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# Decay to equilibrium for energy-reaction-diffusion systems

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## Abstract

We derive thermodynamically consistent models of reaction-diffusion equations coupled to a heat equation. While the total energy is conserved, the total entropy serves as a driving functional such that the full coupled system is a gradient flow. The novelty of the approach is the Onsager structure, which is the dual form of a gradient system, and the formulation in terms of the densities and the internal energy. In these variables it is possible to assume that the entropy density is strictly concave such that there is a unique maximizer (thermodynamical equilibrium) given linear constraints on the total energy and suitable density constraints.

We consider two particular systems of this type, namely, a diffusion-reaction bipolar energy transport system, and a drift-diffusion-reaction energy transport system with confining potential. We prove corresponding entropy-entropy production inequalities with explicitly calculable constants and establish the convergence to thermodynamical equilibrium, at first in entropy and further in  $L^1$  using Csiszár-Kullback-Pinsker type inequalities.

MSC:

Keywords: Gradient flows, Onsager system, thermodynamical reaction-diffusion systems, maximum entropy principle.

## 1 Introduction

The idea of this paper is to formulate the coupling between a reaction-drift-diffusion system and a heat equation in terms of a gradient flow system. For reaction-diffusion systems a full gradient structure was established only recently in [Mie11b], including the non-isothermal case with a heat equation. The latter work was largely inspired by the modeling paper [AGH02] and the abstract theory on metric gradient flows, see e.g.

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[Ott01, AGS05, LiM13]. We also refer to [Mie13] for more details on Allen-Cahn or Cahn-Hilliard type systems coupled to heat equations. However, the coupling of different gradient systems is non-trivial and the main observation of the latter paper is that the coupling is largely simplified if we consider the dual formulation, where the inverse  $\mathbb{K}$  of the Riemannian metric tensor  $\mathbb{G}$  is used. We call the symmetric and positive (semi)definite operator  $\mathbb{K}$  an *Onsager operator*, and the triple  $(\mathbf{X}, \Phi, \mathbb{K})$  is called an *Onsager system*, where the state space  $\mathbf{X}$  is a convex subset of a Banach space and  $\Phi : \mathbf{X} \rightarrow \mathbb{R} \cup \{\infty\}$  is the functional generating the evolutionary system

$$\dot{u} = -\mathbb{K}(u)D\Phi(u) \quad \iff \quad \mathbb{G}(u)\dot{u} = -D\Phi(u).$$

We call the triple  $(\mathbf{X}, \Phi, \mathbb{G})$  the associated gradient system.

A major advantage of the Onsager form is its flexibility in modeling. This is due to the fact that the Onsager operator can be decomposed into additive parts that account for different physical phenomena - in our case, diffusion, heat transfer, and reaction. In most applications the Onsager operator for non-isothermal systems has a special structure (cf. [Edw98, Ött05, Mie11a]) with the free entropy being the correct driving potential for the non-temperature part of the system, see (2.4).

We use the Onsager structure to prove convergence to equilibrium by an application of the entropy method in two particular systems with semiconductor-type reaction inspired by the Read-Shockley-Hall term, see [MRS90]. First, we study a diffusion-reaction bipolar energy transport system, and second, a drift-diffusion-reaction energy transport system with confining potential. In particular, we prove entropy production inequalities with explicitly calculable constants, using a generalization of the approach of [DFM08, MHM15], where the isothermal reaction-diffusion system was considered. This entails convergence to an entropy minimizing equilibrium state, at first in entropy and further in  $L^1$  norm using Csiszár-Kullback-Pinsker type inequalities, see e.g. [UA\*00]. The entropy approach is per se a nonlinear method avoiding any kind of linearization and capable of providing explicitly computable convergence rates. Moreover, being based on functional inequalities rather than particular differential equations, it has the advantage of being quite robust with respect to model variations.

To introduce the main ideas and notations we consider a simplified but still nontrivial example, namely the reaction diffusion system

$$\dot{u} = \delta\Delta u + \kappa(e^\alpha - u^\beta), \tag{1.1a}$$

$$\dot{e} = \delta\Delta e, \tag{1.1b}$$

where  $u(t, x) > 0$  is the density of a chemical species  $X_u$  and  $e(t, x) > 0$  is the internal energy. The chemical species can be absorbed by or generated from the background according to the mass action law  $\beta X_u \rightleftharpoons \emptyset$ , where the equilibrium state  $w$  depends on the internal energy, namely  $w(e) = e^{\alpha/\beta}$ . This system can be written as a gradient flow for the entropy functional  $\mathcal{S}$  and the total conserved energy (assuming no-flux boundary conditions):

$$\begin{aligned} \mathcal{S}(u, e) &= \int_{\Omega} S(u(x), e(x)) dx \quad \text{and} \quad \mathcal{E}(u, e) = \int_{\Omega} e(x) dx, \quad \text{with} \\ S(u, e) &= s(e) - w(e)\lambda_B\left(\frac{u}{w(e)}\right) = \widehat{s}(e) - \lambda_B(u) + u \ln w(e), \end{aligned}$$

where  $\lambda_B(\nu) := \nu \ln \nu - \nu + 1 \geq 0$  with  $\lambda_B(1) = 0$  and  $\widehat{s}(e) = s(e) - w(e) + 1$ . Assuming that  $\widehat{s}$  is strictly increasing and that  $\widehat{s}$  and  $w$  are concave (i.e.  $\alpha \leq \beta$ ), implies that  $S : [0, \infty]^2 \rightarrow \mathbb{R}$  is concave, which is expected from thermodynamical models. Moreover, the temperature  $\theta = 1/\partial_e S(u, e)$  is positive.

The gradient structure follows from the fact that the Onsager system  $(\mathbf{X}, \Phi, \mathbb{K})$  generates (1.1) if we choose

$$\mathbb{K}(u, e) \begin{pmatrix} \eta \\ \varepsilon \end{pmatrix} := -\operatorname{div} \left( \mathbb{M}(u, e) \nabla \begin{pmatrix} \eta \\ \varepsilon \end{pmatrix} \right) + \begin{pmatrix} \mathbb{H}(u, e) & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \eta \\ \varepsilon \end{pmatrix},$$

where  $\mathbb{M}(u, e) = \delta(-D^2 S(u, e))^{-1}$  and  $\mathbb{H}(u, e) = \kappa \frac{w(e)^\beta - u^\beta}{\ln w(e) - \ln u} > 0$ .

With this choice we easily see that (1.1) takes the form

$$\frac{d}{dt} \begin{pmatrix} u \\ e \end{pmatrix} = \mathbb{K}(u, e) D\mathcal{S}(u, e) \quad \text{and that } \mathbb{K}(u, e) D\mathcal{E}(u, e) = 0,$$

where the last relation leads to energy conservation, i.e. every solution  $t \mapsto (u(t), e(t))$  satisfies  $\mathcal{E}(u(t), e(t)) = \mathcal{E}(u(0), e(0)) =: E_0$ .

Because of the strict concavity of  $\mathcal{S}$ , we expect that the solutions  $(u(t), e(t))$  converge to the unique maximizer of  $\mathcal{S}$  under the constraint  $\mathcal{E}(u, e) = E_0$ , namely  $(u_*, e_*)$  where  $e_* = E_0/\operatorname{vol}(\Omega)$  and  $u_* = w(e_*)$ . Thus, we can define the non-negative and convex relative entropy

$$\mathcal{H}(u, e) = \mathcal{S}(u_*, e_*) + D_e \mathcal{S}(u_*, e_*)[e - e_*] - \mathcal{S}(u, e),$$

which satisfies  $\mathcal{H}(u, e) \geq \mathcal{H}(u_*, e_*) = 0$ .

The convergence to equilibrium is now controlled by the entropy production  $\mathcal{P}$  defined as follows, where we reduce to the case  $\alpha = 1 < \beta$  and  $\widehat{s}(e) = \sigma e^{1/\beta}$  with  $\sigma > 0$  for notational simplicity:

$$-\frac{d}{dt} \mathcal{H}(u(t), e(t)) = \mathcal{P}(u(t), e(t)) = \delta \mathcal{P}_{\text{diff}}(u(t), e(t)) + \kappa \mathcal{P}_{\text{react}}(u(t), e(t)),$$

where  $\mathcal{P}_{\text{diff}}(u, e) = \int_{\Omega} \left\{ \frac{\beta-1}{\beta} \frac{|\nabla u|^2}{u} + \frac{4e}{\beta} \left| \nabla \sqrt{\frac{u}{e}} \right|^2 + \sigma \frac{\beta-1}{\beta^2} \frac{|\nabla e|^2}{e^{2-1/\beta}} \right\} dx$

and  $\mathcal{P}_{\text{react}}(u, e) = \int_{\Omega} \mathbb{H}(u, e) (\ln(u/w(e)))^2 dx = \int_{\Omega} \frac{1}{\beta} (u^\beta - e) (\ln u^\beta - \ln e) dx$ .

After this modeling steps are done, the main task is to derive an entropy production estimate in the form

$$\mathcal{P}(u, e) \geq K(e_*) \mathcal{H}(u, e) \quad \text{for all } (u, e) \text{ with } \mathcal{E}(u, e) = e_* \operatorname{vol}(\Omega), \quad (1.2)$$

which then leads, via  $\frac{d}{dt} \mathcal{H}(u, e) \leq -K(e_*) \mathcal{H}(u, e)$ , to the exponential decay estimate

$$\mathcal{H}(u(t), e(t)) \leq \exp(-K(e_*)t) \mathcal{H}(u(0), e(0)) \quad \text{for } t > 0,$$

where  $e_* = \mathcal{E}(u(0), e(0))/\operatorname{vol}(\Omega)$ .

In fact, we are not able to prove (1.2) in the general form given here, but refer to [MHM15] for such results in the isothermal case. As in this work the general strategy

is (i) to exploit  $\mathcal{P}_{\text{diff}}$  to estimate the distance between  $(u, e)$  and its averages  $(\bar{u}, e_*)$  and (ii) to exploit  $\mathcal{P}_{\text{react}}$  to estimate  $\bar{u} - u_*$ . For (i), we see that the first and third term in  $\mathcal{P}_{\text{diff}}$  allow a first estimate, but because of the special structure of  $S$  which couples  $u$  and  $e$  non-trivially, we also need the second term, which gives a log-Sobolev estimate for  $u/e$  with respect to the measure  $\frac{e}{e_*} dx$  such that we have to impose bounds of the form  $0 < \underline{e} \leq e(t, x) \leq \bar{e} < \infty$  for showing (1.2), see Propositions 6.2 and 6.8.

The structure of the paper is as follows: In Section 2 we provide a general review on gradient and Onsager systems and introduce non-isothermal systems. In Section 3 we present the Onsager structure for a wide class of isothermal reaction-diffusion systems based on the assumption of detailed balance for the reaction system, cf. [Mie11b]. Reaction and diffusion can be discussed as separate dissipative processes giving  $\mathbb{K} = \mathbb{K}_{\text{diff}} + \mathbb{K}_{\text{react}}$ . In Section 4 we follow [Mie13] for the modeling of non-isothermal reaction-diffusion systems and provide the corresponding Onsager operator. As in example (1.1) we will see that it is advantageous to use the internal energy  $e$  as variable instead of the more common temperature  $\theta = 1/\partial_e S(\mathbf{u}, e)$ . This is even more evident in the analysis in Sections 5 and 6. In Section 4.4 we also compare the general form of these systems with the energy-transport models derived in [Jün09, Jün10] from a diffusive scaling of the semiconductor Boltzmann equation. In Section 5 we derive special instances of the general system, in particular, a diffusion-reaction bipolar energy-transport system, and a drift-diffusion-reaction energy transport system with confining potential  $V(x)$ . In Section 6, we apply the entropy entropy-production method to study the convergence to equilibrium for the two systems, where the focus is to derive the estimate (1.2). The first model is posed on a  $d$ -dimensional torus of homogeneous material, i.e. the constitutive functions  $w$ ,  $s$ , and hence  $S$  are independent of  $x$ . The second model is considered in the full space setting, where  $w_i(x, e) = C_i \sqrt{e} \exp(-V(x))$  and  $\hat{s}(x, e) = c \sqrt{e} \exp(-V(x))$ . Now the entropy entropy-production estimate (1.2) can be derived in suitably weighted spaces, see Proposition 6.8. Finally, in Appendix A we provide an overview of auxiliary results that we use throughout the paper.

## 2 Gradient systems including heat equations

In this section we discuss some general background about gradient systems and address the general question how the temperature or other thermodynamic variables such as the internal energy  $e$  or the entropy  $s$  can be included. We follow the ideas developed in [Mie11a, Mie13]. Instead of the metric tensor  $\mathbb{G}$  which is in the origin of the name gradient system, we will use its inverse  $\mathbb{K} = \mathbb{G}^{-1}$  which we call Onsager operator, as it was Onsager's fundamental contribution in [Ons31] to show that the matrix or operator  $\mathbb{K}$  that maps thermodynamic driving forces into rates should be symmetric (called reciprocal relation at that time) and positive semidefinite. Throughout our arguments are formal and assume sufficient smoothness of the potentials as well as the solutions (which is the common approach in thermomechanics).

### 2.1 General modeling with gradient systems

A gradient system is a triple  $(\mathbf{X}, \Phi, \mathbb{G})$  where  $\mathbf{X}$  is the state space containing the states  $U \in \mathbf{X}$ . For simplicity we assume that  $\mathbf{X}$  is a reflexive Banach space with dual  $\mathbf{X}^*$ . The

driving functional  $\Phi : \mathbf{X} \rightarrow \mathbb{R} \cup \{\infty\}$  is assumed to be differentiable (in a suitable way) such that the potential restoring force is given by  $-\mathrm{D}\Phi(U) \in \mathbf{X}^*$ . The third ingredient is a metric tensor  $\mathbb{G}$ , i.e.  $\mathbb{G}(U) : \mathbf{X} \rightarrow \mathbf{X}^*$  is linear, symmetric and positive (semi-)definite. Indeed, in a proper manifold setting,  $\mathbb{G}$  maps the tangent space  $\mathrm{T}_U\mathbf{X}$  into the cotangent space  $\mathrm{T}_U^*\mathbf{X} = (\mathrm{T}_U\mathbf{X})^*$ . The gradient flow associated with  $(\mathbf{X}, \Phi, \mathbb{G})$  is the (abstract) force balance

$$\mathbb{G}(U)\dot{U} = -\mathrm{D}\Phi(U) \quad \iff \quad \dot{U} = -\nabla_{\mathbb{G}}\Phi(U) =: -\mathbb{K}(U)\mathrm{D}\Phi(U), \quad (2.1)$$

where we recall that the “gradient”  $\nabla_{\mathbb{G}}\Phi$  of the functional  $\Phi$  is an element of  $\mathbf{X}$  (in contrast to the differential  $\mathrm{D}\Phi(U) \in \mathbf{X}^*$ ) and is calculated via  $\mathbb{K}(U)\mathrm{D}\Phi(U)$  with  $\mathbb{K}(U) := \mathbb{G}(U)^{-1}$ . The left equation in (2.1) is an abstract force balance, since  $\mathbb{G}(U)\dot{U} \in \mathbf{X}^*$  can be seen as a viscous force arising from the motion of  $U$ . The equation on the right-hand side is a rate equation, where the equality is formulated in the tangent space  $\mathbf{X}$ .

The symmetries of  $\mathbb{G}$  and  $\mathbb{K}$  allow us to define the associated primal and dual *dissipation potentials*  $\Psi : \mathbf{X} \times \mathbf{X} \rightarrow [0, \infty]$  and  $\Psi^* : \mathbf{X} \times \mathbf{X}^* \rightarrow [0, \infty]$ , respectively, via

$$\Psi(U, V) = \frac{1}{2}\langle \mathbb{G}(U)V, V \rangle \quad \text{and} \quad \Psi^*(U, \Xi) = \frac{1}{2}\langle \Xi, \mathbb{K}(U)\Xi \rangle,$$

where  $\Psi^*(U, \cdot)$  is the Fenchel–Legendre transform of  $\Psi(U, \cdot)$ . If  $\Phi$  is the negative total entropy, then  $\Psi$  is called the *entropy production potential*.

Hence, using  $\mathrm{D}_V\Psi(U, V) = \mathbb{G}(U)V$  and  $\mathrm{D}_{\Xi}\Psi^*(U, \Xi) = \mathbb{K}(U)\Xi$  the equations in (2.1) can be written as

$$0 = \mathrm{D}_V\Psi(U, \dot{U}) + \mathrm{D}\Phi(U) \quad \iff \quad \dot{U} = \mathrm{D}_{\Xi}\Psi^*(U, -\mathrm{D}\Phi(U)),$$

which are also the correct forms for so-called generalized gradient systems, where  $\Psi(U, \cdot)$  and  $\Psi^*(U, \cdot)$  are not quadratic, see [Mie16, LM\*15].

The importance of gradient systems is clearly motivated in the theory of thermodynamics, namely by the *Onsager symmetry principle*, see [Ons31, DeM84]. Strictly speaking, this principle is only derived for systems close to thermodynamic equilibrium, see [Ött05] for physical justifications to use these principles in a wider range. The symmetry principle has two forms, both of which are important for reaction-diffusion systems. (I) In the first case one considers a spatially homogeneous system described by a state vector  $z$ , which is a small perturbation of the equilibrium. Then, its macroscopic rate  $\dot{z}$  is given in the form  $-\mathbb{H}\zeta$ , where  $\zeta = -\mathrm{D}S(z)$  is the thermodynamically conjugate driving force and  $S$  is the entropy. The symmetry relation states that the matrix  $\mathbb{H}$  has to be symmetric, while the entropy production principle  $\frac{d}{dt}S(z(t)) = \mathrm{D}S(z) \cdot \mathbb{H}\mathrm{D}S(z) \geq 0$  implies that  $\mathbb{H}$  has to be positive semidefinite. (II) In the second case one considers a spatially extended system with densities  $u_i > 0$  defining a vector  $\mathbf{u} = (u_i)_{i=1, \dots, I} : \Omega \rightarrow ]0, \infty[^I$  and a total entropy  $\mathcal{S}(\mathbf{u}) = \int_{\Omega} S(x, \mathbf{u}(x)) dx$ . If each total mass  $m_i := \int_{\Omega} u_i(x) dx$  is conserved, then the densities satisfy a balance equation of the form

$$\dot{\mathbf{u}} + \mathrm{div} \mathbf{j}_{\mathbf{u}} = 0 \quad \text{with} \quad \mathbf{j}_{\mathbf{u}} = \mathbb{M}\nabla\boldsymbol{\mu},$$

where the vector  $\boldsymbol{\mu}$  of the chemical potentials is given by  $\boldsymbol{\mu} = \mathrm{D}\mathcal{S}(\mathbf{u})$ , i.e.  $\mu_i(x) = \partial_{u_i}S(x, \mathbf{u}(x))$ . Again, the symmetry and entropy principle imply that  $\mathbb{M}$  is a symmetric and positive semidefinite tensor (of fourth order), see [Ons31].

Note that in this work we will call  $\boldsymbol{\mu} = \text{D}\mathcal{S}$  the thermodynamic driving force (rather than a potential). In our approach the driving force is lying in the dual space of the variable (here  $\mathbf{u}$ ), while  $\nabla\mu_j$  relates to gradient in the physical domain  $\Omega$ . However, more importantly, we will couple the equation  $\dot{\mathbf{u}} + \text{div}(\mathbb{M}\nabla\boldsymbol{\mu}) = 0$  with  $\boldsymbol{\mu} = \text{D}\mathcal{S}$  in the form  $\dot{\mathbf{u}} = \mathbb{K}(\mathbf{u})\text{D}\mathcal{S}$ , where  $\mathbb{K}(u) = -\text{div}(\mathbb{M}\nabla\Box)$  is a symmetric operator.

