ESAIM: M2AN 52 (2018) 2357–2408
https://doi.org/10.1051/m2an/2018042

ESAIM: Mathematical Modelling and Numerical Analysis
www.esaim-m2an.org

ON CONVERGENT SCHEMES FOR TWO-PHASE FLOW OF DILUTE POLYMERIC SOLUTIONS

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Abstract. We construct a Galerkin finite element method for the numerical approximation of weak solutions to a recent micro-macro bead-spring model for two-phase flow of dilute polymeric solutions derived by methods from nonequilibrium thermodynamics ([Grün, Metzger, *M3AS* **26** (2016) 823–866]). The model consists of Cahn–Hilliard type equations describing the evolution of the fluids and the unsteady incompressible Navier–Stokes equations in a bounded domain in two or three spatial dimensions for the velocity and the pressure of the fluids with an elastic extra-stress tensor on the right-hand side in the momentum equation which originates from the presence of dissolved polymer chains. The polymers are modeled by dumbbells subjected to a finitely extensible, nonlinear elastic (FENE) spring-force potential. Their density and orientation are described by a Fokker–Planck type parabolic equation with a center-of-mass diffusion term. We perform a rigorous passage to the limit as the spatial and temporal discretization parameters simultaneously tend to zero, and show that a subsequence of these finite element approximations converges towards a weak solution of the coupled Cahn–Hilliard–Navier–Stokes–Fokker–Planck system. To underline the practicality of the presented scheme, we provide simulations of oscillating dilute polymeric droplets and compare their oscillatory behaviour to the one of Newtonian droplets.

Mathematics Subject Classification. 35Q30, 35Q35, 35Q84, 65M12, 65M60, 76A05, 82D60, 76T99.

Received April 19, 2017. Accepted June 25, 2018.

1. Introduction

In this paper, we present a stable, fully discrete finite-element scheme for a diffuse interface model for two-phase flow of dilute polymeric solutions and establish convergence for the case of equal fluid mass densities. Allowing for different solubility properties which are modelled by some phase dependent cost functional β, the presented model covers the case of two dilute polymeric solutions as well as the case of one dilute polymeric solution and one pure Newtonian fluid. In contrast to other approaches (see *e.g.* [7, 8]) our scheme solely relies on standard finite element functions. In particular, it does not include simplices with curved edges or faces. The presented results are excerpts from the author's Ph.D. thesis [25].

Keywords and phrases. Convergence of finite-element schemes, existence of weak solutions, polymeric flow model, two-phase flow, diffuse interface models, Navier–Stokes equations, Fokker–Planck equations, Cahn–Hilliard equations, FENE.

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The aforementioned model derived by G. Grün and S. Metzger ([18]) combines a diffuse interface model for two-phase flow of incompressible, viscous fluids (*cf.* [1]) for the description of the immiscible fluids in an open domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3, with a FENE-dumbbell description of the dissolved polymer chains. That is a polymer chain is represented by two beads connected by a massless spring (*cf.* [5, 22]) and can be described by the position of its barycenter and the configurational vector $\mathbf{q}$ connecting the beads. Using the so called FENE spring potential (FENE: acronym for *f*initely *e*xtensible, *n*onlinear *e*lastic), which reads

$$U\left(\tfrac{1}{2}|\mathbf{q}|^2\right) = -\tfrac{Q_{\max}^2}{2}\ln\left(1-\tfrac{|\mathbf{q}|^2}{Q_{\max}^2}\right), \tag{1.1}$$

restricts the admissible polymer elongations to

$$\mathbf{q} \in D := B(0, Q_{\max}), \tag{1.2}$$

where $B(0, Q_{\max})$ is a bounded, open, origin centered ball with radius $Q_{\max}$. Associated with the potential, there comes the Maxwellian

$$M(\mathbf{q}) := \frac{\exp\left(-U\left(\frac{1}{2}|\mathbf{q}|^2\right)\right)}{\int_D \exp\left(-U\left(\frac{1}{2}|\overline{\mathbf{q}}|^2\right)\right)\,\mathrm{d}\overline{\mathbf{q}}}, \tag{1.3}$$

which provides the energetically most favorable probability density of the elongation of a polymer chain. A straight forward computation shows that

$$M\nabla_{\mathbf{q}}M^{-1} = -M^{-1}\nabla_{\mathbf{q}}M = U'\mathbf{q}. \tag{1.4}$$

As shown in [5], the FENE-potential defined in (1.1) and the Maxwellian satisfy the following properties on the corresponding set of admissible elongations D.

