

ON DIFFUSION INDUCED SEGREGATION IN TIME-DEPENDENT DOMAINS

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Abstract. This article is concerned with the derivation and analysis of a model for diffusion induced segregation phenomena in the physically relevant case that the domain representing the crystal grows in time. A mathematical model is formulated where the phase parameter is a function of bounded variation and the equations are completed with the Gibbs-Thomson law. Based on suitable a-priori bounds, methods from geometric measure theory are applied to derive suitable compactness properties which allow to show the existence of weak solutions in three space dimensions.

Key words. phase transitions, dynamics of phase boundary, Gibbs-Thomson law

AMS subject classifications. 49Q20, 74N20, 80A22

1. Introduction. Diffusion induced segregation (DIS) processes represent a particular class of phase change problems in solids that has been widely studied in mineralogy and crystallography. Typical of DIS, the segregation only starts after the concentration of one selected component that diffuses into the single crystal from outside exceeds a certain threshold. DIS phenomena are very interesting for geological applications as the segregation is irreversible and rock samples with DIS can be regarded as a natural geologic clock. One prominent application is the attempt to estimate the time scale for magma ascending from the earth's mantle by the investigation of specimen with the so-called chalcopyrite disease within sphalerite. Mineralogical experiments on this particular example were first carried out in [2] and [3] under isothermal conditions. These articles explain conclusively the rearrangement of the lattice as well as the qualitative mechanism responsible for DIS.

A collection of experiments revealing DIS phenomena is available in [2] and [3], and the results are compared with geological observations of DIS.

In order to get a better understanding of chalcopyrite disease within sphalerite, a first phase-field model based on partial differential equations with a modified Allen-Cahn equation was developed in [4]. More advanced simulations on the related ternary system of sphalerite, chalcopyrite and cubanite are done in [5]. A general existence and uniqueness result for the mathematical formulation derived in [4] is contained in [6]. More sophisticated numerical simulations can be found in [7], where ab-initio methods are used on a large scale to approximately compute the physical free energies. The results of the ab-initio computations are validated with quantum mechanical and molecular dynamics calculations. In particular, the results in [7] provide *quantitative* predictions.

As is explained in [4], the mathematical model developed in earlier articles neglects the attachment of sulphur ions which lead to a growth of the crystal during the experiments. Instead, the domain Ω representing the crystal was assumed time-independent.

In this article we will close this gap. In the model presented in Section 2, boundary conditions on the chemical potential are assumed which are close to the physical reality and which allow the domain to grow. These boundary conditions are connected to a generalized Gibbs-Thomson law. The rest of the paper is devoted to the proof of

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existence of weak solutions. We follow the ansatz in [1] which is classical by now. In Section 4, a time discrete scheme is introduced.

We apply methods from geometric measure theory to show suitable a-priori bounds and to establish the compactness in space and time of the time-discrete solution. Central argument is Lemma 7.7. In the subset of large discrete-interface velocities its proof is based on the construction of a Besicovitch-type covering that fails for space dimensions $n > 3$. In the set of small discrete-interface velocity the proof relies on Bernstein's theorem which is known to hold for space dimensions $n \leq 8$. Due to these restrictions, the main lemmata are formulated $n = 3$. The proof of convergence further requires the technical assumption (8.1) that is needed to prevent a loss of area when passing to the limit.

Finally we mention that the employed techniques and results are related to the Stefan problem and the Mullins-Sekerka flow, see in particular the articles [22], [23] and [19], and also can be transferred to applications in shape optimisation problems.

2. Derivation of the Model. Let $\Omega \subset \mathbb{R}^n$ be a box chosen large such that for times $0 \leq t \leq T$ with given stop time $T > 0$ a time-dependent set $\Omega^I = \Omega^I(t) \subset \mathbb{R}^n$ is contained in Ω . For the proof of existence of weak solutions we will set $n = 3$. We assume that Ω is a bounded domain with Lipschitz boundary. We call the set $\Omega^I(t)$ the *inner domain* as it represents the growing crystal at time t surrounded by a second copper rich mineral. This second phase occupies $\Omega^{II} := \Omega \setminus \overline{\Omega^I}$ which we call the *outer domain*.

We introduce the two space-time cylinders $\Omega_T := \Omega \times (0, T)$, $\Omega_T^I := \Omega^I(t) \times (0, T)$, and by $\theta > 0$ we denote the constant temperature.

We introduce for $1 \leq i \leq 4$ functions $n_i : \Omega_T \rightarrow \mathbb{N}$ which determine the number of lattice positions in Ω_T occupied by species i . The n_i are related to the species by

$$n_1 \dots \text{Fe}^{3+}, \quad n_2 \dots \text{Fe}^{2+}, \quad n_3 \dots \text{Zn}^{2+}, \quad n_4 \dots \text{Cu}^+.$$

Similarly, by n_v we denote the number of vacant lattice positions.

We introduce the vector $m = (m_1, \dots, m_4)$, where

$$m_i(x, t) := \frac{n_i(x, t)}{\sum_{j=1}^4 n_j(x, t) + n_v(x, t)}, \quad 1 \leq i \leq 4$$

is the number density of the i -th constituent in Ω_T . We assume that we have a perfect crystal without impurities such that no further constituents need to be considered.

The variable m_5 specifies the electron density. The condition of electric neutrality leads to the formula

$$(2.1) \quad m_5 = 3m_1 + 2m_2 + 2m_3 + m_4 - 2.$$

The coefficients of m_i in (2.1) refer to the positive ionisation of the i -th constituent and 2 is subtracted in the formula due to the attachment of S^{2-} ions.

In Ω_T^I the free energy density is given by

$$(2.2) \quad f_I(m) = k_B \theta \left[\sum_{i=1}^4 m_i \ln m_i + \left(1 - \sum_{i=1}^4 m_i \right) \ln \left(1 - \sum_{i=1}^4 m_i \right) \right] \\ + \sum_{i=1}^4 \sum_{j=1}^4 \alpha_{ij} m_i m_j + \sum_{i=1}^4 \beta_i m_i.$$

The matrix $A := (\alpha_{ij})_{1 \leq i, j \leq 4}$ is symmetric and positive definite with constant coefficients, β_i are positive enthalpic constants and k_B denotes the Boltzmann constant. The first term $\sum_i m_i \ln m_i$ in (2.2) is the entropic contribution to the free energy as it counts all possible configurations with given vector m . The second summand with coefficients $\alpha_{ij} = \alpha_{ji}$ measures the elastic energy, i.e. $\alpha_{ij} m_i m_j$ is the contribution due to the interaction of ion i with ion j , see [4] for further details.

For the free energy of the outer phase and for given small $\delta > 0$ we make the ansatz

$$(2.3) \quad f_{II}(m) = k_B \theta \left[\sum_{i=1}^4 m_i \ln m_i - (\ln \delta + 1) \sum_{i=1}^2 m_i \right].$$

The chemical potential of the i -th constituent fulfills for $1 \leq i \leq 4$, see (2.13) below,

$$(2.4) \quad \mu_i = \frac{\partial f_I}{\partial m_i}(m) \quad \text{in } \Omega^I, \quad \mu_i = \frac{\partial f_{II}}{\partial m_i}(m) \quad \text{in } \Omega^{II}.$$

Ansatz (2.3) is chosen such that $\mu_i = k_B \theta \ln(m_i/\delta)$ and μ_i is positive in Ω^{II} for $m_i > \delta$ and $i = 1, 2$.

The oxidation process $\text{Fe}^{3+} + e \leftrightarrow \text{Fe}^{2+}$ in Ω_T^I is formally modelled as a reaction. The reaction vector r^I in Ω^I is given by, see [12] for a general explanation,

$$(2.5) \quad r^I = (r_1^I, -r_1^I, 0, 0), \quad r_1^I = r_1^I(m) = k_1 m_2 - k_2 m_5$$

with positive reaction rates k_1, k_2 .

The conservation of mass leads to the formulation $\partial_t m_i = -\text{div}(J_i) + r_i(m)$. Onsager's postulate, [16], [17], states that the thermodynamic flux J 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 [13] p.137,

$$(2.6) \quad J_i = - \sum_{j=1}^4 L_{ij} \nabla \mu_j, \quad 1 \leq i \leq 4,$$

with a mobility tensor $L = (L_{ij})_{1 \leq i, j \leq M}$ that may depend on μ . The Onsager reciprocity law, [16], [17], [13], 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.

The coefficients of L depend on the domain as $L = L^I$ in Ω^I and $L = L^{II}$ in Ω^{II} . The diffusion rates measured for Cu^+ and Zn^{2+} are of the same order and are about 1000 times larger than the diffusivities of Fe^{3+} and Fe^{2+} . Mathematically, we look at an idealised situation where we set $L_{ij}^{II} := 0$ for $i \neq j$ (this means no cross diffusion) and $L_{11}^{II}, L_{22}^{II} \sim \varepsilon$ and $L_{33}^{II}, L_{44}^{II} \sim \frac{1}{\varepsilon}$. For small $\varepsilon > 0$ this gives rise to the boundary conditions on $\partial\Omega^I$

$$(2.7) \quad - \sum_{j=1}^4 L_{ij}^I(\mu) \nabla \mu_j \vec{n} = m_i v \quad \text{for } i = 1, 2,$$

$$(2.8) \quad \mu_i = \varphi_i \quad \text{for } i = 3, 4.$$

The parameter v denotes the speed with which the interface moves outward, \vec{n} is the unit outer normal to Ω^I and φ_1, φ_2 are two given constants invariant in time and space.

We have the diffusion equations

$$(2.9) \quad \partial_t m_i = \operatorname{div} \left(\sum_{j=1}^4 L_{ij}^I \nabla \mu_j \right) + r_i^I(m), \quad \text{in } \Omega^I,$$

$$(2.10) \quad \partial_t m_i = \operatorname{div} \left(L_{ii}^{II} \nabla \mu_i \right) + r_i^{II}(\mu) \quad \text{in } \Omega^{II}.$$

Experimentally it is observed that the outer domain only contains a very small amount of Fe^{3+} , Fe^{2+} except in a small strip near Ω^I . To ensure this condition for the mathematical system if the free boundary $\partial\Omega^I \cap \partial\Omega^{II}$ moves inward, i.e. if $v < 0$, we make the ansatz

$$(2.11) \quad r^{II}(\mu) = -\frac{1}{\gamma}(\mu_1, \mu_2, 0, 0),$$

where $\gamma > 0$ is a small constant related to the thickness of the Fe-containing strip close to Ω^I .

The model is formulated for small positive parameters γ , δ and ε , but we will show in Sections 5 and 7 that the existence theory remains valid in the limit $\gamma, \delta, \varepsilon \searrow 0$, see in particular the assumptions (A1)-(A4) below on the time-discrete problem.

We postulate that for all $0 \leq t < T$ the set $\Omega^I(t)$ has finite perimeter. For the characteristic function $\chi : \Omega_T \rightarrow \{0, 1\}$ of $\Omega^I(t)$ this means

$$\int_{\Omega} |\nabla \chi(t)| = \|\chi(t)\|_{BV(\Omega)} < \infty \quad \text{for all } 0 \leq t \leq T.$$

The condition $\|\chi\|_{BV(\Omega)} < \infty$ means that χ is a function of bounded variation in Ω , see [24], [25]. The symbol $H^{1,2}(\Omega) \subset L^2(\Omega)$ denotes the Sobolev space of functions with first weak derivatives in the Hilbert space $L^2(\Omega)$.

We consider a physical system with surface tension, so the total free energy F is given by

$$(2.12) \quad F(\chi, \mu) := \int_{\Omega} |\nabla \chi| + \int_{\partial\Omega^I} v - \int_{\Omega} \left(\chi f_I^*(\mu) + (1 - \chi) f_{II}^*(\mu) \right).$$

Here, $f_I^*(\mu)$, $f_{II}^*(\mu)$ are the Legendre-Fenchel transforms of $f_I(\mu)$, $f_{II}(\mu)$ defined by

$$f_I^*(\mu) := \sup_m \{ \mu \cdot m - f_I(\mu) \}, \quad f_{II}^*(\mu) := \sup_m \{ \mu \cdot m - f_{II}(\mu) \},$$

In these definitions, \cdot denotes the inner product, i.e. $\mu \cdot m = \sum_{i=1}^4 \mu_i m_i$. If there can be no ambiguity, we drop \cdot and simply write μm in this article.

The mathematical description of the system is completed with the condition

$$(2.13) \quad F(\chi, \mu) \rightarrow \min,$$

where μ is fixed and fulfills the constraints (2.9), (2.10) and the minimum is sought for $\chi \in BV(\Omega; \{0, 1\})$. When restricting to smooth deformations of $\partial\Omega^I(t)$, the stationarity of F with respect to characteristic functions $\chi \in BV(\Omega; \{0, 1\})$ for fixed μ leads to the Gibbs-Thomson law

$$(2.14) \quad H + v = f_I^*(\mu) - f_{II}^*(\mu),$$

and H is the mean curvature of the interface $\partial\Omega^I(t)$. Below, (2.14) is replaced by the weaker condition (W2) that requires less regularity on χ .

The vector m is obtained from μ by the splitting

$$(2.15) \quad m = \chi m_I + (1 - \chi)m_{II},$$

where the mass vector m_I in the inner domain $\Omega^I(t)$ and the mass vector m_{II} in the outer domain are determined implicitly by

$$(2.16) \quad \mu = \frac{\partial f_I}{\partial m}(m_I) \text{ in } \Omega^I(t), \quad \mu = \frac{\partial f_{II}}{\partial m}(m_{II}) \text{ in } \Omega \setminus \Omega^I(t).$$

The free energy densities f_I and f_{II} are convex functions, so (2.16) is meaningful. The decomposition (2.15), (2.16) is essential for the further understanding of this article.

