1)^2}{p^2} z^2$. This provides $\widehat{M}_{p,p+1} = 1/4$, because optimality follows by taking $z \rightarrow 0$. ■

Using this estimate we can now estimate the relative entropies with F_p instead of λ_B , the technique being exactly the same as above.

Theorem 4.10 (Exponential decay of $\mathcal{E}_p(\mathbf{u}(\tau))$) For $\alpha \geq 1$ choose any $p > 0$ with $\alpha - 1 \leq p \leq \max\{\alpha/2, \alpha - 1\}$ and define the relative entropy $E_p(\tau) := \mathcal{E}_p(\mathbf{u}(\tau) | \mathbf{U})$ for the similarity profile $\mathbf{U} = (U, V)^\top$ satisfying (4.3). Then, all solutions $\mathbf{u} = (u, v)^\top$ of the scaled system (4.1) with $E_p(0) < \infty$ satisfy the estimate

$$\frac{d}{d\tau} E_p(\tau) \leq -\left(\frac{1}{2} - \tilde{\mu}_{p,\alpha} e^{-\tau}\right) E_p(\tau) + \tilde{K}_{p,\alpha} e^{-\tau},$$

where the constants $\tilde{\mu}_{p,\alpha}$ and $\tilde{K}_{p,\alpha}$ are given by

$$\text{for } 2 \leq \alpha = p + 1: \quad \tilde{\mu}_{\alpha-1,\alpha} = 0 \text{ and } \tilde{K}_{\alpha-1,\alpha} = \frac{1}{4k} \int_{\mathbb{R}} \frac{\Lambda^2}{U^\alpha} dy,$$

$$\text{for } 1 \leq \alpha < 2: \quad \tilde{\mu}_{p,\alpha} = \frac{\kappa}{k} \widehat{M}_{p,\alpha} \left\| \frac{\Lambda^2}{U^{\alpha+1}} \right\|_{L^\infty} \text{ and } \tilde{K}_{p,\alpha} = \frac{1}{k} \widehat{M}_{p,\alpha} (\kappa F_p^*(\kappa) + 1) \int_{\mathbb{R}} \frac{\Lambda^2}{U^\alpha} dy,$$

where $\kappa = \sqrt{1+p-\alpha}$.

Proof. We continue with estimate (4.8) and obtain

$$\mathcal{I}_{p,\Lambda}(\rho, \zeta) - e^\tau \mathcal{D}_{p,\text{react}}(\rho, \zeta) \leq e^{-\tau} \widehat{M}_{p,\alpha} \int_{\mathbb{R}} \rho^{1+p-\alpha} \frac{\Lambda^2}{k U^\alpha} dy.$$

For $\alpha \geq 2$ we have $p = \alpha - 1$, and the integrand is independent of ρ . Hence, the assertion is clear in this case.

For $\alpha \in [1, 2)$ we observe $\kappa = \sqrt{1+p-\alpha} \in (0, 1]$ and estimate as follows:

$$\rho^{1+p-\alpha} = \rho^{\kappa^2} \leq \kappa^2 \rho + (1 - \kappa^2) \leq \kappa (\kappa \rho) + 1 \leq \kappa (F_p(\rho) + F_p^*(\kappa)) + 1.$$

With this we find

$$\mathcal{I}_{p,\Lambda}(\rho, \zeta) - e^\tau \mathcal{D}_{p,\text{react}}(\rho, \zeta) \leq e^{-\tau} \frac{\widehat{M}_{p,\alpha}}{k} \left(\kappa \left\| \frac{\Lambda^2}{U^{\alpha+1}} \right\|_{L^\infty} \mathcal{E}_p(\mathbf{u}) + (\kappa F_p^*(\kappa) + 1) \int_{\mathbb{R}} \frac{\Lambda^2}{U^\alpha} dy \right),$$

which gives the desired result for $\alpha \in [1, 2)$. ■

The following corollary provides some natural consequences of the above result. First, we show that for $\alpha \geq 3$ we again have exponential decay like $e^{-\tau/2}$ if we use the relative entropy $\mathcal{E}_{\alpha-1}(\mathbf{u} | \mathbf{U})$. This improves the result in Theorem 4.1, where $\mathcal{E}_1 = \mathcal{E}_B$ only decays like $e^{-\tau/(\alpha-1)}$. Second, we show that for the linear case with $\alpha = 1$ we can significantly improve the constants μ_0 and K_0 in Lemma 4.8 by using $\mathcal{E}_{1/2}$ instead of $\mathcal{E}_1 = \mathcal{E}_B$.

