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On reconstitutive phase transitions and the jump of the chemical potential

Thomas Blesgen

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Summary: This article studies diffusion in solids in the case of two phases under isothermal conditions where due to plastic effects the number of vacancies changes when crossing a transition layer, i.e. a reconstitutive phase transition. A segregation model is derived and the equations are studied in the limit of a sharp interface. A Gibbs–Thomson law is derived and it is shown that the vacancy component of the chemical potential jumps across the transition layer thereby explaining recent experimental observations. The thermodynamic correctness of the model is shown as well as the existence of weak solutions with logarithmic free energies.

1 Introduction

The present article is concerned with the influence of phase transitions on diffusion processes in solids close to transition fronts. In particular the model developed here conclusively explains recent experimental results in [29], see also [30], on the ferrite transformation at high temperature in low-carbon steels where a jump of the chemical potential across the interface is observed. This observation is not in agreement with well-established mathematical and physical models for interface dynamics like the Allen–Cahn or phase field equations, [5], the Cahn–Hilliard system, [12], the Stefan problem, [20], or other recent models for phase transitions in solids, see for instance [14, 2], and [3].

In [29] also some numerical simulations are done. They are based on the representation $f_l = \sum_{i=1}^{M} X_{li}\mu_{li}(X_{l1}, \ldots, X_{lM})$ of the free energy density of phase l and a formula for the mass flux J related to the Onsager relation, see (2.5) below. Both crucial identities thus depend on the vector μ of chemical potentials which in turn depends in a complicated way on the molar fractions X_{li}. Explicit formulas for μ as a function of X_{li} are provided by huge data bases in CALPHAD or SGTE, see [17, 15], and `http://www.calphad.org`, `http://www.sgte.org`. In this way, the jump of the chemical potential is captured in the numerical computations in [29], but no further explanation for the jump of μ is given. This is the objective of the present article.

A jump of the chemical potential was also observed numerically in [9] on studies of stress assisted diffusion in Gallium Arsenide single crystals where unwanted liquid droplets grow in the solid surrounding. Because contrary to the solid phase the liquid

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phase does not contain any dislocations and vacancies, this leads to a jump of the chemical potential across the solid-liquid interface. For the chemical potential of the Gallium phase and the Arsenide phase, [9] postulates the constitutive relations

$$\mu_{\mathrm{Ga}} = \mu_{\mathrm{Ga}}^0 + RT\log(1-y) + (L_0 + L_1(3-y))^2,$$
$$\mu_{\mathrm{As}} = \mu_{\mathrm{Ga}}^0 + RT\log(y) + (L_0 + L_1(1-4y))(1-y)^2,$$

where the constants $L_0,\ L_1 > 0$ measure the strength of the mixing energy, T denotes the constant temperature and R is the gas constant. The parameter y denotes the arsenic mole fraction. It is set according to measured values and jumps at the interface.

Key to the mathematical formulation presented here is Equation (2.9) that describes the behaviour of the vacancies as a traveling wave with a non-vanishing velocity only close to the interfacial layer. This ansatz is purely phenomenological. From the mechanical point of view, close to a transition layer the internal forces may be considerably larger than the drag forces of the lattice and the material undergoes a plastic deformation. On the atomistic level, this may be accompanied by the presence of dislocations, by twinning or by the generation of shear bands. In this article no attempt is made to incorporate these phenomena into the model as at present no satisfying theory for the dynamics of lattice dislocations exist (but see [25, 22]).

As we shall see, due to (2.9) the number of vacant lattice positions n_v changes locally. This causes a local change of the concentration vector c which is the reason for the local variation of the free energy with respect to c close to the interface.

The outline of this article is as follows. In Section 2 we introduce some notation and derive the model. A thermodynamic validation follows in Section 3. The mathematical existence proof is subdivided into two parts. The first part in Section 4 deals with the straightforward case of positive mobilities and polynomial free energies. The second part in Section 5 discusses possibly degenerate mobilities and a logarithmic free energy and uses part one. The sharp interface limit is studied in Section 7.

2 Derivation of the model

We consider an isothermal regime with constant temperature θ. Let $\Omega \subset \mathbb{R}^D$ be a bounded domain with Lipschitz boundary that contains $M \geq 1$ different species of molecules.

Let $n_i = n_i(x,t)$ be the number of lattice sites occupied by an atom of species i, $1 \leq i \leq M$ and let $n := (n_1, \ldots, n_M)$. By n_v we denote the number of vacant lattice positions. Due to plastic deformations near the interface the local coordination of the atoms may change irreversibly. Conservation of mass implies that $\int_\Omega n_i(x,t)dx$ are conserved quantities for $1 \leq i \leq M$. Yet, the mass *densities* vary locally when crossing a phase transition due to changes of the lattice geometry. In the following we will take this into account by allowing the vacancy number n_v to change locally. This means that $\int_\Omega n_v(x,t)dx$ is a non-conserved quantity.

Consequently we write

$$N = N(n, n_v) := \sum_{i=1}^{M} n_i + n_v \qquad (2.1)$$

for the available lattice sites in Ω and set $c_i := \frac{n_i}{N}$, $1 \leq i \leq M$ for the concentration of the i-th constituent. The established mathematical models are formulated for the concentration vector $c := (c_1, \ldots, c_M)$ and neglect plastic effects.

As we assume that at most two phases coexist we introduce a phase parameter $\chi = \chi(x,t) \in [0,1]$ which is an indicator function of Phase 1, say. Instead of the common variable c we formulate the model for (n, n_v), as we want to keep track of the change of lattice positions during the reorganisation of the lattice close to the transition layer.

The free energy F of the system is

$$F = F(n, n_v, \chi) = \int_\Omega f(n, n_v, \chi)\, dx$$

with the free energy density $f(n, n_v, \chi)$. For f we make the ansatz

$$f(n, n_v, \chi) = \chi f_1(n, n_v) + (1-\chi) f_2(n, n_v) + \theta\Big(W(\chi) + \frac{\tilde{\gamma}}{2}|\nabla\chi|^2 + \frac{1}{2}|\nabla n_v|^2\Big), \tag{2.2}$$

where the last term is due to the entropy of mixing. Furthermore, $\tilde{\gamma} > 0$ determines the square root of the thickness of the boundary layer between the two phases, and

$$W(\chi) := \chi \ln \chi + (1-\chi)\ln(1-\chi) - \theta_c \chi^2$$

is a double well potential for a large constant $\theta_c > 0$. To simplify notation, we set $\gamma := \theta\tilde{\gamma}$. The unconserved order parameter χ is governed by the Allen–Cahn equation

$$\hat{\tau}\partial_t \chi = -\frac{\partial f}{\partial \chi}(n, n_v, \chi) \tag{2.3}$$

with a positive constant $\hat{\tau} = \hat{\tau}(\theta)$ that adjusts the time scale of the propagation in χ, and $\frac{\partial f}{\partial \chi}$ denotes the first variation of the functional f with respect to χ, i.e.

$$\frac{\partial f}{\partial \chi}(n, n_v, \chi)\zeta = \frac{d}{ds} f(n, n_v, \chi + s\zeta)|_{s=0}.$$

The functions f_l in (2.2) denote the convex and smooth free energy densities of phase l. A possible choice on f_l, $l = 1, 2$ is the purely entropic ansatz

$$f_l(n, n_v) := k_B\theta\Bigg[\sum_{i=1}^{M}\Big(\frac{n_i}{N}\Big)\Big(\ln\Big(\frac{n_i}{N}\Big) + \frac{E_i^l}{k_B\theta}\Big) + \Big(\frac{n_v}{N}\Big)\Big(\ln\Big(\frac{n_v}{N}\Big) + \frac{E_0^l}{k_B\theta}\Big)\Bigg], \tag{2.4}$$

where k_B denotes the Boltzmann constant and $E_i^l > 0$ are enthalpic energy terms.

The conservation of mass leads to the formulation $\partial_t n = -\mathrm{div}(J)$. Onsager's postulate, [23, 24], states that the thermodynamic flux is linearly related to the thermodynamic force. In our case the thermodynamic forces are the negative chemical potential gradients, and we obtain the phenomenological equations, see [18, p. 137],

$$J_i = -\sum_{j=1}^{M} L_{ij} \nabla \mu_j, \quad 1 \le i \le M, \tag{2.5}$$

with a mobility matrix $L = (L_{ij})_{1\le i,j\le M}$ that may depend on the solution vector. The Onsager reciprocity law, [23, 24, 18], states that L has to be symmetric which we assume in the following. To simplify the existence theory we will further assume that L is positive definite. By

$$\mu_i(n, n_v, \chi) = \frac{\partial f}{\partial n_i}(n, n_v, \chi), \quad 1 \le i \le M, \qquad \mu_v(n, n_v, \chi) = \frac{\partial f}{\partial n_v}(n, n_v, \chi)$$

we denote the i-th chemical potential and the vacancy component of the chemical potential, respectively. Furthermore we set $\mu := (\mu_1, \dots, \mu_M)$.

Similar to (2.3) we postulate that n_v is governed by gradient descend dynamics,

$$\partial_t n_v = -V(\chi)\frac{\delta f}{\delta n_v}(n, n_v, \chi) = -V(\chi)\mu_v(n, n_v, \chi),$$

where a physically reasonable ansatz for V is, see [6] and [16],

$$V(\chi) := \chi(1-\chi). \tag{2.6}$$

As a consequence of the evolution laws $\partial_t n = -\text{div}(J)$ and $\partial_t n_v = -V(\chi)\mu_v$, n and n_v are subject to continuous changes and are no integer quantities. Similarly, $N = N(x,t)$ specifies an inverse density.