As was observed in [Mie11b, GIM13, Mie13], it is advantageous to use the Onsager operator  $\mathbb{K}$  for modeling purposes rather than the metric operator  $\mathbb{G} = \mathbb{K}^{-1}$ , so we will also write  $(\mathbf{X}, \Phi, \mathbb{K})$  for the gradient system and call it Onsager system then. The flexibility in modeling arises from the fact that evolutionary systems are often written in rate form where the vector field is additively decomposed into different physical phenomena. This additive split can be also used for the Onsager operator, as long as all the different effects are driven by the same functional  $\Phi$ . Below we will see that  $\mathbb{K}$  takes the additive form

$$\mathbb{K} = \mathbb{K}_{\text{diff}} + \mathbb{K}_{\text{react}} + \mathbb{K}_{\text{heat}},$$

such that the evolution equation reads

$$\dot{U} = -\left(\mathbb{K}_{\text{diff}}\text{D}\Phi + \mathbb{K}_{\text{react}}\text{D}\Phi + \mathbb{K}_{\text{heat}}\text{D}\Phi\right) = -\mathbb{K}\text{D}\Phi.$$

A similar additive split is not possible for the metric  $\mathbb{G}$ , as the inverse operator to a sum of operators is difficult to express.

## 2.2 Non-isothermal Onsager systems

In the isothermal case the functional  $\Phi$  is typically the free energy, and the state  $U$  consists of positive densities  $u_i$  of phase indicators  $\varphi_j$ . In the non-isothermal case the functional  $\Phi$  is the total entropy  $\mathcal{S}$  and an additional scalar thermal variable  $r$  is needed, which can be the absolute temperature  $\theta > 0$ , the internal energy density  $e$ , the entropy density  $s$ , or some variable derived from those. As in [Mie11a, Sect. 2.3] we will keep  $r$  unspecified at this stage, because this elucidates the general structure. Hence the states take the form  $U = (\mathbf{y}, r)$ , and we consider the functionals

$$\mathcal{E}(\mathbf{y}, r) = \int_{\Omega} E(x, \mathbf{y}(x), r(x)) dx \quad \text{and} \quad \mathcal{S}(\mathbf{y}, r) = \int_{\Omega} S(x, \mathbf{y}(x), r(x)) dx, \quad (2.2)$$

where the constitutive functions  $E$  and  $S$  are related by Gibbs formula defining the temperature

$$\theta = \Theta(x, \mathbf{y}, r) := \frac{\partial_r E(x, \mathbf{y}, r)}{\partial_r S(x, \mathbf{y}, r)}.$$

Without loss of generality, we subsequently assume that  $\partial_r E$  and  $\partial_r S$  are positive.

We also argue that physically relevant driving forces should not depend on the choice of  $r \in \{\theta, e, s\}$ . Thus, introducing the Helmholtz free energy  $\psi = e - \theta s$  and the Helmholtz free entropy  $\eta = -\psi/\theta = s - e/\theta$  (also called Massieu potential), we have the formulas

$$\begin{aligned} \psi &= F(x, \mathbf{y}, r) := E(x, \mathbf{y}, r) - \Theta(x, \mathbf{y}, r)S(x, \mathbf{y}, r) \quad \text{and} \\ \eta &= H(x, \mathbf{y}, r) := S(x, \mathbf{y}, r) - \frac{E(x, \mathbf{y}, r)}{\Theta(x, \mathbf{y}, r)}. \end{aligned}$$

The point here is that the driving forces  $\partial_{\mathbf{y}}F$  and  $\partial_{\mathbf{y}}S$  are independent of the choice of  $r$  when the arguments are transformed correspondingly.

In the non-isothermal case the total entropy  $\mathcal{S}$  (with the physically correct sign) is increasing, so  $\Phi = -\mathcal{S}$  is the driving potential for the gradient flow. However, we will not make this distinction in the text; instead, we will always use the corresponding correct signs in the formulas. Our Onsager system  $(\mathbf{X}, \mathcal{S}, \mathbb{K})$  hence gives rise to the equation  $\dot{U} = \mathbb{K}(U)\mathcal{D}\mathcal{S}(U)$ . In order to have energy conservation, we need

$$0 = \frac{d}{dt}\mathcal{E}(U) = \langle \mathcal{D}\mathcal{E}(U), \dot{U} \rangle = \langle \mathcal{D}\mathcal{E}(U), \mathbb{K}(U)\mathcal{D}\mathcal{S}(U) \rangle = \langle \mathbb{K}(U)\mathcal{D}\mathcal{E}(U), \mathcal{D}\mathcal{S}(U) \rangle,$$

where we used  $\mathbb{K} = \mathbb{K}^*$ . Hence, it is sufficient (but not necessary) to impose the condition

$$\mathbb{K}(U)\mathcal{D}\mathcal{E}(U) = 0 \quad \text{for all } U \in \mathbf{X}.$$

In many applications the Onsager operator for non-isothermal systems has a special structure (cf. [Edw98, Ött05, Mie11a]), namely

$$\mathbb{K}(\mathbf{y}, r) = \mathcal{M}_{\mathcal{E}}^* \begin{pmatrix} \mathbb{K}_{\mathbf{y}}^{\text{simple}} & 0 \\ 0 & \mathbb{K}_{\text{heat}}^{\text{simple}} \end{pmatrix} \mathcal{M}_{\mathcal{E}} \quad \text{with} \quad (2.3a)$$

$$\mathbb{K}_{\text{heat}}^{\text{simple}} \rho = -\text{div}(k_{\text{heat}}(\mathbf{y}, r)\nabla\rho) \quad \text{and} \quad \mathcal{M}_{\mathcal{E}} = \begin{pmatrix} I & -\frac{1}{\partial_r \mathcal{E}} \mathcal{D}_{\mathbf{y}} \mathcal{E} \\ 0 & \frac{1}{\partial_r \mathcal{E}} \end{pmatrix}. \quad (2.3b)$$

The definition of  $\mathcal{M}_{\mathcal{E}}$  implies that

$$\mathcal{M}_{\mathcal{E}}\mathcal{D}\mathcal{E} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathcal{M}_{\mathcal{E}}\mathcal{D}\mathcal{S} = \begin{pmatrix} \mathcal{D}_{\mathbf{y}}\mathcal{S} - \frac{1}{\Theta}\mathcal{D}_{\mathbf{y}}\mathcal{E} \\ 1/\Theta \end{pmatrix} = \begin{pmatrix} \mathcal{D}_{\mathbf{y}}\mathfrak{H}(\mathbf{y}, r) \\ 1/\Theta \end{pmatrix},$$

where  $\mathfrak{H}(\mathbf{y}, r) = \int_{\Omega} H(x, \mathbf{y}(x), r(x)) dx$  is the total free entropy. Since  $\mathbb{K}_{\text{heat}}^{\text{simple}} 1 \equiv 0$ , we have the desired relation  $\mathbb{K}\mathcal{D}\mathcal{E} \equiv 0$  for energy conservation. Moreover, the coupled system  $(\dot{\mathbf{y}}, \dot{r}) = \mathbb{K}(\mathbf{y}, r)\mathcal{D}\mathcal{S}(\mathbf{y}, r)$  can be rewritten in the form

$$\dot{\mathbf{y}} = \mathbb{K}_{\mathbf{y}}^{\text{simple}}(\mathbf{y}, r)\mathcal{D}_{\mathbf{y}}\mathfrak{H}(\mathbf{y}, r), \quad \dot{r} = \frac{1}{\partial_r \mathcal{E}} \left( \partial_{\mathbf{y}} \mathcal{E} \cdot \dot{\mathbf{y}} + \mathbb{K}_{\text{heat}}^{\text{simple}}(\mathbf{y}, r)(1/\Theta(\mathbf{y}, r)) \right) \quad (2.4)$$

We conclude that in the non-isothermal case with conserved energy  $\mathcal{E}$  the correct driving potential for the non-temperature part  $\mathbf{y}$  of the system is the free entropy  $\mathfrak{H}(\mathbf{y}, \theta)$ , see also [Mie15]. Nevertheless,  $\mathcal{S}$  is the functional for the Onsager system, the correction  $-\frac{1}{\partial_r \mathcal{E}}\partial_{\mathbf{y}}\mathcal{E}$  arises because of energy conservation, which is encoded in the way  $\mathbb{K}$  is constructed from  $\mathbb{K}_{\mathbf{y}}^{\text{simple}}$  and  $\mathbb{K}_{\text{heat}}^{\text{simple}}$ .

We end this section by observing that the case  $r = e$ , namely  $\widehat{E}(x, \mathbf{y}, e) := e$ , leads to an especially simple case, because  $\partial_e \widehat{E} \equiv 1$  and  $\partial_{\mathbf{y}} \widehat{E}(x, \mathbf{y}, e) \equiv 0$ . Indeed, (2.4) turns into

$$\dot{\mathbf{y}} = \mathbb{K}_{\mathbf{y}}^{\text{simple}}(\mathbf{y}, e)\mathcal{D}_{\mathbf{y}}\mathcal{S}(\mathbf{y}, e), \quad \dot{e} = \mathbb{K}_{\text{heat}}^{\text{simple}}(\mathbf{y}, e)(1/\widehat{\Theta}(\mathbf{y}, e)). \quad (2.5)$$

### 3 Isothermal reaction-diffusion systems

While the gradient structure for scalar diffusion equations (e.g. porous medium equation or the Fokker-Planck equation) is well known (cf. [JKO98, Ott01]), the Onsager



structure for a wider class of reaction-diffusion systems is less known. It was established in a few particular cases (see [Yon08, GrÖ97]), but only highlighted in its own right in [Mie11b, GIM13]. The central point is that in the Onsager form we have an additive splitting of the Onsager operator into a diffusive part and a reaction part, namely  $\dot{\mathbf{u}} = -(\mathbb{K}_{\text{diff}}(\mathbf{u}) + \mathbb{K}_{\text{react}}(\mathbf{u}))\mathcal{F}_{\text{chem}}(\mathbf{u})$ , where  $\mathbf{u} : \Omega \rightarrow ]0, \infty[^I$  is the vector of densities of the species  $X_1, \dots, X_I$ . The free-energy functional  $\mathcal{F}_{\text{chem}}$ , which is also called the relative entropy with respect to the reference density  $\mathbf{u}^*$ , takes the form

$$\mathcal{F}_{\text{chem}}(\mathbf{u}) = \int_{\Omega} \sum_{i=1}^I u_i^* \lambda_{\text{B}}(u_i(x)/u_i^*) dx \quad \text{where} \quad \lambda_{\text{B}}(\nu) := \nu \ln \nu - \nu + 1. \quad (3.1)$$

We will now discuss the diffusive and reactive parts separately.

### 3.1 Diffusion systems

For the gradient structure of diffusion systems  $\dot{\mathbf{u}} = \text{div}(\mathbb{M}(\mathbf{u})\nabla\mathbf{u})$  one might be tempted to use a functional involving the gradient  $\nabla u$ , however we have to use the relative entropy as a driving functional, because we have to use the same functional for modeling the reactions. Hence, we use the Wasserstein approach to diffusion introduced by Otto in [JKO98, Ott01].

The diffusion system will take the form  $\dot{\mathbf{u}} = -\mathbb{K}_{\text{diff}}(\mathbf{u})D\mathcal{F}_{\text{chem}}(\mathbf{u})$  with the Onsager operator  $\mathbb{K}_{\text{diff}}$  given via

$$\mathbb{K}_{\text{diff}}(\mathbf{u})\boldsymbol{\mu} = -\text{div}(\tilde{\mathbb{M}}(\mathbf{u})\nabla\boldsymbol{\mu}),$$

where  $\tilde{\mathbb{M}}(\mathbf{u}) : \mathbb{R}^{m \times d} \rightarrow \mathbb{R}^{m \times d}$  is a symmetric and positive semi-definite tensor of order 4. The Onsager operator can also be implicitly defined via the dual dissipation potential, which will be useful later:

$$\Psi_{\text{Wass}}^*(\mathbf{u}, \boldsymbol{\mu}) = \frac{1}{2} \int_{\Omega} \nabla\boldsymbol{\mu} : \tilde{\mathbb{M}}(\mathbf{u}) \nabla\boldsymbol{\mu} dx,$$

where  $\boldsymbol{\mu} = (\mu_i)_{i=1, \dots, I}$  is the vector of chemical potentials, which occurs as the driving force

$$\boldsymbol{\mu} = D_{\mathbf{u}}\mathcal{F}_{\text{chem}}(\mathbf{u}) = \mathbf{log} \mathbf{u} - \mathbf{log} \mathbf{u}^*.$$

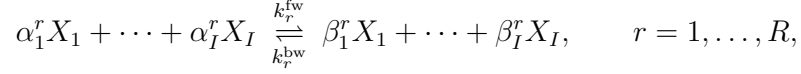
Hence, if the reference densities  $\mathbf{u}^*$  are spatially constant (which is, however, usually not true in heterostructures like semiconductors), the Onsager system leads to the diffusion system

$$\dot{\mathbf{u}} = \text{div}(\tilde{\mathbb{M}}(\mathbf{u})\nabla(\mathbf{log} \mathbf{u} - \mathbf{log} \mathbf{u}^*)) = \text{div}(\mathbb{M}(\mathbf{u})\nabla\mathbf{u}), \quad \text{where} \quad \tilde{\mathbb{M}}(\mathbf{u}) = \mathbb{M}(\mathbf{u})\text{diag}(\mathbf{u}).$$

### 3.2 Chemical reaction kinetics

Chemical reaction systems are ODE systems of the type  $\dot{\mathbf{u}} = \mathbf{R}(\mathbf{u})$ , where often the right-hand side is written in terms of polynomials associated to the reaction kinetics. It was observed in [Mie11b] that under the assumption of detailed balance (also called reversibility) such system have a gradient structure with the relative entropy as the driving

functional. We assume that there are  $R$  reactions of mass-action type (cf. e.g. [DeM84, GIM13]) between the species  $X_1, \dots, X_I$  in the form



where  $k_r^{\text{bw}}$  and  $k_r^{\text{fw}}$  are the backward and forward reaction rates, and the vectors  $\boldsymbol{\alpha}^r, \boldsymbol{\beta}^r \in \mathbb{N}_0^I$  contain the stoichiometric coefficients. For instance, for the chemical reaction  $2 \text{CO} + 1 \text{O}_2 \rightleftharpoons 2 \text{CO}_2$  we have  $\boldsymbol{\alpha} = (2, 1, 0)^\top$  and  $\boldsymbol{\beta} = (0, 0, 2)^\top$ .

The associated reaction system for the densities (in a spatially homogeneous system, where diffusion can be neglected) reads

$$\dot{\mathbf{u}} = \mathbf{R}(\mathbf{u}) := - \sum_{r=1}^R (k_r^{\text{fw}} \mathbf{u}^{\boldsymbol{\alpha}^r} - k_r^{\text{bw}} \mathbf{u}^{\boldsymbol{\beta}^r}) (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r), \quad (3.2)$$

where we use the monomial notation  $\mathbf{u}^\boldsymbol{\alpha} = u_1^{\alpha_1} \dots u_I^{\alpha_I}$ . The main assumption to obtain a gradient structure is that of *detailed balance*, which means that there exists a reference density vector  $\mathbf{u}^*$  such that all  $R$  reactions are balanced individually, namely

$$\exists \mathbf{u}_* \in ]0, \infty[^I \quad \forall r = 1, \dots, R \quad \forall \mathbf{u} \in ]0, \infty[^I : k_r^{\text{fw}}(\mathbf{u}) \mathbf{u}_*^{\boldsymbol{\alpha}^r} = k_r^{\text{bw}}(\mathbf{u}) \mathbf{u}_*^{\boldsymbol{\beta}^r} =: k_r^*(\mathbf{u}). \quad (3.3)$$

Here we used the freedom to let reaction coefficients depend on the densities (and later also on other material properties like temperature).

We now define the Onsager matrix

$$\mathbb{H}(\mathbf{u}) = \sum_{r=1}^R k_r^*(\mathbf{u}) \boldsymbol{\Lambda} \left( \frac{\mathbf{u}^{\boldsymbol{\alpha}^r}}{\mathbf{u}_*^{\boldsymbol{\alpha}^r}}, \frac{\mathbf{u}^{\boldsymbol{\beta}^r}}{\mathbf{u}_*^{\boldsymbol{\beta}^r}} \right) (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \otimes (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \quad \text{with} \quad \boldsymbol{\Lambda}(a, b) = \frac{a - b}{\ln a - \ln b} \quad (3.4)$$

and find, following [Mie11b], that the reaction system (3.2) takes the form

$$\dot{\mathbf{u}} = \mathbf{R}(\mathbf{u}) = -\mathbb{H}(\mathbf{u}) \text{D}\mathcal{F}_{\text{chem}}(\mathbf{u})$$

with  $\mathcal{F}_{\text{chem}}$  given by (3.1). This follows easily by using the definition of  $\boldsymbol{\Lambda}$  and the rules for logarithms, namely  $(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r) \cdot (\boldsymbol{\mu} - \boldsymbol{\mu}^*) = \ln(\mathbf{u}^{\boldsymbol{\alpha}^r} / \mathbf{u}_*^{\boldsymbol{\alpha}^r}) - \ln(\mathbf{u}^{\boldsymbol{\beta}^r} / \mathbf{u}_*^{\boldsymbol{\beta}^r})$ . The quotient  $\boldsymbol{\Lambda}(a, b) = \frac{a - b}{\ln a - \ln b}$  (or variants of it) have occurred occasionally in the modeling of reaction kinetics, see [GrÖ97, Sect. V.B], [EdG08, Ede09], and [Yon08, Sect. 7].

We refer to [LM\*15, MP\*15] for a different gradient structure, where  $\mathcal{F}_{\text{chem}}$  is the same, but the quadratic dual dissipation potential  $\Psi_{\text{quad}}^*(\boldsymbol{\mu}, \boldsymbol{\mu}) = \frac{1}{2} \boldsymbol{\mu} \cdot \mathbb{H}(\boldsymbol{\mu}) \boldsymbol{\mu}$  is replaced by a non-quadratic one that is derived from a large-deviation principle.

### 3.3 Coupling diffusion and reaction

We summarize the previous two subsections by stating the following result derived in [Mie11b].

**Theorem 3.1** *If the reaction-diffusion system*

$$\dot{\mathbf{u}} = \text{div}(\mathbb{M}(\mathbf{u}) \nabla \mathbf{u}) + \mathbf{R}(\mathbf{u}) \quad (3.5)$$

with  $\mathbf{R}(\mathbf{u}) = -\sum_{r=1}^R (k_r^{fw}(\mathbf{u})\mathbf{u}^{\alpha^r} - k_r^{bw}(\mathbf{u})\mathbf{u}^{\beta^r})(\alpha^r - \beta^r)$  satisfies the detailed balance condition (3.3) and  $\tilde{\mathbb{M}}(\mathbf{u}) = \mathbb{M}(\mathbf{u})\text{diag}(\mathbf{u})$  is symmetric and positive semidefinite, then it is an Onsager system  $\dot{\mathbf{u}} = -\mathbb{K}_{\text{RD}}(\mathbf{u})\text{D}\mathcal{F}_{\text{chem}}(\mathbf{u})$  with

$$\mathcal{F}_{\text{chem}}(\mathbf{u}) = \int_{\Omega} \sum_{i=1}^I u_i^* \lambda_{\text{B}}(u_i(x)/u_i^*) dx \quad \text{and} \quad \Psi_{\text{RD}}^*(\mathbf{u}, \boldsymbol{\mu}) = \frac{1}{2} \int_{\Omega} \nabla \boldsymbol{\mu} : \tilde{\mathbb{M}}(\mathbf{u}) : \nabla \boldsymbol{\mu} + \boldsymbol{\mu} \cdot \mathbb{H}(\mathbf{u}) \cdot \boldsymbol{\mu} dx.$$

We mention that many reaction-diffusion systems studied (including semiconductor models involving an elliptic equation for the electrostatic potential) have the gradient structure developed above, see, e.g. [GIH05, DeF06, DeF07, Gli09, BoP11]. So far, the gradient structure was not used explicitly, only the Liapunov property of the free energy (relative entropy) was exploited.