Corollary 4.11 (Decay of \mathcal{E}_p for $\alpha = \beta$) We have the following estimates:

$$\text{For } \alpha \geq 2: \quad \frac{d}{d\tau} \mathcal{E}_{\alpha-1}(\mathbf{u} | \mathbf{U}) \leq -\frac{1}{2} \mathcal{E}_{\alpha-1}(\mathbf{u} | \mathbf{U}) + e^{-\tau} \int_{\mathbb{R}} \frac{\Lambda^2}{4k U^\alpha} dy, \quad (4.10a)$$

$$\text{for } \alpha = 1: \quad \frac{d}{d\tau} \mathcal{E}_{1/2}(\mathbf{u} | \mathbf{U}) \leq -\left(\frac{1}{2} - \tilde{\mu}_*\right) \mathcal{E}_{1/2}(\mathbf{u} | \mathbf{U}) + e^{-\tau} \int_{\mathbb{R}} \frac{11 + \sqrt{2}}{14k} \frac{\Lambda^2}{U} dy, \quad (4.10b)$$

where $\tilde{\mu}_* = \left\| \Lambda/U \right\|_{L^\infty}^2 / (k\sqrt{8})$.

Proof. The estimate in (4.10a) is a simple rewriting of the corresponding case in Theorem 4.10. The second estimate in (4.10b) follows similarly from the case $\alpha = 1$ and $p = 1/2$ by observing $\kappa = \sqrt{1+p-\alpha} = 1/\sqrt{2}$ and $F_{1/2}^*(\zeta) = 2\zeta/(2-\zeta)$. ■

5 Convergence for the case $\alpha > \beta \geq 1$

In this section, we consider the case $\alpha \neq \beta$. Without loss of generality, we assume that $\alpha > \beta$. We aim to show that solutions to the Cauchy problem (3.2),(3.3) converge to the similarity profile $\mathbf{U} = (U, V)^\top$ characterized by the equations (3.4), but in contrast to the special case $\alpha = \beta$, there is no meaningful possibility to simplify the mixed term $\mathcal{I}_\Lambda(\rho, \zeta) = \int_{\mathbb{R}} ((\zeta-1)\beta - (\rho-1)\alpha)\Lambda \, dy$. Let us recall that in this general setting, Λ is given as

$$\Lambda = \frac{1}{\beta}(d_2 V'' + \frac{y}{2} V') = -\frac{1}{\alpha}(d_1 U'' + \frac{y}{2} U'),$$

where the last equality follows by (3.4). As in Section 4.1, we need to control the mixed term \mathcal{I}_Λ in order to estimate the dissipation functional \mathcal{D}_B from Proposition 3.1. The difference to the case $\alpha = \beta$ is that the mixed term \mathcal{I}_Λ cannot be estimated with the reactive dissipation term $-e^\tau \mathcal{D}_{\text{react}}$ alone, but we need to steal parts of the bonus factor $1/2$. More precisely, we do the following

$$\begin{aligned} \mathcal{I}_\Lambda(\rho, \zeta) &= \int_{\mathbb{R}} ((\zeta-1)\beta - (\rho-1)\alpha)\Lambda \, dy \\ &= \int_{\mathbb{R}} (\Psi(\zeta^\beta) - \Psi(\rho^\alpha))\Lambda \, dy + \int_{\mathbb{R}} \left((\zeta-1 - \frac{1}{\beta}\Psi(\zeta^\beta))\beta - (\rho-1 - \frac{1}{\alpha}\Psi(\rho^\alpha))\alpha \right)\Lambda \, dy \\ &=: \mathcal{I}_{\Lambda,1}(\rho, \zeta) + \mathcal{I}_{\Lambda,2}(\rho, \zeta) \end{aligned} \quad (5.1)$$

for a suitable function Ψ that will be selected below. That is, we split the mixed term into the two terms $\mathcal{I}_{\Lambda,1}$ and $\mathcal{I}_{\Lambda,2}$ with the strategy to estimate them separately in the following way:

- 1 We aim to control the integral term $\mathcal{I}_{\Lambda,1}$ with $-e^\tau \mathcal{D}_{\text{react}}$ in a similar way as it is done in Section 4.
- 2 The integral term $\mathcal{I}_{\Lambda,2}$ will be estimated exploiting $-\frac{1}{2}\mathcal{E}_B$. To this end, we need to choose the function Ψ in such a way that we can globally estimate

$$\alpha \left| \rho-1 - \frac{1}{\alpha}\Psi(\rho^\alpha) \right| \leq C_\alpha \lambda_B(\rho) \quad \text{and} \quad \beta \left| \zeta-1 - \frac{1}{\beta}\Psi(\zeta^\beta) \right| \leq C_\beta \lambda_B(\zeta), \quad (5.2)$$

for constants $C_\alpha, C_\beta \geq 0$. Further, the profile functions U and V have to satisfy $\Lambda/U \in L^\infty(\mathbb{R})$ and $\Lambda/V \in L^\infty(\mathbb{R})$. Even more, we need

$$\max \left\{ C_\alpha \|\Lambda/U\|_\infty, C_\beta \|\Lambda/V\|_\infty \right\} < 1/2,$$

where $1/2$ is the bonus factor. This can be achieved if A_- and A_+ are close enough to each other so that the profiles are flat and hence $\|\Lambda\|_\infty$ is small enough, we refer to [MiS23a, Rem. 5.1].

The considerations above lead to the function

$$\Psi(r) := \max\{\alpha, \beta\} (r^{1/\max\{\alpha, \beta\}} - 1) = \alpha (r^{1/\alpha} - 1).$$

First, it satisfies $\Psi(1) = 0$ and $\Psi'(1) = 1$ for all α , which is a necessary condition for the inequalities (5.2). Second, it allows us to use the same technique with the Legendre transform in order to control

$\Psi(\zeta^\beta) - \Psi(\rho^\alpha)$ through $\Gamma(\rho^\alpha, \zeta^\beta)$, as we will see later. Let us start considering point 2. If we insert the ansatz for Ψ , we obtain

$$\alpha \left| \rho - 1 - \frac{1}{\alpha} \Psi(\rho^\alpha) \right| \equiv 0 \quad \text{and} \quad \beta \left| \zeta - 1 - \frac{1}{\beta} \Psi(\zeta^\beta) \right| = \left(\beta - \frac{\beta^2}{\alpha} \right) F_{\beta/\alpha}(\zeta) \leq (\alpha - \beta) \lambda_B(\zeta),$$

where $F_{\beta/\alpha}$ denotes the entropy function defined in (3.8) for $p = \beta/\alpha$ so that we can use the property $F_p(z) \leq \frac{1}{p} F_1(z) = \frac{1}{p} \lambda_B(z)$, see (3.9a). With this, the following lemma is established.

Lemma 5.1 *For all $\alpha > \beta \geq 1$, the second addend $\mathcal{I}_{\Lambda,2}$ of the mixed term \mathcal{I}_Λ can be bounded by*

$$\mathcal{I}_{\Lambda,2}(\rho, \zeta) \leq \theta \mathcal{E}_B(\mathbf{u} | \mathbf{U}), \quad \text{with} \quad \theta = (\alpha - \beta) \|\Lambda/V\|_\infty.$$

After the preliminary considerations, we can formulate the main theorem of this section.

Theorem 5.2 (Convergence for $\alpha > \beta \geq 1$) *Consider the relative Boltzmann entropy $E(\tau) := \mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U})$ for the unique similarity profile $\mathbf{U} = (U, V)^\top$ which is characterized by (3.4). Assume further that $|A_- - A_+|$ is small enough such that*

$$\theta := (\alpha - \beta) \|\Lambda/V\|_\infty < 1/2.$$

Then, for all solutions $\mathbf{u} = (u, v)^\top$ of the Cauchy problem (3.2),(3.3) with finite initial entropy $E(0) < \infty$, the following differential inequalities hold true:

$$\text{For } \alpha \in (1, 2), \text{ it holds} \quad \dot{E}(\tau) \leq -\left(\frac{1}{2} - \theta - \mu_1 e^{-\tau}\right) E(\tau) + K_1 e^{-\tau} \quad \text{for all } \tau > 0, \quad (5.3a)$$

$$\text{and if } \alpha \geq 2, \text{ then} \quad \dot{E}(\tau) \leq -\left(\frac{1}{2} - \theta\right) E(\tau) + K_2 e^{-\tau/(\alpha-1)} \quad \text{for all } \tau > 0, \quad (5.3b)$$

where μ_1, K_1 and K_2 were already defined in Section 4.1, in Lemma 4.5 and 4.7, respectively.