To conclude, we are concerned with the following system of equations:

$$\partial_t n_i = \text{div}\Big(\sum_{j=1}^{M} L_{ij} \nabla \mu_j\Big), \tag{2.7}$$

$$\mu_i = \frac{\partial f}{\partial n_i}(n, n_v, \chi), \tag{2.8}$$

$$\partial_t n_v = -V(\chi)\mu_v(n, n_v, \chi), \tag{2.9}$$

$$\mu_v = \frac{\partial f}{\partial n_v}(n, n_v, \chi), \tag{2.10}$$

$$\hat{\tau}\partial_t \chi = \gamma \triangle \chi + \omega(n, n_v, \chi) \tag{2.11}$$

combined with the initial conditions

$$n_i(\cdot, 0) = n_{i0}, \quad n_v(\cdot, 0) = n_{v0}, \quad \chi(\cdot, 0) = \chi_0 \qquad \text{in } \Omega, \tag{2.12}$$

and the Neumann- and no-flux boundary conditions

$$\nabla n_i \cdot \nu = \nabla \mu_i \cdot \nu = \nabla \mu_v \cdot \nu = \nabla n_v \cdot \nu = \nabla \chi \cdot \nu = 0 \qquad \text{on } \partial\Omega,\ t > 0. \tag{2.13}$$

In this formulation, n_{i0}, n_{v0} and χ_0 are initial values for n_i, n_v and χ, and ν denotes the outer normal to $\partial\Omega$.

A comparison to (2.3) yields

$$\omega(n, n_v, \chi) = (f_2 - f_1)(n, n_v) - \theta W'(\chi).$$

If we multiply (2.9) with a test function, integrate by parts and respect the boundary conditions for ∇n_v, we obtain

$$\partial_t n_v = \operatorname{div}(V(\chi)\theta\nabla n_v) - b(n, n_v, \chi).$$

A comparison with (2.9) and using (2.4) yields for the source term b

$$\begin{aligned} b(n, n_v, \chi) &= V(\chi)\Big(\chi\frac{\partial f_1}{\partial n_v} + (1-\chi)\frac{\partial f_2}{\partial n_v}\Big) \qquad (2.14)\\ &= \frac{k_B\theta}{N}V(\chi)\sum_{i=1}^{M}\Big(\frac{n_i}{N}\Big)\Big[\ln\Big(\frac{n_v}{n_i}\Big) + \chi\frac{E_0^1 - E_i^1}{k_B\theta} + (1-\chi)\frac{E_0^2 - E_i^2}{k_B\theta}\Big], \end{aligned}$$

where we used for $l = 1, 2$

$$\frac{\partial f_l}{\partial n_v}(n, n_v) = \frac{k_B\theta}{N}\sum_{i=1}^{M}\Big(\frac{n_i}{N}\Big)\Big[\ln\Big(\frac{n_v}{n_i}\Big) + \frac{E_0^l - E_i^l}{k_B\theta}\Big].$$

Due to (2.9), the number of vacancies n_v is different in each phase. Therefore, in the limit $\gamma \to 0$, the vacancy component of the chemical potential μ_v jumps at the interface.

3 Thermodynamic validation

We shortly verify the second law of thermodynamics for the equations (2.7)–(2.13). As the temperature θ is kept constant it is enough to show that for a closed system the total free energy decreases with time.

The chain rule yields $\frac{d}{dt} f(n, n_v, \chi) = \sum_{i=1}^M \frac{\partial f}{\partial n_i}\partial_t n_i + \frac{\partial f}{\partial n_v}\partial_t n_v + \frac{\partial f}{\partial \chi}\partial_t\chi$. Thus we have to test $(2.7)_i$ with $\frac{\partial f}{\partial n_i}$, (2.9) with $\frac{\partial f}{\partial n_v}$ and (2.11) with $\frac{\partial f}{\partial \chi}$. After summation, integration over Ω and one integration by parts the result is

$$\frac{d}{dt}\int_\Omega f(n, n_v, \chi) + \int_{\partial\Omega}\sum_{i=1}^{M}\mu_i J_i\cdot\nu - \int_\Omega\Big[\sum_{i=1}^{M}\nabla\mu_i\cdot J_i + \frac{\partial f}{\partial n_v}\partial_t n_v + \frac{\partial f}{\partial\chi}\partial_t\chi\Big] = 0.$$

With the help of (2.3), (2.5) and (2.9) this can be rewritten in the form

$$\begin{aligned} \frac{d}{dt}\int_\Omega f(n, n_v, \chi) &+ \int_\Omega\Big[L\nabla\mu : \nabla\mu + V(\chi)(\mu_v)^2 + \frac{1}{\hat\tau}(\partial_\chi f(n, n_v, \chi))^2\Big]\\ &+ \int_{\partial\Omega}\sum_{i=1}^{M}\mu_i J_i\cdot\nu = 0. \qquad (3.1) \end{aligned}$$

This is the constitutive equality for the Helmholtz free energy. $L\nabla\mu : \nabla\mu$ represents the entropy production due to mass fluxes of constituents 1 to M, $V(\chi)\mu_v(n, n_v, \chi)^2$ is the production due to the vacancy flux and finally $\frac{1}{\tau}(\partial_\chi f(n, n_v, \chi))^2$ the production due to reorganisation of the phases. In Section 5 we will show that $0 < \chi < 1$ almost everywhere in Ω. Thus all production terms are non-negative yielding for a thermodynamically closed system the crucial estimate $\frac{d}{dt}\int_\Omega F(n(x,t), n_v(x,t), \chi(x,t))\,dx \le 0$.

4 Existence result for positive mobilities

In this section we study a regularisation of System (2.7)–(2.13) with a mobility V that is bounded away from zero. In Section 5 we will use this result to generalise to the regularised system with possibly degenerate mobility. The regularised problem is obtained after adding an artificial viscosity term $\frac{\kappa}{2}\big(\sum_{i=1}^{M}|\nabla(n_i/N)|^2 + |\nabla(n_v/N)|^2\big)$ to the free energy for small $\kappa > 0$. Later we will derive uniform estimates independent of κ that allow us to pass to the limit $\kappa \searrow 0$.

We apply techniques from [19] and [31], see also [27], originally developed for the Navier–Stokes equations. Related mathematical methods for estimating degenerate parabolic equations can be found in [7, 10], and [8].

For a stop time $T > 0$ let $\Omega_T := \Omega \times (0, T)$. By $C^k(\Omega)$ we denote the k-times continuously differentiable functions in Ω and by $H^m(\Omega) = H^{m,2}(\Omega)$ for $m \in \mathbb{N}$ the Sobolev space of m-times weakly differentiable functions, i.e. the space of functions u for which $\partial^\alpha u$ exists in the Hilbert space $L^2(\Omega)$ in the weak sense for any $\alpha \in \mathbb{R}^n$ with $|\alpha| \le m$. For later use in Theorem 6.2 we also need to extend this definition of $H^s(\Omega)$ to general real $s > 0$. To this end let $s = m + \sigma$ with $m \in \mathbb{N}$ and $0 < \sigma < 1$. We then introduce (see [1, Theorem 7.48] for details)

$$\|u\|_{H^s(\Omega)} := \left(\|u\|^2_{H^m(\Omega)} + \sum_{|\alpha|=m}\int_\Omega\int_\Omega \frac{|\partial^\alpha u(x) - \partial^\alpha u(y)|^2}{|x-y|^{n+2\sigma}}\,dx\,dy\right)^{1/2}$$

such that

$$H^s(\Omega) := \{u \in L^2(\Omega) \mid \|u\|_{H^s(\Omega)} < \infty\}.$$

We are going to impose growth conditions on (compare with (2.2))

$$\overline{f}(n, n_v, \chi) := \chi f_1(n, n_v) + (1-\chi) f_2(n, n_v) + \theta W(\chi)$$

and it is convenient to rewrite $\overline{f}$ by setting

$$\overline{f}(n, n_v, \chi) = \hat{f}\Big(\frac{n}{N}, \frac{n_v}{N}, \chi\Big) =: \hat{f}(c, c_v, \chi)$$

and state conditions for $\hat{f}$. With this definition in mind, we make the following assumptions to show existence of weak solutions (a *weak solution* to (2.7)–(2.13) is defined as in (4.1)–(4.7) with arbitrary test functions $\varphi \in H^1(\Omega)$):

(A0) $\Omega \subset \mathbb{R}^D$ is a bounded domain with Lipschitz boundary.

(A1) The initial values fulfill $n_0 \in H^1(\Omega; \mathbb{R}^M)$; $\chi_0,\ n_{v0} \in H^1(\Omega)$ such that

$$f(n_0, n_{v0}, \chi_0) + \frac{\kappa}{2}\left(\sum_{i=1}^{M}\left|\nabla\left(\frac{n_{i0}}{N_0}\right)\right|^2 + \left|\nabla\left(\frac{n_{v0}}{N_0}\right)\right|^2\right) < \infty.$$

(A2) The free energy density f fulfills $f \in C^1(\mathbb{R}^M \times \mathbb{R}^+ \times \mathbb{R}; \mathbb{R})$. Furthermore, for all $\delta > 0$ there exists a constant $C_\delta > 0$ such that for all (n, n_v) with $N(n, n_v) \neq 0$ and $\chi \in \mathbb{R}$

$$\left|\partial_\chi \hat{f}\left(\frac{n}{N}, \frac{n_v}{N}, \chi\right)\right| \leq \delta \hat{f}\left(\frac{n}{N}, \frac{n_v}{N}, \chi\right) + C_\delta.$$

(A3) $V : \mathbb{R} \to \mathbb{R}^+$ is a continuous function and there exist constants $v_1,\ v_0 > 0$ such that

$$v_0 \leq |V(\chi)| \leq v_1 \quad \text{for all } \chi \in \mathbb{R}.$$

(A4) The mobility matrix L is a symmetric, positive definite tensor with constant entries.

We remark that by Assumption (A2) any polynomial growth is allowed for $\hat{f}$, whereas exponential growth is not.
In particular, (A2) with $\delta = 1$ yields the existence of a constant $C_1 > 0$ such that $f \geq -C_1$.