In summary, we are concerned with the free energy minimisation (2.13) under the constraints

$$(2.17) \quad \partial_t(\chi m) = \operatorname{div}(\chi L^I(\mu)\nabla\mu) + \chi r^I(m) \quad \text{in } \Omega, t > 0,$$

$$(2.18) \quad \partial_t((1 - \chi)m) = \operatorname{div}((1 - \chi)L^{II}(\mu)\nabla\mu) + (1 - \chi)r^{II}(\mu) \quad \text{in } \Omega, t > 0$$

with r^I, r^{II} given by (2.5), (2.11), where $m(t)$ fulfills (2.15), (2.16), and equipped with the initial conditions

$$(2.19) \quad \chi(\cdot, 0) = \chi_0 \quad \text{in } \Omega,$$

$$(2.20) \quad \mu(\cdot, 0) = \mu_0 \quad \text{in } \Omega.$$

The Equation (2.20) also determines $m(t = 0)$ with (2.16). The functions of initial data $\chi_0 \in BV(\Omega)$ and $\mu_0 \in H^{1,2}(\Omega)$ fulfill the compatibility conditions

$$(2.21) \quad \mu_{01} = \mu_{02} = 0 \quad \text{in } \left\{x \in \Omega \mid \operatorname{dist}(x, \overline{\Omega^I(t=0)}) \geq \sqrt{\varepsilon}\right\},$$

$$(2.22) \quad \mu_{03} = \psi_3, \quad \mu_{04} = \psi_4 \quad \text{in } \Omega \setminus \overline{\Omega^I(t=0)},$$

where $\psi_3, \psi_4 \in H^{1,2}(\Omega \setminus \overline{\Omega^I(t=0)})$. As the free energy in the outer phase depends on the parameter $\delta > 0$, we demand that for a constant C independent of δ

$$(2.23) \quad \int_{\Omega \setminus \overline{\Omega^I(t=0)}} f_{II}(m(t=0)) \leq C \quad \text{uniformly in } \delta > 0.$$

The system is subject to the boundary conditions (2.7), (2.8) and

$$(2.24) \quad \mu_i = 0 \quad \text{for } i = 1, 2 \quad \text{on } \partial\Omega \times (0, T),$$

$$(2.25) \quad \mu_i = \varphi_i \quad \text{for } i = 3, 4 \quad \text{on } \partial\Omega \times (0, T).$$

For later use we want to introduce some notations. Let

$$\mu^N := (\mu_1, \mu_2), \quad \mu^D := (\mu_3, \mu_4).$$

The vector m is decomposed in m^N, m^D accordingly.

We define $f_{II}^{D,*}(m^N, \mu^D)$ as the partial Legendre-Fenchel transformation of $f_{II}(m)$ with respect to m , that is

$$f_{II}^{D,*}(m^N, \mu^D) := \sup_{m^D} \{\mu^D m^D - f_{II}(m)\}.$$

Due to the form of f_{II} we may write

$$f_{II}^{D,*}(m^N, \mu^D) = f_{II}^{D,*}(\mu^D) - f_{II}^N(m^N),$$

where we introduced the functions

$$\begin{aligned} f_{II}^N(m^N) &:= k_B \theta \left(\sum_{i=1}^2 m_i \ln m_i - \sum_{i=1}^2 (\ln \delta + 1) m_i \right), \\ f_{II}^{D,*}(\mu^D) &:= \sup_{m^D} \left\{ \mu^D m^D - f_{II}^D(m^D) \right\}, \\ f_{II}^D(m^D) &:= k_B \theta \left(\sum_{i=1}^2 m_i \ln m_i \right). \end{aligned}$$

As a prerequisite to existence theory we remark the validity of the second law of thermodynamics, which in the isothermal setting reads

$$\frac{d}{dt} F(\chi, \mu) \leq 0.$$

For a direct proof of this inequality see [6]. So it holds

$$\begin{aligned} -\partial_t \int_{\Omega} \left[\chi(f_I(\mu) - m\varphi) + (1-\chi)(f_{II}(\mu) - m\varphi) \right] &\geq \partial_t \int_{\Omega} |\nabla \chi| + \partial_t \int_{\partial\Omega^I} v \\ (2.26) \quad &+ \int_{\Omega} \left(\chi L^I(\mu) + (1-\chi)L^{II}(\mu) \right) |\nabla \mu|^2 - \int_{\Omega} (\chi r^I(m) + (1-\chi)r^{II}(\mu)) \mu. \end{aligned}$$

We remark that in (2.26) it holds

$$(2.27) \quad - \int_{\Omega} r \mu := - \int_{\Omega} (\chi r^I + (1-\chi)r^{II}) \mu \geq 0.$$

Physically, $-\int_{\Omega} r \mu$ is the production of entropy due to chemical reactions.

In order to show (2.27), we compute with (2.5)

$$(2.28) \quad - \sum_{i=1}^4 r_i^I \mu_i = r_1^I (\mu_2 - \mu_1) = q_I(r_1^I, m_2) + q_I^*(\mu^N, m_2),$$

where

$$\begin{aligned} q_I(r_1^I, m_2) &:= k_B \theta \left[(k_1 m_2 - r_1^I) \ln \left(1 - \frac{r_1^I}{k_1 m_2} \right) + r_1^I \right], \\ q_I^*(\mu^N, m_2) &:= k_1 m_2 \left[\mu_2 - \mu_1 + k_B \theta \left(\exp \left(\frac{\mu_1 - \mu_2}{k_B \theta} \right) - 1 \right) \right]. \end{aligned}$$

The function q_I^* denotes as above the Legendre-Fenchel transform of q_I . We can check elementary that the functions q_I and q_I^* are non-negative which proves (2.27).

Motivated by Equation (2.11) we define for further use (see (2.26) and (4.3) below)

$$q_{II}^*(\mu^N) := -\frac{1}{2\gamma} |\mu^N|^2.$$

With (2.28) we have found a general formulation for the reaction terms based on duality. We remark that Condition (2.27) can also be derived from an Arrhenius ansatz for the reaction rates, see [6], [8].

Integrating (2.26) with respect to time we get the a-priori estimate

$$\begin{aligned}
& \sup_{t \in (0, T)} |\nabla \chi(t)| + \int_{\Omega_T} (\chi L^I(\mu) + (1 - \chi) L^{II}(\mu)) |\nabla \mu|^2 - \int_{\Omega_T} (\chi r^I(m) + (1 - \chi) r^{II}(\mu)) \mu \\
& + \int_0^T \int_{\partial \Omega^I(t)} v \leq \int_{\Omega} (\chi f_I(m) + (1 - \chi) f_{II}(m))(t = 0) + \int_{\Omega} m(T) \varphi - \int_{\Omega} m(0) \varphi \\
(2.29) \quad & - \int_{\Omega} (\chi f_I(m) + (1 - \chi) f_{II}(m))(t = T).
\end{aligned}$$

Since $f_{II}(t = 0)$ is bounded due to Estimate (2.23) we get the boundedness of the right hand side of (2.29). As L^I, L^{II} are positive definite, we obtain estimates for the functions χ, μ and velocity v . These estimates will be improved later.

3. Weak solutions. We want to shortly specify the class of solutions we are looking for. We call the triple (m, μ, χ) a *weak solution* of the system (2.17)-(2.24) if (2.13) holds, $m = m(\mu)$ is given by (2.15), (2.16), and if (μ, χ) solve the following weak formulations (W1)-(W3):

(W1) For all $\xi \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\xi(T) = 0$ it holds

$$\begin{aligned}
& - \int_{\Omega_T} \chi m \partial_t \xi = - \int_{\Omega_T} \chi L^I(\mu) \nabla \mu \nabla \xi + \int_{\Omega_T} \chi f_I(m) \xi + \int_{\Omega} \chi(t=0) m(t=0) \xi(t=0), \\
& - \int_{\Omega_T} (1 - \chi) m \partial_t \xi = - \int_{\Omega_T} (1 - \chi) L^{II}(\mu) \nabla \mu \nabla \xi + \int_{\Omega_T} (1 - \chi) f_{II}(m) \xi \\
& \quad + \int_{\Omega} (1 - \chi(t=0)) m(t=0) \xi(t=0).
\end{aligned}$$

(W2) For all $\zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial \Omega \times (0, T)$ it holds

$$\int_{\Omega_T} \left(\operatorname{div} \zeta - \frac{\nabla \chi}{|\nabla \chi|} \nabla \zeta \frac{\nabla \zeta}{|\nabla \zeta|} \right) |\nabla \chi| + \int_{\Omega_T} v \zeta \nabla \chi = \int_{\Omega_T} (f_I^*(\mu) - f_{II}^*(\mu)) \zeta \nabla \chi.$$

(W3) For all $\xi \in C^1([0, T] \times \bar{\Omega}; \mathbb{R})$ with $\xi = 0$ on $\partial \Omega \times (0, T)$ and $\xi(T) = 0$ it holds

$$\int_{\Omega_T} \chi \partial_t \xi + \int_{\Omega} \chi_{\Omega_0} \xi(0) = - \int_{\Omega_T} v \xi |\nabla \chi|.$$

4. Time discrete scheme. For fixed $h > 0$ we consider in Ω the time-discrete scheme

$$\begin{aligned}
(4.1) \quad & \chi(t) m(t) - \chi(t-h) m(t-h) = h \operatorname{div} [\chi(t-h) L^I(\mu(t-h)) \nabla \mu(t)] \\
& \quad + \chi(t-h) h r^I(m(t)), \\
(4.2) \quad & (1 - \chi(t)) m(t) - (1 - \chi(t-h)) m(t-h) = h \operatorname{div} [(1 - \chi(t-h)) L^{II}(\mu(t-h)) \nabla \mu(t)] \\
& \quad + (1 - \chi(t-h)) h r^{II}(\mu(t)).
\end{aligned}$$

This is an implicit time discretisation except for the coefficients $L^I(\mu)$, $L^{II}(\mu)$ and χ that are treated explicitly. Also we wrote $\mu(t)$ shortly for $\mu(\chi(t))$ and set $\chi(t) := \chi_0$, $m(t) := m(t=0)$ for $-h \leq t < 0$.

For given $\chi(t-h)$, $\mu(t-h)$, let the discrete free energy functional be given by

$$\begin{aligned}
F_h(\chi(t), \mu(t)) &= \int_{\Omega} |\nabla \chi(t)| + \int_{\Omega^I(t) \Delta \Omega^I(t-h)} \frac{1}{h} \text{dist}(\cdot, \partial \Omega^I(t-h)) + \int_{\Omega} m(t-h) \mu(t) \\
&\quad - \int_{\Omega} \left[\chi(t) f_I^*(\mu(t)) + (1 - \chi(t)) f_{II}^*(\mu(t)) \right] \\
&\quad - h \int_{\Omega} \left[\chi(t-h) L^I(\mu(\chi(t-h))) + (1 - \chi(t-h)) L^{II}(\mu(\chi(t-h))) \right] |\nabla \mu(t)|^2 \\
(4.3) \quad &\quad - \int_{\Omega} \chi(t-h) h q_I^*(\mu^N(t), m_2(t)) + \int_{\Omega} (1 - \chi(t-h)) h q_{II}^*(\mu^N(t)).
\end{aligned}$$

Here we used the notation $A \Delta B := (A \setminus B) \cup (B \setminus A)$ for the symmetrised difference of two sets A and B .

We construct the time-discrete solution $\chi_h \in L^\infty(0, T; BV(\Omega; \{0, 1\}))$ in the following way. Let $T = hN$. At time $t = 0$, $\Omega^I(t=0)$ and μ_0 are given. For discrete time values $t = kh$, $k = 1, \dots, N$, the function $\chi_h(t)$ with $\mu_h(t) = \mu_h(\chi_h(t))$ fulfilling the constraints (4.1), (4.2) iteratively solves the energy minimisation problem

$$(4.4) \quad F_h(\chi_h(t), \mu_h) \rightarrow \min$$

in the class $BV(\Omega; \{0, 1\})$. The discrete mapping m_h is computed from χ_h , μ_h with the help of (2.15), (2.16). We continue χ_h to arbitrary $t \in (0, T)$ by setting

$$\chi_h(t) := \chi_h(kh) \quad \text{for } t \in ((k-1)h, kh].$$

We introduce the discrete velocity of the interface by

$$(4.5) \quad v_h(x) := \frac{1}{h} \text{dist}(x, \partial \Omega^I(t-h)).$$

The following result is well known.

LEMMA 4.1 (Weak mean curvature equation). *The minimum (χ_h, μ_h) of F_h satisfies the weak mean curvature equation*

$$\int_{\Omega} \left(\text{div} \zeta - \frac{\nabla \chi_h}{|\nabla \chi_h|} \nabla \zeta \frac{\nabla \chi_h}{|\nabla \chi_h|} \right) |\nabla \chi_h| + \int_{\Omega} v_h \zeta \nabla \chi_h = \int_{\Omega} \left(f_I^*(\mu_h(\chi_h)) - f_{II}^*(\mu_h(\chi_h)) \right) \zeta \nabla \chi_h$$

for all $\zeta \in C_0^1(\Omega; \mathbb{R}^3)$.

Proof. We compute the first variation of F_h with respect to deformations of $\Omega^I(t)$, i.e. we compute

$$\left. \frac{d}{ds} F_h(\chi_h \circ \zeta_s, \mu_h(\chi_h \circ \zeta_s)) \right|_{s=0}$$

for all $\zeta \in C_0^1(\Omega; \mathbb{R}^3)$ with $\zeta_0(x) = x$, $\partial_s \zeta_s(x) = \zeta(\zeta_s(x))$. With $\chi_h := \chi_h(t)$ we obtain

$$\int_{\Omega} \left(\text{div} \zeta - \frac{\nabla \chi_h}{|\nabla \chi_h|} \nabla \zeta \frac{\nabla \chi_h}{|\nabla \chi_h|} \right) |\nabla \chi_h| + \int_{\Omega} v_h \zeta \nabla \chi_h - \int_{\Omega} \left(f_I^*(\mu_h(\chi_h)) - f_{II}^*(\mu_h(\chi_h)) \right) \zeta \nabla \chi_h$$

$$\begin{aligned}
&= \int_{\Omega} m_h \mu_{\zeta} - \int_{\Omega} m_h(t-h) \mu_{\zeta} \\
&\quad - h \int_{\Omega} \operatorname{div} \left[\left(\chi_h(t-h) L^I(\mu_h(\chi_h(t-h))) + (1-\chi_h(t-h)) L^{II}(\mu_h(\chi_h(t-h))) \right) \nabla \mu_h(\chi_h) \right] \mu_{\zeta} \\
&\quad - h \int_{\Omega} \left(\chi_h(t-h) r^I(m_h) + (1-\chi_h(t-h)) r^{II}(\mu_h(\chi_h)) \right) \mu_{\zeta},
\end{aligned}$$

where $\mu_{\zeta} := \mu_h(\chi_h(\zeta(\zeta_s)))$. As the right hand side is zero, the lemma is proved. \square

5. A priori estimates. In this section we show a-priori estimates for the time-discrete solution. Together with the compactness results they are the main ingredients for the existence proof.