(P1) $\mathbf{q} \mapsto U\left(\frac{1}{2}|\mathbf{q}|^2\right) \in C^\infty(D)$, nonnegative;

(P2) $\mathbf{q} \mapsto U'\left(\frac{1}{2}|\mathbf{q}|^2\right)$ is positive on D;

(P3) there exist constants $c_i > 0$ $(i = 1, \ldots, 5)$ such that for $\kappa = \frac{Q_{\max}^2}{2}$ the following inequalities hold true:

$$c_1[\operatorname{dist}(\mathbf{q}, \partial D)]^\kappa \le M(\mathbf{q}) \le c_2[\operatorname{dist}(\mathbf{q}, \partial D)]^\kappa \qquad \forall \mathbf{q} \in D,$$
$$c_3 \le [\operatorname{dist}(\mathbf{q}, \partial D)]U'\left(\tfrac{1}{2}|\mathbf{q}|^2\right) \le c_4, \qquad [\operatorname{dist}(\mathbf{q}, \partial D)]^2\left|U''\left(\tfrac{1}{2}|\mathbf{q}|^2\right)\right| \le c_5 \qquad \forall \mathbf{q} \in D,$$

(P4) $\int_D \left[1 + \left(1+|\mathbf{q}|^2\right)\left((U)^2 + |\mathbf{q}|^2 (U')^2\right)\right] M\,\mathrm{d}\mathbf{q} < \infty.$

Under the additional assumption $Q_{\max} > \sqrt{2}$, the FENE-potential additionally satisfies the following estimates:

(P5) There exist constants c_6, $c_7 > 0$, such that for $B(0, (\frac{d}{c_7})^{1/2}) \subset\subset D$

$$(U')^2 - U'' \ \ge c_6 \quad \forall \mathbf{q} \in D \qquad \text{and} \qquad (U')^2 - U'' \ge 2c_7U' \quad \forall \mathbf{q} \in D : |\mathbf{q}|^2 \ge \tfrac{d}{c_7}.$$

In [18], spatial distribution and configuration of the polymer chains is described by the configurational density $\psi : \Omega \times D \times \mathbb{R}_0^+ \to \mathbb{R}_0^+$. Following the approach in [7], we define the scaled configurational density function $\hat{\psi} := \frac{\psi}{M}$. As the scaled configurational density is defined on the product space of the spatial domain Ω and the configurational space D, we introduce two different variables, $\mathbf{x} \in \Omega$ and $\mathbf{q} \in D$, to determine the position in the spatial domain Ω and the configurational space D. Consequently, we denote the gradient and the divergence operators with respect to $\mathbf{x}$ and $\mathbf{q}$ by $\nabla_{\mathbf{x}}$, $\nabla_{\mathbf{q}}$, $\operatorname{div}_{\mathbf{x}}$, and $\operatorname{div}_{\mathbf{q}}$. Using this notation, the model reads as follows:

$$\partial_t\phi + \mathbf{u}\cdot\nabla_{\mathbf{x}}\phi - \operatorname{div}_{\mathbf{x}}\left\{m(\phi)\nabla_{\mathbf{x}}\mu_\phi\right\} = 0, \tag{1.5a}$$

$$\mu_\phi = -\delta\sigma\Delta_{\mathbf{x}}\phi + \tfrac{\sigma}{\delta}W'(\phi) + \beta'(\phi)\mathcal{J}_\varepsilon\left\{\int_D M\hat{\psi}\right\}, \tag{1.5b}$$