Lemma 4.1 *Let (A0)–(A4) hold. Then there exists* $(n, n_v, \mu, \mu_v, \chi)$ *which satisfies (2.7)–(2.13) in the weak sense such that for any* $0 < q < 1$

(i) $n \in L^\infty(0, T;\ H^1(\Omega; \mathbb{R}^M)) \cap C^0([0, T];\ H^q(\Omega; \mathbb{R}^M))$,
$\partial_t n \in L^2(0, T; (H^1(\Omega; \mathbb{R}^M))')$,

(ii) $n_v \in L^\infty(0, T;\ H^1(\Omega)) \cap C^0([0, T];\ H^q(\Omega))$, $\partial_t n_v \in L^2(\Omega_T)$,

(iii) $\chi \in L^\infty(0, T;\ H^1(\Omega)) \cap C^0([0, T];\ H^q(\Omega))$, $\partial_t \chi \in L^2(0, T;\ (H^1(\Omega))')$,

(iv) $\mu \in L^2(0, T;\ H^1(\Omega; \mathbb{R}^M))$, $\mu_v \in L^2(\Omega_T)$,

(v) $(n, n_v, \chi)(t = 0) = (n_0, n_{v0}, \chi_0)$.

Proof: Let $\{\varphi_i\}_{i\in\mathbb{N}}$ be the eigenfunctions of the Laplace operator with Neumann boundary conditions, i.e. for associated eigenvalues $(\lambda_i)_{i\in\mathbb{N}} \in \mathbb{R}^+$

$$\begin{aligned} -\triangle\varphi_i &= \lambda_i\varphi_i && \text{in } \Omega,\\ \nabla\varphi_i \cdot \nu &= 0 && \text{on } \partial\Omega. \end{aligned}$$

The functions $\{\varphi_i\}_{i\in\mathbb{N}}$ form an orthogonal system in $L^2(\Omega)$ and $H^1(\Omega)$. We can normalise them such that $(\varphi_i, \varphi_j)_{L^2(\Omega)} = \delta_{ij}$. Additionally we may assume $\lambda_1 = 0$, $\varphi_1 = \text{const}$.

For $K \in \mathbb{N}$ we consider the Galerkin approach

$$
\begin{aligned}
n_i^K(x,t) &= \sum_{k=1}^{K} \alpha_{ik}^K(t)\varphi_k(x), \quad \mu_i^K(x,t) = \sum_{k=1}^{K} \beta_{ik}^K(t)\varphi_k(x), \quad 1 \le i \le M,\\
n_v^K(x,t) &= \sum_{k=1}^{K} \gamma_k^K(t)\varphi_k(x), \quad \mu_v^K(x,t) = \sum_{k=1}^{K} \delta_k^K(t)\varphi_k(x),\\
\chi^K(x,t) &= \sum_{k=1}^{K} \varepsilon_k^K(t)\varphi_k(x).
\end{aligned}
$$

These functions solve

$$
\int_\Omega \partial_t n_i^K \varphi_l = -\int_\Omega \sum_{j=1}^{M} L_{ij} \nabla \mu_j^K \cdot \nabla \varphi_l \quad \text{for } 1 \le i \le M, \tag{4.1}
$$

$$
\int_\Omega \mu_i^K \varphi_l = \int_\Omega \frac{\partial f}{\partial n_i}(n^K, n_v^K, \chi^K)\varphi_l + \kappa \int_\Omega \nabla(n_i^K/N^K) \cdot \nabla(\varphi_l/N^K), \tag{4.2}
$$

$$
\int_\Omega \partial_t n_v^K \varphi_l = -\int_\Omega V(\chi^K)\mu_v^K \varphi_l, \tag{4.3}
$$

$$
\int_\Omega \mu_v^K \varphi_l = \int_\Omega \frac{\partial f}{\partial n_v}(n^K, n_v^K, \chi^K)\varphi_l + \kappa \int_\Omega \nabla(n_v^K/N^K) \cdot \nabla(\varphi_l/N^K), \tag{4.4}
$$

$$
\hat{\tau} \int_\Omega \partial_t \chi^K \varphi_l = \int_\Omega \omega(n^K, n_v^K, \chi^K)\varphi_l - \int_\Omega \gamma \nabla \chi^K \cdot \nabla \varphi_l, \tag{4.5}
$$

$$
n_i^K(0) = \Pi^K n_{i0} := \sum_{k=1}^{K} (n_{i0}, \varphi_k)_{L^2(\Omega)} \varphi_k, \quad 1 \le i \le M, \tag{4.6}
$$

$$
n_v^K(0) = \Pi^K n_{v0}, \quad \chi^K(0) = \Pi^K \chi_0. \tag{4.7}
$$

Here we introduced the projection $\Pi^K : L^2(\Omega) \to \operatorname{span}\{\varphi_1, \ldots, \varphi_K\}$.

The coefficient functions $\alpha_{il}^K(t)$, $\beta_{il}^K(t)$, $\gamma_l^K(t)$, $\delta_l^K(t)$ and $\varepsilon_l^K(t)$ for $1 \le i \le M$, $1 \le l \le K$ solve the following initial value problem for a system of ordinary differential equations

$$\partial_t \alpha_{il}^K = -\lambda_l \sum_{j=1}^{M} L_{ij} \beta_{jl}^K \int_\Omega \varphi_l, \tag{4.8}$$

$$\begin{aligned}\beta_{il}^K = &\int_\Omega \frac{\partial f}{\partial n_i}\Big(\sum_{j=1}^K \alpha_{1j}^K\varphi_j, \dots, \sum_{j=1}^K \alpha_{Mj}^K\varphi_j, \sum_{j=1}^K \gamma_j^K\varphi_j, \sum_{j=1}^K \varepsilon_j^K\varphi_j\Big)\varphi_l \\ &+\kappa\lambda_l\alpha_{il}^K\Big[\int_\Omega \frac{\varphi_l}{(N^K)^2} + \Big(\sum_{m=1}^M \alpha_{ml}^K\Big)^2 \int_\Omega \frac{\varphi_l}{(N^K)^4} - 2\sum_{m=1}^M \alpha_{ml}^K \int_\Omega \frac{\varphi_l}{(N^K)^3}\Big],\end{aligned} \tag{4.9}$$

$$\partial_t \gamma_l^K = -\int_\Omega V\Big(\sum_{j=1}^K \varepsilon_j^K\varphi_j\Big)\delta_l^K, \tag{4.10}$$

$$\begin{aligned}\delta_{il}^K = &\int_\Omega \frac{\partial f}{\partial n_v}\Big(\sum_{j=1}^K \alpha_{1j}^K\varphi_j, \dots, \sum_{j=1}^K \alpha_{Mj}^K\varphi_j, \sum_{j=1}^K \gamma_j^K\varphi_j, \sum_{j=1}^K \varepsilon_j^K\varphi_j\Big)\varphi_l \\ &+\kappa\lambda_l\gamma_{il}^K\Big[\int_\Omega \frac{\varphi_l}{(N^K)^2} + \Big(\sum_{m=1}^M \gamma_{ml}^K\Big)^2 \int_\Omega \frac{\varphi_l}{(N^K)^4} - 2\sum_{m=1}^M \gamma_{ml}^K \int_\Omega \frac{\varphi_l}{(N^K)^3}\Big],\end{aligned} \tag{4.11}$$

$$\begin{aligned}\hat\tau\partial_t\varepsilon_l^K = &\int_\Omega \omega\Big(\sum_{j=1}^K \alpha_{1j}^K\varphi_j, \dots, \sum_{j=1}^K \alpha_{Mj}^K\varphi_j, \sum_{j=1}^K \gamma_j^K\varphi_j, \sum_{j=1}^K \varepsilon_j^K\varphi_j\Big)\varphi_l \\ &-\gamma\lambda_l\varepsilon_l^K,\end{aligned} \tag{4.12}$$

$$\alpha_{il}^K(0) = (n_{i0}, \varphi_l)_{L^2(\Omega)} \quad \text{for } 1 \le i \le M, \tag{4.13}$$

$$\gamma_l^K(0) = (n_{v0}, \varphi_l)_{L^2(\Omega)}, \quad \varepsilon_l^K(0) = (\chi_0, \varphi_l)_{L^2(\Omega)}. \tag{4.14}$$

In (4.10), (4.12) we used the abbreviation

$$N^K = N^K\big((\alpha_{il}^K)_{il}\big) := \sum_{m=1}^M \sum_{k=1}^K \alpha_{mk}^K \varphi_k.$$

Due to Peano's theorem this initial value problem has a local solution as the right hand side depends continuously on the coefficients α_{il}^K, β_{il}^K, γ_l^K, δ_l^K and ε_l^K.

Equation (3.1) is also valid for the regularised system, where the term

$$\frac{\kappa}{2}\Big(\sum_{i=1}^M |\nabla(n_i/N)|^2 + |\nabla(n_v/N)|^2\Big)$$

has been added to the energy functional if we adapt μ_i and μ_v accordingly. After integration in time from 0 to $t \le T$ we obtain the a-priori estimate

$$\begin{aligned}
&\int_\Omega \Big(f(n, n_v, \chi) + \frac{\kappa}{2} \sum_{i=1}^{M} \Big|\nabla\Big(\frac{n_i}{N}\Big)\Big|^2 + \frac{\kappa}{2}\Big|\nabla\Big(\frac{n_v}{N}\Big)\Big|^2\Big)(t) \\
&\quad + \int_{\Omega_t} \Big(L\nabla\mu : \nabla\mu + \frac{1}{\hat{\tau}}|\partial_\chi f|^2 + v_0\theta|\mu_v|^2\Big) \\
&\quad \le \int_\Omega \Big(f(n_0, n_{v0}, \chi_0) + \frac{\kappa}{2} \sum_{i=1}^{M} \Big|\nabla\Big(\frac{n_{i0}}{N_0}\Big)\Big|^2 + \frac{\kappa}{2}\Big|\nabla\Big(\frac{n_{v0}}{N_0}\Big)\Big|^2\Big) \le C. \qquad (4.15)
\end{aligned}$$

With (2.2), the fact that L is positive definite, (A0), (A2) and the Poincaré inequality this implies

$$\begin{aligned}
&\operatorname{ess\,sup}_{0\le t\le T}\big(\|n^K(t)\|_{H^1} + \|n_v^K(t)\|_{H^1} + \|\chi^K(t)\|_{H^1}\big) \\
&\qquad + \|\mu^K\|_{L^2(0,T;\, H^1(\Omega;\mathbb{R}^M))} + \|\mu_v^K\|_{L^2(\Omega_T)} \le C. \qquad (4.16)
\end{aligned}$$

Consequently, the coefficients α_{il}^K, β^K, γ^K, δ^K and ε^K are bounded and a global solution to the initial value problem (4.8)–(4.14) exists.