Generically, we denote by C various constants that may change from estimate to estimate.

LEMMA 5.1 (A-priori estimates for the time-discrete solution).

(i) *The following a-priori estimate holds:*

$$\begin{aligned}
&\sup_{t \in (0, T)} \int_{\Omega} |\nabla \chi_h(t)| + \frac{1}{h^2} \int_0^T \int_{\Omega^I(t) \Delta \Omega^I(t-h)} \operatorname{dist}(\cdot, \partial \Omega^I(t-h)) + \frac{1}{2\gamma} \int_{\Omega_T} (1-\chi_h(t-h)) |\mu_h^N|^2 \\
&+ \int_{\Omega_T} \left(\chi_h(t-h) L^I(\mu_h(\chi_h(t-h))) + (1-\chi_h(t-h)) L^{II}(\mu_h(\chi_h(t-h))) \right) |\nabla \mu_h(\chi_h)|^2 \\
(5.1) \quad &\leq \int_{\Omega} \left(\chi_h f_I(m_h) + (1-\chi_h) f_{II}(m_h) \right) (t=0) - \int_{\Omega} \left(\chi_h f_I(m_h) + (1-\chi_h) f_{II}(m_h) \right) (t=T).
\end{aligned}$$

(ii) *For the chemical potential and the time derivative of m it holds:*

$$(5.2) \quad \int_{\Omega_T} \chi_h(t-h) |\nabla \mu_h(t)|^2 \leq C,$$

$$(5.3) \quad \int_{\Omega_T} (1-\chi_h(t-h)) |\nabla \mu_h^N(t)|^2 \leq C\varepsilon^{-1},$$

$$(5.4) \quad \int_{\Omega_T} (1-\chi_h(t-h)) |\nabla \mu_h^D(t)|^2 \leq C\varepsilon,$$

$$(5.5) \quad \int_{\Omega_T} (1-\chi_h(t-h)) |\mu_h^N(t)|^2 \leq C\gamma,$$

$$(5.6) \quad \int_{\Omega_T} \|\chi_h \partial_t^h m_h\|_{H^{-1}(\Omega)}^2 \leq C.$$

Proof. (i) Due to the minimality of (χ_h, μ_h) with respect to F_h we have

$$(5.7) \quad F_h(\chi_h(t), \mu_h(t)) \leq F_h(\chi, \mu_h(\tilde{\chi})) \quad \text{for all } \tilde{\chi} \in BV(\Omega; \{0, 1\}).$$

When choosing $\tilde{\chi} := \chi_h(t-h)$ in (5.7) we find

$$\begin{aligned}
& \int_{\Omega} |\nabla \chi_h(t)| + \int_{\Omega^I(t) \Delta \Omega^I(t-h)} \frac{1}{h} \text{dist}(\cdot, \partial\Omega(t-h)) + \int_{\Omega} m_h(t-h) \mu_h(\chi_h(t)) \\
& + \int_{\Omega} \left[\chi_h f_I(m_h(t)) + (1 - \chi_h(t)) f_{II}(m_h(t)) - m_h(t) \mu_h(\chi_h(t)) \right] \\
& - h \int_{\Omega} \left[\chi_h(t-h) L^I(\mu_h(\chi_h(t-h))) + (1 - \chi_h(t-h)) L^{II}(\mu_h(\chi_h(t-h))) \right] |\nabla \mu_h(\chi_h(t))|^2 \\
& - h \int_{\Omega} \chi_h(t-h) q_I^*(\mu_h^N(\chi_h(t)), m_{h,2}(t)) + h \int_{\Omega} (1 - \chi_h(t-h)) q_{II}^*(\mu_h^N(\chi_h(t))) \\
& \leq \int_{\Omega} |\nabla \chi_h(t-h)| + \int_{\Omega} \left[\chi_h(t-h) f_I(m_h(t-h)) + (1 - \chi_h(t-h)) f_{II}(m_h(t-h)) \right] \\
& - h \int_{\Omega} \left[\chi_h(t-h) L^I(\mu_h(\chi_h(t-h))) + (1 - \chi_h(t-h)) L^{II}(\mu_h(\chi_h(t-h))) \right] |\nabla \mu_h(\chi_h(t-h))|^2 \\
& - h \int_{\Omega} \chi_h(t-h) q_I^*(\mu_h^N(\chi_h(t-h)), m_{h,2}(t-h)) + h \int_{\Omega} (1 - \chi_h(t-h)) q_{II}^*(\mu_h^N(\chi_h(t-h))).
\end{aligned}$$

We rewrite this and first observe that $q_I, q_I^* \geq 0, q_{II}^* \leq 0$. Additionally,

$$\begin{aligned}
& \int_{\Omega} \chi_h(t) f_I(m_h(t)) - \chi_h(t-h) f_I(m_h(t-h)) \\
& + \int_{\Omega} (1 - \chi_h(t)) f_{II}(m_h(t)) - (1 - \chi_h(t-h)) f_{II}(m_h(t-h)) \\
& = \int_{\Omega} \left[\chi_h(t) (f_I(m_h(t)) - f_I(m_h(t-h))) + (1 - \chi_h(t)) (f_{II}(m_h(t)) - f_{II}(m_h(t-h))) \right] \\
& + \int_{\Omega} h \partial_t^h \chi_h(t) (f_I(m_h(t-h)) - f_{II}(m_h(t-h))).
\end{aligned}$$

The second integral on the right is non-positive due to (4.4). The first integral on the right, from the definition of the chemical potential μ , can be estimated from above by

$$\int_{\Omega} \mu_h(\chi_h(t)) m_h(t-h).$$

With this result, $F_h(\chi_h(t), \mu_h(t)) \leq F_h(\chi_h(t-h), \mu_h(\chi_h(t-h)))$ finally becomes

$$\begin{aligned}
& \partial_t^h \int_{\Omega} |\nabla \chi_h| + \frac{1}{h^2} \int_{\Omega^I(t) \Delta \Omega^I(t-h)} \text{dist}(\cdot, \partial\Omega(t-h)) + \frac{1}{2\gamma} \int_{\Omega} (1 - \chi_h(t-h)) |\mu_h^N|^2 \\
& + \int_{\Omega} \left(\chi_h(t-h) L^I(\mu_h(\chi_h(t-h))) + (1 - \chi_h(t-h)) L^{II}(\mu_h(\chi_h(t-h))) \right) |\nabla \mu_h(\chi_h)|^2 \\
(5.8) \quad & \leq -\partial_t^h \left(\int_{\Omega} \chi_h f_I(m_h) \right) + \int_{\Omega} (1 - \chi_h) f_{II}(m_h).
\end{aligned}$$

Integration in time proves (i).

(ii) This follows directly from (i) and (4.1), (4.2). \square

6. A density lemma. Now we show a density lemma that establishes a strong geometric property of the sets $\Omega^I(t)$.

LEMMA 6.1. *For any $\mu \in H^{1,2}(\Omega; \mathbb{R}^4)$ it holds*

$$\|f_I^*(\mu) - f_{II}^*(\mu)\|_{L^\infty(\Omega_T)} \leq \|f_I\|_{L^\infty((0,T) \times \mathbb{R}^4)} + \|f_{II}\|_{L^\infty((0,T) \times \mathbb{R}^4)}.$$

Proof. Directly from the definitions of f_I^* and f_{II}^* we see

$$f_I^*(\mu) - f_{II}^*(\mu) = \sup_{\tilde{m}} \{\tilde{m} \cdot \mu - f_I(\tilde{m})\} - \sup_{\tilde{m}} \{\tilde{m} \cdot \mu - f_{II}(\tilde{m})\} \leq f_{II}(m) - f_I(m).$$

The analogous estimate of $f_{II}^*(\mu) - f_I^*(\mu)$ gives

$$\|f_{II}^*(\mu) - f_I^*(\mu)\|_{L^\infty} \leq \|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty}$$

which proves the lemma. \square

We recall the following results from geometric measure theory. For a proof see for instance [24], [10].

THEOREM 6.2 (Trace Operator in BV). *Let $\Omega \subset \mathbb{R}^n$ be an open bounded set and $\partial\Omega$ Lipschitz. Then there exists a trace operator $\text{tr} : BV(\Omega) \rightarrow L^1(\partial\Omega, d\mathcal{H}^{n-1})$ such that for given $f \in BV(\Omega)$*

$$\int_{\Omega} f \text{div} \varphi = - \int_{\Omega} \varphi \cdot \nabla f + \int_{\partial\Omega} \text{tr} f(\varphi \cdot \vec{n}) d\mathcal{H}^{n-1} \quad \text{for all } \varphi \in C^1(\mathbb{R}^n, \mathbb{R}^n),$$

where \vec{n} is the unit outer normal to $\partial\Omega$. Furthermore

$$\lim_{\varrho \searrow 0} \left(\varrho^{-n} \int_{B_\varrho(x) \cap \Omega} |f(y) - \text{tr} f(x)| dy \right) = 0 \quad \text{for } d\mathcal{H}^{n-1} - \text{almost all } x \in \partial\Omega.$$

If $E \subset\subset \Omega$ is an open set with Lipschitz boundary, then $f|_E \in BV(E)$ and $f|_{\Omega \setminus \bar{E}} \in BV(\Omega \setminus \bar{E})$ have traces on ∂E . In the sequel we write $f_E^- := \text{tr}(f|_E)$ and $f_E^+ := \text{tr}(f|_{\Omega \setminus \bar{E}})$. We remark for later use the equality

$$(6.1) \quad \int_{\partial E} |f_E^- - f_E^+| d\mathcal{H}^{n-1} = \int_{\partial E} |\nabla f| d\mathcal{H}^{n-1}.$$

Finally, by χ_E we denote the characteristic function of a set E .

THEOREM 6.3 (Isoperimetric Inequalities). *Let $\Omega \subset \mathbb{R}^n$ be a bounded set with $\chi_\Omega \in BV(\mathbb{R}^n)$. Then it holds*

$$(6.2) \quad \gamma_n \left(\int_{\mathbb{R}^n} \chi_\Omega \right)^{\frac{n-1}{n}} \leq \int_{\mathbb{R}^n} |\nabla \chi_\Omega|,$$

$$(6.3) \quad \min \left\{ \left(\int_{B_\varrho(x)} \chi_\Omega \right)^{\frac{n}{n-1}}, \left(\int_{B_\varrho(x)} \chi_\Omega^c \right)^{\frac{n}{n-1}} \right\} \leq C(n) \int_{B_\varrho(x)} |\nabla \chi_\Omega| \quad \text{for all } B_\varrho(x) \subset \mathbb{R}^n,$$

where $\gamma_n := n\omega_n^{\frac{1}{n}}$ and $\omega_n := \mathcal{L}^n(B_1(0))$ are dimensional constants.

Now we show the following geometric property of the sets $\Omega^I(t)$:

LEMMA 6.4 (Density Lemma). *Let $\kappa_1 := \frac{1}{4^3}$ and let $\chi_h(t)$ be a minimiser of the functional $F_h(\chi_h(t), \mu_h(\chi_h(t)))$. Then for all $x \in \partial\Omega^I(t)$ and for all $\varrho > 0$ which satisfy*

$$(6.4) \quad \varrho \leq \frac{\gamma_3}{2\omega_3^{\frac{1}{3}}(\|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty} + h^{-1}\|\text{dist}(\cdot, \partial\Omega^I(t-h))\|_{L^\infty(\Omega^I(t)\Delta\Omega^I(t-h))})}$$

it holds

$$(6.5) \quad \kappa_1 \leq \omega_3^{-1}\varrho^{-3} \int_{B_\varrho(x)} \chi_h(t) \leq 1 - \kappa_1.$$

Proof. (i) Estimate from below.

Let $x \in \partial\Omega^I(t)$ and $\varrho > 0$ be given which satisfies (6.4). Recall that $\chi_{\Omega^I(t)} = \chi_h(t)$ and recall the notions χ_h^+ , χ_h^- introduced after Theorem 6.2. Consider generally $\Omega \subset \mathbb{R}^n$.

First we show that $\Omega^I(t) \cap B_\varrho(x)$ consists of only one radial component, i.e.

$$(6.6) \quad \int_{\partial B_r(x)} \chi_h^- d\mathcal{H}^{n-1} + \int_{\partial B_r(x)} \chi_h^+ d\mathcal{H}^{n-1} > 0 \quad \text{for all } 0 < r < \varrho.$$

Assume (6.6) does not hold for a radius $r \in (0, \varrho)$. We use (5.7) with $\tilde{\chi} := \chi_{\Omega^I(t) \setminus B_r(x)}$ and find

$$(6.7) \quad \begin{aligned} \int_{\Omega} |\nabla \chi_h(t)| - \int_{\Omega} |\nabla \tilde{\chi}| &\leq \int_{B_r(x)} \frac{1}{h} \|\text{dist}(\cdot, \partial\Omega^I(t-h))\|_{L^\infty(\Omega^I \Delta \Omega^I(t-h))} \\ &\quad + \int_{B_r(x)} \left(f_I^*(\mu_h(\chi_h(t))) - f_{II}(\mu_h(\chi_h(t))) \right) \chi_h(t) \\ &\leq \int_{B_r(x)} C_1(h) \chi_h(t), \end{aligned}$$

where led by Lemma 6.1 we introduced the constant

$$C_1(h) := \|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty} + h^{-1}\|\text{dist}(\cdot, \partial\Omega^I(t-h))\|_{L^\infty(\Omega^I(t)\Delta\Omega^I(t-h))}.$$

Now we use the equalities

$$\begin{aligned} \int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t) \cap B_r(x)}| &= \int_{B_r(x)} |\nabla \chi_{\Omega^I(t)}| + \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1}, \\ \int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t) \setminus B_r(x)}| &= \int_{\mathbb{R}^n \setminus B_r(x)} |\nabla \chi_{\Omega^I(t)}| + \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} \end{aligned}$$

and the isoperimetric inequality (6.2) to conclude

$$\int_{B_r(x)} C_1(h) \chi_{\Omega^I(t)} \geq \int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t)}| - \int_{\mathbb{R}^n \setminus B_r(x)} |\nabla \chi_{\Omega^I(t)}| - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1}$$

$$\begin{aligned}
&= \int_{B_r(x)} |\nabla \chi_{\Omega^I(t)}| - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} \\
&= \int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t) \cap B_r(x)}| - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1} \\
&\geq \gamma_n \left(\int_{B_r(x)} \chi_{\Omega^I(t)} \right)^{\frac{n-1}{n}} - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} - \int_{\partial B_r(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1}.
\end{aligned}$$

Since we assumed that (6.6) is false the last two boundary integrals on the right can be estimated from below by zero and we end up with

$$\gamma_n \leq C_1(h) \left(\int_{B_r(x)} \chi_{\Omega^I(t)} \right)^{\frac{1}{n}} \leq C_1(h) \omega_n^{\frac{1}{n}} \varrho.$$

This is a contradiction to (6.4), so (6.6) is proved.