The proof can be found at the end of this section. Notice that the case $\alpha = 1$ does not occur since $\alpha > \beta \geq 1$. Moreover, we see that we obtain here the same constants μ_1, K_1 and K_2 as in the special case $\alpha = \beta$. But one has to be careful, the constants only coincide if Λ is given in its general form, namely $\Lambda = \frac{1}{\beta}(d_2 V'' + \frac{y}{2} V') = -\frac{1}{\alpha}(d_1 U'' + \frac{y}{2} U')$, while in Section 4 there is the possibility to simplify Λ due to $\alpha = \beta$ and $U = V$.

The fact that they coincide, up to the possible simplification of Λ , already indicates that we can trace a part of the proof back to what we already did in Section 4. In the following, we will find out how it works explicitly.

Thus, we turn our attention to point 1 of our strategy. Luckily, we will see that the function $\Psi(r) = \alpha(r^{1/\alpha} - 1)$ is a well-working function for estimating $\mathcal{I}_{\Lambda,1}$ as well. We aim to estimate the difference $\mathcal{I}_{\Lambda,1} - e^\tau \mathcal{D}_{\text{react}}$ in a suitable way. It holds

$$\begin{aligned} \mathcal{I}_{\Lambda,1}(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &= \int_{\mathbb{R}} (\Psi(\zeta^\beta) - \Psi(\rho^\alpha)) \Lambda - e^\tau k U^\alpha \Gamma(\rho^\alpha, \zeta^\beta) dy \\ &= \int_{\mathbb{R}} \alpha \rho \left(\frac{\zeta^{\beta/\alpha}}{\rho} - 1 \right) \Lambda - e^\tau k U^\alpha \rho^\alpha \left(\frac{\zeta^\beta}{\rho^\alpha} - 1 \right) \log(\zeta^\beta / \rho^\alpha) dy. \end{aligned}$$

Next, we take the very same function Φ_α defined in (4.5). However, in this general case we have to define $z := \frac{\zeta^{\beta/\alpha}}{\rho} - 1$ to ensure everything fits together. This yields

$$\begin{aligned} \mathcal{I}_{\Lambda,1}(\rho, \zeta) - e^\tau \mathcal{D}_{\text{react}}(\rho, \zeta) &= \int_{\mathbb{R}} \alpha \rho \Lambda z - e^\tau k(U\rho)^\alpha \Phi_\alpha(z) dy \\ &\leq \int_{\mathbb{R}} e^\tau k(U\rho)^\alpha \Phi_\alpha^* \left(\tilde{\Lambda} \rho^{1-\alpha} e^{-\tau} \right) dy, \quad \text{with} \quad \tilde{\Lambda} := \frac{\alpha \Lambda}{kU^\alpha} = -\frac{d_1 U'' + \frac{y}{2} U'}{kU^\alpha}. \end{aligned} \quad (5.4)$$

Comparing this estimate above with that from Section 4, we realize that we end up with the same inequality like in (4.6), with the only difference that Λ is in its general setting. With this, we can easily proof the following by replicating the steps of Lemma 4.7 and 4.8.

Lemma 5.3 *Under the assumptions of Theorem 5.2, for the inequality (5.4) the following bounds from below hold true for all $\tau > 0$:*

$$\text{For } \alpha \in (1, 2), \text{ we have} \quad \mathcal{I}_{\Lambda,1} - e^\tau \mathcal{D}_{\text{react}} \leq \mu_1 e^{-\tau} \mathcal{E}_B(\mathbf{u} | \mathbf{U}) + K_1 e^{-\tau} \quad (5.5a)$$

$$\text{and for } \alpha \geq 2, \text{ it holds} \quad \mathcal{I}_{\Lambda,1} - e^\tau \mathcal{D}_{\text{react}} \leq K_2 e^{-\tau/(\alpha-1)}, \quad (5.5b)$$

with μ_1, K_1 and K_2 precisely defined in Lemma 4.7 and 4.8, respectively.

We are now ready to prove the main theorem of this section.