For $\varphi \in L^2(0, T;\ H^1(\Omega))$ we have

$$\begin{aligned}
\Big|\int_{\Omega_T} \partial_t n_i^K \varphi\Big| &= \Big|\int_{\Omega_T} \sum_{j=1}^{M} L_{ij}\nabla\mu_j^K \cdot \nabla\Pi^K\varphi\Big| \\
&\le C \sup_{1\le j\le M} \|\nabla\mu_j^K\|_{L^2(\Omega_T)}\|\nabla\Pi^K\varphi\|_{L^2(\Omega_T)} \le C\|\nabla\varphi\|_{L^2(\Omega_T)}, \\
\Big|\int_{\Omega_T} \partial_t\chi^K\varphi\Big| &\le \int_{\Omega_T} \Big|\omega(n^K, n_v^K, \chi^K)\Pi^K\varphi\Big| + \gamma\int_{\Omega_T}\Big|\nabla\chi^K\cdot\nabla\Pi^K\varphi\Big| \\
&\le C\|\varphi\|_{L^2(\Omega_T)} + \gamma\|\nabla\chi^K\|_{L^2(\Omega_T)}\|\nabla\varphi\|_{L^2(\Omega_T)} \\
&\le C\|\varphi\|_{L^2(0,T;\, H^1(\Omega))}, \\
\Big|\int_{\Omega_T} \partial_t n_v^K\varphi\Big| &\le \int_{\Omega_T}\Big|V(\chi^K)\Big|\Big|\mu_v^K\Pi^K\varphi\Big| \le C(v_1)\|\varphi\|_{L^2(\Omega_T)}.
\end{aligned}$$

This implies

$$\|\partial_t n^K\|_{L^2(0,T;\,(H^1(\Omega;\,\mathbb{R}^M))')} + \|\partial_t n_v^K\|_{L^2(\Omega_T)} + \|\partial_t\chi^K\|_{L^2(0,T;\,(H^1(\Omega))')} \le C. \qquad (4.17)$$

Additionally, the boundedness of $\partial_t n_v^K$ implies the well-definedness of $b(n^K, n_v^K, \chi^K)$ and the boundedness of f yields that expressions like $\frac{n_i^K}{N^K}$ are not singular.

The uniform boundedness of the time derivatives allows us to apply compactness results from [19, 31]. When passing to a subsequence (denoted as the original sequence) we thus find for $1 \le i \le M$ as $K \to \infty$

$$
\begin{aligned}
n_i^K &\overset{*}{\rightharpoonup} n_i &&\text{in} \quad L^\infty(0,T;\ H^1(\Omega)),\\
n_i^K &\to n_i &&\text{in} \quad C^0([0,T];\ H^q(\Omega)) \quad \text{for any } q<1,\\
\partial_t n_i^K &\rightharpoonup \partial_t n_i &&\text{in} \quad L^2(0,T;\ (H^1(\Omega))').
\end{aligned}
$$

These statements hold analogously for χ^K and n_v^K (except $\partial_t n_v^K \rightharpoonup \partial_t n_v$ in $L^2(\Omega_T)$). Finally we have

$$
\begin{aligned}
\mu_i^K &\rightharpoonup \mu_i &&\text{in} \quad L^2(0,T;\ H^1(\Omega)),\\
\mu_v^K &\rightharpoonup \mu_v &&\text{in} \quad L^2(\Omega_T).
\end{aligned}
$$

For a subsequence also $n_i^K \to n_i$, $n_v^K \to n_v$ and $\chi^K \to \chi$ almost everywhere in Ω_T. By (A2), $\partial_n f$, $\partial_{n_v} f$ and $\partial_\chi f$ are continuous, thus

$$
\left.
\begin{aligned}
\partial_n f(n^K, n_v^K, \chi^K) &\to \partial_n f(n, n_v, \chi)\\
\partial_{n_v} f(n^K, n_v^K, \chi^K) &\to \partial_{n_v} f(n, n_v, \chi)\\
\partial_\chi f(n^K, n_v^K, \chi^K) &\to \partial_\chi f(n, n_v, \chi)
\end{aligned}
\right\} \quad \text{almost everywhere in } \Omega_T.
$$

The growth condition (A2) on $\hat{f}$ implies for all $\delta > 0$ and all measurable $E \subset \Omega$

$$
\begin{aligned}
\int_E |\partial_\chi \overline{f}(n^K, n_v^K, \chi^K) &= \int_E \left|\partial_\chi \hat{f}\Big(\frac{n^K}{N^K}, \frac{n_v^K}{N^K}, \chi^K\Big)\right|\\
&\le \delta \int_E \hat{f}\Big(\frac{n^K}{N^K}, \frac{n_v^K}{N^K}, \chi^K\Big) + C_\delta |E|\\
&\le \delta C + C_\delta |E|.
\end{aligned}
$$

Therefore $\int_E |\partial_\chi \overline{f}(n^K, n_v^K, \chi^K)| \to 0$ as $|E| \to 0$ uniformly in K and by Vitali's theorem, $\partial_\chi \overline{f}(n^K, n_v^K, \chi^K) \to \partial_\chi \overline{f}(n, n_v, \chi)$ in $L^1(\Omega_T)$ as $K \in \mathbb{N}$ tends to infinity.

This convergence property permits to carry out the limit for ω and to pass to $K \to \infty$ in (4.1)–(4.7). The limit $(n, n_v, \mu, \mu_v, \chi)$ is a weak solution of (2.7)–(2.13).
By Parseval's representation we have $\Pi^K w \to w$ in $L^2(\Omega)$ for any $w \in L^2(\Omega)$. Because of $n_i^K \to n_i$, $n_v^K \to n_v$, $\chi^K \to \chi$ in $C^0([0,T];\ L^2(\Omega))$ we find $(n, n_v, \chi)(t=0) = (n_0, n_{v0}, \chi_0)$. □

5 Existence result for degenerate mobility

We exploit the result of the previous section to show existence to the regularised system with V given by (2.6). The difficulty is that the mobility might vanish and the system becomes degenerate. Thus we introduce for $\varepsilon > 0$ the extended mobility V_ε by

$$
V_\varepsilon(\chi) := \begin{cases} V(\chi) & \text{if } \varepsilon < \chi < 1-\varepsilon,\\ V(\varepsilon) & \text{if } \chi \le \varepsilon,\\ V(1-\varepsilon) & \text{if } \chi \ge 1-\varepsilon. \end{cases} \tag{5.1}
$$

This ansatz implies $V_\varepsilon : \mathbb{R} \to \mathbb{R}_{>0}$ and $V_\varepsilon(\chi)$ fulfills (A3) for any $\chi \in \mathbb{R}$.

For $d > 0$ we define the convex function

$$\psi(d) := d \ln d$$

and for $\varepsilon > 0$ its regularisation (defined for all $d \in \mathbb{R}$)

$$\psi_\varepsilon(d) := \begin{cases} d \ln d & \text{if } d \geq \varepsilon, \\ d \ln \varepsilon - \frac{\varepsilon}{2} + \frac{d^2}{2\varepsilon} & \text{if } d < \varepsilon \end{cases}$$

The regularised free energy functional is defined in such a way that $\psi_\varepsilon \in C^2$ and the derivative ψ_ε' is monotone increasing. This ansatz goes back to [11].

For later use we introduce $\varphi_\varepsilon := (\psi_\varepsilon)'$. Since φ_ε will be singular as $\varepsilon \to 0$ we introduce for $r > 0$

$$\varphi_\varepsilon^r(d) := \begin{cases} \varphi_\varepsilon(d)|\varphi_\varepsilon(d)|^{r-1} & \text{if } \varphi_\varepsilon(d) \neq 0, \\ 0 & \text{if } \varphi_\varepsilon(d) = 0. \end{cases}$$

By definition, $\varphi_\varepsilon^r \in C^0(\mathbb{R})$. For $0 < r < 1$, φ_ε^r is not differentiable at the zero point of φ_ε. To overcome this difficulty, for $\varrho > 0$ we introduce the function $\varphi_\varepsilon^{r,\varrho}$ with $\varphi_\varepsilon^{r,\varrho} = \varphi_\varepsilon^r$ in $\mathbb{R} \setminus [0, 1]$ and define $\varphi_\varepsilon^{r,\varrho}$ in $[0, 1]$ such that $\varphi_\varepsilon^{r,\varrho}$ is a C^1 function, monotone increasing and $\varphi_\varepsilon^{r,\varrho} \to \varphi_\varepsilon^r$ in $C^0(\mathbb{R})$ as $\varrho \searrow 0$.

The definition of ψ_ε allows us to introduce the following regularisation of f,

$$\begin{aligned} f_\varepsilon(n, n_v, \chi) := k_B\theta\Big[&\sum_{i=1}^{M} \Big(\psi_\varepsilon\Big(\frac{n_i}{N}\Big) + \Big(\frac{n_i}{N}\Big)\frac{\chi E_i^1 + (1-\chi)E_i^2}{k_B\theta}\Big) + \psi_\varepsilon\Big(\frac{n_v}{N}\Big) \\ &+ \Big(\frac{n_v}{N}\Big)\frac{\chi E_0^1 + (1-\chi)E_0^2}{k_B\theta}\Big] + \theta[\psi_\varepsilon(\chi) + \psi_\varepsilon(1-\chi) - \theta_c\chi^2] \\ &+ \frac{\gamma}{2}|\nabla\chi|^2 + \frac{\theta}{2}|\nabla n_v|^2. \end{aligned} \tag{5.2}$$

For the requirements of the logarithmic f we replace the assumptions of Section 4:

(A1') Assumption (A1) remains valid. Additionally, the initial data n_0, n_{v0}, χ_0 fulfills

$$\int_\Omega n_{i0} > 0 \quad \text{for } 1 \leq i \leq M, \quad \int_\Omega n_{v0} > 0, \quad \int_\Omega \chi_0 > 0, \int_\Omega (1-\chi_0) > 0.$$

(A2') f is given by (5.2) with positive constants θ, θ_c and γ.