A similar technique is now used for proving the bound from below in (6.5). This time we use in (5.7) the comparison function

$$\tilde{\chi} := \chi_{\Omega^I(t) \setminus (B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x))}$$

with $0 < \sigma < \frac{\varrho}{2}$. Let

$$V(\sigma) := \mathcal{L}^n \left(\Omega^I(t) \cap (B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x)) \right).$$

With this choice of $\tilde{\chi}$ Equation (5.7) yields

$$(6.8) \quad \int_{\Omega} |\nabla \chi_{\Omega^I(t)}| - \int_{\Omega} |\nabla \tilde{\chi}| \leq C_1(h) V(\sigma).$$

Similar to above we have the identities

$$\begin{aligned}
\int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t) \cap (B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x))}| &= \int_{B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x)} |\nabla \chi_{\Omega^I(t)}| + \int_{\partial B_{\frac{\varrho}{2}+\sigma}(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1} \\
&\quad + \int_{\partial B_{\frac{\varrho}{2}-\sigma}(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1}, \\
\int_{\mathbb{R}^n} |\nabla \chi_{\Omega^I(t) \setminus (B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x))}| &= \int_{\mathbb{R}^n \setminus (B_{\frac{\varrho}{2}+\sigma}(x) \setminus B_{\frac{\varrho}{2}-\sigma}(x))} |\nabla \chi_{\Omega^I(t)}| + \int_{\partial B_{\frac{\varrho}{2}+\sigma}(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} \\
&\quad + \int_{\partial B_{\frac{\varrho}{2}-\sigma}(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1}.
\end{aligned}$$

With these two equalities and (6.8) we compute

$$C_1(h) V(\sigma) \geq \gamma_n V(\sigma)^{\frac{n-1}{n}} - \int_{\partial B_{\frac{\varrho}{2}+\sigma}(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1} - \int_{\partial B_{\frac{\varrho}{2}-\sigma}(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1}$$

$$(6.9) \quad - \int_{\partial B_{\frac{\varrho}{2} + \sigma}(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} - \int_{\partial B_{\frac{\varrho}{2} - \sigma}(x)} \chi_{\Omega^I(t)}^- d\mathcal{H}^{n-1}$$

$$(6.10) \quad = \gamma_n V(\sigma)^{\frac{n-1}{n}} - 2 \frac{d}{d\sigma} V(\sigma).$$

The last equality holds for almost all $0 < \sigma < \frac{\varrho}{2}$.

From the definition of $V(\sigma)$ and the upper bound (6.4) on ϱ we directly find

$$V(\sigma) \leq \omega_n \varrho^n \leq \frac{\gamma_n^n}{((n-1)C_1(h))^n},$$

implying at once

$$C_1(h) \leq \frac{\gamma_n}{(n-1)V(\sigma)^{\frac{1}{n}}}.$$

Using the last inequality in (6.10) finally shows the crucial estimate

$$(6.11) \quad \frac{d}{d\sigma} V(\sigma) \geq \frac{\gamma_n}{2} V(\sigma)^{\frac{n-1}{n}} - \frac{C_1(h)}{2} V(\sigma) \geq \frac{\gamma_n}{2} \frac{n-2}{n-1} V(\sigma)^{\frac{n-1}{n}}.$$

We integrate (6.11) from $0 < \sigma < \frac{\varrho}{2}$. We see directly

$$\int_0^{\frac{\varrho}{2}} \frac{d}{d\sigma} V(\sigma) d\sigma = V(\varrho/2) - V(0) = \int_{B_\varrho(x)} \chi_h(t).$$

For $n = 3$ the integration of (6.11) therefore yields

$$\int_{B_\varrho(x)} \chi_h(t) \geq \frac{\omega_n}{4^3} \varrho^3 = \kappa_1 \omega_3 \varrho^3,$$

which proves the lower bound in (6.5).

(ii) The upper bound in (6.5) can be derived in the same way as in (i) by replacing $\Omega^I(t)$ by its complement. Obviously,

$$\int_{\Omega} |\nabla \chi_{\Omega^I(t)}| = \int_{\Omega} |\nabla \chi_{\mathbb{R}^n \setminus \Omega^I(t)}|.$$

Now we consider minimisers $\tilde{\chi}(t)$ of $\tilde{F}_h(\tilde{\chi}, \tilde{\mu}(\tilde{\chi}))$, where the functional \tilde{F}_h is defined as F_h in (4.3) but with χ being replaced by $1 - \chi$ and $1 - \chi$ being replaced by χ .

Then we redo the proof of (i), now for the functional \tilde{F}_h . We obtain

$$\omega_n^{-1} \varrho^{-n} \int_{B_\varrho(x)} \chi_h(t) \leq 1 - \kappa_1.$$

This shows the bound from above in (6.5) and ends the proof. \square

COROLLARY 6.5. *Let $\chi_h := \chi_{\Omega^I(t)}$ be a minimiser of the functional $F_h(\chi, \mu(\chi))$ and let $\kappa_2 := \frac{1}{2^3}$. Then for any $\varrho > 0$ and any pair (x, y) with $x \in \partial\Omega^I(t)$, $y \in B_\varrho(x)$ and*

$$(6.12) \quad \|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty} \leq \frac{1}{h} \text{dist}(y, \partial\Omega^I(t-h))$$

it holds

$$\begin{aligned} \kappa_2 &\leq \omega_3^{-1} \varrho^{-3} \int_{B_\varrho(x)} \chi_h(t) && \text{if } x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h), \\ \omega_3^{-1} \varrho^{-3} \int_{B_\varrho(x)} \chi_h(t) &\leq 1 - \kappa_2 && \text{if } x \in \Omega^I(t-h) \setminus \overline{\Omega^I(t)}. \end{aligned}$$

The assertion remains valid if the assumption $x \in \partial\Omega^I(t)$ is replaced by $x \in \Omega$.

Proof. The proof is again similar to the proof of Lemma 6.4. Let $\varrho > 0$ satisfy (6.12). First we consider the case $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$ and show that (6.6) holds. First consider generally $\Omega \subset \mathbb{R}^n$. We exploit (5.7) with $\tilde{\chi} := \chi_{\overline{\Omega^I(t)} \setminus B_\varrho(x)}$. Assuming that (6.6) is violated for a radius $r \in (0, \varrho)$ we obtain analogous to (6.7)

$$(6.13) \quad \int_{\Omega} |\nabla \chi_{\Omega^I(t)}| - \int_{\Omega} |\nabla \tilde{\chi}| \leq \int_{B_r(x)} C_2(h, y) \chi_{\Omega^I(t)} dy \leq 0,$$

where we have according to (6.12)

$$C_2(h, y) := \|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty} - \frac{1}{h} \text{dist}(y, \partial\Omega^I(t-h)) \leq 0.$$

From (6.13) and (6.2) we conclude

$$\gamma_n \left(\int_{B_\varrho(x)} \chi_{\Omega^I(t)} \right)^{\frac{n-1}{n}} \leq 0,$$

a contradiction.

The analogon to (6.9) is

$$\gamma_n V(\sigma)^{\frac{n-1}{n}} - \int_{\partial B_{\frac{\varrho}{2} + \sigma}(x)} \left(\chi_{\Omega^I(t)}^- + \chi_{\Omega^I(t)}^+ \right) d\mathcal{H}^{n-1} - \int_{\partial B_{\frac{\varrho}{2} - \sigma}(x)} \left(\chi_{\Omega^I(t)}^- + \chi_{\Omega^I(t)}^+ \right) d\mathcal{H}^{n-1} \leq 0$$

and from that we can proceed as in the proof of Lemma 6.4.

The other case $x \in \Omega^I(t-h) \setminus \overline{\Omega^I(t)}$ is treated alike by considering the functional \tilde{F} on the complementary set $(\Omega^I(t))^C$. \square

COROLLARY 6.6. *Under the assumptions of Corollary 6.5 there exists a constant C independent of h such that for all $\varrho > 0$*

$$(6.14) \quad \int_{B_\varrho(x)} |\nabla \chi_h| \leq C \varrho^2.$$

Proof. The proof is analogous to Corollary 6.5. Let $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$. We use (5.7) with $\tilde{\chi} := \chi_{\overline{\Omega^I(t)} \setminus \Omega(t-h)}$. With Condition (6.12) we find

$$\int_{B_\varrho(x)} |\nabla \chi_{\Omega^I(t)}| \leq \int_{\partial B_\varrho(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^2,$$

therefore

$$\int_{B_\varrho(x)} |\nabla \chi_{\Omega^I(t)}| \leq \mathcal{H}^2(\partial B_\varrho(x)) \leq C\varrho^2.$$

The other case $x \in \Omega^I(t-h) \setminus \Omega^I(t)$ can be proved in the same way. \square

The model (2.17)-(2.24) was formulated for small positive parameters γ , δ and ε . As will become clear in the sequel, the existence theory remains valid if $\gamma = \gamma(h)$, $\delta = \delta(h)$ and $\varepsilon = \varepsilon(h)$ are functions that tend to 0 as $h \searrow 0$. The convergence of the discrete solution to the limit problem can be ensured provided the following three conditions are met:

The functions $\delta(h) > 0$ and $\varepsilon(h) > 0$ fulfill

$$(A1) \quad \lim_{h \searrow 0} h^{\frac{1}{2}} \ln(\delta(h)) = 0,$$

$$(A2) \quad \lim_{h \searrow 0} (\delta(h)\varepsilon^{-1}(h)) = 0,$$

$$(A3) \quad \lim_{h \searrow 0} (h^{\frac{1}{4}}\varepsilon^{-\frac{3}{4}}(h)) = 0,$$

$$(A4) \quad \lim_{h \searrow 0} (h^{\frac{1}{3}}\varepsilon^{-1}) = 0.$$

Now we can formulate an estimate on the discrete velocity of the interface.

LEMMA 6.7 (*L^∞ -bound on the discrete velocity*). *For any $h > 0$ there exists a positive constant C independent of h such that*

$$\left\| \frac{1}{h} \text{dist}(\cdot, \partial\Omega(t-h)) \right\|_{L^\infty(\Omega^I(t) \Delta \Omega^I(t-h))} < Ch^{-\frac{1}{2}}$$

uniformly in time.

Proof. Without loss of generality we restrict to the case $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$. The other case $x \in \Omega^I(t-h) \setminus \Omega^I(t)$ is treated correspondingly.

The proof is done by contradiction. Assume that there exists a $x \in \partial\Omega^I(t)$ such that

$$(6.15) \quad \frac{1}{h} \text{dist}(x, \partial\Omega^I(t-h)) \geq lh^{-\frac{1}{2}} \quad \text{for all } l \in \mathbb{N}.$$

We use again (5.7) with $\tilde{\chi} := \chi_{\Omega^I(t) \setminus B_{\frac{l}{2}\sqrt{h}}(x)}$ to find

$$(6.16) \quad \begin{aligned} \int_{\Omega} |\nabla \tilde{\chi}| - \int_{\Omega} |\nabla \chi_{\Omega^I(t)}| &\geq \int_{\Omega^I(t) \cap B_{\frac{l}{2}\sqrt{h}}(x)} \frac{1}{h} \text{dist}(\cdot, \partial\Omega^I(t-h)) \\ &- \int_{B_{\frac{l}{2}\sqrt{h}}(x)} (\|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty}) \chi_{\Omega^I(t)}. \end{aligned}$$

The left hand side of (6.16) can be estimated from above,

$$\begin{aligned} \int_{\Omega} |\nabla \chi_{\Omega^I(t) \setminus B_{\frac{l}{2}\sqrt{h}}(x)}| - \int_{\Omega} |\nabla \chi_{\Omega^I(t)}| &= - \int_{B_{\frac{l}{2}\sqrt{h}}(x)} |\nabla \chi_{\Omega^I(t)}| + \int_{\partial B_{\frac{l}{2}\sqrt{h}}(x)} \chi_{\Omega^I(t)}^+ d\mathcal{H}^{n-1} \\ &\leq \mathcal{H}^{n-1}(\partial B_{\frac{l}{2}\sqrt{h}}(x)) = n \left(\frac{l}{2} \sqrt{h} \right)^{n-1} \omega_n. \end{aligned}$$

By Assumption (6.15) the last estimate applied to (6.16) yields

$$\frac{l}{2} h^{-\frac{1}{2}} \int_{B_{\frac{l}{2}\sqrt{h}}(x)} \chi_{\Omega^I(t)} \leq n \left(\frac{l}{2} \sqrt{h} \right)^{n-1} \omega_n + (\|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty}) \left(\frac{l}{2} \sqrt{h} \right)^n.$$

From Assumption (A1), it follows that Condition (6.12) is fulfilled. For $n = 3$ we apply Corollary 6.5 and find

$$\frac{l}{2}h^{-\frac{1}{2}}\kappa_2\left(\frac{l}{2}\sqrt{h}\right)^3\omega_3 \leq 3\left(\frac{l}{2}\sqrt{h}\right)^2\omega_3 + \left(\|f_I\|_{L^\infty} + \|f_{II}\|_{L^\infty}\right)\left(\frac{l}{2}\sqrt{h}\right)^3.$$

This is a contradiction for sufficiently large l . \square

LEMMA 6.8 (Improved density lemma). *Let $\chi_h(t)$ be a minimiser of the functional $F_h(\chi_h, \mu_h(\chi_h))$. Then there exists a constant C independent of h such that for all $\varrho > 0$ with $\varrho \leq C\sqrt{h}$*

$$(6.17) \quad \kappa_1 \leq \omega_3^{-1}\varrho^{-3} \int_{B_\varrho(x)} \chi_h(t) \leq 1 - \kappa_1 \quad \text{for all } x \in \partial\Omega^I(t).$$

Proof. This follows directly from Lemma 6.4 and Lemma 6.7. \square

7. Compactness properties of the discrete solution. We proceed with compactness properties of the time-discrete solution χ_h .