Proof of Theorem 5.2. Denote the relative Boltzmann entropy by $E(\tau) := \mathcal{E}_B(\mathbf{u}(\tau) | \mathbf{U})$ and use Proposition 3.1 together with the nonnegativity of the Fisher information which yield

$$\frac{d}{d\tau} E = -\mathcal{D}_B \quad \text{with} \quad \mathcal{D}_B \geq \frac{1}{2} E + e^\tau \mathcal{D}_{\text{react}} - \mathcal{I}_\Lambda.$$

In this general setting, the mixed term is given by $\mathcal{I}_\Lambda(\rho, \zeta) = \int_{\mathbb{R}} ((\zeta-1)\beta - (\rho-1)\alpha) \Lambda dy$. So, in (5.1) we split \mathcal{I}_Λ into $\mathcal{I}_{\Lambda,1}$ and $\mathcal{I}_{\Lambda,2}$ and estimated both addends separately. First, using Lemma 5.1 yields $\mathcal{I}_{\Lambda,2} \leq \theta E(\tau)$ for all $\alpha > \beta \geq 1$. Second, Lemma 5.3 provides in both cases $\alpha \in (1, 2)$ and $\alpha \geq 2$ that $\mathcal{I}_{\Lambda,1} - e^\tau \mathcal{D}_{\text{react}} \leq \mu_j e^{-\tau} E(\tau) + K_j e^{-\sigma_j \tau}$ for $j = 1, 2$, with $\mu_2 = 0$. Inserting all estimates, we obtain (5.3) as claimed. ■

This proof concludes the section and therefore also completes the new results we can formulate on the convergence towards similarity profiles. Through this, it provides a qualitative statement on the long-time behavior of solutions to the given reaction-diffusion system under the difficulty of considering the whole space, i.e. unbounded domains, and infinite mass. In the current paper, new approaches are used which allow to treat these difficulties. In particular, this means the transformation of the system into parabolic scaling variables, which generates the bonus factor $d/2$ and thus allows the energy-dissipation estimates (of Boltzmann type), that are well-studied on bounded domains, to be applied to the whole space. In the case $\alpha \neq \beta$, we have seen that additional restrictions must hold on the similarity profile, namely that $|A_- - A_+|$ is sufficiently small. The question, whether the convergence holds true for solutions with arbitrary boundary values, remains open. Furthermore, the considered system, especially the reaction $\alpha X_1 \rightleftharpoons \beta X_2$, is still very simple. Perhaps, the methods presented above provide a starting point for more complicated systems admitting a family of steady-states.

Our approach based on energy-dissipation estimates seems to be flexible enough to treat more complicated reaction-diffusion systems, where more species and more reactions can be involved. For the general setup we refer to [MiS23a] where the existence result for similarity profiles is proved for these general situations. The main task is then the control of the mixed term \mathcal{I}_Λ , which may now involve more than one Lagrange multiplier.

A Appendices

In this appendix, we will give the omitted proofs of auxiliary results we used throughout this paper.

Proof of Lemma 3.3. The given differential inequality is of the form

$$\frac{d}{d\tau} E(\tau) \leq -a(\tau) E(\tau) + b(\tau) \quad \text{for } a(\tau) := \eta - \mu e^{-\tau} \text{ and } b(\tau) := K e^{-\gamma\tau}.$$

A direct application of the differential version of Grönwall's lemma yields

$$E(\tau) \leq E(0) e^{-\int_0^\tau a(r) dr} + \int_0^\tau b(s) e^{-\int_s^\tau a(r) dr} ds. \quad (\text{A.1})$$

First, we estimate the integral $\int_s^\tau a(r) dr$ roughly but sufficiently as we will see. We have

$$-\int_s^\tau a(r) dr = \int_s^\tau \mu e^{-r} - \eta dr = \mu(e^{-s} - e^{-\tau}) - \eta(\tau - s) \leq \mu - \eta(\tau - s)$$

since $s \geq 0$. Inserting this into (A.1) and using the monotonicity of the exponential function gives

$$\begin{aligned} E(\tau) &\leq E(0) e^{\mu - \eta\tau} + K e^{\mu - \eta\tau} \int_0^\tau e^{(\eta - \gamma)s} ds = e^\mu \left(E(0) e^{-\eta\tau} + \frac{K}{\eta - \gamma} (e^{-\gamma\tau} - e^{-\eta\tau}) \right) \\ &\leq e^{-\min\{\eta, \gamma\}\tau + \mu} \left(E(0) + \frac{2K}{|\eta - \gamma|} \right) \quad \text{if } \eta \neq \gamma. \end{aligned}$$

In case $\eta = \gamma$, the integrand above is identically 1, which gives the result. ■

We now give the proof of Lemma 4.4, which provides the necessary upper estimates of the functions Φ_α .