(A3') V_ε is defined by (5.1).

For $\varepsilon < \varepsilon_0$, f_ε is bounded from below. For a proof see [11, Lemma 2.1]. Thus f_ε fulfills all assumptions of Section 4. With the help of Lemma 4.1 we therefore obtain the existence of a weak solution $(n_\varepsilon, n_{v\varepsilon}, \mu_\varepsilon, \mu_{v\varepsilon}, \chi_\varepsilon)$ to the system

$$\partial_t n_{i\varepsilon} = \operatorname{div}\Big(\sum_{j=1}^{M} L_{ij} \nabla \mu_{j\varepsilon}\Big), \tag{5.3}$$

$$\mu_{i\varepsilon} = \frac{\partial f_\varepsilon}{\partial n_i}(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon) - \frac{\kappa}{N_\varepsilon}\triangle\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big), \tag{5.4}$$

$$\partial_t n_{v\varepsilon} = -V_\varepsilon(\chi_\varepsilon)\mu_{v\varepsilon}(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon), \tag{5.5}$$

$$\mu_{v\varepsilon} = \frac{\partial f_\varepsilon}{\partial n_v}(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon) - \frac{\kappa}{N_\varepsilon}\triangle\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big), \tag{5.6}$$

$$\hat{\tau}\partial_t \chi_\varepsilon = \gamma\triangle\chi_\varepsilon + \omega_\varepsilon(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon) \tag{5.7}$$

with initial values (2.12) and Neumann boundary conditions (2.13) and where

$$\omega_\varepsilon(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon) = -\theta\Big[\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon) - 2\theta_c\chi_\varepsilon\Big] + \sum_{i=1}^{M}\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)(E_i^2 - E_i^1) + \Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)(E_0^2 - E_0^1).$$

Lemma 5.1 *Let (A1')–(A3'), (A4) hold and let $\varepsilon < \varepsilon_0$.*
(i) There exists a weak solution $(n_\varepsilon, n_{v\varepsilon}, \mu_\varepsilon, \mu_{v\varepsilon}, \chi_\varepsilon)$ of (5.3)–(5.7) with f given by (5.2). Further there exists a constant $C > 0$ independent of ε such that

$$\operatorname{ess\,sup}_{0\le t\le T}\big(\|n_\varepsilon(t)\|_{H^1} + \|n_{v\varepsilon}(t)\|_{H^1} + \|\chi_\varepsilon(t)\|_{H^1}\big) + \|\mu_\varepsilon\|_{L^2(0,T;\,H^1(\Omega;\mathbb{R}^M))} + \|\mu_{v\varepsilon}\|_{L^2(\Omega_T)} \le C,$$

$$\|\partial_t n_\varepsilon\|_{L^2(0,T;\,(H^1(\Omega;\,\mathbb{R}^M))')} + \|\partial_t n_{v\varepsilon}\|_{L^2(\Omega_T)} + \|\partial_t\chi_\varepsilon\|_{L^2(0,T;\,(H^1(\Omega))')} \le C.$$

(ii) One can find subsequences $(n_\varepsilon)_{\varepsilon\in P}$, $(n_{v\varepsilon})_{\varepsilon\in P}$, $(\mu_\varepsilon)_{\varepsilon\in P}$, $(\mu_{v\varepsilon})_{\varepsilon\in P}$, $(\chi_\varepsilon)_{\varepsilon\in P}$ where $P \subset (0, \varepsilon_0)$ is a countable set with 0 as the only accumulation point such that

$n_{i\varepsilon} \overset{*}{\rightharpoonup} n_i,\ n_{v\varepsilon} \overset{*}{\rightharpoonup} n_v,\ \chi_\varepsilon \overset{*}{\rightharpoonup} \chi$	*in* $L^\infty(0,T;\ H^1(\Omega))$,
$n_{i\varepsilon} \to n_i,\ n_{v\varepsilon} \to n_v,\ \chi_\varepsilon \to \chi$	*in* $C^0([0,T];\ H^q(\Omega))$ *for any* $q < 1$,
$n_{i\varepsilon} \to n_i,\ n_{v\varepsilon} \to n_v,\ \chi_\varepsilon \to \chi$	*a.e. in* Ω_T *and* $0 \le \frac{n_i}{N},\ \frac{n_v}{N},\ \chi \le 1$,
$\partial_t n_{i\varepsilon} \rightharpoonup \partial_t n_i,\ \partial_t\chi_\varepsilon \rightharpoonup \partial_t\chi$	*in* $L^2(0,T;\ (H^1(\Omega))')$,
$\partial_t n_{v\varepsilon} \rightharpoonup \partial_t n_v$	*in* $L^2(\Omega_T)$,
$\mu_{i\varepsilon} \rightharpoonup \mu_i$	*in* $L^2(0,T;\ H^1(\Omega))$,
$\mu_{v\varepsilon} \rightharpoonup \mu_v$	*in* $L^2(\Omega_T)$

as $\varepsilon \in P$ tends to 0.
(iii) There exists a number $s > 1$ and a constant $C > 0$ independent of ε such that

$$\|\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon)\|_{L^s(\Omega_T)} \le C,$$

$$\sum_{i=1}^{M}\Big\|\varphi_\varepsilon\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\Big\|_{L^s(\Omega_T)} + \Big\|\varphi_\varepsilon\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)\Big\|_{L^s(\Omega_T)} \le C.$$

Proof: (i) This follows from Lemma 4.1 and (4.16), (4.17).
(ii) The convergence properties are shown as in the proof of Lemma 4.1. The estimates $0 \le \frac{n_i}{N}, \frac{n_v}{N}, \chi \le 1$ follow from the estimate of $f_\varepsilon(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon)$, see (4.15) with v_0 being replaced by $V_\varepsilon(\chi_\varepsilon) > 0$, and (A1).
(iii) The weak formulation of (5.7) in Ω_T reads

$$\theta \int_{\Omega_T} \big(\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon)\big)\eta + \gamma \int_{\Omega_T} \nabla\chi_\varepsilon \cdot \nabla\eta$$
$$= 2\theta\theta_c \int_{\Omega_T} \chi_\varepsilon \eta - \hat{\tau} \int_{\Omega_T} \partial_t \chi_\varepsilon \eta + \int_{\Omega_T} \Big[\sum_{i=1}^M \Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)(E_i^2 - E_i^1) + \Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)(E_0^2 - E_0^1)\Big]\eta$$

for test functions $\eta \in L^2(0,T;H^1(\Omega))$. We choose $\eta := \varphi_\varepsilon^{r,\varrho}(\chi_\varepsilon) + \varphi_\varepsilon^{r,\varrho}(1-\chi_\varepsilon)$ which is admissible for all $0 < r \le 1$. Due to $(\varphi_\varepsilon^{r,\varrho})' \ge 0$ we find

$$\int_{\Omega_T} \gamma \nabla\chi_\varepsilon \cdot \nabla\big(\varphi_\varepsilon^{r,\varrho}(\chi_\varepsilon) - \varphi_\varepsilon^{r,\varrho}(1-\chi_\varepsilon)\big) \ge 0.$$

With (i) we thus obtain

$$\begin{aligned}
&\int_{\Omega_T} \Big(\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon)\Big)\big(\varphi_\varepsilon^{r,\varrho}(\chi_\varepsilon) + \varphi_\varepsilon^{r,\varrho}(1-\chi_\varepsilon)\big)\\
&\quad \le C\|\varphi_\varepsilon^{r,\varrho}(\chi_\varepsilon) + \varphi_\varepsilon^{r,\varrho}(1-\chi_\varepsilon)\|_{L^2(\Omega_T)}\\
&\qquad \cdot\Big(\|\chi\|_{L^2(\Omega_T)} + \|\partial_t\chi\|_{L^2(\Omega_T)} + \Big\| \sum_{i=1}^M \Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\Big\|_{L^2(\Omega_T)} + \Big\|\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)\Big\|_{L^2(\Omega_T)}\Big),
\end{aligned} \tag{5.8}$$

where the constant C depends on θ, θ_c and on $E_0^1,\ E_0^2,\ E_1^1,\ E_1^2, \ldots, E_M^1,\ E_M^2$.
Because of (ii) we have $0 \le \frac{n_{v\varepsilon}}{N_\varepsilon}, \frac{n_{i\varepsilon}}{N_\varepsilon} \le 1$, thus the right hand side of (5.8) is bounded independently of ε. After taking the limit $\varrho \searrow 0$ we have for the left hand side of (5.8)

$$C \ge \int_{\Omega_T} \big(\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon)\big)\big(\varphi_\varepsilon^r(\chi_\varepsilon) + \varphi_\varepsilon^r(1-\chi_\varepsilon)\big) \ge \int_{\Omega_T} |\varphi_\varepsilon(\chi_\varepsilon) + \varphi_\varepsilon(1-\chi_\varepsilon)|^{r+1}.$$

In order to show the second part we consider the weak formulation of (5.4) in Ω_T,

$$\begin{aligned}
\int_{\Omega_T} \mu_{i\varepsilon}\xi &= \int_{\Omega_T} \frac{k_B\theta}{N_\varepsilon}\Big[\sum_{j=1}^M \Big(\varphi_\varepsilon\Big(\frac{n_{j\varepsilon}}{N_\varepsilon}\Big) + \frac{\chi_\varepsilon E_j^1 + (1-\chi_\varepsilon)E_j^2}{k_B\theta}\Big)\frac{\delta_{ij}N_\varepsilon - n_{j\varepsilon}}{N_\varepsilon}\\
&\quad - \Big(\varphi_\varepsilon\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big) + \frac{\chi_\varepsilon E_0^1 + (1-\chi_\varepsilon)E_0^2}{k_B\theta}\Big)\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)\Big]\xi + \kappa\int_{\Omega_T} \nabla\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\cdot\nabla\Big(\frac{\xi}{N_\varepsilon}\Big)
\end{aligned}$$

for $\xi \in L^2(0,T;H^1(\Omega))$. We choose $\xi := N_\varepsilon \varphi_\varepsilon^{r,\varrho}(n_{i\varepsilon}/N_\varepsilon)$ and remark that as above

$$\kappa \int_{\Omega_T} \nabla\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\cdot\nabla\varphi_\varepsilon^{r,\varrho}\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big) \ge 0.$$