LEMMA 7.1 (Compactness in space). *For every unit vector $e \in \mathbb{R}^3$ it holds uniformly in h*

$$(7.1) \quad \lim_{s \searrow 0} \int_{\Omega_T} |\chi_h(x + se, t) - \chi_h(x, t)| = 0.$$

Proof. The claim follows from the a-priori estimate (5.1) after observing that

$$\int_{\Omega} |\chi(\cdot + se) - \chi| \leq s \int_{\Omega} |\nabla \chi|$$

for arbitrary functions $\chi \in BV(\Omega)$. \square

LEMMA 7.2 (Compactness of χ_h in time I). *There exists a constant C such that the discrete solution χ_h satisfies*

$$\int_0^{T-\tau} \int_{\Omega} |\chi_h(x, t + \tau) - \chi_h(x, t)| < c\tau \quad \text{for any } \tau > 0.$$

Proof. First we consider the case $\tau = kh$ for $k \in \mathbb{N}$. Writing the integrand as a telescopic sum we see

$$\begin{aligned} \int_0^{T-\tau} \int_{\Omega} |\chi_h(x, t + \tau) - \chi_h(x, t)| &\leq \int_0^{T-\tau} \int_{\Omega} \sum_{l=1}^k |\chi_h(x, t + lh) - \chi_h(x, t + (l-1)h)| \\ &= \int_0^{T-\tau} \int_{\Omega} \sum_{l=1}^k h |\partial_t^{-h} \chi_h(x, t + lh)| \leq \tau \int_0^T \int_{\Omega} |\partial_t^{-h} \chi_h(x, t)|. \end{aligned}$$

Consequently the proof is finished if we can show that

$$(7.2) \quad \int_{\Omega_T} |\partial_t^{-h} \chi_h| = \sum_{k=1}^N |\Omega^I(kh) \Delta \Omega^I((k-1)h)| < C$$

for a constant C which is independent of h . In order to prove (7.2) we notice

$$\begin{aligned} \Omega^I(t) \Delta \Omega^I(t-h) &\subset \left\{ x \in \Omega^I(t) \Delta \Omega^I(t-h) \mid \text{dist}(x, \partial \Omega(t-h)) > c_1 h \right\} \\ &\quad \cup \left\{ x \in \Omega^I(t) \Delta \Omega^I(t-h) \mid \text{dist}(x, \partial \Omega(t-h)) \leq c_1 h \right\} \\ &=: E_1(t) \cup E_2(t), \end{aligned}$$

where c_1 is a small positive constant. It remains to show that the sets $E_1(t)$, $E_2(t)$ for $t = lh$ and $1 \leq l \leq N$ are bounded. For $E_1(t)$ we have as a consequence of the free energy inequality (2.26)

$$\begin{aligned} |E_1(t)| &< \frac{1}{2c_1} \int_{\Omega^I(t) \Delta \Omega^I(t-h)} \text{dist}(\cdot, \Omega^I(t-h)) \\ &\leq -h \partial_t^h \left[\int_{\Omega} \left(\chi_h f_I(m_h) + (1 - \chi_h) f_{II}(m_h) \right) \right] (t). \end{aligned}$$

Discrete integration in time gives

$$\begin{aligned} \sum_{l=1}^N |E_1(lh)| &\leq \int_{\Omega} \left(\chi_h f_I(m_h) + (1 - \chi_h) f_{II}(m_h) \right) (t=0) \\ &\quad - \int_{\Omega} \left(\chi_h f_I(m_h) + (1 - \chi_h) f_{II}(m_h) \right) (t=T) \leq C. \end{aligned}$$

In order to show that $E_2(t)$ is bounded, we cover $E_2(t)$ with a family \mathcal{B} of balls with radius $2c_1 h$ and center points $x \in \partial \Omega^I(t-h)$. The Besicovitch-Covering-Lemma assures that the covering can be chosen such that any point in $E_2(t)$ is contained in at most M different balls in \mathcal{B} , where $M \in \mathbb{N}$ is a fixed number.

With the help of the Density-Lemma 6.8 we see that there exists a constant $c_2 > 0$ such that

$$(7.3) \quad \int_{B_\varrho(x)} \chi_{\Omega^I(t) \Delta \Omega^I(t-h)} \leq \omega_3 \varrho^3 \leq c_2 \varrho \min \left\{ \left(\int_{B_\varrho(x)} \chi_{\Omega^I(t-h)} \right)^{\frac{2}{3}}, \left(\int_{B_\varrho(x)} \chi_{\mathbb{R}^3 \setminus \Omega^I(t-h)} \right)^{\frac{2}{3}} \right\}.$$

The right hand side of (7.3) can be bounded with the help of the isoperimetric inequality (6.3) which proves

$$\int_{B_\varrho(x)} \chi_{\Omega^I(t) \Delta \Omega^I(t-h)} \leq c_2 \varrho \int_{B_\varrho(x)} |\nabla \chi_{\Omega^I(t-h)}|.$$

This estimate holds for each ball $B \in \mathcal{B}$ and the union over all elements of \mathcal{B} yields

$$|E_2(lh)| \leq c_1 c_2 M h \int_{\Omega} |\nabla \chi_{\Omega^I((l-1)h)}|.$$

After summation we get

$$\sum_{l=1}^N |E_2(lh)| \leq \sum_{l=1}^N c_2 h \int_{\Omega} |\nabla \chi_{\Omega^I((l-1)h)}| \leq C.$$

The generalisation to arbitrary $\tau \in (0, T)$ is straightforward. \square

LEMMA 7.3 (Compactness of χ_h in time II). *The discrete solution χ_h fulfills*

$$\int_{\Omega} |\chi_h(x, t + \tau) - \chi_h(x, t)| \leq C\tau^{\frac{1}{2}}$$

for all $h \leq \tau \leq T - t$.

Proof. Assume that $\tau = kh$ and $t = mh$ for $k, m \in \mathbb{N}$. As in Lemma 7.2 we conclude

$$\begin{aligned} \int_{\Omega} |\chi_h(x, t + \tau) - \chi_h(x, t)| &\leq \int_{\Omega} \sum_{l=0}^{k-1} |\chi_h(x, (m+l+1)h) - \chi_h(x, (m+l)h)| \\ &= \sum_{l=0}^{k-1} |\Omega^I((m+l+1)h) \Delta \Omega^I((m+l)h)|. \end{aligned}$$

Therefore it is enough to prove

$$\sum_{l=0}^{k-1} |\Omega^I((m+l+1)h) \Delta \Omega^I((m+l)h)| \leq C\tau^{\frac{1}{2}}.$$

Here we consider the decomposition

$$\begin{aligned} \Omega^I(t) \Delta \Omega^I(t-h) &\subset \left\{ x \in \Omega^I(t) \Delta \Omega^I(t-h) \mid \text{dist}(x, \partial\Omega(t-h)) > \frac{c_2}{4} h^{\frac{3}{2}} \right\} \\ &\cup \left\{ x \in \Omega^I(t) \Delta \Omega^I(t-h) \mid \text{dist}(x, \partial\Omega(t-h)) \leq \frac{c_2}{4} h^{\frac{3}{2}} \right\}, \end{aligned}$$

where c_2 is the constant of (7.3). The proof follows like in Lemma 7.2 where we can invoke Lemma 6.8 with $\varrho = \frac{c_2}{2} h^{\frac{1}{2}}$. We obtain

$$\sum_{l=0}^{k-1} |\Omega^I((m+l+1)h) \Delta \Omega^I((m+l)h)| \leq c_2 h^{\frac{1}{2}} \leq C\tau^{\frac{1}{2}}.$$

The generalisation to arbitrary τ and t is straightforward. \square

THEOREM 7.4 (Compactness of χ_h). *There exists a subsequence of χ_h and a function $\chi \in L^1(\Omega_T, \{0, 1\})$ such that*

$$\chi_h \rightarrow \chi \quad \text{in } L^1(\Omega_T).$$

For almost all $t \in (0, T)$ the function $\chi(t)$ is in $BV(\Omega)$ and is a characteristic function of a set $\Omega^I(t) \subset \Omega$. Additionally, we have the convergence of the Radon measures

$$\nabla \chi_h \rightharpoonup \nabla \chi \quad \text{in } \text{rca}(\Omega_T).$$

Proof. This is a direct consequence of the compactness properties established in Lemma 7.1 and Lemma 7.2. \square

LEMMA 7.5 (Estimate of the discrete velocity I). *There exists a constant C such that for sufficiently large speed s*

$$\int_{\{|v_h| > s\} \cap \Omega_T} |v_h| |\nabla \chi_h| < Cs^{-1}.$$

Proof. We restrict the proof to the case $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$, the other case $x \in \Omega^I(t-h) \setminus \Omega^I(t)$ can be proved accordingly.

Let $t = kh$ with $k \in \mathbb{N}$. For given $s > 0$ we fix $l \in \mathbb{N}$ and consider those $x \in \partial\Omega^I(t)$ with $x \in \partial\Omega^I(t) \cap \{2^l s < |v_h| \leq 2^{l+1} s\}$.

We cover the set

$$\partial\Omega^I(t) \cap \left\{ z \in \Omega \mid 2^l s < |v_h(z, t)| \leq 2^{l+1} s \right\}$$

with a family of balls $B \in \mathcal{B}_l$, each ball having a center $x \in \partial\Omega^I(t)$ and a radius $\frac{hs}{2}$.

By construction it holds

$$\begin{aligned} \int_{(\Omega^I(t) \setminus \Omega^I(t-h)) \cap B_{\frac{hs}{2}}(x)} |v_h| &\geq \int_{(\Omega^I(t) \setminus \Omega^I(t-h)) \cap B_{\frac{hs}{2}}(x)} \left(2^l s - \frac{1}{2} sh \right) \\ &> \int_{(\Omega^I(t) \setminus \Omega^I(t-h)) \cap B_{\frac{hs}{2}}(x)} C 2^l s \\ &= \int_{\Omega^I(t) \cap B_{\frac{hs}{2}}(x)} C 2^l s = C 2^l s \int_{B_{\frac{hs}{2}}(x)} \chi_h(t). \end{aligned}$$

With Corollary 6.5 this implies the estimate

$$\int_{(\Omega^I(t) \setminus \Omega^I(t-h)) \cap B_{\frac{hs}{2}}(x)} |v_h| > C 2^l s^4 h^3.$$

With $|v_h| < 2^{l+1} s$ and Corollary 6.6 we find the upper estimate

$$\int_{B_{\frac{hs}{2}}(x)} |v_h| |\nabla \chi_h| < \int_{B_{\frac{hs}{2}}(x)} 2^{l+1} s |\nabla \chi_h| \leq C 2^{l+1} s^3 h^2.$$

Consequently

$$\int_{B_{\frac{hs}{2}}(x)} |v_h| |\nabla \chi_h| < C h^{-1} s^{-1} \int_{(\Omega^I(t) \setminus \Omega^I(t-h)) \cap B_{\frac{hs}{2}}(x)} |v_h|$$

for every ball $B \in \mathcal{B}_l$. When taking the union of all balls in \mathcal{B}_l we arrive at

$$\int_{\{2^l s < |v_h| \leq 2^{l+1} s\}} |v_h| |\nabla \chi_h| < C s^{-1} h^{-1} \int_{\{(2^l - \frac{1}{2})s < |v_h| < (2^{l+1} + \frac{1}{2})s\} \cap (\Omega^I(t) \Delta \Omega^I(t-h))} |v_h|.$$

Summation over all $l \in \mathbb{N}$ yields

$$\int_{\{|v_h| > s\} \cap \Omega^I(t)} |v_h| |\nabla \chi_h| < C h^{-1} s^{-1} \int_{\Omega^I(t) \Delta \Omega^I(t-h)} |v_h|$$

and after integration in time

$$\int_{\{|v_h|>s\}\cap\Omega_T} |v_h|\|\nabla\chi_h\| < Ch^{-1}s^{-1} \int_0^T \int_{\Omega^I(t)\Delta\Omega^I(t-h)} |v_h| \leq Cs^{-1}.$$

The last inequality follows from the a-priori estimate (5.1) in Lemma 5.1. \square

LEMMA 7.6 (Estimate on the discrete velocity II). *There exists a constant C such that*

$$\int_{\Omega_T} v_h^2 \|\nabla\chi_h\| < C.$$

Proof. We only need to prove the assertion if $|v_h| > s$ for some $s > 0$ chosen large. As in Lemma 7.5 let $t = kh$ for $k = 1, \dots, N$ and $x \in \partial\Omega^I(t) \cap \{2^l s < |v_h| \leq 2^{l+1} s\}$ for fixed $l \in \mathbb{N}$. Again we restrict the proof to the case $x \in \Omega^I(t) \setminus \Omega^I(t-h)$.

We cover the set $\partial\Omega^I(t) \cap \{2^l s < |v_h| \leq 2^{l+1} s\}$ by a family of balls $B \in \mathcal{B}_l$ each with radius $2^{l-1}sh$ and center points $x \in \partial\Omega^I(t)$. As in Lemma 7.5 we find

$$\int_{(\Omega^I(t)\setminus\Omega^I(t-h))\cap B_{2^{l-1}sh}(x)} |v_h| > \int_{(\Omega^I(t)\setminus\Omega^I(t-h))\cap B_{2^{l-1}sh}(x)} C2^l s \geq C2^{4l-3}h^3 s^4.$$

On the other hand,

$$\int_{B_{2^{l-1}sh}(x)} v_h^2 \|\nabla\chi_h\| \leq C(2^{l+1}s)^2(2^{l-1}sh)^2 = C2^{4l-6}h^2 s^4.$$

A comparison yields

$$\int_{B_{2^{l-1}sh}(x)} v_h^2 \|\nabla\chi_h\| < Ch^{-1} \int_{(\Omega^I(t)\setminus\Omega^I(t-h))\cap B_{2^{l-1}sh}(x)} |v_h|.$$

Now we can proceed as in Lemma 7.5. \square

LEMMA 7.7 (Error in the discrete velocity). *For all test functions $\xi \in C_0^0(\Omega_T; \mathbb{R})$ it holds*

$$\lim_{h \searrow 0} \int_{\Omega_T} \left(\frac{1}{h} \text{dist}(\cdot, \partial\Omega^I(t-h)) \|\nabla\chi_h\| - \partial_t^{-h}\chi_h \right) \xi = 0$$

Proof. The principle of the proof is taken from [15], see also [21] and [20].