As we assume throughout that our system (3.5) has no-flux boundary conditions, we may have additional conservation laws, often called conservation of atomic mass. With

$$\mathbb{S} := \text{span}\{ \boldsymbol{\alpha}^r - \boldsymbol{\beta}^r \mid r = 1, \dots, R \} \subset \mathbb{R}^I \quad \text{and} \quad \mathbb{S}^{\perp} := \{ \mathbf{p} \in \mathbb{R}^I \mid \mathbf{p} \cdot \boldsymbol{\gamma} = 0 \text{ for all } \boldsymbol{\gamma} \in \mathbb{S} \},$$

we denote the stoichiometric subspace  $\mathbb{S}$  associated to the reaction system (3.2) and its orthogonal complement. From  $\mathbb{H}(\mathbf{u})\mathbf{p} \equiv 0$  for all  $\mathbf{p} \in \mathbb{S}^{\perp}$  we conclude that the functionals  $\mathcal{C}_{\mathbf{p}}(\mathbf{u}) := \int_{\Omega} \mathbf{p} \cdot \mathbf{u}(x) dx$  are conserved along solutions of the reaction-diffusion system. Defining by  $\mathbb{P} : \mathbb{R}^I \rightarrow \mathbb{R}^I$  the orthogonal projection onto  $\mathbb{S}^{\perp}$ , we obtain that

$$\mathcal{C}_{\mathbb{S}^{\perp}}(\mathbf{u}) := \int_{\Omega} \mathbb{P}\mathbf{u}(x) dx \in \mathbb{S}^{\perp} \tag{3.6}$$

is conserved along solutions of (3.5).

## 4 Non-isothermal reaction-diffusion systems

We now restrict ourselves to a system described by  $(\mathbf{u}, r)$  with the total energy and entropy functionals

$$\mathcal{E}(\mathbf{u}, r) = \int_{\Omega} E(x, \mathbf{u}(x), r(x)) dx \quad \text{and} \quad \mathcal{S}(\mathbf{u}, r) = \int_{\Omega} S(x, \mathbf{u}(x), r(x)) dx,$$

where the integrands are strictly local, i.e. they do not depend on  $\nabla \mathbf{u}$  and  $\nabla r$ . Recall that  $r$  is a scalar thermodynamical variable such as  $\theta$ ,  $e$ , or  $s$ . Throughout the paper, the densities may explicitly depend on the material point, but we will omit this dependence in the sequel. The energy density  $E$  and the entropy density  $S$  satisfy the Gibbs relation  $\partial_r E(\mathbf{u}, r) = \Theta(\mathbf{u}, r) \partial_r S(\mathbf{u}, r)$  and the positivity of the specific heat  $\partial_{\theta} E > 0$ .

The dual entropy production potential  $\Psi^*$  will depend on the state  $(\mathbf{u}, r)$  and the thermodynamic conjugate variables  $(\boldsymbol{\mu}, \rho)$ . In principle,  $\Psi^*$  will contain three parts, namely a diffusion part, a reaction part, and a part for heat conduction. However, the heat conduction and the diffusion can be joined into one quadratic form on  $(\nabla \boldsymbol{\mu}, \nabla \rho)$ , thus allowing for ‘‘cross-diffusion’’ effects between chemical diffusion and heat transfer, which is needed to model thermophilic or thermophobic materials occurring for instance in polymers, see e.g. [AnW12].

To guarantee energy conservation, we follow [Mie11b, Sect.3.6] in using the special form (2.3) and consider

$$\Psi^*(\mathbf{u}, r; \boldsymbol{\mu}, \rho) = \tilde{\Psi}^*(\mathbf{u}, r; \boldsymbol{\mu} - \frac{\rho}{\partial_r E} \partial_{\mathbf{u}} E, \frac{\rho}{\partial_r E}) \quad (4.1a)$$

$$\text{with } \tilde{\Psi}^*(\mathbf{u}, r; \tilde{\boldsymbol{\mu}}, \tilde{\rho}) = \frac{1}{2} \int_{\Omega} (\nabla \tilde{\boldsymbol{\mu}}, \nabla \tilde{\rho}) : \tilde{\mathbb{M}}(\mathbf{u}, r) (\nabla \tilde{\boldsymbol{\mu}}, \nabla \tilde{\rho}) + \tilde{\boldsymbol{\mu}} \cdot \mathbb{H}(\mathbf{u}, r) \tilde{\boldsymbol{\mu}} dx, \quad (4.1b)$$

where  $\mathbb{H}$  is given as in (3.4). The mobility tensor  $\mathbb{M}(\mathbf{u}, r) : \mathbb{R}^{I \times d} \times \mathbb{R}^d \rightarrow \mathbb{R}^{I \times d} \times \mathbb{R}^d$  is symmetric and positive semidefinite and has the block structure

$$\mathbb{M}(\mathbf{u}, r) = \begin{pmatrix} \mathbb{M}_{uu}(\mathbf{u}, r) & \mathbb{M}_{ur}(\mathbf{u}, r) \\ \mathbb{M}_{ur}^*(\mathbf{u}, r) & \mathbb{M}_{rr}(\mathbf{u}, r) \end{pmatrix}.$$

The associated Onsager operator  $\mathbb{K}$  satisfies  $\mathbb{K}D\mathcal{E} \equiv 0$ , and we see that  $\Psi^*$  only depends on

$$D_{\mathbf{u}}S - \frac{1}{\theta} D_{\mathbf{u}}\mathcal{E} = \partial_{\mathbf{u}}S - \frac{1}{\Theta} \partial_{\mathbf{u}}E = \partial_{\mathbf{u}}H \quad \text{and} \quad \frac{\partial_{\theta}S}{\partial_{\theta}E} = \frac{1}{\Theta},$$

where  $H = -\psi/\theta = -F(\mathbf{u}, \Theta)/\Theta = S - E/\Theta$  is the free entropy.

## 4.1 Reaction-diffusion systems with temperature

For completeness and for the comparison with our modeling based on the internal energy, we also consider the choice  $r = \theta$ , which leads to the following system for  $(\mathbf{u}, \theta)$ :

$$\begin{aligned} \dot{\mathbf{u}} &= -\operatorname{div} \mathbf{j}_{\mathbf{u}} + \mathbb{H}(\mathbf{u}, \theta) (\partial_{\mathbf{u}} \bar{S}(\mathbf{u}, \theta) - \frac{1}{\theta} \partial_{\mathbf{u}} \bar{E}(\mathbf{u}, \theta)), \\ \dot{\theta} &= -\frac{1}{\partial_{\theta} E} \operatorname{div} \mathbf{j}_{\theta} + \frac{1}{\partial_{\theta} E} \partial_{\mathbf{u}} \bar{E} \cdot (\operatorname{div} \mathbf{j}_{\mathbf{u}} - \mathbb{H}(\mathbf{u}, \theta) (\partial_{\mathbf{u}} \bar{S}(\mathbf{u}, \theta) - \frac{1}{\theta} \partial_{\mathbf{u}} \bar{E}(\mathbf{u}, \theta))), \end{aligned}$$

with the fluxes

$$\begin{aligned} \mathbf{j}_{\mathbf{u}} &= \mathbb{M}_{uu}(\mathbf{u}, \theta) \nabla (\partial_{\mathbf{u}} \bar{S}(\mathbf{u}, \theta) - \frac{1}{\theta} \partial_{\mathbf{u}} \bar{E}(\mathbf{u}, \theta)) + \mathbb{M}_{u\theta}(\mathbf{u}, \theta) \nabla (1/\theta), \\ \mathbf{j}_{\theta} &= \mathbb{M}_{u\theta}^*(\mathbf{u}, \theta) \nabla (\partial_{\mathbf{u}} \bar{S}(\mathbf{u}, \theta) - \frac{1}{\theta} \partial_{\mathbf{u}} \bar{E}(\mathbf{u}, \theta)) + \mathbb{M}_{\theta\theta}(\mathbf{u}, \theta) \nabla (1/\theta). \end{aligned}$$

In the examples below, we will see that the formulation in terms of  $(\mathbf{u}, e)$  gives a much simpler system. Moreover, in general the function  $s = \bar{S}(\mathbf{u}, \theta)$  does not enjoy any concavity properties, in contrast to the function  $s = \widehat{S}(\mathbf{u}, e)$ .

## 4.2 Reaction-diffusion systems with internal energy

According to [AGH02, Mie11b], it is more convenient to study energy-reaction-diffusion systems with the choice  $r = e$ , for the following two reasons. First, it is physically reasonable to assume that

$$s = \widehat{S}(x, \mathbf{u}, e)$$

is a strictly concave function in the extensive variables  $\mathbf{u}$  and  $e$ . Second,

$$\widehat{\mathcal{E}}(\mathbf{u}, e) = \int_{\Omega} e(x) dx$$

provides a linear functional to express energy conservation. Thus, the energy and entropy functionals are

$$\widehat{\mathcal{E}}(\mathbf{u}, e) = \int_{\Omega} e(x) dx \quad \text{and} \quad \widehat{\mathcal{S}}(\mathbf{u}, e) = \int_{\Omega} \widehat{S}(x, \mathbf{u}(x), e(x)) dx.$$

Now the Gibbs relation leads to the definition of temperature as

$$\theta = \widehat{\Theta}(x, \mathbf{u}, e) := 1/\partial_e \widehat{S}(x, \mathbf{u}, e),$$

where the relation  $\partial_e \widehat{S}(\mathbf{u}, e) > 0$  is imposed.

The driving force through the free entropy is most simple, as  $\partial_{\mathbf{u}} H = \partial_{\mathbf{u}} \widehat{S}$ , since using  $\widehat{E}(\mathbf{u}, e) := e$  we have  $\partial_{\mathbf{u}} \widehat{E} \equiv 0$ . Thus, the dual entropy-production potential in terms of  $(\mathbf{u}, e)$  takes the form

$$\widehat{\Psi}^*(\mathbf{u}, e; \boldsymbol{\mu}, \varepsilon) = \frac{1}{2} \int_{\Omega} (\nabla \boldsymbol{\mu}, \nabla \varepsilon) : \widehat{\mathbb{M}}(\mathbf{u}, e) (\nabla \boldsymbol{\mu}, \nabla \varepsilon) + \boldsymbol{\mu} \cdot \widehat{\mathbb{H}}(\mathbf{u}, e) \boldsymbol{\mu} dx, \quad (4.2)$$

where  $\widehat{\mathbb{M}}$  and  $\widehat{\mathbb{H}}$  are positive semidefinite. As a consequence of the simple form of  $\widehat{\mathcal{E}}$ , and hence of  $\widehat{\Psi}^*$ , the evolution equations for  $(\mathbf{u}, e)$  take the simple form

$$\begin{pmatrix} \dot{\mathbf{u}} \\ \dot{e} \end{pmatrix} = -\operatorname{div} \left( \widehat{\mathbb{M}}(\mathbf{u}, e) \nabla \begin{pmatrix} \partial_{\mathbf{u}} \widehat{S}(\mathbf{u}, e) \\ \partial_e \widehat{S}(\mathbf{u}, e) \end{pmatrix} \right) + \begin{pmatrix} \widehat{\mathbb{H}}(\mathbf{u}, e) \partial_{\mathbf{u}} S(\mathbf{u}, e) \\ 0 \end{pmatrix}. \quad (4.3)$$

This form has the major advantage that we easily see the parabolic nature. Moreover, there are no source terms in the energy equation.

### 4.3 Two examples

The major modeling issue in non-isothermal reaction-diffusion system is the fact that the thermodynamical equilibrium satisfying the detailed-balance condition (3.3) should depend on the temperature. In our modeling we will make it dependent on the internal energy  $e$  and write  $\mathbf{u} = \mathbf{w}(x, e) = (w_1(x, e), \dots, w_I(x, e))$  for the equilibrium. Obviously, this equilibrium is obtained by maximizing  $\widehat{S}(x, \mathbf{u}, e)$  with respect to  $\mathbf{u}$ . Note that we always assume that  $\widehat{S}(x, \cdot, \cdot)$  is strictly concave, so a maximizer is unique.

We give two examples of relevant entropy functions  $\widehat{S}$ . The first one depends on  $e$  in the form  $\ln e$  like for gases, while in the second one can choose  $\widehat{S}$  such that it stays finite at  $e = 0$  which corresponds to  $\theta = 0$ , which is suitable for modeling solids, i.e. electrochemical species diffusing and reacting inside a solid. Both examples use an additive form of the entropy, which is a good model only in the case of low densities; of course also entropies with strong coupling between the components  $u_1, \dots, u_I$  could be considered.

**Example 1** has the form

$$\widehat{S}_1(x, \mathbf{u}, e) = \sum_{i=1}^I \left( c_i u_i \ln e - u_{*,i} \lambda_B(u_i/u_{*,i}) \right),$$

where  $c_i \geq 0$  and  $u_{*,i} > 0$  may depend on  $x \in \Omega$ . Using  $\lambda'_B(\nu) = \ln \nu$  we find that  $\partial_{\mathbf{u}} \widehat{S}_1(u, e) = 0$  for

$$\mathbf{u} = \mathbf{w}(e) = (u_{*,i} e^{c_i})_{i=1, \dots, I}.$$

Gibbs relation gives the relation between internal energy and temperature in the form

$$\frac{1}{\theta} = \frac{1}{\widehat{\Theta}(\mathbf{u}, e)} = \frac{\mathbf{c} \cdot \mathbf{u}}{e} \quad \text{or} \quad e = \overline{E}(\mathbf{u}, \theta) = \theta \mathbf{c} \cdot \mathbf{u}, \quad \text{where } \mathbf{c} = (c_1, \dots, c_I).$$

For the second derivative of  $\widehat{S}_1$  we have the relation

$$\begin{aligned} -\left(\frac{\boldsymbol{\mu}}{\varepsilon}\right) \cdot \partial^2 \widehat{S}_1(\mathbf{u}, e)\left(\frac{\boldsymbol{\mu}}{\varepsilon}\right) &= \sum_{i=1}^I \frac{\mu_i^2}{u_i} - 2 \frac{\mathbf{c} \cdot \boldsymbol{\mu}}{e} \varepsilon + \frac{\mathbf{c} \cdot \mathbf{u}}{e^2} \varepsilon^2 \\ &\stackrel{(1)}{\geq} \sum_{i=1}^I \frac{\mu_i^2}{u_i} - \frac{(\mathbf{c} \cdot \boldsymbol{\mu})^2}{\mathbf{c} \cdot \mathbf{u}} \stackrel{(2)}{\geq} \sum_{i=1}^I \frac{\mu_i^2}{u_i} - \sum_{i=1}^I \frac{c_i \mu_i^2}{u_i}, \end{aligned}$$

where we minimized over  $\varepsilon$  to obtain  $\stackrel{(1)}{\geq}$ , while  $\stackrel{(2)}{\geq}$  follows using the Cauchy-Schwarz estimate. Thus, we see that concavity of  $\widehat{S}_1$  holds if and only if all  $c_i$  lie in  $[0, 1]$ .

However, inserting  $e = \overline{E}(\mathbf{u}, \theta)$  into  $\widehat{S}_1$ , we see that  $\overline{S}_1(\mathbf{u}, \theta) = \widehat{S}_1(\mathbf{u}, \overline{E}(\mathbf{u}, \theta))$  is not concave in general. Indeed, in the case  $I = 1$  with  $u_* = 1$  we have

$$\overline{S}(u, \theta) = cu \ln \theta - (1-c)u \ln u + (1+c \ln c)u - 1$$

which is concave if and only if  $c \in [0, 1/2]$ .

For **Example 2**, we allow for general functions  $w_i(e)$  and assume that  $\widehat{S}_2$  has the form

$$\widehat{S}_2(\mathbf{u}, e) = s(e) - \sum_{i=1}^I w_i(e) \lambda_B(u_i/w_i(e)) = \widehat{s}(e) - \sum_{i=1}^I \left( \lambda_B(u_i) - u_i \ln w_i(e) \right), \quad (4.4)$$

where  $\widehat{s}(e) = s(e) + I - \sum_{i=1}^I w_i(e)$ . Since  $\lambda_B'(\nu) = \ln \nu = 0$  if and only if  $\nu = 1$ , the reference densities in the detailed balance condition (3.3) are exactly  $\mathbf{w}(e)$ . In addition to the dependence on the internal energy (i.e. on the temperature), they may vary with  $x \in \Omega$ . The concavity can be checked by calculating

$$-\left(\frac{\boldsymbol{\mu}}{\varepsilon}\right) \cdot \text{D}^2 \widehat{S}_2(\mathbf{u}, e)\left(\frac{\boldsymbol{\mu}}{\varepsilon}\right) = \sum_{i=1}^I u_i \left( \frac{\mu_i}{u_i} - \varepsilon \frac{w_i'(e)}{w_i(e)} \right)^2 + \varepsilon^2 \left( -\widehat{s}''(e) - \sum_{i=1}^I u_i \frac{w_i''(e)}{w_i(e)} \right).$$

Thus, we have strict concavity on the whole domain  $]0, \infty[^I \times ]e_0, \infty[$  if and only if  $\widehat{s}''(e) < 0$  and  $w_i''(e) \leq 0$  for all  $i$ .

Thus, the form (4.4) provides a quite general form to model suitable temperature-dependent reaction-diffusion systems. A simple choice for  $s(e)$  and  $\mathbf{w}(e)$  are therefore given by

$$\begin{aligned} \widehat{s}(e) &= c \ln e \text{ for } c > 0 \quad \text{or} \quad \widehat{s}(e) = ce^\sigma \text{ for } \sigma \in ]0, 1[, \\ w_i(e) &= u_{*,i} e^{b_i} \quad \text{for some } u_{*,i} > 0 \text{ and } b_i \in [0, 1]. \end{aligned} \quad (4.5)$$

In the case  $s(e) = c \ln e$  we find the simple relation  $1/\theta = \partial_e \widehat{S}(\mathbf{u}, e) = (c + \mathbf{b} \cdot \mathbf{u})/e$ , where  $\mathbf{b} = (b_i)_{i=1, \dots, I}$ , and we have the nice linear relation

$$e = \overline{E}(\mathbf{u}, \theta) = (c + \mathbf{b} \cdot \mathbf{u}) \theta.$$

## 4.4 Comparison with energy transport models derived from the semiconductor Boltzmann equation

In the context of semiconductor modeling, energy transport equations were derived in the diffusive scaling limit of the Boltzmann equation, see, e.g. [Jün09, Jün10]. The general (unipolar) form obtained by this procedure is

$$\dot{n} = \operatorname{div} \bar{\mathbf{j}}_n, \quad (4.6a)$$

$$\dot{e} = \operatorname{div} \mathbf{j}_e - \mathbf{j}_n \cdot \nabla_x V - W, \quad (4.6b)$$

with  $n$  and  $e$  the electron position and electron energy densities, respectively. The term  $W$  describes averaged inelastic particle scattering and  $V$  is the electrostatic potential. The particle and energy current densities  $\bar{\mathbf{j}}_n$  and  $\mathbf{j}_e$  are expressed as functions of the chemical potential  $\mu$  and electron temperature  $\theta$ ,

$$\bar{\mathbf{j}}_n = D_{00} \left( \nabla_x \left( \frac{\mu}{\theta} \right) - \frac{\nabla_x V}{\theta} \right) - D_{01} \nabla_x \left( \frac{1}{\theta} \right), \quad (4.6c)$$

$$\mathbf{j}_e = D_{10} \left( \nabla_x \left( \frac{\mu}{\theta} \right) - \frac{\nabla_x V}{\theta} \right) - D_{11} \nabla_x \left( \frac{1}{\theta} \right), \quad (4.6d)$$

where  $D_{ij} = D_{ij}(\mu, \theta)$ ,  $i, j \in \{0, 1\}$ , defines the symmetric and positive definite diffusion matrix. For the sake of the comparison with our formulation (4.3) we set  $W = 0$ .