Due to the uniform boundedness of the terms $\frac{n_{j\varepsilon}}{N_\varepsilon}\varphi_\varepsilon\Big(\frac{n_{j\varepsilon}}{N_\varepsilon}\Big)$, $\frac{n_{v\varepsilon}}{N_\varepsilon}\varphi_\varepsilon\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)$ we obtain for $C = C(k_B\theta, \|\mu_{i\varepsilon}\|_{L^2(\Omega_T)}, \|\varphi_\varepsilon^{r,\varrho}(n_{i\varepsilon}/N_\varepsilon)\|_{L^2(\Omega_T)}, E_0^1, E_1^1, \dots, E_M^1, E_0^2, E_1^2, \dots, E_M^2)$ with (ii) in the limit $\varrho \searrow 0$

$$C \geq \int\limits_{\Omega_T} \varphi_\varepsilon\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\varphi_\varepsilon^r\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big) \geq \int\limits_{\Omega_T} \Big|\varphi_\varepsilon\Big(\frac{n_{i\varepsilon}}{N_\varepsilon}\Big)\Big|^{r+1}.$$

Equation (5.5) is treated alike, choosing $\varphi_\varepsilon^{r,\varrho}(n_{v\varepsilon}/N_\varepsilon)$ as test function. We end up with

$$C \geq \int\limits_{\Omega_T} \varphi_\varepsilon\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)\varphi_\varepsilon^r\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big) \geq \int\limits_{\Omega_T} \Big|\varphi_\varepsilon\Big(\frac{n_{v\varepsilon}}{N_\varepsilon}\Big)\Big|^{r+1},$$

where $C = C(k_B\theta, \|\partial_t n_v\|_{L^2(\Omega_T)}, \|\varphi_\varepsilon^{r,\varrho}(\frac{n_{v\varepsilon}}{N_\varepsilon})\|_{L^2(\Omega_T)}, E_0^1, \dots, E_M^1, E_0^2, \dots, E_M^2)$. □

Lemma 5.1 (iii) shows in particular $0 < \chi < 1$, so $V(\chi)$ remains positive.

6 The limit equations

It remains to pass to the limit $\kappa \to 0$. This step is straightforward and is done in much the same way as before by showing a-priori estimates and employing compactness results.

Lemma 6.1 *(a) Let (A0), (A1')–(A3'), (A4) hold. Then for $\kappa > 0$ there exists a weak solution $(n^\kappa, n_v^\kappa, \mu^\kappa, \mu_v^\kappa, \chi^\kappa)$ of (5.3)–(5.7) which fulfills for a constant C which is independent of κ*

$$\begin{aligned} &\operatorname{ess\,sup}_{0\leq t\leq T}\big(\|n^\kappa\|_{H^1}(t) + \|n_v^\kappa(t)\|_{H^1} + \|\chi^\kappa(t)\|_{H^1}\big) \\ &\qquad\qquad + \|\mu^\kappa\|_{L^2(0,T;\,H^1(\Omega;\mathbb{R}^M))} + \|\mu_v^\kappa\|_{L^2(\Omega_T)} \leq C, \\ &\|\partial_t n^\kappa\|_{L^2(0,T;\,(H^1(\Omega;\,\mathbb{R}^M))')} + \|\partial_t n_v^\kappa\|_{L^2(\Omega_T)} + \|\partial_t \chi^\kappa\|_{L^2(0,T;\,(H^1(\Omega))')} \leq C. \end{aligned}$$

(b) One can extract subsequences $(n^\kappa)_\kappa$, $(n_v^\kappa)_\kappa$, $(\mu^\kappa)_\kappa$, $(\mu_v^\kappa)_\kappa$ and $(\chi^\kappa)_\kappa$ such that

$$\begin{array}{ll} n_i^\kappa \overset{*}{\rightharpoonup} n_i,\, n_v^\kappa \overset{*}{\rightharpoonup} n_v,\, \chi^\kappa \overset{*}{\rightharpoonup} \chi & \text{in} \quad L^\infty(0,T;\ H^1(\Omega)), \\ n_i^\kappa \to n_i,\, n_v^\kappa \to n_v,\, \chi^\kappa \to \chi & \text{in} \quad C^0([0,T];\ H^q(\Omega)) \text{ for any } q < 1, \\ n_i^\kappa \to n_i,\, n_v^\kappa \to n_v,\, \chi^\kappa \to \chi & \text{a.e. in } \Omega_T \text{ and } 0 \leq \frac{n_i}{N},\ \frac{n_v}{N},\ \chi \leq 1, \\ \partial_t n_i^\kappa \rightharpoonup \partial_t n_i,\, \partial_t\chi^\kappa \rightharpoonup \partial_t\chi & \text{in} \quad L^2(0,T;\ (H^1(\Omega))'), \\ \partial_t n_v^\kappa \rightharpoonup \partial_t n_v & \text{in} \quad L^2(\Omega_T), \\ \mu_i^\kappa \rightharpoonup \mu_i & \text{in} \quad L^2(0,T;\ H^1(\Omega)), \\ \mu_v^\kappa \rightharpoonup \mu_v & \text{in} \quad L^2(\Omega_T) \end{array}$$

as κ tends to zero.

Proof: By Lemma 5.1, a weak solution for fixed κ exists. The estimates are a direct consequence of Lemma 5.1. Since $F^\kappa(n_0, n_{v0}, \chi_0)$ can be estimated independently of κ, the constant C on the right hand side does not depend on κ. This shows (a).
Part(b) is proved by Lemma 5.1. □

The following theorem is now clear.

Theorem 6.2 *Let the assumptions (A0), (A1)', (A2)‘, (A3)', (A4) hold. Then there exists a weak solution* $(n, n_v, \mu, \mu_v, \chi)$ *of (2.7)–(2.13) with the logarithmic free energy given by (2.2) such that for* $1 \le i \le M$

(i) $n_i,\ n_v,\ \chi \in L^\infty(0,T;\ H^1(\Omega)) \cap C^0([0,T];\ H^q(\Omega))$ *for any* $q < 1$,
$\mu_i \in L^2(0,T;\ H^1(\Omega))$, $\mu_v \in L^2(\Omega_T)$,
(ii) $\partial_t n,\ \partial_t \chi \in L^2(0,T_0;\ (H^1(\Omega))')$, $\partial_t n_v \in L^2(\Omega_T)$.
(iii) There exists a $s > 1$ *such that* $\ln(n_j/N),\ \ln(n_v/N),\ \ln\chi \in L^s(\Omega_T)$ *for* $1 \le j \le M$, *and in particular* $0 < \frac{n_j}{N},\ \frac{n_v}{N},\ \chi < 1$ *almost everywhere in* Ω.

7 Interface dynamics

In this section we are going to analyse the dynamics of the interface Γ of χ and Λ of $n_{v\varepsilon}$ in the limit $\gamma \searrow 0$. For simplicity we will restrict to the two-dimensional case as this already shows all the interesting features.

Subsequently we study formal expansions of the solution n, n_v and χ assuming that these functions as well as all other functions and functionals are sufficiently regular. For the analysis we consider the most interesting case where bulk diffusion and movement of the transition layers occur on the same time scale. Therefore we rescale the problem by setting $\gamma \rightsquigarrow \varepsilon^2$, $\theta_c = \frac{1}{\varepsilon}$, $F \rightsquigarrow \frac{1}{\varepsilon}F$, $L_{ij} := \varepsilon\delta_{ij}$ and set for simplicity $\hat\tau := 1$. We consider a parabolic scaling where space and time are weighted equally. The dependence of the solution vector on ε is emphasized in the following by a subscript ε.

So we are concerned with $(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon)$ solving

$$\varepsilon\partial_t\chi_\varepsilon = \varepsilon\triangle\chi_\varepsilon - \frac{1}{\varepsilon}\partial_\chi H(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon), \tag{7.1}$$

$$\varepsilon\partial_t n_{v\varepsilon} = \varepsilon\,\mathrm{div}(V(\chi_\varepsilon)\theta\nabla n_{v\varepsilon}) - \frac{1}{\varepsilon}b(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon), \tag{7.2}$$

$$\varepsilon\partial_t n_{i\varepsilon} = \frac{1}{\varepsilon}\triangle\partial_{n_i}H(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon). \tag{7.3}$$

Here we used the definition

$$H(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon) := \varepsilon\chi_\varepsilon f_1(n_\varepsilon, n_{v\varepsilon}) + \varepsilon(1-\chi_\varepsilon) f_2(n_\varepsilon, n_{v\varepsilon}) + \theta W(\chi_\varepsilon).$$

System (7.1)–(7.3) is completed with initial values (2.12) and boundary conditions (2.13).

7.1 Bulk expansion

First we are concerned with the behaviour of the solution in the bulk away from $\partial\Omega$. We consider expansions of the form

$$\begin{aligned} \chi_\varepsilon(x,t) &= \overline{\chi}(x,t) + \varepsilon\overline{\overline{\chi}}(x,t) + \mathcal{O}(\varepsilon^2), \\ n_\varepsilon(x,t) &= \overline{n}(x,t) + \varepsilon\overline{\overline{n}}(x,t) + \mathcal{O}(\varepsilon^2), \\ n_{v\varepsilon}(x,t) &= \overline{n}_v(x,t) + \varepsilon\overline{\overline{n}}_v(x,t) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Substituting into (7.1)–(7.3) we find to leading order:

$$W'(\overline{\chi}) = 0, \qquad b(\overline{n}, \overline{n}_v, \overline{\chi}) = 0, \qquad \triangle\mu(\overline{n}, \overline{n}_v, \overline{\chi}) = 0. \tag{7.4}$$

Here, as in the first part of this paper, we set

$$\mu(n, n_v, \chi) := \partial_n f(n, n_v, \chi) = \chi\partial_n f_1(n, n_v) + (1-\chi)\partial_n f_2(n, n_v)$$

for the chemical potential.