$$M\partial_t\hat{\psi} + M\mathbf{u}\cdot\nabla_{\mathbf{x}}\hat{\psi} + \operatorname{div}_{\mathbf{q}}\left\{M\hat{\psi}\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q}\right\} \\ = \operatorname{div}_{\mathbf{q}}\left\{c_{\mathbf{q}}M\nabla_{\mathbf{q}}\hat{\psi}\right\} + \operatorname{div}_{\mathbf{x}}\left\{c_{\mathbf{x}}M\hat{\psi}\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\right\}, \tag{1.5c}$$

$$\rho(\phi)\partial_t\mathbf{u} + ((\rho(\phi)\mathbf{u} - m(\phi)\rho'\nabla_{\mathbf{x}}\mu_\phi)\cdot\nabla_{\mathbf{x}})\mathbf{u} - \operatorname{div}_{\mathbf{x}}\{2\eta(\phi)\mathbf{D}\mathbf{u}\} + \nabla_{\mathbf{x}}p \\ = \mu_\phi\nabla_{\mathbf{x}}\phi + \int_D M\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\nabla_{\mathbf{x}}\hat{\psi} + \operatorname{div}_{\mathbf{x}}\left\{\mathfrak{J}_\varepsilon\left\{\int_D M\nabla_{\mathbf{q}}\hat{\psi}\otimes\mathbf{q}\right\}\right\}, \tag{1.5d}$$

$$\operatorname{div}_{\mathbf{x}}\mathbf{u} = 0 \tag{1.5e}$$

on $\Omega\times\mathbb{R}^+$ (or $\Omega\times D\times\mathbb{R}^+$, respectively) with the boundary conditions

$$\nabla_{\mathbf{x}}\phi\cdot\mathbf{n}_{\mathbf{x}} = 0 \qquad \text{on } \partial\Omega\times\mathbb{R}^+, \tag{1.5f}$$

$$\nabla_{\mathbf{x}}\mu_\phi\cdot\mathbf{n}_{\mathbf{x}} = 0 \qquad \text{on } \partial\Omega\times\mathbb{R}^+, \tag{1.5g}$$

$$M\hat{\psi}\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\cdot\mathbf{n}_{\mathbf{x}} = 0 \qquad \text{on } \partial\Omega\times D\times\mathbb{R}^+, \tag{1.5h}$$

$$\Big(M\hat{\psi}\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q} - c_{\mathbf{q}}M\nabla_{\mathbf{q}}\hat{\psi}\Big)\cdot\mathbf{n}_{\mathbf{q}} = 0 \qquad \text{on } \Omega\times\partial D\times\mathbb{R}^+, \tag{1.5i}$$

$$\mathbf{u} = 0 \qquad \text{on } \partial\Omega\times\mathbb{R}^+. \tag{1.5j}$$

The Cahn–Hilliard type phase-field equations (1.5a) and (1.5b) describe the evolution of two immiscible fluids in terms of the phase-field parameter ϕ and its chemical potential μ_ϕ. Thereby, m is the mobility and W is a double-well potential with minima in ± 1, representing the pure phases $\phi\equiv\pm 1$. The parameters σ and δ denote the surface tension and the width of the diffuse interface, respectively. Throughout this paper, we will set $\sigma=\delta=1$ for the ease of notation and assume a constant mobility, *i.e.* $m\equiv 1$. In contrast to other publications (see *e.g.* [23, 24]), the coefficient $c_{\mathbf{x}}$ of the center-of-mass diffusion term is kept as it guarantees parabolicity of the Fokker–Planck type equation (1.5c) (*cf.* [5]). The tuple $(\mathbf{u},p)$ stands for the velocity and pressure field, respectively, and

$$\rho(\phi) := \frac{\tilde{\rho}_2+\tilde{\rho}_1}{2} - \frac{\tilde{\rho}_2-\tilde{\rho}_1}{2}\phi \tag{1.6}$$

is the phase-field dependent mass density of the fluids, where $\tilde{\rho}_1$ and $\tilde{\rho}_2$ denote the mass densities of the pure phases.