Under reasonable simplifying assumptions [Jün09, Jün10] the extensive variables  $(n, e)$  and the intensive variables  $(\mu, \theta)$  are related by the formulas

$$n = N_0 \theta^{3/2} \exp(\mu/\theta) \quad \text{and} \quad e = \frac{3}{2} n \theta, \quad (4.7)$$

where  $N_0 \theta^{3/2}$  is the scaled density of states. The diffusion matrix  $(D_{ij})$  then becomes

$$(D_{ij}) = \mu_0 \Gamma(2-\beta) n \theta^{1/2-\beta} \begin{pmatrix} 1 & (2-\beta)\theta \\ (2-\beta)\theta & (3-\beta)(2-\beta)\theta^2 \end{pmatrix},$$

where  $\mu_0 > 0$  comes from the elastic scattering rate and  $\Gamma$  denotes the Gamma function. Typical choices for  $\beta$  are  $\beta = 1/2$  (nonpolar phonon scattering),  $\beta = 0$  (acoustic phonon scattering) and  $\beta = -1/2$  (diffusion approximation of the hydrodynamic semiconductor model), see [Jün10].

We now show that the above system (4.6) is consistent with our modeling scheme with

$$\mathcal{S}(n, e) = \int_{\Omega} \widehat{S}(n(x), e(x)) \, ds \quad \text{and} \quad \mathcal{E}(n, e) = \int_{\Omega} e(x) - n(x)V(x) \, dx,$$

where using the relation  $\mu = -\theta \partial_n \widehat{S}(n, e)$  the choice

$$\widehat{S}(n, e) = \frac{3}{2} n \ln e - \frac{5}{2} (n \ln n - n) + n \ln (N_0 (2/3)^{3/2})$$

is consistent with (4.7). Example 1 in Section 4.3 shows that  $\widehat{S}$  is concave. We define the dual entropy-production potential via

$$\Psi^*(n, e; \nu, \varepsilon) = \frac{1}{2} \int_{\Omega} \begin{pmatrix} \nabla \nu + \varepsilon \nabla V \\ \nabla \varepsilon \end{pmatrix} \cdot \begin{pmatrix} D_{00} & D_{01} \\ D_{10} & D_{11} \end{pmatrix} \begin{pmatrix} \nabla \nu + \varepsilon \nabla V \\ \nabla \varepsilon \end{pmatrix} \, dx,$$

where we emphasize that the term  $\varepsilon \nabla V$  (in contrast to  $\nabla(\varepsilon V)$ ) is important to obtain the above model. Using  $\Psi^*(n, e; D\mathcal{E}(n, e)) = 0$  we conclude that the associated Onsager operator  $\mathbb{K}(n, e) = D^2\Psi(n, e)$  satisfies the energy conservation  $\mathbb{K}(n, e)D\mathcal{E}(n, e) = 0$ . Indeed, we have

$$\mathbb{K}(n, e) \begin{pmatrix} \nu \\ \varepsilon \end{pmatrix} = \begin{pmatrix} -\operatorname{div}(D_{00}(\nabla\nu + \varepsilon\nabla V) + D_{01}\nabla\varepsilon) \\ -\operatorname{div}(D_{10}(\nabla\nu + \varepsilon\nabla V) + D_{11}\nabla\varepsilon) + \nabla V \cdot (D_{00}(\nabla\nu + \varepsilon\nabla V) + D_{01}\nabla\varepsilon) \end{pmatrix}.$$

Inserting  $\nu = -\mu/\theta = \partial_n \widehat{S}(n, e)$  and  $\varepsilon = \partial_e \widehat{S}(n, e) = 1/\theta$ , we see that system (4.6) with  $W \equiv 0$  is a gradient system for the entropy  $\mathcal{S}$  and the Onsager operator  $\mathbb{K}$ .

## 5 Maximum principle and evolution for explicit and special cases

### 5.1 Maximum entropy principle

For the general system we may consider all conservation laws using the projection  $\mathcal{C}_{\mathbb{S}^\perp}$  as defined in (3.6). Hence, for given values of

$$\mathcal{C}_{\mathbb{S}^\perp}(\mathbf{u}) = \int_{\Omega} \mathbf{P}\mathbf{u}(x) dx =: \mathbf{C}_0 \in \mathbb{S}^\perp \quad \text{and} \quad \mathcal{E}(\mathbf{u}, e) = \int_{\Omega} e(x) dx =: E_0 \quad (5.1)$$

we maximize the concave function

$$(\mathbf{u}, e) \mapsto \widehat{S}(\mathbf{u}, e).$$

Under reasonable weak additional assumptions, we obtain a unique maximizer  $(\mathbf{u}^*, e^*)$ , called thermodynamical equilibrium.

If  $\mathbf{w}(e)$  is independent of  $x \in \Omega$ , then  $(\mathbf{u}^*, e^*)$  is spatially constant. If  $\mathbf{w}$  and hence  $\widehat{S}(x, \mathbf{u}, e)$  depends on  $x \in \Omega$ , then  $(\mathbf{u}^*, e^*)$  is a nonconstant function on  $\Omega$ . Nevertheless, the temperature  $\theta^*$  is constant as

$$\partial_{\mathbf{u}} \widehat{S}(x, \mathbf{u}^*(x), e^*(x)) = \boldsymbol{\Sigma}_{\mathbf{u}} \mathbf{P} \quad \text{and} \quad 1/\theta^* = \partial_e \widehat{S}(x, \mathbf{u}^*(x), e^*(x)) = \Sigma_e, \quad (5.2)$$

where  $\boldsymbol{\Sigma}_{\mathbf{u}} \in \mathbb{S}^\perp$  is the constant Lagrange multiplier associated with  $\mathcal{C}_{\mathbb{S}^\perp}$  and  $\Sigma_e \in \mathbb{R}$  is the constant Lagrange multiplier associated with  $\mathcal{E}(\mathbf{u}, e) = \int_{\Omega} e(x) dx = E_0$ .

### 5.2 The case of $x$ -independent $\mathbf{w}(e)$

The simplest reaction-diffusion system is obtained if we choose the mobility tensor  $\widehat{\mathbb{M}} = -\kappa(D^2\widehat{S})^{-1}$ , where  $\kappa > 0$  is a scalar. Note that  $\widehat{\mathbb{M}}$  has to be a symmetric tensor (of order 4), so we are not able to choose  $\kappa$  to be a symmetric tensor not commuting with  $D^2\widehat{S}$ . Of course  $\kappa$  may depend on  $x$ , but we assume it to be constant for simplicity. Inserting this mobility tensor into (4.3) we obtain the system

$$\begin{aligned} \dot{\mathbf{u}} &= \kappa \Delta \mathbf{u} + \widehat{\mathbb{H}}(\mathbf{u}, e) \partial_{\mathbf{u}} \widehat{S}(\mathbf{u}, e), \\ \dot{e} &= \kappa \Delta e. \end{aligned} \quad (5.3)$$



Thus, our model, which is thermodynamically consistent, predicts that the internal energy diffuses independently of the densities  $u_i$ , however, there may still be a strong dependence of the reactions on the internal energy.

We note that the reaction terms are given via  $\widehat{\mathbb{H}}$  as in (3.4), where  $\mathbf{u}^*$  is replaced by  $\mathbf{w}(e)$  and  $k_r^*$  can be chosen arbitrarily as a function of  $(\mathbf{u}, e)$ , giving

$$\widehat{\mathbb{H}}(\mathbf{u}, e) \partial_{\mathbf{u}} \widehat{\mathcal{S}}(\mathbf{u}, e) = - \sum_{r=1}^R k_r^*(\mathbf{u}, e) \left( \frac{\mathbf{u}^{\alpha^r}}{\mathbf{w}(e)^{\alpha^r}} - \frac{\mathbf{u}^{\beta^r}}{\mathbf{w}(e)^{\beta^r}} \right) (\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r). \quad (5.4)$$

Imposing sufficient decay to  $k_r^*(\mathbf{u}, e)$ , it is possible to make these terms globally Lipschitz if necessary.

The constant steady state is determined as the maximum of  $\widehat{\mathcal{S}}$  subject to the conservation properties (5.1). With  $\widehat{\mathcal{S}}$  given by (4.4), the relations (5.2) become

$$\begin{aligned} \ln \frac{u_i^*}{w_i(e^*)} &= -(\boldsymbol{\Sigma}_{\mathbf{u}} \mathbb{P})_i =: \ln \widetilde{C}_i \\ s'(e^*) + \sum_{i=1}^I u_i^* \frac{w'_i(e^*)}{w_i(e^*)} &= \Sigma_e \end{aligned}$$

Inserting the first relation into the second one we obtain

$$s'(e^*) + \frac{\mathbf{u}^* \cdot \mathbf{b}}{e^*} = s'(e^*) + \sum_{i=1}^I \widetilde{C}_i w'_i(e^*) = \Sigma_e.$$

The conservation property of the internal energy determines  $e^*$ , which then sets the Lagrange multiplier  $\Sigma_e$ . The other Lagrange multipliers  $\boldsymbol{\Sigma}_{\mathbf{u}}$ , and therefore  $\widetilde{C}_i$ , are determined through the conservation law for  $\mathbb{P}\mathbf{u}$ . The relative entropy functional

$$\mathcal{H}(\mathbf{u}, e) = -\widehat{\mathcal{S}}(\mathbf{u}, e) + \widehat{\mathcal{S}}(\mathbf{u}^*, e^*) + \boldsymbol{\Sigma}_{\mathbf{u}} \int_{\Omega} \mathbb{P}(\mathbf{u} - \mathbf{u}^*) dx + \Sigma_e \int_{\Omega} (e - e^*) dx$$

decays until the steady state  $(\mathbf{u}^*, e^*)$  is reached. Using the relations for the Lagrange multipliers we can reformulate  $\mathcal{H}$  as follows

$$\begin{aligned} \mathcal{H}(\mathbf{u}, e) &= \sum_{i=1}^I \int_{\Omega} \widetilde{C}_i w_i(e) \lambda_B \left( \frac{u_i}{\widetilde{C}_i w_i(e)} \right) dx - \sum_{i=1}^I \int_{\Omega} \widetilde{C}_i (w_i(e) - w_i(e^*) - w'_i(e^*)(e - e^*)) dx \\ &\quad - \sum_{i=1}^I \int_{\Omega} (s(e) - s(e^*) - s'(e^*)(e - e^*)) dx. \end{aligned}$$

This relation holds generally for the entropy  $\widehat{\mathcal{S}}$  with steady states being the maximizers under the conservation laws (5.1). We see that due to the concavity of  $s$  and  $w_i$  with respect to  $e$  also the last two terms give nonnegative contributions to the relative entropy.

With the particular choice

$$w_i(e) = C_i e^{b_i}, \quad s(e) = c e^{\sigma},$$

we can simplify the relative entropy to

$$\begin{aligned} \mathcal{H}(\mathbf{u}, e) &= \sum_{i=1}^I \int_{\Omega} \tilde{C}_i w_i(e) \lambda_{\mathbb{B}}\left(\frac{u_i}{\tilde{C}_i w_i}\right) dx + \sum_{i=1}^I \int_{\Omega} \frac{C_i}{(e^*)^{1-b_i}} (b_i e - e^{b_i} (e^*)^{b_i-1} + (1-b_i) e^*) dx \\ &\quad + \int_{\Omega} \frac{c}{(e^*)^{1-\sigma}} (\sigma e - e^{\sigma} (e^*)^{\sigma-1} + (1-\sigma) e^*) dx, \end{aligned} \quad (5.5)$$

where the nonnegativity of the last two integrands can be checked directly by applying Young's inequality.

### 5.3 The case of $x$ -dependent $w(x, e)$

We let again  $\widehat{S}$  be of the form (4.4), where we now assume

$$w_i(x, e) = \exp(-V_i(x)) e^{b_i}, \quad (5.6)$$

for suitable potentials  $V_i : \Omega \rightarrow \mathbb{R}$  with  $\Omega \subset \mathbb{R}^d$ . In the case of potentials being involved, the stationary state is not constant anymore. Therefore an appropriate choice of the energy density  $s(x, e)$  is more delicate. In order for  $\widehat{S}$  to possess a maximum satisfying the required conservation properties, we need the equations (5.2) to hold for the steady state. As above the  $x$ -dependent stationary state  $(n^*, p^*, e^*)$  has to satisfy

$$\ln \frac{u_i^*}{w_i(x, e^*)} = -(\Sigma_{\mathbf{u}} \mathbb{P})_i =: \ln \tilde{C}_i, \quad (5.7)$$

$$s'(x, e^*) + \sum_{i=1}^I \tilde{C}_i w'_i(x, e^*) = \Sigma_e, \quad (5.8)$$

where here and in the following  $s'(x, e) = \partial_e s(x, e)$  and  $w'_i(x, e) = \partial_e w_i(x, e)$ . We give two generalizations for  $s(x, e)$  of the power law form in (4.5) that allow us to deduce the existence of a maximizer of the entropy  $\widehat{S}$ . The first one is given by

$$s(x, e) = c e^{\sigma} \gamma^{1-\sigma}, \quad \sigma \in (0, 1), \quad (5.9)$$

where  $\gamma(x) \geq 0$  is integrable and w.l.o.g. assumed to be normalized such that

$$\int_{\Omega} \gamma(x) dx = \int_{\Omega} e dx = E_0. \quad (5.10)$$

Then condition (5.8) becomes

$$c \sigma \left(\frac{e^*}{\gamma}\right)^{1-\sigma} + \sum_{i=1}^I \tilde{C}_i b_i (e^*)^{b_i-1} \exp(-V_i) = \Sigma_e.$$

Both terms on the left hand side are nonnegative. In general the terms cannot balance each other such that the sum of both terms adds up to a constant. Hence each of them will have to be constant individually, showing that

$$e^*(x) = \gamma(x)$$

and restricting the choices of the potentials  $V_i$  and exponents  $b_i$ . This leads to the relative entropy functional

$$\begin{aligned}\mathcal{H}(\mathbf{u}, e) &= \sum_{i=1}^I \int_{\Omega} \tilde{C}_i w_i(x, e) \lambda_{\mathbb{B}}\left(\frac{u_i}{\tilde{C}_i w_i}\right) dx \\ &+ \sum_{i=1}^I \int_{\Omega} \exp(-V_i(x)) (e^*)^{b_i-1} (b_i e - e^{b_i} (e^*)^{b_i-1} + (1-b_i)e^*) dx \\ &+ c \int_{\Omega} (\sigma e - e^{\sigma} (e^*)^{\sigma-1} + (1-\sigma)e^*) dx.\end{aligned}\quad (5.11)$$

Another generalization of the power law in (4.5) motivated by (5.8) is given by

$$s(x, e) = \sum_{i=1}^I c_i w_i(x, e), \quad \text{for } c_i \geq 0.$$

The steady state relation (5.8) then reduces to

$$\sum_{i=1}^I (c_i + \tilde{C}_i) w_i'(e^*, x) = \sum_{i=1}^I (c_i + \tilde{C}_i) b_i e^{b_i-1} \exp(-V_i) = \Sigma_e, \quad (5.12)$$

which relates the stationary state  $e^*$  to the potentials  $V_i$  and, again, induces a restriction on the choices of  $b_i$  and  $V_i$ . Relation (5.12) allows us to rewrite the relative entropy as follows

$$\begin{aligned}\mathcal{H}(\mathbf{u}, e) &= -\widehat{\mathcal{S}}(\mathbf{u}, e) + \widehat{\mathcal{S}}(\mathbf{u}^*, e^*) + \Sigma_u \int_{\mathbb{R}^d} \mathbb{P}(\mathbf{u} - \mathbf{u}^*) dx + \Sigma_e \int_{\mathbb{R}^d} (e - e^*) dx \\ &= \sum_{i=1}^I \int_{\Omega} \tilde{C}_i w_i(e) \lambda_{\mathbb{B}}\left(\frac{u_i}{\tilde{C}_i w_i(e)}\right) dx \\ &+ \sum_{i=1}^I (c_i + \tilde{C}_i) \int_{\mathbb{R}^d} (e^*)^{b_i-1} \exp(-V_i) (b_i e - e^{b_i} (e^*)^{b_i-1} + (1-b_i)e^*) dx\end{aligned}$$

Assuming now that  $s(x, e)$  is chosen appropriately such that the entropy  $\widehat{\mathcal{S}}$  can be maximized under the conservation laws, we derive the corresponding evolutionary system according to (4.3). We therefore first differentiate

$$\nabla \begin{pmatrix} \partial_{\mathbf{u}} \widehat{\mathcal{S}}(x, \mathbf{u}, e) \\ \partial_e \widehat{\mathcal{S}}(x, \mathbf{u}, e) \end{pmatrix} = D^2 \widehat{\mathcal{S}}(x, \mathbf{u}, e) \nabla \begin{pmatrix} \mathbf{u} \\ e \end{pmatrix} + \nabla_{(x)} \begin{pmatrix} -\mathbf{V} \\ s'(x, e) \end{pmatrix},$$

where  $D^2 \widehat{\mathcal{S}}$  denotes as above the Hessian of  $\widehat{\mathcal{S}}$  with respect to  $(\mathbf{u}, e)$  and here and in the following we denote

$$\nabla_{(x)} = \nabla \Big|_{e=\text{const.}}.$$

The choice  $\widehat{\mathbb{M}} = -\kappa(D^2 \widehat{\mathcal{S}})^{-1}$  for the mobility tensor leads to the system

$$\begin{aligned}\dot{\mathbf{u}} &= \kappa(\Delta \mathbf{u} + \text{div } \mathbf{D}^u) + \widehat{\mathbb{H}}(\mathbf{u}, e) \partial_{\mathbf{u}} \widehat{\mathcal{S}}(\mathbf{u}, e), \\ \dot{e} &= \kappa(\Delta e + \text{div } \mathbf{d}^e),\end{aligned}\quad (5.13)$$

where the drift fluxes  $\mathbf{D}^u$  and  $\mathbf{d}^e$  have the form

$$\begin{aligned}\mathbf{D}_{ik}^u &= u_i(\partial_{x_k} V_i + \sum_{j=1}^J \frac{u_j b_j b_i}{M(\mathbf{u}, e)} \partial_{x_k} V_j - b_i \frac{e}{M(\mathbf{u}, e)} \partial_{(x_k)} s'(x, e)) \\ \mathbf{d}_k^e &= e \sum_{j=1}^I \frac{b_j u_j}{M(\mathbf{u}, e)} \partial_{x_k} V_j - \frac{e^2}{M(\mathbf{u}, e)} \partial_{(x_k)} s'(x, e).\end{aligned}$$

Here and in the following  $M(\mathbf{u}, e) = -e^2 s''(e) + \sum_{i=1}^I u_i (b_i - b_i^2)$  and, as above,  $\partial_{(x_k)} s'(x, e)$  denotes the partial derivative of  $s'$  with respect to  $x_k$  while  $e$  is kept constant. To see how the drift fluxes arise, we note that

$$-\mathbf{D}^2 \widehat{S} = \begin{pmatrix} \delta(\mathbf{u})^{-1} & -\frac{1}{e} \mathbf{b} \\ -\frac{1}{e} \mathbf{b}^\top & \frac{-e^2 s''(e) + \mathbf{b} \cdot \mathbf{u}}{e^2} \end{pmatrix}$$

with  $\delta(\mathbf{u}) = \text{diag}(\mathbf{u}) \in \mathbb{R}^{I \times I}$ . The inverse can then be calculated as

$$-(\mathbf{D}^2 \widehat{S})^{-1} = \begin{pmatrix} \delta(\mathbf{u}) + \frac{1}{M(\mathbf{u}, e)} (\delta(\mathbf{u}) \mathbf{b}) \otimes (\delta(\mathbf{u}) \mathbf{b}) & \frac{e}{M(\mathbf{u}, e)} \delta(\mathbf{u}) \mathbf{b} \\ \frac{e}{M(\mathbf{u}, e)} (\delta(\mathbf{u}) \mathbf{b})^\top & \frac{e^2}{M(\mathbf{u}, e)} \end{pmatrix}.$$

## 5.4 An $x$ -dependent bipolar model with semiconductor-type reactions

We now write down the simplest system with two species, electrons and holes, with the semiconductor-type reaction  $X_n + X_p \rightleftharpoons \emptyset$ . The variables  $n, p$  and  $e$  stand for the density of electrons, holes, and the internal energy. We set

$$w_n(x, e) = \exp(-V_n(x)) \sqrt{e}, \quad w_p(x, e) = \exp(-V_p(x)) \sqrt{e},$$

and obtain, using  $b \lambda_B(a/b) = \lambda_B(a) - a \ln b + b - 1$ ,

$$\begin{aligned}\widehat{S}(x, n, p, e) &= s(x, e) - w_n(x, e) \lambda_B\left(\frac{n}{w_n(x, e)}\right) - w_p(x, e) \lambda_B\left(\frac{p}{w_p(x, e)}\right) \\ &= \widehat{s}(x, e) + \frac{1}{2}(n+p) \ln e - \lambda_B(n) - \lambda_B(p) - V_n(x)n - V_p(x)p,\end{aligned}\tag{5.14}$$

where  $\widehat{s}(x, e) = s(x, e) - w_n(x, e) - w_p(x, e) + 2$ . The conserved quantities we denote by

$$\mathcal{C}(n, p, e) = \int_{\Omega} (n-p) \, dx =: \mathbf{C}_0 \quad \text{and} \quad \mathcal{E}(n, p, e) = \int_{\Omega} e \, dx =: E_0.\tag{5.15}$$

For given  $\mathbf{C}_0, E_0 > 0$  and an appropriate choice of  $s(x, e)$  as discussed above, there is a unique maximizer of  $\widehat{S}(n, p, e) = \int_{\Omega} \widehat{S}(x, n, p, e) \, dx$  subject to the constraint  $\mathcal{C}(n, p, e) = \mathbf{C}_0$  and  $\mathcal{E}(n, p, e) = E_0$ .