We subdivide the proof into two parts, the first part studies the region where the discrete velocity is high. We will show the Lemma for $\Omega \subset \mathbb{R}^3$, the following proof fails for space dimensions $n \geq 4$.

We cover the set $\Omega^I(t)\Delta\Omega^I(t-h)$ by a family $\mathcal{B}(t)$ of balls, each with radius $h^{\frac{1}{2}}$ and with center $x \in \Omega^I(t)\Delta\Omega^I(t-h)$. Let

$$\mathcal{B} := \mathcal{B}(h) \cup \mathcal{B}(2h) \cup \dots \cup \mathcal{B}(Nh).$$

(i) By $\mathcal{B}_1 \subset \mathcal{B}$ we denote that subfamily of \mathcal{B} with the property that for every ball B in \mathcal{B}_1 there exists a $z \in B \cap (\Omega^I(t) \Delta \Omega^I(t-h))$ with

$$(7.4) \quad \text{dist}(z, \Omega^I(t-h)) > h^{\frac{9}{16}}.$$

Again it is enough to consider the case $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$. We fix a ball B in \mathcal{B}_1 . With Corollary 6.5 and (7.4) we obtain

$$\int_{B_{\frac{1}{2}h^{9/16}}(x) \cap (\Omega^I(t) \setminus \Omega^I(t-h))} |v_h| > C \frac{h^{-\frac{7}{16}}}{2} \left(\frac{h^{\frac{9}{16}}}{2}\right)^3 = Ch^{\frac{5}{4}}.$$

This implies

$$(7.5) \quad \begin{aligned} \int_{B_{\sqrt{h}}(x)} |\partial_t^{-h} \chi_h| &\leq C \int_{B_{\sqrt{h}}(x)} \frac{1}{h} \leq Ch^{\frac{1}{2}} \leq Ch^{-\frac{3}{4}} \int_{B_{\frac{1}{2}h^{9/16}}(z) \cap (\Omega^I(t) \setminus \Omega^I(t-h))} |v_h| \\ &\leq ch^{-\frac{3}{4}} \int_{B_{2\sqrt{h}}(x) \cap (\Omega^I(t) \setminus \Omega^I(t-h))} |v_h|. \end{aligned}$$

The last estimate (7.5) holds because

$$B_{\frac{1}{2}h^{9/16}}(z) \subset B_{2\sqrt{h}}(x).$$

A further bound can be obtained from Lemma 6.7 and Corollary 6.6,

$$(7.6) \quad \begin{aligned} \int_{B_{\sqrt{h}}(x)} |v_h| |\nabla \chi_h| &\leq Ch^{-\frac{1}{2}} (h^{\frac{1}{2}})^2 \leq Ch^{\frac{1}{2}} \\ &\leq Ch^{-\frac{3}{4}} \int_{B_{2\sqrt{h}}(x) \cap (\Omega^I(t) \setminus \Omega^I(t-h))} |v_h|. \end{aligned}$$

When combining the estimates (7.5) and (7.6) we obtain after taking the union of all balls $B \in \mathcal{B}_1$ and after integration in time

$$(7.7) \quad \int_0^T \int_{\mathcal{B}_1} \left(|\partial_t^{-h} \chi_h| + |v_h| |\nabla \chi_h| \right) \leq Ch^{-\frac{3}{4}} \int_0^T \int_{\Omega^I(t) \setminus \Omega^I(t-h)} |v_h| \leq Ch^{\frac{1}{4}}.$$

The last inequality in (7.7) is a consequence of the a-priori estimate on v_h found in Lemma 5.1. With (7.7) the Lemma is shown for the regions with fast discrete velocity v_h and $x \in \overline{\Omega^I(t)} \setminus \Omega^I(t-h)$.

(ii) Now we discuss the regions in Ω with small discrete velocity. Let $\mathcal{B}_2 := \mathcal{B} \setminus \mathcal{B}_1$. By construction,

$$(7.8) \quad \text{dist}(z, \partial\Omega^I(t-h)) \leq h^{\frac{9}{16}}$$

for any ball $B \in \mathcal{B}_2$ and any $z \in B$. Let $\beta := \frac{17}{32}$.

For $t = kh$, $1 \leq k \leq N$ we consider the subcover $\tilde{\mathcal{B}}_2(t)$ of $\mathcal{B}_2(t)$ with balls of radius $h^\beta = h^{\frac{17}{32}}$ and center $x \in \partial\Omega^I(t)$. Also, let $\tilde{\mathcal{B}}_2 := \cup_{k=1}^N \tilde{\mathcal{B}}_2(kh)$.

The following strong assumption is sufficient to proof part (ii):
For every ball $B \in \tilde{\mathcal{B}}_2$ there exists a $\nu \in S^2$ such that

$$(7.9) \quad \max \left\{ \|\nu_1 - \nu\|_{L^\infty(B)}, \|\nu_2 - \nu\|_{L^\infty(B)} \right\} \leq \omega(h),$$

where ν_1, ν_2 denote the unit outer normals to $\Omega^I(t)$ and $\Omega^I(t-h)$, respectively. The function $\omega(h)$ converges uniformly to 0 in every ball $B \in \tilde{\mathcal{B}}_2$.

It is evident that (7.9) implies the assertion of the lemma. Indeed, (7.9) is a very strong condition as it controls the variation of the normals, thus we obtain directly

$$\left| \int_B \partial_t^{-h} \chi_h - v_h |\nabla \chi_h| \right| \leq \omega(h) \int_B |\partial_t^{-h} \chi_h|$$

for all balls $B \in \tilde{\mathcal{B}}_2$. Taking the union over all balls in $\tilde{\mathcal{B}}_2(t)$ and discrete integration in time yields for a test function $\xi \in C^0(\Omega_T; \mathbb{R})$

$$\left| \int_0^T \int_{\tilde{\mathcal{B}}_2(t)} \left(\partial_t^{-h} \chi_h - v_h |\nabla \chi_h| \right) \xi \right| \leq \|\xi\|_{L^\infty(\Omega_T)} \omega(h) \int_{\Omega_T} |\partial_t^{-h} \chi_h| \leq C\omega(h).$$

The last estimate follows from the bound on $\|\partial_t^{-h} \chi_h\|_{L^1(\Omega_T)}$ provided in Lemma 7.2.

So it remains to proof (7.9). We will use Bernstein's theorem, see [11], [10], and [9] for $n = 8$.

Assume that (7.9) does not hold. Then there exists a subsequence of balls $B_{h^\beta}(x_h)$ such that for all ν the norms $\|\nu_{\Omega^I(t)} - \nu\|_{L^\infty(B)}$, $\|\nu_{\Omega^I(t-h)} - \nu\|_{L^\infty(B)}$ do not converge to 0. We blow up the balls $B_{\sqrt{h}}(x_h)$ with a factor $h^{-\beta}$ and shift them, such that we obtain a sequence of balls with radius $h^{\frac{1}{2}-\beta}$ and center at 0. These scaled and translated balls will be denoted by $\Omega_h^\beta(t)$. The characteristic functions to $\Omega_h^\beta(t)$ are minimisers of the scaled functional F_h given by (4.3). The compactness of $BV(\Omega)$ with respect to L^1 -convergence implies that we can find a subsequence of $\chi_{\Omega_h^\beta(t)}$ and a subsequence of $\chi_{\Omega_h^\beta(t-h)}$ (denoted both as the original sequence) such that

$$\chi_h^\beta(t) := \chi_{\Omega_h^\beta(t)} \rightarrow \chi_{\mathcal{T}_1}, \quad \chi_{\Omega_h^\beta(t-h)} \rightarrow \chi_{\mathcal{T}_2} \quad \text{in } L_{\text{loc}}^1(\mathbb{R}^3)$$

for two sets $\mathcal{T}_1, \mathcal{T}_2$. Since the velocity term in the rescaled functional is scaled by a factor $h^{2\beta}$, we find due to Lemma 6.7

$$h^{2\beta} \int_{\Omega_h^\beta(t) \Delta \Omega_h^\beta(t-h)} \frac{1}{h} \text{dist}(\cdot, \partial \Omega^\beta(t-h)) \leq Ch^{2\beta} h^{-\frac{1}{2}} h^{-\beta} = Ch^{\beta-\frac{1}{2}}.$$

This shows that the velocity term in the rescaled functional converges to 0 for $h \searrow 0$. Due to (5.8), this also holds for the other terms in the scaled functional except for the area term $\int_{\Omega_h^\beta} |\nabla \chi_h^\beta|$. This implies that the sets $\mathcal{T}_1, \mathcal{T}_2$ are area-minimising in \mathbb{R}^3 . Bernstein's theorem thus yields that \mathcal{T}_i are half-spaces.

From the bound on the discrete velocity (7.8) we learn

$$\text{dist}(\cdot, \partial \Omega_h^\beta(t-h)) \leq h^{\frac{9}{16}} h^{-\beta} \rightarrow 0 \quad \text{on } B_{h^{\frac{1}{2}-\beta}}(x_h) \cap (\Omega_h^\beta(t) \Delta \Omega_h^\beta(t-h)).$$

This gives $\mathcal{T}_1 = \mathcal{T}_2 =: \mathcal{T}$ and $0 \in \partial\mathcal{T}$. Without loss of generality we may assume

$$\mathcal{T} = \{z \in \mathbb{R}^3 \mid z_3 < 0\}$$

implying $\nu = (0, 0, 1)$ for the normal to the minimising set \mathcal{T} .

Let $\varrho > 0$ be fixed. Our construction implies

$$\lim_{h \searrow 0} \varrho^{-3} \int_{B_\varrho(z)} |\nu_1 - \nu|^2 |\nabla \chi_h^\beta| = 0 \quad \text{uniformly for } z \in B_1(0) \cap \partial\Omega_h^\beta(t).$$

Now we apply the Excess-decay-lemma, see for instance [24]. It states

$$\lim_{h \searrow 0} |\nu_1(z) - \nu| = 0 \quad \text{uniformly for } z \in B_1(0) \cap \partial\Omega_h^\beta(t).$$

The same statement holds for ν_2 and $\Omega_h^\beta(t-h)$. Thus, after rescaling with factor h^β , this gives a contradiction and (7.9) is proved. \square

8. Convergence of the discrete solution. We still have to verify that the discrete solutions converge to the solution of the continuous equations. We will prove this in a series of lemmata.

From Theorem 7.4 does not follow

$$|\nabla \chi_h| \rightharpoonup |\nabla \chi| \quad \text{in rca}(\Omega_T).$$

For the proofs of this section we therefore make the following assumption

$$(8.1) \quad \int_{\Omega_T} |\nabla \chi_h| \rightarrow \int_{\Omega_T} |\nabla \chi| \quad \text{as } h \searrow 0,$$

where χ is the function of Theorem 7.4.

First we show the existence of a velocity v that satisfies (W3).

LEMMA 8.1 (Existence of limit velocity). *Let χ be the characteristic function specified in Theorem 7.4. Then there exists a velocity function v which satisfies*

$$v \in L^1((0, T); L^1(\Omega; |\nabla \chi(t)|))$$

such that (W3) is fulfilled.

Proof. Discrete integration by parts yields

$$(8.2) \quad \int_{\Omega_T} \xi \partial_t^{-h} \chi_h + \frac{1}{h} \int_{\Omega} \int_0^h \chi_{\Omega_0} \xi = - \int_{\Omega_T} \chi_h \partial_t^h \xi$$

for all $\xi \in C^\infty(\bar{\Omega} \times [0, T]; \mathbb{R})$ with $\xi(T) = 0$.

As was shown in Lemma 7.2 there exists a constant C independent of h such that

$$\int_{\Omega_T} |\partial_t^{-h} \chi_h| < C.$$

Therefore there exists a subsequence of $\partial_t^{-h} \chi_h$ with

$$\partial_t^{-h} \chi_h \rightharpoonup \nu \quad \text{in rca}(\Omega_T).$$

With Lemma 7.7 we find at once

$$(8.3) \quad v_h |\nabla \chi_h| \rightharpoonup \nu \quad \text{in rca}(\Omega_T).$$

We prove now that ν is absolutely continuous with respect to the measure $|\nabla \chi|$. Let $E \subset \Omega_T$ with $|\nabla \chi(E)| = 0$. From our assumption (8.1) we infer that there exists a function $g : \mathbb{R} \rightarrow \mathbb{R}$ with $g(h) \searrow 0$ as $h \searrow 0$ such that

$$|\nabla \chi_h(E)| \leq g(h).$$

Due to Lemma 7.5 it follows

$$\begin{aligned} \int_E |v_h| |\nabla \chi_h| &= \int_{\{|v_h| \leq s\} \cap E} |v_h| |\nabla \chi_h| + \int_{\{|v_h| > s\} \cap E} |v_h| |\nabla \chi_h| \\ &\leq sg(h) + Cs^{-1}. \end{aligned}$$

The right hand side of this estimate can be made arbitrarily small for small h , thus

$$\lim_{h \searrow 0} \int_E |v_h| |\nabla \chi_h| = 0.$$

This shows that $\nu(E) = 0$ and proves the absolute continuity of ν . The existence of $v \in L^1(0, T); L^1(\Omega; |\nabla \chi(t)|)$ satisfying

$$(8.4) \quad \nu = v |\nabla \chi|$$

follows now from the Radon-Nikodym theorem.

The measures $v_h |\nabla \chi_h|$ and $v |\nabla \chi|$ are absolutely continuous in time, furthermore we can approximate ξ in (8.2) by functions with compact support. Passing to the limit $h \searrow 0$ gives (W3). \square

LEMMA 8.2 (Convergence of advection term in weak curvature equation). *Let χ be the characteristic function specified in Theorem 7.4 and v be the function specified in Lemma 8.1. Then it holds*

$$\lim_{h \searrow 0} \int_{\Omega_T} v_h \zeta \nabla \chi_h = \int_{\Omega_T} v \zeta \nabla \chi$$

for all $\zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$.