7.2 Expansion close to the interfaces

Now we deal with the asymptotic behaviour of n_ε, $n_{v\varepsilon}$, χ_ε close to the interface $\Gamma(t)$ of χ and the interface $\Lambda(t)$ of n_v away from $\partial\Omega$. We allow for possibly anisotropic surface energies. Therefore we do not only expand the spatial coordinates in the normal directions of the interfaces, as is done in [26]. Instead we also take the tangential components of $\Gamma(t)$ and $\Lambda(t)$ into account.

We introduce arc-length parametrisations $\sigma \mapsto \varphi(\sigma, t)$ of $\Gamma(t)$ and $\varrho \mapsto \psi(\varrho, t)$ of $\Lambda(t)$ for suitable functions φ and ψ. In a sufficiently small strip $Q(t)$ around the regular curves $\Gamma(t)$ and $\Lambda(t)$ we introduce the two projections

$$\Pi_{\Gamma(t)}(x) := \varphi(\sigma(x,t), t), \qquad \Pi_{\Lambda(t)}(x) := \psi(\varrho(x,t), t),$$

mapping $x \in Q(t)$ onto $\Gamma(t)$ and $\Lambda(t)$, respectively.

The unit tangent vectors τ_Γ to $\Gamma(t)$ in the point $\Pi_{\Gamma(t)}(x)$ and τ_Λ to $\Lambda(t)$ in $\Pi_{\Lambda(t)}(x)$ are defined by

$$\tau_\Gamma(x,t) := \varphi'(\sigma(x,t), t), \qquad \tau_\Lambda(x,t) := \psi'(\varrho(x,t), t).$$

The unit normal vector $\nu_\Gamma(x,t)$ in $\Pi_{\Gamma(t)}(x)$ is the vector orthogonal to $\tau_\Gamma(x,t)$ for which $(\nu_\Gamma(x,t), \tau_\Gamma(x,t))$ is positively oriented; the unit normal vector $\nu_\Lambda(x,t)$ to $\Lambda(t)$ in $\Pi_{\Lambda(t)}(x)$ is the vector orthogonal to $\tau_\Lambda(x,t)$ for which $(\nu_\Lambda(x,t), \tau_\Lambda(x,t))$ is positively oriented.

In the strip $Q(t)$ we introduce two sets of new coordinates (u, σ, t) and (v, ϱ, t) that replace (x, t). We stretch the distance in normal directions setting

$$u(x,t) := \frac{1}{\varepsilon}\text{dist}(x, \Gamma(t)), \qquad v(x,t) := \frac{1}{\varepsilon}\text{dist}(x, \Lambda(t)). \tag{7.5}$$

Here, $\text{dist}(x, \Gamma(t))$ denotes the Euclidean distance of x to $\Gamma(t)$ in the direction of ν_Γ and $\text{dist}(x, \Lambda(t))$ is the Euclidean distance of x to $\Lambda(t)$ in the direction of ν_Λ.

We compute

$$\nabla u(x,t) = \frac{1}{\varepsilon}\nu_\Gamma(x,t), \qquad \nabla v(x,t) = \frac{1}{\varepsilon}\nu_\Lambda(x,t), \tag{7.6}$$

$$\nabla \sigma(x,t) = \tau_\Gamma(x,t) + \mathcal{O}(\varepsilon), \qquad \nabla \varrho(x,t) = \tau_\Lambda(x,t) + \mathcal{O}(\varepsilon). \tag{7.7}$$

For n_ε, $n_{v\varepsilon}$ and χ_ε we consider the expansions

$$\chi_\varepsilon(x,t) = \chi^0(u,\sigma,t) + \varepsilon\chi^1(u,\sigma,t) + \mathcal{O}(\varepsilon^2), \tag{7.8}$$

$$n_\varepsilon(x,t) = n^0(v,\varrho,t) + \varepsilon n^1(v,\varrho,t) + \mathcal{O}(\varepsilon^2), \tag{7.9}$$

$$n_{v\varepsilon}(x,t) = n_v^0(v,\varrho,t) + \varepsilon n_v^1(v,\varrho,t) + \mathcal{O}(\varepsilon^2). \tag{7.10}$$

We assume that these expansions are valid in a sufficiently small strip $Q(t)$ around the interfaces $\Gamma(t)$ and $\Lambda(t)$.

We insert (7.8)–(7.10) into System (7.1)–(7.3). For the time derivatives we observe

$$\begin{aligned}
\varepsilon\frac{d}{dt}\chi^0(u,\sigma,t) &= \varepsilon\partial_u\chi^0(u,\sigma,t)\partial_t u + \varepsilon\partial_\sigma\chi^0(u,\sigma,t) + \varepsilon\partial_t\chi^0(u,\sigma,t)\\
&= \partial_u\chi^0(u,\sigma,t)\,\partial_t \mathrm{dist}(x,\Gamma(t)) + \mathcal{O}(\varepsilon),\\
\varepsilon\frac{d}{dt}n^0_{(v)}(v,\varrho,t) &= \partial_v n^0_{(v)}(v,\varrho,t)\,\partial_t \mathrm{dist}(x,\Lambda(t)) + \mathcal{O}(\varepsilon).
\end{aligned}$$

It remains to calculate the spatial derivatives. We start with (7.1). Using (7.6) and (7.7) we find

$$\begin{aligned}
\varepsilon\triangle\chi_\varepsilon &= \varepsilon\,\mathrm{div}_x(\nabla\chi^0(u(x,t),\sigma(x,t)) + \varepsilon\nabla\chi^1(u(x,t),\sigma(x,t)) + \mathcal{O}(\varepsilon))\\
&= \varepsilon\,\mathrm{div}\Big(\frac{1}{\varepsilon}\partial_u\chi^0\nu_\Gamma + \partial_\sigma\chi^0\tau_\Gamma + \partial_u\chi^1\nu_\Gamma + \mathcal{O}(\varepsilon)\Big).
\end{aligned}$$

To compute this further and for later use we observe the identities

$$\begin{aligned}
\mathrm{div}\,h(u(x),\sigma(x)) &= \frac{1}{\varepsilon}\partial_u h(u(x),\sigma(x))\nu_\Gamma + \partial_\sigma h(u(x),\sigma(x))\tau_\Gamma,\\
\mathrm{div}\,\tilde h(v(x),\varrho(x)) &= \frac{1}{\varepsilon}\partial_v \tilde h(v(x),\varrho(x))\nu_\Lambda + \partial_\varrho \tilde h(v(x),\varrho(x))\tau_\Lambda,
\end{aligned}$$

which hold for differentiable functions $h(u,\sigma)$ and $\tilde h(v,\varrho)$. With these formulas we end up with

$$\varepsilon\triangle\chi_\varepsilon = \frac{1}{\varepsilon}\partial_{uu}\chi^0 + \partial_{uu}\chi^1 + 2\partial_{u\sigma}\chi^0\nu_\Gamma\tau_\Gamma + \mathcal{O}(\varepsilon).$$

In the analogous discussion of the spatial derivatives in (7.2) and (7.3), mixed expressions arise depending simultaneously on both coordinate systems (u,σ,t) and (v,ϱ,t). In order to be able to compare both coordinate systems the following structural assumption is made for the further mathematical treatment:
There exist functions $\tilde\chi^0 = \tilde\chi^0(v,\varrho,t)$ and $\tilde\chi^1 = \tilde\chi^1(v,\varrho,t)$ such that

$$\chi^l(u,\sigma,t) = \tilde\chi^l(v,\varrho,t), \quad l = 1,2. \tag{7.11}$$

Using Taylor expansions of $W(\chi_\varepsilon)$ and $b(n_\varepsilon, n_{v\varepsilon}, \chi_\varepsilon)$, we obtain for (7.1), (7.2) to leading order $\mathcal{O}(\varepsilon^{-1})$

$$-\partial_{uu}\chi^0 + \theta W'(\chi^0) \;=\; 0, \tag{7.12}$$

$$-\frac{d}{dv}(V(\tilde{\chi}^0)\theta\partial_v n_v^0) + b(n^0, n_v^0, \tilde{\chi}^0) \;=\; 0. \tag{7.13}$$

The discussion of Equation (7.3) leads in highest order to the trivial statement

$$\frac{d^2}{dv^2}\partial_n(\theta W(\tilde{\chi}^0)) = 0.$$

To analyse the conditions (7.12), (7.13) near the interface we follow Sternberg [28] and multiply (7.12) by $\partial_u\chi^0$. Integration from $u = -\infty$ to $u = +\infty$ yields

$$\theta\Big[W(\chi^0)\Big]_\Gamma = \frac{1}{2}\Big[(\partial_u\chi^0)^2\Big]_\Gamma. \tag{7.14}$$

Here, the jump $[W]_\Gamma$ of W across $\Gamma(t)$ in direction ν_Γ is defined by

$$\Big[W(\chi^0)\Big]_\Gamma := \int_{-\infty}^{+\infty} \frac{d}{du}(W(\chi^0))du.$$

Multiplying (7.13) by $\theta V(\tilde{\chi}^0)\partial_v n_v^0$ and integrating from $v = -\infty$ to $v = +\infty$, we obtain with the help of (2.14) for fixed n^0

$$\frac{1}{2}\Big[(V(\tilde{\chi}^0)\theta\partial_v n_v^0)^2\Big]_\Lambda = \int_{-\infty}^{+\infty} (\theta V(\tilde{\chi}^0))^2\bigg(\tilde{\chi}^0\frac{d}{dv}f_1(n^0, n_v^0) + (1-\tilde{\chi}^0)\frac{d}{dv}f_2(n^0, n_v^0)\bigg)dv. \tag{7.15}$$

Identity (7.14) was found before when studying the Allen–Cahn system and is referred to in the literature as equipartition of energy across the interface, see [21].