We choose the mobility tensor as  $\widehat{\mathbb{M}} = -\kappa(\mathbf{D}^2 \widehat{S})^{-1}$ . To close the dynamics it remains to set up the reaction terms. The typical form of the semiconductor reactions is given by the Read-Shockley-Hall term  $k(n_I^2 - np)$  with  $k = k(x, n, p, \theta)$  the positive reaction rate and  $n_I = n_I(\theta)$  the intrinsic carrier density, see [MRS90]. The dependence of the intrinsic density on the temperature is modeled as  $n_I(\theta) = c_1 \theta^{3/2} \exp(-c_2/\theta)$  for some positive

constants  $c_1, c_2$ . Observe that  $n_I$  is an increasing function of  $\theta$ . For the sake of simplicity of our forthcoming analysis, we set  $n_I$  to depend linearly on  $e$ . This leads to the form

$$k(e - \rho(x)np), \quad \text{with} \quad \rho(x) = \exp(V_n(x) + V_p(x)).$$

In order to see that this reactive term corresponds to the symmetric form  $\widehat{\mathbb{H}}\boldsymbol{\mu}$  as in (5.4), where we recall the notation  $\boldsymbol{\mu} = \partial_{(n,p)}\widehat{\mathcal{S}}$ , we first rewrite

$$k(\rho(x)np - e) = r_0(n, p, e) \left( \ln \frac{n}{w_n(e)} + \ln \frac{p}{w_p(e)} \right), \quad \text{with} \quad r_0 = ke \left( \frac{np}{w_n w_p} - 1 \right) / \ln \frac{np}{w_n w_p} \geq 0.$$

Thus, we have

$$k(e - \rho(x)np) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \widehat{\mathbb{H}}\boldsymbol{\mu}, \quad \text{where} \quad \widehat{\mathbb{H}} = r_0 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

and we obtain the evolution equations

$$\begin{aligned} \dot{n} &= \kappa \left( \Delta n + \operatorname{div} \left( n \nabla V_n + \frac{n}{N} (n \nabla V_n + p \nabla V_p - 2e \nabla_{(x)} s'(x, e)) \right) \right) + k(x, n, p, e) (e - \rho(x)np), \\ \dot{p} &= \kappa \left( \Delta p + \operatorname{div} \left( p \nabla V_p + \frac{p}{N} (n \nabla V_n + p \nabla V_p - 2e \nabla_{(x)} s'(x, e)) \right) \right) + k(x, n, p, e) (e - \rho(x)np), \\ \dot{e} &= \kappa \left( \Delta e + \operatorname{div} \left( \frac{2e}{N} (n \nabla V_n + p \nabla V_p - 2e \nabla_{(x)} s'(x, e)) \right) \right), \\ 0 &= \nabla p \cdot \boldsymbol{\nu} = \nabla n \cdot \boldsymbol{\nu} = \nabla e \cdot \boldsymbol{\nu} \quad \text{on } \partial\Omega, \end{aligned} \tag{5.16}$$

where  $N(n, p, e) = 4M(n, p, e) = -4e^2 s''(x, e) + n + p$  and  $\rho(x) = \exp(V_n(x) + V_p(x))$ . The reaction terms arise as in (5.4) using  $\boldsymbol{\alpha}_r = (1, 1)^T, \boldsymbol{\beta}_r = (0, 0)^T$ . The reaction coefficient  $k(x, n, p, e) > 0$  can be chosen arbitrarily, for instance the Read-Shockley-Hall generation-recombination model gives  $k = k_0 / (1 + c_n n + c_p p)$  for positive constants  $k_0, c_n$ , and  $c_p$ .

## 6 Global existence of solutions and convergence to equilibrium for particular systems

In this section we derive entropy entropy-production inequalities to prove convergence towards the stationary state in two particular systems. Our approach is inspired by the work [DFM08] and uses logarithmic Sobolev inequalities to bound the entropy in terms of the entropy production. With the known functional inequalities this is, even in the  $x$ -independent case, not possible for an entropy term of the form  $s(e) = c \ln e$ . However, the alternative choice  $s(e) = ce^\sigma$  with  $c \geq 0$  satisfies all required thermodynamical properties and allows us to establish exponential decay of the corresponding relative entropy. In the following we therefore focus on the cases

$$s(e) = c\sqrt{e}, \quad \text{resp.} \quad s(x, e) = c\sqrt{e}\sqrt{\gamma}, \tag{6.1}$$

where  $\gamma(x) \geq 0$  verifying (5.10) corresponds to  $e^*(x)$  in the  $x$ -dependent case.

## 6.1 Global existence and long time behavior in the $x$ -independent case

### 6.1.1 Steady states, relative entropy and evolution equations

We consider a bipolar model with the semiconductor-type reaction  $X_n + X_p \rightleftharpoons \emptyset$ . We put  $\mathbf{u} = (n, p)$ , so that the variables are  $(n, p, e)$  for the density of electrons, holes, and internal energy, respectively. For  $C_p, C_n > 0$  we set

$$w_n(e) = C_n \sqrt{e}, \quad w_p(e) = C_p \sqrt{e}.$$

The derivation of the evolutionary equations from the entropy functional leads to the following semilinear reaction-diffusion system

$$\partial_t n = \kappa \Delta n + k(e - np), \quad (6.2a)$$

$$\partial_t p = \kappa \Delta p + k(e - np), \quad (6.2b)$$

$$\partial_t e = \kappa \Delta e \quad (6.2c)$$

for the constant diffusion coefficient  $\kappa > 0$ . The system is posed on the  $d$ -dimensional torus  $\mathcal{T}^d$  (i.e., with periodic boundary conditions), rescaled such that  $|\mathcal{T}^d| = 1$ .

We shall now investigate the steady states and define the relative entropy. We therefore maximize the entropy

$$\widehat{S}(n, p, e) = c\sqrt{e} - \lambda_B(n) - \lambda_B(p) + n \ln w_n(e) + p \ln w_p(e)$$

on  $\mathcal{T}^d$  under the conservation laws

$$\int_{\mathcal{T}^d} (n - p) dx = \int_{\mathcal{T}^d} (n_0 - p_0) dx = \mathbf{C}_0, \quad \int_{\mathcal{T}^d} e dx = \int_{\mathcal{T}^d} e_0 dx = E_0. \quad (6.3)$$

Introducing the Lagrange multipliers  $\Sigma_0$  and  $\Sigma_e$ , the steady state  $(n^*, p^*, e^*)$  is determined via

$$-\partial_n \widehat{S} + \Sigma_0 = 0, \quad -\partial_p \widehat{S} - \Sigma_0 = 0, \quad -\partial_e \widehat{S} + \Sigma_e = 0,$$

implying the following relations

$$\begin{aligned} n^* &= w_n(e^*) \exp(-\Sigma_0) = C_n \sqrt{e^*} \exp(-\Sigma_0) = \widetilde{C}_n C_n \sqrt{e^*}, \\ p^* &= w_p(e^*) \exp(\Sigma_0) = C_p \sqrt{e^*} \exp(\Sigma_0) = \widetilde{C}_p C_p \sqrt{e^*}, \\ \frac{n^* + p^*}{2e^*} + \frac{c}{2\sqrt{e^*}} &= \Sigma_e. \end{aligned}$$

The detailed balance condition requires

$$n^* p^* = e^*, \quad \text{implying } C_n C_p = 1. \quad (6.4)$$

Moreover, from the conservation property of  $n - p$  we have

$$\frac{1}{2\sqrt{e^*}} (n^* - p^*) = \frac{1}{2} \left( \exp(\ln C_n - \Sigma_0) - \exp(-(\ln C_n - \Sigma_0)) \right) = \sinh(-\ln C_n + \Sigma_0) = \frac{\mathbf{C}_0}{2\sqrt{e^*}}.$$

We note that the pair of constants  $C_n \widetilde{C}_n = C_n \exp(-\Sigma_0)$ ,  $C_p \widetilde{C}_p = C_p \exp(\Sigma_0)$  satisfies the detailed balance condition (6.4). Therefore we shall in the following assume w.l.o.g.

$\tilde{C}_n = \tilde{C}_p = 1$ , which amounts to setting  $\Sigma_0 = 0$ . This can be understood in the sense that the constants  $C_n$  and  $C_p = C_n^{-1}$  are already the right weights in  $w_n$  and  $w_p$  for the stationary states  $n^*$  and  $p^*$ , i.e.

$$n^* = C_n \sqrt{e^*}, \quad p^* = C_p \sqrt{e^*}.$$

The constant steady state, and therefore also the constants  $C_n$  and  $C_p$ , are uniquely determined through the conservation laws and the detailed balance condition, since

$$e^* = E_0, \quad C_n - C_p = C_n - \frac{1}{C_n} = \frac{C_0}{\sqrt{e^*}}.$$

The Lagrange multiplier  $\Sigma_e$  is given by

$$\Sigma_e = \frac{C_n + C_p + c}{2\sqrt{e^*}}. \quad (6.5)$$

Recalling  $\Sigma_0 = 0$ , the convex relative entropy reads as follows

$$\mathcal{H}(n, p, e) = -\widehat{S}(n, p, e) + \widehat{S}(n^*, p^*, e^*) + \Sigma_e \int_{\mathcal{T}^d} (e - e^*) dx, \quad (6.6)$$

which has the crucial property  $\mathcal{H}(n, p, e) \geq \mathcal{H}(n^*, p^*, e^*) = 0$ . Direct computation or using  $\tilde{C}_i = 1, \sigma = b_i = 1/2$  in (5.5) shows that it can also be formulated as

$$\mathcal{H}(n, p, e) = \int_{\mathcal{T}^d} w_n(e) \lambda_B\left(\frac{n}{w_n(e)}\right) + w_p(e) \lambda_B\left(\frac{p}{w_p(e)}\right) + \frac{c+C_n+C_p}{2\sqrt{e^*}} (\sqrt{e} - \sqrt{e^*})^2 dx. \quad (6.7)$$

Note that one can equivalently derive the evolution equations (6.2) starting from  $-\mathcal{H}(n, p, e)$  instead of  $\widehat{S}(n, p, e)$ .

We will prove exponential convergence of solutions to (6.2) based on the dissipation relation

$$\frac{d}{dt} \mathcal{H}(n, p, e) = -\mathcal{P}(n, p, e), \quad (6.8)$$

where the entropy production potential (4.2) reduces to

$$\mathcal{P}(n, p, e) := \int_{\mathcal{T}^d} \kappa \left( n \left| \nabla \ln \frac{n}{\sqrt{e}} \right|^2 + p \left| \nabla \ln \frac{p}{\sqrt{e}} \right|^2 + \frac{N}{4} \left| \frac{\nabla e}{e} \right|^2 \right) + k(np - e) \ln \frac{np}{e} dx,$$

with  $N = N(n, p, e) = n + p + c\sqrt{e}$ .

### 6.1.2 Global existence of solutions

We prove global well-posedness of the system (6.2) on the torus  $\mathcal{T}^d$  subject to the nonnegative initial datum  $(n_0, p_0, e_0) \in L^\infty(\mathcal{T}^d)^3$  and the conservation laws (6.3) with  $E_0 = e^*$ . For the forthcoming analysis we make the assumption that the initial energy is bounded from above and away from zero, i.e. we assume there exist constants  $0 < \underline{e} < \bar{e}$  such that

$$0 < \underline{e} \leq e_0(x) \leq \bar{e} \quad \text{for all } x \in \mathcal{T}^d. \quad (6.9)$$

Then the maximum principle for the solutions  $e$  of (6.2c) implies

$$0 < \underline{e} \leq e(t, x) \leq \bar{e} \quad \text{for all } t \geq 0 \text{ and } x \in \mathcal{T}^d. \quad (6.10)$$

We moreover let the reaction coefficient be bounded from above and away from zero by

$$0 < \underline{k} \leq k \leq \bar{k}.$$

Solutions of the system (6.2) preserve nonnegativity since the nonlinearities on the right-hand side satisfy the *quasi-positivity* condition, see e.g. Lemma 1.1 of [Pie10]. The maximum principle for

$$\partial_t(n + p) - \kappa \Delta(n + p) = 2k(e - np) \leq 2\bar{k}\bar{e}$$

gives

$$\sup_{t \in [0, T]} \|n(t) + p(t)\|_{L^\infty(\mathcal{T}^d)} \leq 2\bar{k}\bar{e}T \|n_0 + p_0\|_{L^\infty(\mathcal{T}^d)},$$

and by nonnegativity,

$$\sup_{t \in [0, T]} \max\{\|n(t)\|_{L^\infty(\mathcal{T}^d)}, \|p(t)\|_{L^\infty(\mathcal{T}^d)}\} \leq 2\bar{k}\bar{e}T \|n_0 + p_0\|_{L^\infty(\mathcal{T}^d)}.$$

This immediately implies the existence of global classical solutions, see [Pie10]. Moreover, the following slightly refined analysis shows that the  $L^1$ -norms of  $n$  and  $p$  are uniformly bounded.

**Lemma 6.1** *Let  $(n, p, e)$  be a solution of the system (6.2) subject to the nonnegative initial data  $(n_0, p_0, e_0)$  satisfying assumption (6.9), the normalizations (6.3) and  $\mathcal{H}(n_0, p_0, e_0) < \infty$ . Then*

$$\sup_{t \geq 0} (\|n\|_{L^1(\mathcal{T}^d)} + \|p\|_{L^1(\mathcal{T}^d)}) < \infty. \quad (6.11)$$

**Proof:** Defining  $\xi := n - p$ , equations (6.2) give

$$\partial_t \xi = \kappa \Delta \xi. \quad (6.12)$$

Therefore, we may write (6.2b) as  $\partial_t p = \kappa \Delta p + k(e - p(p + \xi))$ , and an integration over  $\mathcal{T}^d$  gives

$$\frac{d}{dt} \int_{\mathcal{T}^d} p \, dx = k \left( e^* - \int_{\mathcal{T}^d} p(p + \xi) \, dx \right),$$

where we used the mass conservation of  $e$ . The Cauchy-Schwarz inequality  $\int_{\mathcal{T}^d} p \, dx \leq (\int_{\mathcal{T}^d} p^2 \, dx)^{1/2}$  and the global boundedness  $|\xi(t, x)| \leq C$  (note that  $\xi$  solves the heat equation (6.12)) gives

$$\frac{d}{dt} \int_{\mathcal{T}^d} p \, dx \leq k \left[ e^* - \left( \int_{\mathcal{T}^d} p \, dx \right)^2 + C \int_{\mathcal{T}^d} p \, dx \right],$$

which implies  $\sup_{t \geq 0} \int_{\mathcal{T}^d} p \, dx < \infty$ . Repeating the same steps for  $n$ , we obtain (6.11). ■



### 6.1.3 Convergence to equilibrium

In order to prove the convergence of solutions to the stationary state we have to show the decay of the relative entropy. We shall therefore split the dissipation term into four nonnegative parts, where the ones resulting from the diffusion terms in the dynamics are related to  $-\mathcal{H}$  by using the logarithmic Sobolev type of inequalities (A.1) and the Sobolev imbedding theorems (A.4), where care has to be taken since the norms  $\|n\|_{L^1}$ ,  $\|p\|_{L^1}$  are not conserved (in contrast to  $\|e\|_{L^1}$ ), see also [MHM15, DFM08]. In particular, the difficulty of treating the new mixed dissipation terms arising here involving the heat component is overcome by applying the log-Sobolev inequality with respect to the measure  $edx$ . This clearly requires  $e$  to be bounded uniformly from above and below by a positive constant. In order to control the resulting remainder of the reactive term we proceed in a similar fashion to [DFM08], where the case of a semiconductor reaction-diffusion system with a confining potential but without a heat component was investigated.

**Proposition 6.2 (Entropy entropy-production estimate I)** *For all nonnegative  $(n, p, e)$ , for which  $\mathcal{H}(n, p, e)$ ,  $\mathcal{P}(n, p, e) < \infty$  and  $e$  satisfies (6.10), there exists a  $K$ ,*

$$K = K(\kappa, \|n\|_{L^1}, \|p\|_{L^1}, n^*, p^*, \underline{e}, \bar{e}, e^*) > 0$$

such that the following estimate holds

$$\mathcal{H}(n, p, e) \leq K\mathcal{P}(n, p, e). \quad (6.13)$$

The explicit dependence of  $K$  on its arguments is given in (6.26).