Proof. As $|\nabla \chi|$ is a Radon measure there exists for any $\varepsilon > 0$ a vector-valued mapping $g_\varepsilon \in C^0(\Omega_T; \mathbb{R}^3)$, $|g_\varepsilon| \leq 1$ such that

$$\int_{\Omega_T} |\nabla \chi| - \int_{\Omega_T} g_\varepsilon \nabla \chi < \varepsilon.$$

Consequently,

$$(8.5) \quad \lim_{h \searrow 0} \left(\int_{\Omega_T} |\nabla \chi_h| - \int_{\Omega_T} g_\varepsilon \nabla \chi_h \right) = \int_{\Omega_T} |\nabla \chi| - \int_{\Omega_T} g_\varepsilon \nabla \chi < \varepsilon.$$

With the notations

$$\nu_h := \frac{\nabla \chi_h}{|\nabla \chi_h|}, \quad \nu := \frac{\nabla \chi}{|\nabla \chi|}$$

we find

$$\begin{aligned} \int_{\Omega_T} (\nu_h - g_\varepsilon)^2 |\nabla \chi_h| &= \int_{\Omega_T} (1 - 2g_\varepsilon \nu_h + g_\varepsilon^2) |\nabla \chi_h| = \int_{\Omega_T} (2 - 2g_\varepsilon \nu_h + g_\varepsilon^2 - 1) |\nabla \chi_h| \\ &\leq 2 \int_{\Omega_T} (1 - g_\varepsilon \nu_h) |\nabla \chi_h|. \end{aligned}$$

This estimate in combination with (8.5) yields

$$(8.6) \quad \lim_{h \searrow 0} \int_{\Omega_T} (\nu_h - g_\varepsilon)^2 |\nabla \chi_h| < 2\varepsilon.$$

This result together with Hölder's inequality and the boundedness of $(\int_{\Omega_T} |\nabla \chi_h|)^{\frac{1}{2}}$ implies

$$\lim_{h \searrow 0} \int_{\Omega_T} |\nu_h - g_\varepsilon| |\nabla \chi_h| \leq C \lim_{h \rightarrow 0} \left(\int_{\Omega_T} (\nu_h - g_\varepsilon)^2 |\nabla \chi_h| \right)^{\frac{1}{2}} \leq C(2\varepsilon)^{\frac{1}{2}}.$$

In the same way we compute with Lemma 7.6 and Hölder's inequality

$$(8.7) \quad \begin{aligned} \lim_{h \searrow 0} \int_{\Omega_T} |v_h| |g_\varepsilon - \nu_h| |\nabla \chi_h| &\leq \left(\int_{\Omega_T} |v_h|^2 |\nabla \chi_h| \right)^{\frac{1}{2}} \left(\int_{\Omega_T} (\nu_h - g_\varepsilon)^2 |\nabla \chi_h| \right)^{\frac{1}{2}} \\ &\leq C(2\varepsilon)^{\frac{1}{2}}. \end{aligned}$$

Now we are prepared to show the assertion of the lemma. We see

$$\begin{aligned} \left| \int_{\Omega_T} v_h \zeta \nabla \chi_h - v \zeta \nabla \chi \right| &= \left| \int_{\Omega_T} v_h \zeta \nu_h |\nabla \chi_h| - v \zeta \nu |\nabla \chi| \right| \\ &\leq \left| \int_{\Omega_T} v_h \zeta \nu_h |\nabla \chi_h| - v \zeta g_\varepsilon |\nabla \chi| \right| + \left| \int_{\Omega_T} v \zeta g_\varepsilon |\nabla \chi| - v \zeta \nu |\nabla \chi| \right| \\ &=: I_1(\varepsilon, h) + I_2(\varepsilon). \end{aligned}$$

We estimate I_1 and I_2 independently. For the first integral we have

$$(8.8) \quad I_1(\varepsilon, h) \leq \int_{\Omega_T} |v_h| |\zeta| |\nu_h - g_\varepsilon| |\nabla \chi_h| + \left| \int_{\Omega_T} v_h \zeta g_\varepsilon |\nabla \chi_h| - v \zeta g_\varepsilon |\nabla \chi| \right|.$$

Estimate (8.7) confirms the convergence of the first integral in (8.8), the properties (8.3) and (8.4) lead to the convergence of the second integral, so

$$\lim_{\varepsilon \searrow 0} \lim_{h \searrow 0} I_1(\varepsilon, h) \leq \lim_{\varepsilon \searrow 0} C\varepsilon^{\frac{1}{2}} = 0.$$

For the integral $I_2(\varepsilon)$ we get directly

$$I_2(\varepsilon) \leq \omega(\varepsilon)$$

for a function $\omega(\varepsilon)$ that tends to 0 as ε tends to 0. In conclusion we have found

$$\lim_{h \searrow 0} \left| \int_{\Omega_T} v_h \zeta \nabla \chi_h - v \zeta \nabla \chi \right| = 0$$

and the proof is finished. \square

LEMMA 8.3 (Convergence of the weak curvature term). *Let χ be the characteristic function specified in Theorem 7.4. Then it holds*

$$\lim_{h \searrow 0} \int_{\Omega_T} \nu_h \nabla \zeta \nu_h |\nabla \chi_h| = \int_{\Omega_T} \nu \nabla \zeta \nu |\nabla \chi|$$

for all $\zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$.

Proof. For $\varepsilon > 0$ and the family g_ε of mappings introduced in Lemma 8.2 one has

$$\begin{aligned} \left| \int_{\Omega_T} \nu_h \nabla \zeta \nu_h |\nabla \chi_h| - \int_{\Omega_T} \nu \nabla \zeta \nu |\nabla \chi| \right| &\leq \left| \int_{\Omega_T} \nu_h \nabla \zeta \nu_h |\nabla \chi_h| - \int_{\Omega_T} g_\varepsilon \nabla \zeta g_\varepsilon |\nabla \chi_h| \right| \\ &\quad + \left| \int_{\Omega_T} g_\varepsilon \nabla \zeta g_\varepsilon |\nabla \chi_h| - \int_{\Omega_T} g_\varepsilon \nabla \zeta g_\varepsilon |\nabla \chi| \right| \\ &\quad + \left| \int_{\Omega_T} g_\varepsilon \nabla \zeta g_\varepsilon |\nabla \chi| - \int_{\Omega_T} \nu \nabla \zeta \nu |\nabla \chi| \right|. \end{aligned}$$

With the help of (8.6) and (8.1) we see that the right hand side of this estimate converges to 0 as $h \searrow 0$ and $\varepsilon \searrow 0$. \square

It is well known that Condition (8.1) together with the convergence of $\chi_h \rightarrow \chi$ in $L^1(\Omega_T)$ as stated in Theorem 7.4 implies the convergence of the mean curvature term. This is a consequence of the Lemma of Reshetnyak, which we state for the reader's convenience.

LEMMA 8.4 (Lemma of Reshetnyak). *Let μ_h be a sequence of vector-valued measures in $\Omega \subset \mathbb{R}^n$ with*

$$\mu_h \rightarrow \mu \quad \text{in } \text{rca}(\Omega; \mathbb{R}^n)$$

and

$$|\mu_h|(\Omega) \rightarrow |\mu|(\Omega).$$

Then for all bounded continuous functions in $S^{n-1} \times \Omega$ it holds

$$f\left(\frac{\mu_h}{|\mu_h|}, \cdot\right) |\mu_h| \rightarrow f\left(\frac{\mu}{|\mu|}, \cdot\right) |\mu| \quad \text{in } \text{rca}(\Omega; \mathbb{R}^n),$$

where $\frac{\mu}{|\mu|}$ is defined by the Radon-Nikodym theorem.

Proof. The proof is similar to the proof of Lemma 8.3, see [18]. \square

Now we discuss the convergence of the discrete chemical potentials.

LEMMA 8.5 (Convergence of μ_h^D). *There exists a function $\mu^D \in L^2(0, T; H^{1,2}(\Omega))$ and a subsequence μ_h^D such that for $h \searrow 0$*

$$\mu_h^D \rightharpoonup \mu^D \quad \text{in } L^2(0, T; H^{1,2}(\Omega))$$

and

$$(1 - \chi)\mu_D = (1 - \chi)\varphi \quad \text{for almost every } (x, t) \in \Omega_T.$$

We recall that φ are the boundary conditions on μ^D given by (2.25).

Proof. Due to the a-priori estimates we have for a constant C independent of h

$$\int_{\Omega_T} |\nabla \mu_h^D|^2 \leq C.$$

Together with the boundary conditions for μ_h^D and the Poincaré inequality this yields

$$\|\mu_h^D\|_{L^2(0, T; H^{1,2}(\Omega))} \leq C.$$

The second assertion of the lemma follows directly from the a-priori estimate which ensures

$$\int_{\Omega_T} (1 - \chi_h(t - h)) |\nabla \mu_h^D|^2 \rightarrow 0 \quad \text{for } h \searrow 0.$$

This proves the lemma. \square

LEMMA 8.6 (Convergence of μ_h^N). *There exists a function $\mu^N \in L^2(0, T; H^{1, \frac{3}{2}}(\Omega))$ and a subsequence μ_h^N such that for $h \searrow 0$*

$$\mu_h^N \rightharpoonup \mu^N \quad \text{in } L^2(0, T; L^{\frac{3}{2}}(\Omega)),$$

with

$$(1 - \chi)\mu^N = 0 \quad \text{for almost every } (x, t) \in \Omega_T.$$

Proof. For any $h > 0$ let $\alpha = \alpha(h) > 0$ be a small real number with $\alpha(h) \searrow 0$ as $h \searrow 0$. We define the mapping $\mu_h^{N, \alpha}$ by

$$\mu_h^{N, \alpha} := \begin{cases} (|\mu_h^N| - \alpha)_+ \frac{\mu_h^N}{|\mu_h^N|} & \text{if } \mu_h^N \neq 0, \\ 0 & \text{else.} \end{cases}$$

For this truncated chemical potential we compute with the chain rule

$$\begin{aligned} \int_{\Omega_T} (1 - \chi_h(t - h)) |\nabla \mu_h^{N, \alpha}|^{\frac{3}{2}} &= \int_{\Omega_T \cap \{|\mu_h^{N, \alpha}| > \alpha\}} (1 - \chi_h(t - h)) |\nabla \mu_h^{N, \alpha}|^{\frac{3}{2}} \\ &\leq \int_{\Omega_T \cap \{|\mu_h^{N, \alpha}| > \alpha\}} (1 - \chi_h(t - h)) |\nabla ((\mu_h^{N, \alpha})^{\frac{5}{4}})|^{\frac{3}{2}} \alpha^{-\frac{3}{8}} \\ &\leq \alpha^{-\frac{3}{8}} \left(\int_{\Omega_T} (1 - \chi_h(t - h)) |\nabla \mu_h^{N, \alpha}|^2 \right)^{\frac{3}{4}} \left(\int_{\Omega_T} (1 - \chi_h(t - h)) |\mu_h^{N, \alpha}|^{\frac{3}{2}} \right)^{\frac{1}{4}}, \end{aligned}$$

where Hölder's inequality was used to get the last line.

We apply the a-priori estimates (5.3) and (5.5) and obtain

$$\int_{\Omega_T} (1 - \chi_h(t-h)) |\nabla \mu_h^{N,\alpha}|^{\frac{3}{2}} \leq C \alpha^{-\frac{3}{8}} \varepsilon^{-\frac{3}{4}} \gamma^{\frac{3}{16}} \leq C.$$

Here we chose $\alpha(h)$ such that $\alpha^{-\frac{3}{8}} \varepsilon^{-\frac{3}{4}} \gamma^{\frac{3}{16}}$ is bounded uniformly in h . So we have found

$$\int_{\Omega_T} |\nabla \mu_h^{N,\alpha}|^{\frac{3}{2}} \leq C.$$

With the boundary conditions for μ_h^N this ensures the existence of a subsequence, again denoted by $\mu_h^{N,\alpha}$, and the existence of a function $\mu^{N,\alpha} \in L^2(0, T; H^{1, \frac{3}{2}}(\Omega))$ with

$$\mu_h^{N,\alpha} \rightharpoonup \mu^{N,\alpha} \quad \text{in } L^2(0, T; H^{1, \frac{3}{2}}(\Omega)).$$

Also we can pick a subsequence $\alpha(h)$ with

$$\mu^{N,\alpha} \rightharpoonup \mu^N \quad \text{in } L^2(0, T; H^{1, \frac{3}{2}}(\Omega))$$

for a suitable $\mu^N \in L^2(0, T; H^{1, \frac{3}{2}}(\Omega))$.

Finally, by definition of $\mu_h^{N,\alpha}$, we have for every $\alpha \geq 0$ and every $h > 0$

$$\|\mu_h^N - \mu_h^{N,\alpha}\|_{L^2(0, T; L^{\frac{3}{2}}(\Omega))} \leq C\alpha.$$

By construction it thus holds for $h \searrow 0$

$$\mu_h^N \rightharpoonup \mu^N \quad \text{in } L^2(0, T; L^{\frac{3}{2}}(\Omega)).$$

The second claim of the lemma is again a consequence of the a-priori estimate (5.5) which shows as $\gamma(h) \searrow 0$ for $h \searrow 0$

$$\int_{\Omega_T} (1 - \chi_h(t-h)) |\mu_h^N|^2 \rightarrow 0 \quad \text{as } h \searrow 0.$$

This ends the proof. \square

LEMMA 8.7. *Let χ be the characteristic function specified in Theorem 7.4. Then it holds*

$$\lim_{h \searrow 0} \int_{\Omega_T} f_{II}^*(\mu_h) \zeta \nabla \chi_h = \int_{\Omega_T} K \zeta \nabla \chi$$

for all $\zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$, where $K := f_{II}^{D,*}(\varphi)$.