The dynamic behaviour of $\Gamma(t)$ and $\Lambda(t)$ is revealed by considering the next order of expansions. For Equation (7.3) we have

$$\partial_t \mathrm{dist}(x, \Lambda(t))\partial_v n^0 = \frac{d^2}{dv^2}(\mu(n^0, n_v^0, \tilde{\chi}^0)).$$

The conditions (7.4) in the bulk provide the boundary conditions $\frac{d^2}{dv^2}\mu = 0$ at $v = \pm\infty$, and $\mu(n^0, n_v^0, \tilde{\chi}^0) \equiv \text{const}$ for $|v| \to \infty$. More precisely, since $(v = -\infty, v = +\infty)$ is an unbounded domain and from the regularity of μ, we have $\mu(n^0, n_v^0, \tilde{\chi}^0) = 0$ for $|v| \to \infty$. Hence $[\frac{d}{dv}\mu]_\Lambda = 0$ and

$$\partial_t \mathrm{dist}(x, \Lambda(t))\Big[n^0\Big]_\Lambda = \Big[\frac{d}{dv}\mu(n^0, n_v^0, \tilde{\chi}^0)\Big]_\Lambda = 0. \tag{7.16}$$

Below in (7.19) we will see that in general $\partial_t \mathrm{dist}(x, \Lambda(t)) \neq 0$, therefore (7.16) yields

$$\left[n^0\right]_\Lambda = 0. \tag{7.17}$$

As $\partial_v n^0 = 0$ and f is smooth, $\mu = \frac{\partial f}{\partial n}$ does not jump across $\Lambda(t)$, in contrast to $\mu_v = \frac{\partial f}{\partial n_v}$ as we will learn from (7.26).

The expansions of (7.1), (7.2), proceeding as in (7.12) and (7.13), lead in order ε^0 to

$$\partial_t \mathrm{dist}(x, \Gamma(t)) \partial_u \chi^0 = -2\partial_{u\sigma}\chi^0 \tau_\Gamma \nu_\Gamma - \partial_{uu}\chi^1 + \theta W''(\chi^0)\chi^1, \tag{7.18}$$

$$\begin{aligned} \partial_t \mathrm{dist}(x, \Lambda(t)) \partial_v n_v^0 = & -\frac{d}{dv}(V(\tilde{\chi}^0)\theta\partial_\varrho n_v^0)\tau_\Lambda \nu_\Lambda - \frac{d}{dv}(V(\tilde{\chi}^0)\theta\partial_v n_v^1) \\ & - \frac{d}{dv}(V'(\tilde{\chi}^0)\theta\partial_v n_v^0 \tilde{\chi}^1)\nu_\Lambda - \frac{d}{d\varrho}(V(\tilde{\chi}^0)\theta\partial_v n_v^0)\tau_\Lambda \nu_\Lambda \\ & + \partial_n b(n^0, n_v^0, \tilde{\chi}^0) n^1 + \partial_{n_v} b(n^0, n_v^0, \tilde{\chi}^0) n_v^1 \\ & + \partial_\chi b(n^0, n_v^0, \tilde{\chi}^0)\tilde{\chi}^1. \end{aligned} \tag{7.19}$$

To further examine the movement of the fronts we again multiply (7.18) by $\partial_u \chi^0$ and integrate from $u = -\infty$ to $u = +\infty$. The result is

$$\partial_t \mathrm{dist}(x, \Gamma(t)) \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 du \tag{7.20}$$

$$= -\int_{-\infty}^{+\infty} 2\partial_{u\sigma}\chi^0 \nu_\Gamma \partial_u \chi^0 \tau_\Gamma \, du - \int_{-\infty}^{+\infty} \partial_{uu}\chi^1 \partial_u \chi^0 \, du + \int_{-\infty}^{+\infty} \theta W''(\chi^0) \partial_u \chi^0 \chi^1 \, du.$$

The last integral on the right hand side of (7.21) can be reformulated. Using Identity (7.12) and after integration by parts we see

$$\int_{-\infty}^{+\infty} \chi^1 \theta \frac{d}{du}\big(W'(\chi^0)\big) \, du = -\int_{-\infty}^{+\infty} \partial_u \chi^1 \partial_{uu}\chi^0 \, du = \int_{-\infty}^{+\infty} \partial_{uu}\chi^1 \partial_u \chi^0 \, du. \tag{7.21}$$

With this result and taking into account that

$$\int_{-\infty}^{+\infty} 2\partial_{u\sigma}\chi^0 \nu_\Gamma \partial_u \chi^0 \tau_\Gamma \, du = \frac{d}{d\sigma} \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \nu_\Gamma \tau_\Gamma \, du,$$

Equation (7.21) simplifies to

$$\partial_t \mathrm{dist}(x, \Gamma(t)) \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \, du = -\frac{d}{d\sigma} \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \nu_\Gamma \tau_\Gamma \, du. \tag{7.22}$$

The last integral on the right can be related to the surface energy s_Γ of Γ. For a vector $l \in \mathbb{R}^2 \setminus \{0\}$ we set

$$s_\Gamma(l) := \inf\left\{\int_{-1}^{+1} 2\sqrt{\theta W(p(z))}\,|p'(z)l|dz \,\middle|\, p : [-1, +1] \to [0, 1] \text{ is Lipschitz continuous}\right\}.$$

In this definition, the geodesic curve p connects two minima of W at $z = \pm 1$, i.e. two solutions to (7.4). Equation (7.14) implies $2\theta W(\chi^0) = (\partial_u \chi^0)^2$, and after reparametrisation we obtain, see [28] for details,

$$s_\Gamma(\nu_\Gamma) := \int_{-\infty}^{+\infty} \left(\partial_u \chi^0 \nu_\Gamma\right)^2 du.$$

By straightforward calculations we compute

$$\frac{d}{d\sigma} \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \nu_\Gamma \tau_\Gamma \, du = \mathrm{div}_T D s_\Gamma(\nu_\Gamma), \tag{7.23}$$

where div_T is the surface divergence. In two space dimensions, for a differentiable function h on the interface $\Gamma(t)$, the surface divergence is defined by

$$\mathrm{div}_T h = (\partial_\sigma h)\tau_\Gamma.$$

A well-known fact is the relation of $\mathrm{div}_T D s_\Gamma(\nu_\Gamma)$ to the curvature $\kappa_\Gamma := \mathrm{div}_T \nu_\Gamma$ of $\Gamma(t)$. As is shown for the isotropic case in [28] and [26], it holds

$$\mathrm{div}_T D s_\Gamma(\nu_\Gamma) = s_\Gamma \kappa_\Gamma. \tag{7.24}$$

Exploiting (7.23) and (7.24), Equation (7.22) finally reads

$$\partial_t \mathrm{dist}(x, \Gamma(t)) \int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \, du = -s_\Gamma \kappa_\Gamma. \tag{7.25}$$

Equation (7.25) is an isotropic Gibbs–Thomson law and controls the movement of $\Gamma(t)$. The integral $\int_{-\infty}^{+\infty} (\partial_u \chi^0)^2 \, du$ defines the surface mobility.

The discussion of (7.19) is very similar to the treatment of (7.18). We multiply (7.19) by $\partial_v n_v^0$ and integrate from $v = -\infty$ to $v = +\infty$. Then, analogous to (7.21), we integrate by parts the term $\int_{-\infty}^{+\infty} \partial_v (V(\tilde{\chi}^0)\theta \partial_v \tilde{\chi}^1) \partial_v n_v^0 \, dv$ where we use (7.13). We arrive at

$$\partial_t \mathrm{dist}(x, \Lambda(t)) \int_{-\infty}^{+\infty} (\partial_v n_v^0)^2 dv = -\frac{d}{d\varrho} \int_{-\infty}^{+\infty} (V(\tilde{\chi}^0)\theta \partial_v n_v^0) \partial_v n_v^0 \tau_\Lambda \nu_\Lambda \, dv$$
$$+ \int_{-\infty}^{+\infty} \Big(\partial_n b(n^0, n_v^0, \tilde{\chi}^0) n^1 + \partial_{n_v} b(n^0, n_v^0, \tilde{\chi}^0) n_v^1\Big) \partial_v n_v^0 \, dv.$$

We can simplify the last integral. Because of $\partial_v n^0 = 0$ and the regularity of f we have

$$\int_{-\infty}^{+\infty} \partial_n b(n^0, n_v^0, \tilde{\chi}^0) n^1 \partial_v n_v^0 \, dv = \int_{-\infty}^{+\infty} V(\tilde{\chi}^0) \partial_{n_v} \partial_n \overline{f}(n^0, n_v^0) n^1 \partial_v n_v^0 \, dv = 0.$$

Finally, similar to (7.25), the surface energy of the interface Λ is given by

$$s_\Lambda(\nu_\Lambda) := \int_{-\infty}^{+\infty} \theta V(\tilde{\chi}^0)(\partial_v n_v^0 \nu_\Lambda)^2 \, dv,$$

such that the first integral on the right hand side of (7.26) becomes

$$\frac{d}{d\varrho} \int_{-\infty}^{+\infty} (V(\tilde{\chi}^0)\theta \partial_v n_v^0) \partial_v n_v^0 \tau_\Lambda \nu_\Lambda \, dv = \mathrm{div}_T D s_\Lambda(\nu_\Lambda).$$

So we obtain, if κ_Λ denotes the curvature of $\Lambda(t)$,

$$\partial_t \mathrm{dist}(x, \Lambda(t)) \int_{-\infty}^{+\infty} (\partial_v n_v^0)^2 dv = -s_\Lambda \kappa_\Lambda + \int_{-\infty}^{+\infty} \partial_{n_v} b(n^0, n_v^0, \tilde{\chi}^0) \partial_v n_v^0 n_v^1 \, dv. \qquad (7.26)$$

Equation (7.26) is the isotropic Gibbs–Thomson law for the interface $\Lambda(t)$. The integral on the right in (7.26) is related to the jump of $b = V(\tilde{\chi}^0)\partial_{n_v}\overline{f}$ across $\Lambda(t)$. But here we observe that the source term couples to the other variables and depends on n_v^0, n_v^1 and on $\tilde{\chi}^0$ and n^0.

In the limit $\varepsilon \searrow 0$, Equation (7.26) states that n_v and consequently $\mu_v = \frac{\partial f}{\partial n_v}$ jumps across $\Lambda(t)$.

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Thomas Blesgen
Max-Planck Institute for Mathematics in the Sciences
Inselstrasse 22
04103 Leipzig
Germany
blesgen@mis.mpg.de