Note that due to Lemma 6.1,  $K$  is uniformly bounded along solutions, i.e.

$$\sup_{t>0} K(\kappa, \|n\|_{L^1}(t), \|p\|_{L^1}(t), n^*, p^*, \underline{e}, \bar{e}, e^*) =: \widehat{K} < \infty. \quad (6.14)$$

**Proof:** Let us denote

$$\bar{n} := \int_{\mathcal{T}^d} n dx, \quad \bar{p} := \int_{\mathcal{T}^d} p dx.$$

Using the identity

$$\int_{\mathcal{T}^d} n \ln \left( \frac{n\sqrt{e^*}}{n^*\sqrt{e}} \right) dx = \frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{n}{\bar{n}} dx + \frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{ne^*}{\bar{n}e} dx + \bar{n} \ln \frac{\bar{n}}{n^*}$$

and its analog for  $p$ , we reformulate the relative entropy (6.7) as

$$\begin{aligned} \mathcal{H}(n, p, e) &= \frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{n}{\bar{n}} dx + \frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{ne^*}{\bar{n}e} dx + n^* \lambda_B \left( \frac{\bar{n}}{n^*} \right) \\ &\quad + \frac{1}{2} \int_{\mathcal{T}^d} p \ln \frac{p}{\bar{p}} dx + \frac{1}{2} \int_{\mathcal{T}^d} p \ln \frac{pe^*}{\bar{p}e} dx + p^* \lambda_B \left( \frac{\bar{p}}{p^*} \right) \\ &\quad + \frac{c}{2\sqrt{e^*}} \int_{\mathcal{T}^d} (\sqrt{e} - \sqrt{e^*})^2 dx. \end{aligned} \quad (6.15)$$

Moreover, we split the entropy production into

$$\mathcal{P}(n, p, e) = \kappa(\mathcal{P}_n + \mathcal{P}_p + \mathcal{P}_e) + \mathcal{P}_R,$$

with

$$\begin{aligned}\mathcal{P}_n &= 2 \int_{\mathcal{T}^d} |\nabla \sqrt{n}|^2 dx + 2 \int_{\mathcal{T}^d} \left| \nabla \sqrt{\frac{ne^*}{e}} \right|^2 \frac{e}{e^*} dx, & \mathcal{P}_e &= 4c \int_{\mathcal{T}^d} |\nabla \sqrt[4]{e}|^2 dx, \\ \mathcal{P}_p &= 2 \int_{\mathcal{T}^d} |\nabla \sqrt{p}|^2 dx + 2 \int_{\mathcal{T}^d} \left| \nabla \sqrt{\frac{pe^*}{e}} \right|^2 \frac{e}{e^*} dx, & \mathcal{P}_R &= - \int_{\mathcal{T}^d} k(e - np) \ln \frac{np}{e} dx.\end{aligned}$$

We apply the log-Sobolev inequality (A.1) to estimate the first two terms of  $\mathcal{H}(n, p, e)$  as

$$\frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{n}{\bar{n}} dx \leq \frac{C_{LS}}{2} \int_{\mathcal{T}^d} |\nabla \sqrt{n}|^2 dx,$$

and, using the fact that  $\frac{e dx}{e^*}$  is a probability measure on  $\mathcal{T}^d$ , the generalized log-Sobolev inequality (see e.g. [AM\*01]) to obtain

$$\frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{ne^*}{\bar{n}e} dx \leq \frac{C_{LS}(e/e^*)}{2} \int_{\mathcal{T}^d} \left| \nabla \sqrt{\frac{ne^*}{e}} \right|^2 \frac{e}{e^*} dx.$$

Here  $C_{LS}(e/e^*)$  is the log-Sobolev constant for the probability measure  $\frac{e dx}{e^*}$ , which depends on  $\bar{e}$  and  $\underline{e}$  and approaches the classical log-Sobolev constant  $C_{LS}$  as  $e$  converges to the stationary state. Consequently, we have the bound

$$\frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{n}{\bar{n}} dx + \frac{1}{2} \int_{\mathcal{T}^d} n \ln \frac{ne^*}{\bar{n}e} dx \leq C_{LS}(e/e^*) \mathcal{P}_n,$$

and the same estimate for the  $p$ -terms.

We now turn to the entropy term for the energy and first note that by the mass conservation law for  $e$  we have

$$\frac{c}{2\sqrt{e^*}} \int_{\mathcal{T}^d} (\sqrt{e} - \sqrt{e^*})^2 dx = \frac{c}{\sqrt{e^*}} \int_{\mathcal{T}^d} (e^* - \sqrt{e}\sqrt{e^*}) dx = c \int_{\mathcal{T}^d} (\sqrt{e^*} - \sqrt{e}) dx. \quad (6.16)$$

Moreover, the Jensen inequality gives

$$\int_{\mathcal{T}^d} \sqrt{e^*} dx \leq \left( \int_{\mathcal{T}^d} e^* dx \right)^{1/2} = \left( \int_{\mathcal{T}^d} e dx \right)^{1/2} = \|\sqrt[4]{e}\|_{L^4(\mathcal{T}^d)}^2,$$

and, subsequently, with the Sobolev imbedding (A.4) of the Appendix,

$$\|\sqrt[4]{e}\|_{L^4(\mathcal{T}^d)}^2 \leq C_S \|\nabla \sqrt[4]{e}\|_{L^2(\mathcal{T}^d)}^2 + \|\sqrt[4]{e}\|_{L^2(\mathcal{T}^d)}^2 = \frac{C_S}{4c} \mathcal{P}_e + \int_{\mathcal{T}^d} \sqrt{e} dx.$$

This implies the bound for the last term of  $\mathcal{H}(n, p, e)$  in (6.15),

$$\frac{c}{2\sqrt{e^*}} \int_{\mathcal{T}^d} (\sqrt{e} - \sqrt{e^*})^2 dx \leq \frac{C_S}{4} \mathcal{P}_e. \quad (6.17)$$

For bounding the remaining two terms of  $\mathcal{H}(n, p, e)$  we first apply the auxiliary Lemma (A.4) of the Appendix to get

$$n^* \lambda_B\left(\frac{\bar{n}}{n^*}\right) + p^* \lambda_B\left(\frac{\bar{p}}{p^*}\right) \leq C_0(n^*, p^*, \bar{n}, \bar{p}) \left(\sqrt{\frac{\bar{n}\bar{p}}{n^*p^*}} - 1\right)^2, \quad (6.18)$$

where  $C_0$  satisfies (A.6) and is uniformly bounded. Now the idea is to bound this right hand side further, where we use the dissipation term  $\mathcal{P}_R$  resulting from the reactive terms. We therefore employ the elementary inequality

$$\ln(y)(y-1) \geq 4(\sqrt{y}-1)^2 \quad (6.19)$$

and Jensen's inequality,

$$\begin{aligned} \mathcal{P}_R &= \int_{\mathcal{T}^d} k \ln \frac{np}{e} \left( \frac{np}{e} - 1 \right) e \, dx \geq 4k_0 \int_{\mathcal{T}^d} \left( \sqrt{\frac{np}{e}} - 1 \right)^2 e \, dx \\ &\geq 2k_0 \left( \int_{\mathcal{T}^d} \sqrt{np} - \sqrt{e^*} \, dx \right)^2 - 4k_0 \int_{\mathcal{T}^d} \left( \sqrt{e} - \sqrt{e^*} \right)^2 \, dx \\ &\geq 2k_0 \left( \int_{\mathcal{T}^d} \sqrt{np} - \sqrt{e^*} \, dx \right)^2 - \frac{2C_S k_0 \sqrt{e^*}}{c} \mathcal{P}_e. \end{aligned} \quad (6.20)$$

Inspired by [DFM08], we define

$$\delta_n := \sqrt{n} - \int_{\mathcal{T}^d} \sqrt{n} \, dx, \quad \delta_p := \sqrt{p} - \int_{\mathcal{T}^d} \sqrt{p} \, dx, \quad (6.21)$$

and obtain

$$\begin{aligned} \mathcal{P}_R + \frac{2C_S k_0 \sqrt{e^*}}{c} \mathcal{P}_e &\geq 2k_0 \left( \int_{\mathcal{T}^d} \sqrt{n} \, dx \int_{\mathcal{T}^d} \sqrt{p} \, dx + \int_{\mathcal{T}^d} \delta_n \delta_p \, dx - \sqrt{e^*} \right)^2 \\ &\geq k_0 \left( \int_{\mathcal{T}^d} \sqrt{n} \, dx \int_{\mathcal{T}^d} \sqrt{p} \, dx - \sqrt{e^*} \right)^2 - \frac{k_0}{2} \left( \int_{\mathcal{T}^d} (\delta_n^2 + \delta_p^2) \, dx \right)^2 \\ &\geq k_0 \left( \int_{\mathcal{T}^d} \sqrt{n} \, dx \int_{\mathcal{T}^d} \sqrt{p} \, dx - \sqrt{e^*} \right)^2 - \frac{k_0}{2} (\bar{n} + \bar{p}) \int_{\mathcal{T}^d} (\delta_n^2 + \delta_p^2) \, dx, \end{aligned}$$

where we used

$$\int_{\mathcal{T}^d} \delta_n^2 \, dx = \int_{\mathcal{T}^d} n \, dx - \left( \int_{\mathcal{T}^d} \sqrt{n} \, dx \right)^2 \leq \bar{n} \quad (6.22)$$

and its analog for  $p$ . We can now further apply the Poincaré inequality

$$\int_{\mathcal{T}^d} \delta_n^2 \, dx \leq C_P \int_{\mathcal{T}^d} |\nabla \sqrt{n}|^2 \, dx \leq \frac{C_P}{2} \mathcal{P}_n, \quad (6.23)$$

implying

$$\mathcal{P}_R + \frac{2C_S k_0 \sqrt{e^*}}{c} \mathcal{P}_e \geq k_0 \left( \int_{\mathcal{T}^d} \sqrt{n} \, dx \int_{\mathcal{T}^d} \sqrt{p} \, dx - \sqrt{e^*} \right)^2 - \frac{k_0 C_P}{4} (\bar{n} + \bar{p}) (\mathcal{P}_n + \mathcal{P}_p).$$

We are therefore left to “interchange square roots and integration” in order to connect with (6.18) and complete the estimation of  $\mathcal{H}(n, p, e)$  in terms of the entropy production. We rewrite

$$\int_{\mathcal{T}^d} \sqrt{n} \, dx = \sqrt{\bar{n}} - R_n \int_{\mathcal{T}^d} \delta_n^2 \, dx \quad \text{with} \quad R_n := \left( \sqrt{\bar{n}} + \int_{\mathcal{T}^d} \sqrt{n} \, dx \right)^{-1}. \quad (6.24)$$

Note that  $R_n$  is unbounded if and only if  $\sqrt{\bar{n}} \geq \int_{\mathcal{T}^d} \sqrt{n} dx$  vanishes. We circumvent here the procedure of distinguishing between different cases as in [DFM08] by estimating more directly

$$\begin{aligned} & \left( \int_{\mathcal{T}^d} \sqrt{n} dx \int_{\mathcal{T}^d} \sqrt{p} dx - \sqrt{e^*} \right)^2 \\ & \geq \frac{1}{2} (\sqrt{\bar{n}\bar{p}} - \sqrt{e^*})^2 - \left( R_n \int_{\mathcal{T}^d} \delta_n^2 dx \sqrt{\bar{p}} + R_p \int_{\mathcal{T}^d} \delta_p^2 dx \sqrt{\bar{n}} - R_n R_p \int_{\mathcal{T}^d} \delta_n^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \\ & \geq \frac{1}{2} (\sqrt{\bar{n}\bar{p}} - \sqrt{e^*})^2 - 2C_P(\bar{n} + \bar{p})(\mathcal{P}_n + \mathcal{P}_p) \end{aligned}$$

The derivation of the last inequality is carried out in Lemma A.5 of the Appendix giving

$$\begin{aligned} n^* \lambda_B \left( \frac{\bar{n}}{n^*} \right) + p^* \lambda_B \left( \frac{\bar{p}}{p^*} \right) & \leq C_1(\bar{n}, \bar{p}, n^*, p^*, e^*) \mathcal{P}, \quad \text{where} \quad (6.25) \\ C_1(\bar{n}, \bar{p}, n^*, p^*, e^*) & = \frac{2}{e^* k_0} C_0(\bar{n}, \bar{p}, n^*, p^*) \max \left\{ 1, \frac{2C_S k_0 \sqrt{e^*}}{c\kappa}, \frac{1}{\kappa} \left( \frac{k_0}{4} + 4 \right) C_p(\bar{n} + \bar{p}) \right\}. \end{aligned}$$

Therefore, we can close the chain of inequalities (6.15)–(6.25) and conclude

$$\begin{aligned} \mathcal{H}(n, p, e) & \leq K \mathcal{P}(n, p, e) \quad \text{with} \\ K(\kappa, \bar{n}, \bar{p}, n^*, p^*, e^*, \bar{e}, \underline{e}) & = \kappa^{-1} \max \left\{ \kappa C_1(\bar{n}, \bar{p}, n^*, p^*, e^*), C_{LS}(e/e^*), \frac{C_S}{4} \right\}. \quad (6.26) \end{aligned}$$

Thus the proof of Proposition 6.2 is complete.  $\blacksquare$

Using Proposition 6.2, we are now ready to prove the main result about exponential convergence towards the steady state.

**Theorem 6.3 (Exponential convergence to equilibrium)** *Let  $(n, p, e)$  be a solution to the system (6.2) subject to the nonnegative initial data  $(n_0, p_0, e_0)$  satisfying  $\mathcal{H}(n_0, p_0, e_0) < \infty$ , the normalizations (6.3) and assumption (6.9). Then, the solution converges exponentially fast to the unique constant equilibrium state  $(n^*, p^*, e^*)$ ,*

$$\|n - n^*\|_{L^1(\mathcal{T}^d)}^2 + \|p - p^*\|_{L^1(\mathcal{T}^d)}^2 + \|\sqrt{e} - \sqrt{e^*}\|_{L^2(\mathcal{T}^d)}^2 \leq C(\bar{n}, \bar{p}, n^*, p^*) \mathcal{H}(n_0, p_0, e_0) \exp(-\widehat{K}t),$$

where  $\widehat{K}$  is given by (6.14) and

$$C(\bar{n}, \bar{p}, n^*, p^*) = \max \left\{ \frac{2}{3} (2(\bar{n} + \bar{p}) + 4(C_n + C_p) \|\sqrt{e}\|_{L^1(\mathcal{T}^d)}), \frac{2\sqrt{e^*}}{c + C_n + C_p} (1 + 2C_n^2 + 2C_p^2) \right\}$$

is uniformly bounded.

**Proof:** The entropy entropy-production inequality (6.13) from Proposition 6.2 together with the dissipation relation (6.8) imply the exponential convergence of the relative entropy with exponent  $\widehat{K}$  in (6.14),

$$\mathcal{H}(n, p, e) \leq \mathcal{H}(n_0, p_0, e_0) \exp(-\widehat{K}t). \quad (6.27)$$

It therefore remains to derive the decay estimates for  $n, p, e$  by bounding the relative entropy from below. We first note that

$$\begin{aligned} \|n - n^*\|_{L^1(\mathcal{T}^d)}^2 & \leq 2 \left( \|n - C_n \sqrt{e}\|_{L^1(\mathcal{T}^d)}^2 + C_n^2 \|\sqrt{e} - \sqrt{e^*}\|_{L^1(\mathcal{T}^d)}^2 \right) \\ & \leq 2 \left( \|n - C_n \sqrt{e}\|_{L^1(\mathcal{T}^d)}^2 + C_n^2 \|\sqrt{e} - \sqrt{e^*}\|_{L^2(\mathcal{T}^d)}^2 \right), \end{aligned}$$

and use the Csiszár-Kullback-Pinsker inequality (A.3) of the Appendix,

$$\begin{aligned} \|n - C_n \sqrt{e}\|_{L^1(\mathcal{T}^d)}^2 &\leq \frac{1}{3} \left( 2 \|n\|_{L^1(\mathcal{T}^d)} + 4C_n \|\sqrt{e}\|_{L^1(\mathcal{T}^d)} \right) \int_{\mathcal{T}^d} C_n \sqrt{e} \lambda_B\left(\frac{n}{C_n \sqrt{e}}\right) dx \\ &\leq \frac{1}{3} \left( 2\bar{n} + 4C_n \|\sqrt{e}\|_{L^1(\mathcal{T}^d)} \right) \mathcal{H}(n, p, e). \end{aligned}$$

The analogous estimate holds for  $p$ . The proof is concluded by observing that the term  $\|\sqrt{e} - \sqrt{e^*}\|_{L^2(\mathcal{T}^d)}^2$  is a component of  $\mathcal{H}(n, p, e)$  and using the decay (6.27).  $\blacksquare$

## 6.2 Global existence and long-time behavior in the $x$ -dependent case

### 6.2.1 Steady states, relative entropy and evolution equations

As in Section 5.4 we now consider the case of potentials being involved in the dynamics. In the spirit of semiconductor modeling, the potentials are given by

$$V_n = V_{\text{conf}} + V_{\text{el}}, \quad V_p = V_{\text{conf}} - V_{\text{el}}$$

where  $V_{\text{conf}}$  represents confinement of the carriers and  $V_{\text{el}}$  is the electrostatic potential. However, due to technical difficulties in the derivation of an entropy-entropy-production inequality, we only study a simplified model with  $V_{\text{el}} \equiv 0$  here, i.e., we set  $V_n = V_p = V : \mathbb{R}^d \rightarrow \mathbb{R}$  ( $d \leq 4$ ) on the whole space  $\mathbb{R}^d$ . In particular, we assume that

$$V \in C^2(\mathbb{R}^d) \quad \text{is an } L^\infty\text{-perturbation of a uniformly convex function.} \quad (6.28)$$

In this section we shall not keep as close track of the constants arising as in Section 6.1. Moreover, instead of working on a torus, we consider the full space setting on  $\mathbb{R}^d$ . Note that the presence of the confining potential can be loosely interpreted as a model for a bounded domain.

We start from an entropy relation (5.14) but choose  $s$ ,  $w_n$ , and  $w_p$  depending on  $x$ . To simplify notation and without loss of generality we normalize

$$\int_{\mathbb{R}^d} e \, dx = \int_{\mathbb{R}^d} e_0 \, dx = 1.$$

As in [MHM15, Eqn. (5.5)] we choose  $w_n$  and  $w_p$  linearly dependent in the form

$$w_n(x, e) = C_n \sqrt{e} \exp(-V), \quad w_p(x, e) = C_p \sqrt{e} \exp(-V)$$

for some constants  $C_n, C_p > 0$ . Moreover, for  $c > 0$  we let

$$\widehat{s}(x, e) = c \sqrt{e} \exp(-V) \quad \text{giving } s(x, e) = (c + C_n + C_p) \sqrt{e} \exp(-V(x)).$$

Throughout, we assume the potential to be normalized such that

$$\int_{\mathbb{R}^d} \exp(-2V) \, dx = 1.$$

The steady state is again determined by maximizing the entropy  $\widehat{S}$  under the conservation laws (5.15). Setting the Lagrangian multiplier for the conservation law of  $n - p$  to 0, i.e.  $\Sigma_0 = 0$ , we get

$$\begin{aligned} n^*(x) &= w_n(x, e^*(x)) = C_n \exp(-V(x)) \sqrt{e^*(x)}, \\ p^*(x) &= w_p(x, e^*(x)) = C_p \exp(-V(x)) \sqrt{e^*(x)}. \end{aligned}$$

For the Lagrangian multiplier  $\Sigma_e$  corresponding to the conservation of energy we obtain

$$\Sigma_e = \frac{C_n + C_p + c}{2} \frac{\exp(-V(x))}{\sqrt{e^*}}.$$

Due to the normalizations of  $e$  and  $V$  we have then

$$e^*(x) = \exp(-2V(x)) \quad \text{for } x \in \mathbb{R}^d.$$

Thus, we arrive at the following expression for the relative entropy  $\mathcal{H}$ :

$$\begin{aligned} \mathcal{H}(n, p, e) &= \int_{\mathbb{R}^d} w_n(x, e) \lambda_B\left(\frac{n}{w_n(x, e)}\right) dx + \int_{\mathbb{R}^d} w_p(x, e) \lambda_B\left(\frac{p}{w_p(x, e)}\right) dx \\ &\quad + \frac{c+C_n+C_p}{2} \int_{\mathbb{R}^d} \left(\sqrt{e} - \sqrt{e^*(x)}\right)^2 dx. \end{aligned} \quad (6.29)$$

It is important to realize that no  $x$ -dependent factor  $\mu = \exp(-V(x))$  shows up in the last integral, because  $\mu(x) = \sqrt{e^*(x)}$  gives  $s(x, e) = (c+C_n+C_p)\sqrt{e e^*(x)}$ ; hence

$$\frac{s(x, e^*(x)) - \partial_e s(x, e^*(x))(e - e^*(x)) - s(x, e)}{c+C_n+C_p} = e^*(x) - \frac{1}{2}(e - e^*(x)) - \sqrt{e e^*(x)} = \frac{1}{2}(\sqrt{e} - \sqrt{e^*(x)})^2.$$

The corresponding gradient system takes the form

$$\partial_t n = \nabla \cdot (\nabla n + 2n \nabla V) + k(e - \rho(x)np), \quad (6.30a)$$

$$\partial_t p = \nabla \cdot (\nabla p + 2p \nabla V) + k(e - \rho(x)np), \quad (6.30b)$$

$$\partial_t e = \nabla \cdot (\nabla e + 2e \nabla V). \quad (6.30c)$$

Let us summarize for completeness,

$$\begin{aligned} \rho(x) &= \exp(2V), & w_n &= C_n \exp(-V) \sqrt{e}, & w_p &= C_p \exp(-V) \sqrt{e}, \\ e^* &= \exp(-2V), & n^* &= C_n \exp(-2V), & p^* &= C_p \exp(-2V). \end{aligned}$$

The constants  $C_n, C_p$  are determined by the relations

$$C_n C_p = 1, \quad C_n - C_p = (C_n - C_p) \int_{\mathbb{R}^d} \exp(-2V) dx = \int_{\mathbb{R}^d} (n^* - p^*) dx = \mathbf{C}_0.$$

The entropy production reads

$$\begin{aligned} \mathcal{P}(n, p, e) &= \int_{\mathbb{R}^d} \left( n \left| \nabla \ln \frac{n}{w_n} \right|^2 + p \left| \nabla \ln \frac{p}{w_p} \right|^2 \right) dx + \int_{\mathbb{R}^d} \frac{N}{4} \left| \nabla \ln \frac{e}{e^*} \right|^2 dx \\ &\quad + \int_{\mathbb{R}^d} k e \left( \frac{np}{w_n w_p} - 1 \right) \ln \frac{np}{w_n w_p} dx \\ &= \frac{1}{2} \int_{\mathbb{R}^d} \left( n \left| \nabla \ln \frac{n}{e^*} \right|^2 + n \left| \nabla \ln \frac{n}{e} \right|^2 \right) dx + \frac{1}{2} \int_{\mathbb{R}^d} \left( p \left| \nabla \ln \frac{p}{e^*} \right|^2 + p \left| \nabla \ln \frac{p}{e} \right|^2 \right) dx \\ &\quad + (C_n + C_p + c) \int_{\mathbb{R}^d} \sqrt{\frac{e}{e^*}} \left| \nabla \ln \sqrt{\frac{e}{e^*}} \right|^2 dx + \int_{\mathbb{R}^d} k e \left( \frac{np}{w_n w_p} - 1 \right) \ln \frac{np}{w_n w_p} dx \end{aligned} \quad (6.31)$$

where  $N = n + p + c\sqrt{e}\sqrt{e^*}$ .