Proof of Lemma 4.4. Throughout we use $\alpha \geq 1$ and write $\Phi_\alpha = g_\alpha h_\alpha$ with

$$g_\alpha(z) = \begin{cases} |\log(z+1)^\alpha| & \text{for } z > -1, \\ \infty & \text{for } z \leq -1, \end{cases} \quad \text{and} \quad h_\alpha(z) = \begin{cases} |(z+1)^\alpha - 1| & \text{for } z \geq -1, \\ \infty & \text{for } z < -1. \end{cases}$$

To obtain upper bounds for Φ_α^* , we derive lower bounds for Φ_α . We do the estimates for $z \geq 0$ and $z \leq 0$ separately.

For $z \leq 0$ it suffices to consider $z \in (-1, 0)$. First observe $g_\alpha(z) \geq -\alpha z$ by convexity. Next, we have $h_\alpha(z) = 1 - (z+1)^\alpha$, which is concave because of $\alpha \geq 1$. Hence, $h_\alpha(0) = 0$ and $h_\alpha(1) = 1$ imply $h_\alpha(z) \geq -z$ for $z \in [-1, 0]$. Together we find

$$\Phi_\alpha(z) \geq \alpha z^2 \quad \text{for } z \in [-1, 0], \quad \Phi_\alpha(z) = \infty \quad \text{for } z < -1.$$

For $z \geq 0$ we use $\log 2 > 1/2$ which implies $\log y \geq \min\{(y-1)/2, 1/2\}$ for $y \geq 1$. We find

$$g_\alpha(z) = \alpha \log(z+1) \geq \alpha \min\{z/2, 1/2\}.$$

For h_α we obtain $h_\alpha(z) = (z+1)^\alpha - 1 \geq z^\alpha$, which follows by observing that the derivative of both sides satisfy the same inequality and a subsequent integration. Moreover, $h_\alpha(z) \geq \alpha z$ by convexity. Hence, $h_\alpha(z) \geq \max\{\alpha z, z^\alpha\}$, and we arrive at

$$\Phi_\alpha(z) \geq \frac{\alpha}{2} \max\{\alpha|z|, |z|^\alpha\} \min\{|z|, 1\} \quad \text{for } z \geq 0.$$

For $\alpha = 1$ the above estimate is too weak. To obtain a better estimate we observe that $F_0(\rho) = \rho - \log \rho - \rho \geq 0$, see (3.8). Hence, setting $z = \rho - 1$ we have

$$\Phi_1(z) = (\rho - 1) \log \rho = \lambda_B(\rho) + F_0(\rho) \geq \lambda_B(\rho) = \lambda_B(z + 1) \quad \text{for } z \geq -1.$$

To obtain upper estimates for Φ_α^* we use now again that the Legendre transform is order reversing and the fact that for a family of functions $(f_i)_{i \in I}$ the equality $(\inf_i f_i)^* = \sup_i (f_i^*)$ holds true, which is a direct consequence of the definition (see [Pey15, Prop. 3.50]).

For $\alpha = 1$ this gives

$$\Phi_1^*(\xi) \leq \sup (\xi z - \lambda_B(z + 1)) = -\xi + \lambda_B^*(\xi) = e^\xi - \xi - 1 \quad \text{for all } \xi \in \mathbb{R}.$$

For $\alpha \in [1, 2]$ the above estimates give $\Phi_\alpha(z) \geq \min \left\{ \frac{\alpha}{2} |z|^\alpha, \frac{\alpha}{2} z^2 \right\}$, and we obtain

$$\Phi_\alpha^*(\xi) \leq \max \left\{ \tilde{c}_\alpha |\xi|^{\alpha/(\alpha-1)}, \frac{1}{2\alpha} \xi^2 \right\}.$$

In the case $\alpha \geq 2$ we have $|z|^\alpha \leq |z|^2$ for $|z| \leq 1$ and find $\Phi_\alpha(z) \geq \frac{\alpha}{2} |z|^\alpha$, which gives the desired result.

Finally, we observe that for all $\alpha \geq 1$ we have $\Phi_\alpha(z) \geq \frac{\alpha}{2} z^2$ for $|z| \leq 1$, which implies $\Phi_\alpha^*(\xi) \leq \frac{1}{2\alpha} \xi^2$ for $|\xi| \leq \alpha$. ■

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