Proof. We reformulate the left hand side. For a test function $\zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$ we compute

$$\begin{aligned} \int_{\Omega_T} f_{II}^*(\mu_h) \zeta \nabla \chi_h &= \int_{\Omega_T} (1 - \chi_h) f_{II}^{D,*}(\mu_h^D) \operatorname{div}(\zeta) + \int_{\Omega_T} (1 - \chi_h) m_h^D \nabla \mu_h^D \zeta \\ &\quad + \int_{\Omega_T} (1 - \chi_h) f_{II}^{N,*}(\mu_h^N) \operatorname{div}(\zeta) + \int_{\Omega_T} (1 - \chi_h) m_h^N \nabla \mu_h^N \zeta \\ &=: I_1 + I_2 + I_3 + I_4. \end{aligned}$$

Using the convexity of $f_{II}^{D,*}$ and Lemma 8.5 we have for I_1

$$\lim_{h \searrow 0} \int_{\Omega_T} (1 - \chi_h) f_{II}^{D,*}(\mu_h^D) \operatorname{div}(\zeta) = \int_{\Omega_T} (1 - \chi) f_{II}^{D,*}(\varphi) \operatorname{div}(\zeta).$$

So it remains to show that $I_k \rightarrow 0$ as $h \searrow 0$ for $k = 2, 3, 4$. For I_2 this results from

$$|I_2| \leq C \int_{\Omega_T} |\chi_h(t-h) - \chi_h| |\nabla \mu_h^D| |\zeta| + \int_{\Omega_T} (1 - \chi_h(t-h)) |\nabla \mu_h^D| |\zeta|,$$

and the a-priori estimates and Lemma 7.2 yield as desired $|I_2| \searrow 0$ as $h \searrow 0$.

From $\mu = \frac{\partial f_{II}}{\partial m}$ in $\Omega \setminus \overline{\Omega^I}$ we get

$$m_i^N = \exp(\mu_i^N) \delta \quad \text{for } i = 1, 2$$

and consequently

$$f_{II}^{N,*}(\mu_h^N) = k_B \theta \delta \sum_{i=1}^2 \exp\left(\frac{\mu_{h,i}^N}{k_B \theta}\right).$$

Lemma 8.6 therefore implies $|I_3| \searrow 0$ as $\delta(h) \searrow 0$.

Finally,

$$|I_4| = C \left| \int_{\Omega_T} \delta(1 - \chi_h) \exp(\mu^N) \nabla \mu_h^N \right| \leq C \delta \varepsilon^{-1},$$

where we use again the a-priori estimates and Hölder's inequality. With Assumption (A2) we obtain $|I_2| \searrow 0$ as $h \searrow 0$ and the lemma is proved. \square

LEMMA 8.8. *Let χ be the characteristic function specified in Theorem 7.4. Then it holds*

$$\lim_{h \searrow 0} \int_{\Omega_T} f_I^*(\mu_h) \zeta \nabla \chi_h = \int_{\Omega_T} f_I^*(\mu) \zeta \nabla \chi$$

for all $\zeta \in C^1([0, T] \times \overline{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$, where $\mu = (\mu^N, \mu^D)$.

Proof. We reformulate the left hand side. For a test function $\zeta \in C^1([0, T] \times \overline{\Omega}; \mathbb{R}^3)$ with $\zeta = 0$ on $\partial\Omega \times (0, T)$ we compute

$$(8.9) \quad \int_{\Omega_T} f_I^*(\mu_h) \zeta \nabla \chi_h = - \int_{\Omega_T} \chi_h f_I^*(\mu_h) \operatorname{div}(\zeta) - \int_{\Omega_T} \chi_h m_h \nabla \mu_h \zeta.$$

From the convexity of f_I^* together with Lemma 8.5 and Lemma 8.6 it follows directly

$$\lim_{h \searrow 0} \int_{\Omega_T} \chi_h f_I^*(\mu_h) \operatorname{div}(\zeta) = \int_{\Omega_T} \chi_h f_I^*(\mu^N, \mu^D) \operatorname{div}(\zeta).$$

The proof is finished if we can show the convergence of the second integral on the right in (8.9) for $h \searrow 0$, but this is quite involved.

We use the definition

$$m_h^\beta := \begin{cases} m_h & \text{if } \beta < |m_h| < 1 - \beta, \\ 0 & \text{else.} \end{cases}$$

to reformulate the second integral on the right in (8.9). Since $\frac{\partial f_I^*}{\partial \mu}(\mu)$ is locally a Lipschitz function, we have for arbitrary vectors μ_1, μ_2

$$\left| \frac{\partial f_I^*}{\partial \mu}(\mu_1) - \frac{\partial f_I^*}{\partial \mu}(\mu_2) \right| \leq C|\mu_1 - \mu_2|,$$

where C depends on μ_1, μ_2 and $C \rightarrow \infty$ for $\mu_1, \mu_2 \rightarrow \infty$. So we can estimate

$$\begin{aligned} \int_{\Omega_T} \chi_h |\nabla m_h^\beta|^{\frac{3}{2}} &\leq \int_{\Omega_T} \chi_h(t-h) |\nabla m_h^\beta|^{\frac{3}{2}} + \int_{\Omega_T} |\chi_h - \chi_h(t-h)| |\nabla m_h^\beta|^{\frac{3}{2}} \\ &\leq C \left(\int_{\Omega_T} \chi_h(t-h) |\nabla m_h^\beta|^2 \right)^{\frac{3}{4}} + C \left(\int_{\Omega_T} |\chi_h - \chi_h(t-h)| \right)^{\frac{1}{4}} \left(\int_{\Omega_T} |\nabla m_h^\beta|^2 \right)^{\frac{3}{4}} \\ &\leq C(\varepsilon^{-\frac{3}{4}} h^{\frac{1}{4}} + 1). \end{aligned}$$

Due to Assumption (A3) the right hand side converges to 0 as $h \searrow 0$.

For functions $\varphi, \psi \in C^\infty(B_1(0); \mathbb{R}^+)$ we introduce mollifiers φ_ϱ and ψ_σ by setting $\varphi_\varrho(x) := \varrho^{-3}\varphi(x/\varrho)$ and $\psi_\sigma(t) := \sigma^{-3}\psi(t/\sigma)$. It holds $\text{supp } \varphi_\varrho \subset B_\varrho(0)$, $\text{supp } \psi_\sigma \subset B_\sigma(0)$. We consider sequences (ϱ, σ) with $\sigma^{\frac{1}{2}}\varrho^{-1} \rightarrow 0$. Then we have the estimate

$$\begin{aligned} \int_{\Omega_T} |(\chi_h m_h^\beta) * \varphi_\varrho * \psi_\sigma - \chi_h m_h^\beta| &\leq \int_{\Omega_T} |(\chi_h m_h^\beta) * \varphi_\varrho * \psi_\sigma - (\chi_h m_h^\beta) * \varphi_\varrho| \\ &\quad + \int_{\Omega_T} |(\chi_h m_h^\beta) * \varphi_\varrho - \chi_h m_h^\beta| \\ &\leq C\sigma^{\frac{1}{2}}\varrho^{-1} \|\partial_t^h(\chi_h m_h^\beta)\|_{L^2(0,T; H^{-1,2}(\Omega))} + C\varrho \left(\int_{\Omega_T} |\nabla(\chi_h m_h^\beta)| + 1 \right). \end{aligned}$$

Taking (5.6) into account we arrive at

$$\int_{\Omega_T} |(\chi_h m_h^\beta) * \varphi_\varrho * \psi_\sigma - \chi_h m_h^\beta| \leq C(\sigma^{\frac{1}{2}}\varrho^{-1} + \varrho),$$

which holds uniformly in h . It follows that there exists a subsequence of $\chi_h m_h^\beta$ (denoted as the original sequence) and a function $\Gamma \in L^1(\Omega_T)$ such that

$$(8.10) \quad \chi_h m_h^\beta \rightarrow \Gamma \quad \text{in } L^1(\Omega_T).$$

Additionally,

$$\|\chi_h m_h - \Gamma\|_{L^1(\Omega_T)} \leq \|\chi_h m_h - \chi_h m_h^\beta\|_{L^1(\Omega_T)} + \|\chi_h m_h^\beta - \Gamma\|_{L^1(\Omega_T)},$$

and the right side of this estimate converges to 0 for $h \searrow 0$. With (8.10) this ensures the strong convergence of a subsequence $\chi_h m_h$ in $L^1(\Omega_T)$. Furthermore we know that there exists a subsequence of m_h such that for any $1 \leq p < \infty$

$$m_h \rightarrow m \quad \text{in } L^p(\Omega_T) \text{ for } h \searrow 0.$$

This yields $\chi_h m_h \rightarrow \chi m$ in $L^p(\Omega_T)$ and finally

$$(8.11) \quad \chi_h m_h \rightarrow \chi m \quad \text{in } L^p(\Omega_T) \text{ for } h \searrow 0.$$

Next we will show

$$\chi_h \nabla \mu_h \zeta \rightarrow \chi \nabla \mu \zeta \quad \text{in } L^2(0, T; L^{\frac{6}{5}}(\Omega)).$$

We use again the mapping $\mu_h^{N, \alpha}$ from the proof of Lemma 8.6. We define the mapping $\mu_{h, \alpha}^N$ by

$$\mu_{h, \alpha}^N := \begin{cases} \min\{\alpha, |\mu_h^{N, \alpha}|\} \frac{\mu_h^N}{|\mu_h^N|} & \text{if } \mu_h^N \neq 0, \\ 0 & \text{else.} \end{cases}$$

From the definitions we get

$$\int_{\Omega_T} \chi_h(t-h) \nabla \mu_h^N \zeta = \int_{\Omega_T} \chi_h(t-h) \nabla \mu_{h, \alpha}^{N, \alpha} \zeta + \int_{\Omega_T} \chi_h(t-h) \nabla \mu_{h, \alpha}^N \zeta$$

leading to

$$(8.12) \quad \begin{aligned} \left| \int_{\Omega_T} \chi_h(t-h) \nabla \mu_{h, \alpha}^N \zeta \right| &\leq C \int_{\Omega_T} |\mu_{h, \alpha}^N| |\nabla(\chi_h(t-h)\zeta)| \\ &\leq C\alpha \int_{\Omega_T} |\nabla(\chi_h(t-h)\zeta)| \leq C\alpha. \end{aligned}$$

Also we have the convergence

$$\int_{\Omega_T} \chi_h(t-h) \nabla \mu_{h, \alpha}^{N, \alpha} \zeta \rightarrow \int_{\Omega_T} \chi \nabla \mu^N \zeta$$

which leads with (8.12) to

$$(8.13) \quad \int_{\Omega_T} \chi_h(t-h) \nabla \mu_h^N \zeta \rightarrow \int_{\Omega_T} \chi \nabla \mu^N \zeta$$

From the a-priori estimates we can deduce

$$\chi_h(t-h) \nabla \mu_h^N \rightharpoonup \Lambda \quad \text{in } L^2(0, T; L^2(\Omega)),$$

therefore

$$(8.14) \quad \int_{\Omega_T} \chi_h(t-h) \nabla \mu_h^N \zeta \rightarrow \int_{\Omega_T} \Lambda \zeta \quad \text{for } h \searrow 0.$$

From (8.13) and (8.14) we obtain

$$\int_{\Omega_T} (\chi \nabla \mu^N - \Lambda) \zeta = 0 \quad \text{for all } \zeta \in C^1([0, T] \times \bar{\Omega}; \mathbb{R}^3) \text{ with } \zeta = 0 \text{ on } \partial\Omega \times (0, T).$$

Consequently,

$$\chi \nabla \mu^N = \Lambda \quad \text{for almost every } (x, t) \in \Omega_T.$$

So we have shown

$$\chi_h(t-h) \nabla \mu_h^N \zeta \rightharpoonup \chi \nabla \mu^N \zeta \quad \text{in } L^2(0, T; L^2(\Omega)) \quad \text{for } h \searrow 0.$$

Fix an arbitrary $g \in L^2(0, T; L^6(\Omega))$. We rewrite the integrand in the form

$$\int_{\Omega_T} \chi_h \nabla \mu_h^N \zeta g = \int_{\Omega_T} (\chi_h - \chi_h(t-h)) \nabla \mu_h^N \zeta g + \int_{\Omega_T} \chi_h(t-h) \nabla \mu_h^N \zeta g.$$

With Lemma 7.3 and Hölder's inequality we can find the estimate

$$\begin{aligned} \left| \int_{\Omega_T} (\chi_h - \chi_h(t-h)) \nabla \mu_h^N \zeta g \right| &\leq C \left(\int_{\Omega} |\chi_h - \chi_h(t-h)| \right)^{\frac{2}{3}} \left(\int_{\Omega_T} |\mu_h^N|^2 \right)^{\frac{1}{2}} \|g\|_{L^2(0, T; L^6(\Omega))} \\ &\leq Ch^{\frac{1}{3}} \varepsilon^{-1} \|g\|_{L^2(0, T; L^6(\Omega))}. \end{aligned}$$

With Assumption (A4) this yields

$$(8.15) \quad \chi_h \nabla \mu_h^N \zeta \rightharpoonup \chi \nabla \mu^N \zeta \quad \text{in } L^2(0, T; L^{\frac{6}{5}}(\Omega)) \quad \text{for } h \searrow 0.$$

The statements (8.11) and (8.15) combined give

$$\int_{\Omega_T} \chi_h m_h^N \nabla \mu_h^N \zeta \rightarrow \int_{\Omega_T} \chi m^N \nabla \mu^N \zeta \quad \text{for } h \searrow 0.$$

The proof of convergence for the Dirichlet data is analogous. Now we can pass to the limit $h \searrow 0$ in (8.9). \square

The following theorem is now a direct consequence of the Lemmata shown above.

THEOREM 8.9 (Existence of weak solutions). *Let $\Omega \subset \mathbb{R}^3$ be an open bounded set with Lipschitz boundary and let the no-loss of area condition (8.1) hold. Let $\chi_0 \in BV(\Omega)$, $\mu_0 \in H^{1,2}(\Omega)$. Then there exists (m, μ, χ, v) with*

$$\begin{aligned} \chi &\in L^\infty(0, T; BV(\Omega; \{0, 1\})), \quad \text{supp } \chi(t) \subset\subset \Omega \text{ for all } 0 < t < T, \\ v &\in L^1(0, T; L^1(\Omega; \mathbb{R}; |\nabla \chi(t)|)), \\ \mu &= (\mu^N, \mu^D), \quad \mu^N \in L^2(0, T; H^{1, \frac{3}{2}}(\Omega)), \quad \mu^D \in L^2(0, T; H^{1,2}(\Omega)), \\ (1 - \chi)\mu^N &= 0, \quad (1 - \chi)\mu^D = (1 - \chi)\varphi \quad \text{for almost all } (x, t) \in \Omega_T, \end{aligned}$$

such that (m, μ, χ) is a weak solution in the sense of Section 3.

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