## 6.2.2 Global existence of solutions

We consider the system (6.30) posed in the full space  $\mathbb{R}^d$ , subject to the initial data

$$n(0, x) = n_0(x) \geq 0, \quad p(0, x) = p_0(x) \geq 0, \quad e(0, x) = e_0(x) \geq 0.$$

We first derive an  $L^\infty$ -bound for the solution  $e$  of the Fokker-Planck equation (6.30c), which is decoupled from the evolution of  $n, p$ .

**Lemma 6.4** *Assume that the initial datum  $e_0 \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ . Then the solution  $e$  to (6.30c) satisfies*

$$\sup_{t \geq 0} \|e(t)\|_{L^\infty(\mathbb{R}^d)} < \infty. \quad (6.32)$$

A proof of this Lemma can be found e.g. [DFM08]. For the sake of completeness we summarize the main arguments here.

**Proof:** Let us calculate the evolution of the  $L^{j+1}$  norm of  $e$  via integration by parts,

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} e^{j+1} dx &= -\frac{4j}{j+1} \int_{\mathbb{R}^d} \left| \nabla e^{\frac{j+1}{2}} \right|^2 dx + 2j \int_{\mathbb{R}^d} e^{j+1} \Delta V dx \\ &\leq -\frac{4j}{j+1} \int_{\mathbb{R}^d} \left| \nabla e^{\frac{j+1}{2}} \right|^2 dx + 2j \|\Delta V\|_{L^\infty(\mathbb{R}^d)} \int_{\mathbb{R}^d} e^{j+1} dx. \end{aligned}$$

We now use the classical Nash inequality, see e.g. [Nas58, CaL93], valid for all  $f \in L^1(\mathbb{R}^d) \cap H^1(\mathbb{R}^d)$ ,

$$\|f\|_{L^2(\mathbb{R}^d)}^{\frac{d+2}{d}} \leq C_d \|f\|_{L^1(\mathbb{R}^d)}^{2/d} \|\nabla f\|_{L^2(\mathbb{R}^d)},$$

for  $f = e^{\frac{j+1}{2}}$ , and the Young inequality with the conjugate exponents  $\frac{d+2}{d}$  and  $\frac{d+2}{2}$ , to obtain

$$\int_{\mathbb{R}^d} e^{j+1} dx \leq \varepsilon \int_{\mathbb{R}^d} \left| \nabla e^{\frac{j+1}{2}} \right|^2 dx + \frac{C}{\varepsilon} \left( \int_{\mathbb{R}^d} e^{\frac{j+1}{2}} dx \right)^2.$$

Consequently, for  $\varepsilon$  of the form  $\varepsilon = \varepsilon_j = \frac{A}{j}$  with a suitable constant  $A > 0$ , we have

$$\frac{d}{dt} \int_{\mathbb{R}^d} e^{j+1} dx \leq -\varepsilon_j \int_{\mathbb{R}^d} e^{j+1} dx + Cj(j + \varepsilon_j) \sup_{0 \leq \tau \leq t} \left( \int_{\mathbb{R}^d} e^{\frac{j+1}{2}} dx \right)^2.$$

By an iterative argument (Lemma 4.2 in [DFM08]), this implies the announced bound (6.32).  $\blacksquare$

Next, we derive a uniform  $L^1$  bound for  $n$  and  $p$ .

**Lemma 6.5** *Let  $(n, p, e)$  be a solution to the system (6.30) subject to the nonnegative initial data  $(n_0, p_0, e_0)$  with finite entropy  $\mathcal{H}(n_0, p_0, e_0) < \infty$ , satisfying the normalizations (5.1). Then*

$$\sup_{t \geq 0} \left( \|n\|_{L^1(\mathbb{R}^d)} + \|p\|_{L^1(\mathbb{R}^d)} \right) < \infty. \quad (6.33)$$

**Proof:** We first bound

$$\|n\|_{L^1(\mathbb{R}^d)}^2 \leq 2 \left( \|n - w_n\|_{L^1(\mathbb{R}^d)}^2 + \|w_n\|_{L^1(\mathbb{R}^d)}^2 \right),$$

and deduce from the Csiszár-Kullback-Pinsker inequality (A.3),

$$\begin{aligned} \|n - w_n\|_{L^1(\mathbb{R}^d)}^2 &\leq \frac{1}{3} \left( 2 \|n\|_{L^1(\mathbb{R}^d)} + 4 \|w_n\|_{L^1(\mathbb{R}^d)} \right) \int_{\mathbb{R}^d} \left( n \ln \frac{n}{w_n} - (n - w_n) \right) dx \\ &\leq \frac{1}{3} \left( 2 \|n\|_{L^1(\mathbb{R}^d)} + 4 \|w_n\|_{L^1(\mathbb{R}^d)} \right) \mathcal{H}(n, p, e). \end{aligned}$$

Due to the entropy production  $\mathcal{H}(n, p, e) \leq \mathcal{H}(n_0, p_0, e_0)$  and the mass conservation property for  $e$ , we have

$$\|w_n\|_{L^1(\mathbb{R}^d)} \leq C_n \|\exp(-2V)\|_{L^2(\mathbb{R}^d)} \|\sqrt{e}\|_{L^2(\mathbb{R}^d)} = C_n.$$

Therefore,

$$\|n\|_{L^1(\mathbb{R}^d)}^2 \leq C_1 \|n\|_{L^1(\mathbb{R}^d)} + C_2$$

for some constants  $C_1, C_2 > 0$ , which immediately implies the claim for  $n$ . Repeating the same steps for  $p$ , we conclude.  $\blacksquare$

Finally, we derive uniform  $L^\infty$ -bounds for  $n$  and  $p$ .

**Lemma 6.6** *Assume that the initial data  $(n_0, p_0, e_0)$  are in  $(L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d))^3$  with finite entropy  $\mathcal{H}(n_0, p_0, e_0) < \infty$ . Then the solution  $(n, p, e)$  to the system (6.30) satisfies*

$$\sup_{t \geq 0} \left( \|n(t)\|_{L^\infty(\mathbb{R}^d)} + \|p(t)\|_{L^\infty(\mathbb{R}^d)} \right) < \infty.$$

**Proof:** We use the same Nash-Moser iteration as in the proof of Lemma 6.4, noticing that the only structural difference between the  $e$ -equation (6.30c) and the  $n, p$ -equations (6.30a), (6.30b) is the reaction term. Thus, we only have to use the additional estimate

$$\begin{aligned} \int_{\mathbb{R}^d} (n^j + p^j) k(e - \rho n p) dx &\leq \|k\|_{L^\infty(\mathbb{R}^d)} \|e\|_{L^\infty(\mathbb{R}^d)} \int_{\mathbb{R}^d} (n^j + p^j) dx \\ &\leq C j \int_{\mathbb{R}^d} (n^{j+1} + p^{j+1}) dx + \frac{C}{j}, \end{aligned}$$

where we used the interpolation of Lebesgue spaces in the second line and the uniform boundedness of the  $L^1$ -norms, to derive

$$\frac{d}{dt} \int_{\mathbb{R}^d} (n^{j+1} + p^{j+1}) dx \leq -\varepsilon \int_{\mathbb{R}^d} (n^{j+1} + p^{j+1}) dx + C j(j+\varepsilon) \sup_{0 \leq \tau \leq t} \left( \int_{\mathbb{R}^d} (n^{\frac{j+1}{2}} + p^{\frac{j+1}{2}}) dx \right)^2 + \frac{C}{j}.$$

Again, Lemma 4.2 of [DFM08] gives uniform boundedness of  $n$  and  $p$  in  $L^\infty$ .  $\blacksquare$

Similarly to the  $x$ -independent case we need a comparison principle for  $e$ , which we obtain with respect to the measure  $e^*$  as follows.



**Lemma 6.7** *Let  $e_0 \in L^1(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$  satisfy*

$$\underline{e} e^* \leq e_0(x) \leq \bar{e} e^*, \quad x \in \mathbb{R}^d \quad (6.34)$$

*for some  $0 < \underline{e} \leq \bar{e} < \infty$ . Then the solution  $e$  to (6.30c) remains within these bounds for all times,*

$$\underline{e} e^* \leq e(t, x) \leq \bar{e} e^*, \quad x \in \mathbb{R}^d, t > 0. \quad (6.35)$$

**Proof:** Recalling that  $e^* = \exp(-2V)$  is a probability measure, we introduce

$$f = e \exp(2V) = \frac{e}{e^*}$$

and equation (6.30c) becomes

$$\exp(-2V) \partial_t f = \nabla \cdot (\exp(-2V) \nabla f).$$

Multiplication by the negative part of  $f - \underline{e}$ , i.e.  $(f - \underline{e})_-$ , and integration by parts gives

$$\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} [(f - \underline{e})_-]^2 \exp(-2V) dx = - \int_{\mathbb{R}^d} |\nabla (f - \underline{e})_-|^2 \exp(-2V) dx \leq 0.$$

Since  $(f - \underline{e})_-(t = 0) = 0$ , this property is retained for all times. The upper bound follows using the same argumentation.  $\blacksquare$

### 6.2.3 Convergence to equilibrium

The proof of convergence of the solution towards the stationary state relies on the exponential decay of the negative entropy  $\mathcal{H}$ . This follows, as in Section 6.1.3, from the entropy entropy-production inequality. Additional care has to be taken here due to the  $x$ -dependent stationary states, which requires to work with the reference probability measure  $e^* dx$ .

**Proposition 6.8 (Entropy entropy-production estimate II)** *Let  $(n, p, e)$  be a non-negative solution to (6.30) in  $L^\infty(0, \infty; L^1(\mathbb{R}^d)) \cap L^\infty((0, \infty) \times \mathbb{R}^d)$ , and  $e$  satisfy the bounds (6.35). Then there exists a constant  $K > 0$  such that*

$$\mathcal{H}(n, p, e) \leq K \mathcal{P}(n, p, e). \quad (6.36)$$

**Proof:** We recall that  $e dx$  and  $e^* dx = \exp(-2V) dx$  are probability measures and let

$$\bar{n} = \int_{\mathbb{R}^d} n dx = \|n\|_{L^1}, \quad \bar{p} = \int_{\mathbb{R}^d} p dx = \|p\|_{L^1}.$$

Using the identity

$$\begin{aligned} \int_{\mathbb{R}^d} n \left( \ln \frac{n}{w_n(e)} - 1 \right) dx &= \frac{1}{2} \int_{\mathbb{R}^d} \left( n \ln \frac{n}{C_n^2 e^*} + n \ln \frac{n}{e} \right) dx - \bar{n} \\ &= \frac{1}{2} \int_{\mathbb{R}^d} \left( n \ln \frac{n}{e^* \bar{n}} + n \ln \frac{n}{e \bar{n}} \right) dx + \left( \bar{n} \ln \frac{\bar{n}}{C_n} - \bar{n} \right) \end{aligned}$$

and its equivalent for  $p$ , we rewrite the entropy as follows,

$$\begin{aligned}\mathcal{H}(n, p, e) &= \frac{1}{2} \int_{\mathbb{R}^d} \left( n \ln \frac{n}{e^* \bar{n}} + n \ln \frac{n}{\bar{n} e} \right) dx + C_n \lambda_B \left( \frac{\bar{n}}{C_n} \right) \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} \left( p \ln \frac{p}{e^* \bar{p}} + p \ln \frac{p}{\bar{p} e} \right) dx + C_p \lambda_B \left( \frac{\bar{p}}{C_p} \right) \\ &\quad + \frac{c}{2} \int_{\mathbb{R}^d} \left( \sqrt{e} - \sqrt{e^*} \right)^2 dx,\end{aligned}$$

where we used the identity

$$\int_{\mathbb{R}^d} (w_n + w_p) dx - (C_n + C_p) = -\frac{C_n + C_p}{2} \int_{\mathbb{R}^d} (\sqrt{e} - \sqrt{e^*})^2 dx.$$

We also reformulate the entropy production as  $\mathcal{P}(n, p, e) = \mathcal{P}_n + \mathcal{P}_p + \mathcal{P}_e + \mathcal{P}_R$ , with

$$\begin{aligned}\mathcal{P}_n &= 2 \int_{\mathbb{R}^d} \left| \nabla \sqrt{n/e^*} \right|^2 e^* dx + 2 \int_{\mathbb{R}^d} \left| \nabla \sqrt{n/e} \right|^2 e dx, & \mathcal{P}_e &= 8 \int_{\mathbb{R}^d} \left| \nabla \sqrt[4]{e/e^*} \right|^2 e^* dx, \\ \mathcal{P}_p &= 2 \int_{\mathbb{R}^d} \left| \nabla \sqrt{p/e^*} \right|^2 e^* dx + 2 \int_{\mathbb{R}^d} \left| \nabla \sqrt{p/e} \right|^2 e dx, & \mathcal{P}_R &= \int_{\mathbb{R}^d} k \left( \frac{\rho n p}{e} - 1 \right) \ln \frac{\rho n p}{e} e dx.\end{aligned}$$

The generalized logarithmic Sobolev inequality [AM\*01] with respect to the probability measures  $e^* dx$ ,  $e dx$  directly implies the following bound on the first and third term of  $\mathcal{H}(n, p, e)$ :

$$\int_{\mathbb{R}^d} \left( n \ln \frac{n}{\bar{n} e^*} + n \ln \frac{n}{\bar{n} e} + p \ln \frac{p}{\bar{p} e^*} + p \ln \frac{p}{\bar{p} e} \right) dx \leq C_{LS}(e, e^*) (\mathcal{P}_n + \mathcal{P}_p).$$

Moreover, the Sobolev embedding (A.4) gives

$$1 = \left\| \sqrt[4]{e/e^*} \right\|_{L^4(e^* dx)}^2 \leq C \left\| \nabla \sqrt[4]{e/e^*} \right\|_{L^2(e^* dx)}^2 + \left\| \sqrt[4]{e/e^*} \right\|_{L^2(e^* dx)}^2 = C \mathcal{P}_e + \int_{\mathbb{R}^d} \sqrt{e} \sqrt{e^*} dx.$$

Using again the fact that  $e dx$  and  $e^* dx$  are probability measures, we obtain

$$\mathcal{P}_e \geq C \int_{\mathbb{R}^d} \left( \sqrt{e} - \sqrt{e^*} \right)^2 dx. \quad (6.37)$$

For the entropy terms containing the averages we proceed similarly as in the proof of Proposition 6.2 to obtain

$$\mathcal{H}(n, p, e) \leq C(\mathcal{P}_n + \mathcal{P}_p + \mathcal{P}_e) + C(\bar{n}, \bar{p}) (\sqrt{\bar{n}\bar{p}} - 1)^2, \quad (6.38)$$

Now the idea is to bound the additional terms depending on  $\bar{n}, \bar{p}$  using the entropy-production term  $\mathcal{P}_R$  resulting from the reactive terms. We employ the elementary inequality  $\ln(y)(y-1) \geq 4(\sqrt{y}-1)^2$  and Jensen's inequality, also recalling that  $n^* p^* = e^{-2V} e^* = \rho^{-1} e^* = (e^*)^2$ , to obtain

$$\begin{aligned}\mathcal{P}_R &= \int_{\mathbb{R}^d} k \ln \frac{\rho(x) n p}{e} \left( \frac{\rho(x) n p}{e} - 1 \right) e dx \geq 4k_0 \int_{\mathbb{R}^d} \left( \sqrt{\frac{\rho(x) n p}{e}} - 1 \right)^2 e dx = \\ &= 4k_0 \int_{\mathbb{R}^d} \left( \sqrt{\frac{n p}{n^* p^*}} - \sqrt{\frac{e}{e^*}} \right)^2 e^* dx \geq 4k_0 \left( \int_{\mathbb{R}^d} \left( \sqrt{\frac{n p}{(e^*)^2}} - \sqrt{\frac{e}{e^*}} \right) e^* dx \right)^2.\end{aligned} \quad (6.39)$$

We are therefore left to interchange square roots and integration in order to complete the estimation of  $\mathcal{H}(n, p, e)$  in terms of the entropy production. We shall proceed as in [DFM08] and introduce a generalization of  $\delta_n, \delta_p$  in (6.21) as follows

$$\sqrt{\frac{n}{e^*}} = \int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx + \delta_n, \quad \sqrt{\frac{p}{e^*}} = \int_{\mathbb{R}^d} \sqrt{\frac{p}{e^*}} e^* dx + \delta_p,$$

and  $\delta_e$  as

$$\sqrt{\frac{e}{e^*}} = 1 + \delta_e.$$

Note that, by definition, we have

$$\int_{\mathbb{R}^d} \delta_n e^* dx = 0, \quad \int_{\mathbb{R}^d} \delta_n^2 e^* dx \leq \bar{n}$$

Then, due to the Poincaré inequality, we have

$$\int_{\mathbb{R}^d} \delta_n^2 e^* dx \leq C \left\| \nabla \sqrt{n/e^*} \right\|_{L^2(e^* dx)}^2 \leq C \mathcal{P}_n.$$

Clearly, analogous properties hold for  $\delta_p$ . Moreover, due to (6.37),

$$\frac{1}{2} \int_{\mathbb{R}^d} \delta_e^2 e^* dx = 1 - \int_{\mathbb{R}^d} \sqrt{e} \sqrt{e^*} dx = \frac{1}{2} \int_{\mathbb{R}^d} (\sqrt{e^*} - \sqrt{e})^2 dx \leq C \mathcal{P}_e.$$

We now expand (6.39) as

$$\begin{aligned} \mathcal{P}_R &\geq C \left( \int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx \int_{\mathbb{R}^d} \sqrt{\frac{p}{e^*}} e^* dx - 1 + \int_{\mathbb{R}^d} \delta_n \delta_p e^* dx + \int_{\mathbb{R}^d} \delta_e e^* dx \right)^2 \\ &\geq C \left( \int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx \int_{\mathbb{R}^d} \sqrt{\frac{p}{e^*}} e^* dx - 1 \right)^2 - C \int_{\mathbb{R}^d} (\delta_n^2 + \delta_p^2 + \delta_e^2) e^* dx \\ &\geq C \left( \int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx \int_{\mathbb{R}^d} \sqrt{\frac{p}{e^*}} e^* dx - 1 \right)^2 - C(\mathcal{P}_n + \mathcal{P}_p + \mathcal{P}_e). \end{aligned} \quad (6.40)$$

Introducing  $R_n = (\sqrt{\bar{n}} + \int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx)^{-1}$  and observing that

$$\int_{\mathbb{R}^d} \sqrt{\frac{n}{e^*}} e^* dx = \sqrt{\bar{n}} - R_n \int_{\mathbb{R}^d} \delta_n^2 dx,$$

we proceed as in the proof of Proposition 6.2, using Lemmas A.4 and A.5 of the Appendix, to conclude the desired estimate  $\mathcal{H}(n, p, e) \leq K(\mathcal{P}_n + \mathcal{P}_p + \mathcal{P}_e + \mathcal{P}_R) = K\mathcal{P}(n, p, e)$ .  $\blacksquare$

Using this Lemma we are now able to prove convergence towards the steady state.

**Theorem 6.9 (Exponential convergence towards steady state)** *Let  $(n, p, e)$  be the nonnegative solution of the system (6.30) with nonnegative initial data  $(n_0, p_0, e_0)$  such that the initial entropy  $\mathcal{H}(n_0, p_0, e_0)$  is finite and  $e_0$  satisfies (6.34). Then the solution converges exponentially fast to the steady state  $(n^*, p^*, e^*)$ ,*

$$\|n - n^*\|_{L^1(\mathbb{R}^d)}^2 + \|p - p^*\|_{L^1(\mathbb{R}^d)}^2 + \|\sqrt{e} - \sqrt{e^*}\|_{L^2(\mathbb{R}^d)}^2 \leq C \exp(-Kt) \quad (6.41)$$

with  $C$  a positive constant and  $K > 0$  as in (6.36).

**Proof:** We write

$$\|n - n^*\|_{L^1(\mathbb{R}^d)}^2 \leq 2 \left( \|n - w_n\|_{L^1(\mathbb{R}^d)}^2 + \|w_n - n^*\|_{L^1(\mathbb{R}^d)}^2 \right),$$

and use the Csiszár-Kullback-Pinsker inequality (A.3) of the Appendix,

$$\|n - w_n\|_{L^1(\mathbb{R}^d)}^2 \leq \frac{1}{3} \left( 2 \|n\|_{L^1(\mathbb{R}^d)} + 4 \|w_n\|_{L^1(\mathbb{R}^d)} \right) \int_{\mathbb{R}^d} n \ln \frac{n}{w_n} - (n - w_n) dx.$$

Then, we proceed as in the proof of Theorem 6.3: we combine the uniform boundedness of  $\|n\|_{L^1(\mathbb{R}^d)}$  and  $\|w_n\|_{L^1(\mathbb{R}^d)}$  provided by Lemma 6.5, the dissipation relation (6.8) and the entropy entropy-production estimate of Proposition 6.8 to conclude (6.41).  $\blacksquare$

## A Appendix

A probability measure  $d\nu$  satisfies the logarithmic Sobolev inequality if there exists a constant  $C > 0$  such that

$$\int f \ln \frac{f}{\|f\|_{L^1(d\nu)}} d\nu \leq C \|\nabla \sqrt{f}\|_{L^2(d\nu)}^2 \quad (\text{A.1})$$

for every  $f \in L^1(d\nu)$ . For more details we refer to [AM\*01].

The Csiszár-Kullback inequality, see e.g. [UA\*00], states for the probability densities  $f$  and  $g$  that

$$\|f - g\|_{L^1}^2 \leq C \int g \lambda_B\left(\frac{f}{g}\right) dx. \quad (\text{A.2})$$

A generalization to the case when  $f, g$  are not probability measures is provided by the following Csiszár-Kullback-Pinsker inequality:

**Lemma A.1** *Let  $\Omega$  be a measurable domain in  $\mathbb{R}^d$ . Let  $f, g : \Omega \rightarrow \mathbb{R}_+$  be measurable. Then,*

$$\int_{\Omega} g \lambda_B\left(\frac{f}{g}\right) dx \geq \frac{3}{2 \|f\|_{L^1} + 4 \|g\|_{L^1}} \|f - g\|_{L^1}^2. \quad (\text{A.3})$$

**Proof:** The elementary estimate  $3|u - 1|^2 \leq (2u + 4)\lambda_B(u)$  for  $u \in \mathbb{R}$  (Pinsker) gives

$$\begin{aligned} \|f - g\|_{L^1} &= \int_{\Omega} \left| \frac{f}{g} - 1 \right| g dx \leq \int_{\Omega} \sqrt{2\frac{f}{g} + 4} \sqrt{\lambda_B\left(\frac{f}{g}\right)} \frac{g}{\sqrt{3}} dx \\ &\leq \frac{1}{\sqrt{3}} \sqrt{\int_{\Omega} (2f + 4g) dx} \sqrt{\int_{\Omega} g \lambda_B\left(\frac{f}{g}\right) dx}, \end{aligned}$$

where we used the Cauchy-Schwarz inequality.  $\blacksquare$

**Lemma A.2 (Sobolev imbedding)** *For dimensions  $d \leq 4$  we have for a probability measure  $d\nu$  the Sobolev imbedding*

$$\|f\|_{L^4(d\nu)}^2 \leq C \|\nabla f\|_{L^2(d\nu)}^2 + \|f\|_{L^2(d\nu)}^2. \quad (\text{A.4})$$

Note that in the standard formulation of the Sobolev imbedding the constant  $C$  would multiply the whole right hand side. For our sake it is however important to have the coefficient 1 in front of the  $L^2$ -norm.

**Proof:** Due to the “standard” Sobolev imbedding and the Poincaré inequality,

$$\|f - \bar{f}\|_{L^4(d\nu)} \leq C \|f - \bar{f}\|_{H^1(d\nu)} \leq C \|\nabla f\|_{L^2(d\nu)}$$

Then, since  $\|\bar{f}\|_{L^4(d\nu)} = \bar{f} \leq \|f\|_{L^2(d\nu)}$  for the probability measure  $d\nu$ , we have

$$\|f\|_{L^4(d\nu)} - \|f\|_{L^2(d\nu)} \leq \|f - \bar{f}\|_{L^4(d\nu)} + \|\bar{f}\|_{L^4(d\nu)} - \|f\|_{L^2(d\nu)} \leq \|f - \bar{f}\|_{L^4(d\nu)}.$$

■

**Lemma A.3** For any  $y > 0$  the following inequality holds,

$$\lambda_B(y) \leq 2(1 + |\ln y|)(\sqrt{y} - 1)^2. \quad (\text{A.5})$$

**Proof:** In order to show the nonnegativity of

$$g(y) = 2(1 + |\ln y|)(\sqrt{y} - 1)^2 - \lambda_B(y)$$

we distinguish between the cases  $y \in (0, 1]$  and  $y > 1$ . Note that  $g(1) = 0$ , hence the statement holds true if  $g'(y) \leq 0$  for  $y \in (0, 1]$  and  $g'(y) \geq 0$  for  $y > 1$ .

Case  $y \in (0, 1)$ : Differentiation of  $g$  in this region gives

$$g'(y) = -\frac{2}{y}(\sqrt{y} - 1)^2 + 2(1 - \ln y)\frac{\sqrt{y} - 1}{\sqrt{y}} - \ln y.$$

Inequality (6.19) implies  $-\ln y \geq 4(1 - \sqrt{y})/(1 + \sqrt{y})$  and we obtain

$$g'(y) \geq -\frac{2}{y}(\sqrt{y} - 1)^2 - 2\frac{1 - \sqrt{y}}{\sqrt{y}} h(y) \text{ with } h(y) := 1 - \ln y - \frac{2\sqrt{y}}{\sqrt{y} + 1}.$$

Clearly, the first term is nonpositive. For the second term the same is true as  $h$  is nonnegative, because  $h(0) = \infty$ ,  $h(1) = 0$  and  $h'(y) \leq 0$  for  $y \in (0, 1]$ .

Case  $y \geq 1$ : In this case differentiation of  $g$  gives

$$g'(y) = \frac{2}{y}(\sqrt{y} - 1)^2 + 2(1 + \ln y)\frac{\sqrt{y} - 1}{\sqrt{y}} - \ln y,$$

which we shall prove to be nonnegative. The only negative contribution is due to the last term. Note first that for  $y \geq 4$  we have  $\ln y \left(2\frac{\sqrt{y}-1}{\sqrt{y}} - 1\right) \geq 0$ . Hence, it remains to investigate the case  $y \in [1, 4]$ . Using the elementary inequality  $\ln x \leq x - 1$  applied to  $x = \sqrt{y}$ , we obtain

$$\begin{aligned} g'(y) &\geq \frac{2}{y}(\sqrt{y} - 1)^2 + 2(1 + \ln y)\frac{\sqrt{y} - 1}{\sqrt{y}} - 2(\sqrt{y} - 1) \\ &= 2\frac{\sqrt{y}-1}{y} \left( -(\sqrt{y}-1)^2 + \sqrt{y} \ln y \right) \geq 2\frac{\sqrt{y}-1}{y} (\sqrt{y}-1)^2 \left( -1 + 4\frac{\sqrt{y}}{y-1} \right), \end{aligned}$$

where the second inequality is again due to (6.19). We see that  $g'(y) \geq 0$  also for  $y \in [1, 4]$ .

■

**Lemma A.4** *Let the assumptions of Proposition 6.2 hold and let  $\delta_n, \delta_p$  be defined as in (6.21), then the following estimate holds*

$$n^* \lambda_B\left(\frac{\bar{n}}{n^*}\right) + p^* \lambda_B\left(\frac{\bar{p}}{p^*}\right) \leq C_0(\bar{n}, \bar{p}, n^*, p^*) \left(\sqrt{\frac{\bar{n}\bar{p}}{n^*p^*}} - 1\right)^2,$$

where the factor

$$C_0(\bar{n}, \bar{p}, n^*, p^*) = C_1(\bar{n}, \bar{p}, n^*, p^*) \left( p^* + \frac{(p^*)^2}{n^*} + 2 \frac{n^*}{\max\left\{\frac{\bar{p}}{p^*}, \frac{\bar{n}}{n^*}\right\}} \right) \quad (\text{A.6})$$

is uniformly bounded if  $(\bar{n}, \bar{p}, n^*, p^*)$  are uniformly bounded, with  $C_1$  being explicitly given in (A.7).

**Proof:** Using the elementary inequality (A.5) we obtain

$$n^* \lambda_B\left(\frac{\bar{n}}{n^*}\right) + p^* \lambda_B\left(\frac{\bar{p}}{p^*}\right) \leq C_1(\bar{n}, \bar{p}, n^*, p^*) \left[ n^* \left(\sqrt{\frac{\bar{n}}{n^*}} - 1\right)^2 + p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 \right],$$

where

$$C_1(\bar{n}, \bar{p}, n^*, p^*) = \begin{cases} 2 \max\left\{1 + \left|\ln\left(\frac{\bar{n}}{n^*}\right)\right|, 1 + \left|\ln\left(\frac{\bar{p}}{p^*}\right)\right|\right\} & \text{if } \frac{\bar{p}}{p^*}, \frac{\bar{n}}{n^*} \geq \frac{1}{4} \\ 2 \left(1 + \left|\ln\left(\frac{\bar{p}}{p^*}\right)\right|\right) & \text{if } \frac{\bar{p}}{p^*} \geq \frac{1}{4}, \frac{\bar{n}}{n^*} < \frac{1}{4} \\ 2 \left(1 + \left|\ln\left(\frac{\bar{n}}{n^*}\right)\right|\right) & \text{if } \frac{\bar{n}}{n^*} \geq \frac{1}{4}, \frac{\bar{p}}{p^*} < \frac{1}{4} \end{cases} \quad (\text{A.7})$$

which is uniformly bounded due to Lemma 6.1. We next use the following estimate derived in [DFM08] under the conservation law for  $n - p$ ,

$$n^* \left(\sqrt{\frac{\bar{n}}{n^*}} - 1\right)^2 + p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 \leq C_2(\bar{n}, \bar{p}, n^*, p^*) \left(\sqrt{\frac{\bar{n}\bar{p}}{n^*p^*}} - 1\right)^2. \quad (\text{A.8})$$

In order to keep track of the dependence of the constants on the parameters we give here an explicit bound

$$C_2(n^*, p^*, \bar{n}, \bar{p}) = p^* + \frac{(p^*)^2}{n^*} + 2 \frac{n^*}{\max\left\{\frac{\bar{p}}{p^*}, \frac{\bar{n}}{n^*}\right\}}. \quad (\text{A.9})$$

To see this we first note that the conservation law  $\bar{n} - n^* = \bar{p} - p^*$  can be reformulated as

$$n^* \left(\sqrt{\frac{\bar{n}}{n^*}} - 1\right) \left(\sqrt{\frac{\bar{n}}{n^*}} + 1\right) = p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right) \left(\sqrt{\frac{\bar{p}}{p^*}} + 1\right). \quad (\text{A.10})$$

This allows us to rewrite

$$\begin{aligned} n^* \left(\sqrt{\frac{\bar{n}}{n^*}} - 1\right)^2 + p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 &= p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 \left(\frac{n^* \left(\sqrt{\frac{\bar{n}}{n^*}} - 1\right)^2}{p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2} + 1\right) \\ &= p^* \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 \left(\frac{p^* \left(\sqrt{\frac{\bar{p}}{p^*}} + 1\right)^2}{n^* \left(\sqrt{\frac{\bar{n}}{n^*}} + 1\right)^2} + 1\right) \\ &\leq C_3(n^*, p^*, \bar{n}, \bar{p}) \left(\sqrt{\frac{\bar{p}}{p^*}} - 1\right)^2 \left(\frac{p^* \left(\sqrt{\frac{\bar{p}}{p^*}} + 1\right)}{n^* \left(\sqrt{\frac{\bar{n}}{n^*}} + 1\right)} \sqrt{\frac{\bar{p}}{p^*}} + 1\right)^2 = C_3(n^*, p^*, \bar{n}, \bar{p}) \left(\sqrt{\frac{\bar{n}\bar{p}}{n^*p^*}} - 1\right)^2, \end{aligned}$$

where we applied again (A.10) to see the last equality. The multiplier  $C_3(n^*, p^*, \bar{n}, \bar{p})$  satisfies the bound

$$C_3(n^*, p^*, \bar{n}, \bar{p}) \geq p^* \left( \frac{p^* (\sqrt{\frac{\bar{p}}{p^*} + 1})^2}{n^* (\sqrt{\frac{\bar{n}}{n^*} + 1})^2} + 1 \right) / \left( \frac{p^* (\sqrt{\frac{\bar{p}}{p^*} + 1})}{n^* (\sqrt{\frac{\bar{n}}{n^*} + 1})} \sqrt{\frac{\bar{p}}{p^*} + 1} \right)^2.$$

Distinguishing between the cases  $\sqrt{\frac{\bar{p}}{p^*} + 1} \geq (\leq) \sqrt{\frac{\bar{n}}{n^*} + 1}$ , we see that the choice

$$C_3(n^*, p^*, \bar{n}, \bar{p}) = p^* + \frac{(p^*)^2}{n^*} + 2 \frac{n^*}{\max\{\frac{\bar{p}}{p^*}, \frac{\bar{n}}{n^*}\}}$$

is sufficient and moreover uniformly bounded.  $\blacksquare$

**Lemma A.5** *Let the assumptions of Proposition 6.2 hold and let  $\delta_n, \delta_p$  and  $R_n, R_p$  be defined as in (6.21) and (6.24) accordingly. Then the estimate*

$$\left( R_n \int_{\mathcal{T}^d} \delta_n^2 dx \sqrt{\bar{p}} + R_p \int_{\mathcal{T}^d} \delta_p^2 dx \sqrt{\bar{n}} - R_n R_p \int_{\mathcal{T}^d} \delta_n^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \leq 2C_P(\bar{n} + \bar{p})(\mathcal{P}_n + \mathcal{P}_p)$$

holds.

**Proof:** We first note that

$$\begin{aligned} & \left( R_n \int_{\mathcal{T}^d} \delta_n^2 dx \sqrt{\bar{p}} + R_p \int_{\mathcal{T}^d} \delta_p^2 dx \sqrt{\bar{n}} - R_n R_p \int_{\mathcal{T}^d} \delta_n^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \\ & \leq \max \left\{ \left( R_n \int_{\mathcal{T}^d} \delta_n^2 dx \sqrt{\bar{p}} + R_p \int_{\mathcal{T}^d} \delta_p^2 dx \sqrt{\bar{n}} \right)^2, \left( R_n R_p \int_{\mathcal{T}^d} \delta_n^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \right\} \quad (\text{A.11}) \end{aligned}$$

due to the nonnegativity of both terms. For bounding these terms we will make use of the fact that due to the definition of  $R_n$  and  $\delta_n$  and the bound in (6.22) we have

$$R_n \int_{\mathcal{T}^d} \delta_n^2 dx \leq \sqrt{\bar{n}} \quad \text{and} \quad R_n^2 \int_{\mathcal{T}^d} \delta_n^2 dx \leq \frac{\sqrt{\bar{n}}}{\sqrt{\bar{n} + \int_{\mathcal{T}^d} \delta_n dx}} \leq 1.$$

Using these estimates we can proceed as follows

$$\begin{aligned} & \left( R_n \int_{\mathcal{T}^d} \delta_n^2 dx \sqrt{\bar{p}} + R_p \int_{\mathcal{T}^d} \delta_p^2 dx \sqrt{\bar{n}} \right)^2 \leq 2 \left( R_n^2 \left( \int_{\mathcal{T}^d} \delta_n^2 dx \right)^2 \bar{p} + R_p^2 \left( \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \bar{n} \right) \\ & \leq 2 \left( \bar{p} \int_{\mathcal{T}^d} \delta_n^2 dx + \bar{n} \int_{\mathcal{T}^d} \delta_p^2 dx \right) \leq 2(\bar{n} + \bar{p}) \int_{\mathcal{T}^d} (\delta_n^2 + \delta_p^2) dx. \end{aligned}$$

The second term in (A.11) we now bound by

$$\begin{aligned} & R_n^2 R_p^2 \left( \int_{\mathcal{T}^d} \delta_n^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \\ & = \frac{1}{2} R_n^2 \left( \int_{\mathcal{T}^d} \delta_n^2 dx \right)^2 R_p^2 \int_{\mathcal{T}^d} \delta_p^2 dx \int_{\mathcal{T}^d} \delta_p^2 dx + \frac{1}{2} R_n^2 \int_{\mathcal{T}^d} \delta_n^2 dx R_p^2 \left( \int_{\mathcal{T}^d} \delta_p^2 dx \right)^2 \int_{\mathcal{T}^d} \delta_n^2 dx \\ & \leq \frac{1}{2} \left( \bar{n} \int_{\mathcal{T}^d} \delta_p^2 dx + \bar{p} \int_{\mathcal{T}^d} \delta_n^2 dx \right) \leq \frac{1}{2} (\bar{n} + \bar{p}) \int_{\mathcal{T}^d} (\delta_n^2 + \delta_p^2) dx \end{aligned}$$

Applying finally the Poincaré estimate as in (6.23) completes the proof.  $\blacksquare$

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