Formal computations (*cf.* Lem. B.1) show that the energy

$$\mathcal{E}(\phi,\hat{\psi},\mathbf{u}) := \int_\Omega \tfrac{\sigma\delta}{2}\left|\nabla_{\mathbf{x}}\phi\right|^2 + \int_\Omega \tfrac{\sigma}{\delta}W(\phi) + \int_{\Omega\times D} Mg\Big(\hat{\psi}\Big) + \int_{\Omega\times D} M\mathcal{J}_\varepsilon\{\beta(\phi)\}\hat{\psi} \\ + \int_\Omega \tfrac{1}{2}\rho(\phi)\left|\mathbf{u}\right|^2 \tag{1.7}$$

is not increasing over time. Thereby, the first two terms are the so-called Cahn–Hilliard free energy and describe the contributions of the fluid-fluid contact area. The next two terms describe the properties of the polymers. Introducing the entropic functional $g(s) := s\log s - s$, the first one measures the deviation of the configurational density ψ from the Maxwellian M. The second one, the so-called Henry energy, describes the solubility properties in the different fluids: High values of β indicate a poor solubility of polymers, while low values indicate good solubility properties in the corresponding fluid. The last term in (1.7) is the kinetic energy of the fluids. By $\mathcal{J}_\varepsilon : L^1(\Omega)\to W^{2,\infty}(\Omega)$ (or $\boldsymbol{\mathcal{J}}_\varepsilon : \boldsymbol{L}^1(\Omega)\to\boldsymbol{W}^{2,\infty}(\Omega)$, respectively), we denote the isotropic mollifier which is defined as

$$\mathcal{J}_\varepsilon\{f\}(\mathbf{x}) := \int_\Omega \zeta_\varepsilon(\mathbf{x}-\mathbf{y})f(\mathbf{y})\mathrm{d}\mathbf{y} \qquad \forall\mathbf{x}\in\Omega, \qquad \forall f\in L^1(\Omega), \tag{1.8}$$

where $\zeta_\varepsilon(\mathbf{x}) := \varepsilon^{-d}\zeta(\varepsilon^{-1}\mathbf{x})$ with $\zeta \in W^{2,\infty}(\mathbb{R}^d)$ being nonnegative and rotationally symmetric, satisfying $\operatorname{supp}\zeta \subset \overline{B(0,1)}$ and having mass one. This mollifier satisfies the following properties.

$$\|\mathcal{J}_\varepsilon\{f\}\|_{L^2(\Omega)} \leq \|f\|_{L^2(\Omega)} \qquad \forall f \in L^2(\Omega), \tag{1.9a}$$

$$\|(I-\mathcal{J}_\varepsilon)\{f\}\|_{L^2(\Omega)} \to 0 \quad \text{as } \varepsilon \searrow 0 \qquad \forall f \in L^2(\Omega), \tag{1.9b}$$

$$\int_\Omega \mathcal{J}_\varepsilon\{f\} g \,\mathrm{d}\mathbf{x} = \int_\Omega f \mathcal{J}_\varepsilon\{g\} \,\mathrm{d}\mathbf{x} \qquad \forall f, g \in L^2(\Omega), \tag{1.9c}$$

$$\partial_{x_i}\mathcal{J}_\varepsilon\{f\} = \mathcal{J}_\varepsilon\{\partial_{x_i} f\} \qquad \forall f \in H_0^1(\Omega),\ i = 1,\dots,d, \tag{1.9d}$$

$$\|\mathcal{J}_\varepsilon\{f\}\|_{H^1(\Omega)} \leq \|f\|_{H^1(\Omega)} \qquad \forall f \in H_0^1(\Omega), \tag{1.9e}$$

$$\|\mathcal{J}_\varepsilon\{f\}\|_{W^{2,\infty}(\Omega)} \leq C(\varepsilon)\,\|f\|_{L^1(\Omega)} \qquad \forall f \in L^1(\Omega). \tag{1.9f}$$

Restricting (1.5) to the case of a single-phase flow, *i.e.* ϕ, ρ, and η constant, allows to recover the set of equations derived by Barrett and Süli [5]. Convergent numerical schemes for this single-phase model can be found in [7,8]. Neglecting the mollifier and using simplices with curved edges or faces, J.W. Barrett and E. Süli showed convergence towards weak solutions of a regularized single-phase model (*cf.* [7]) and, by passing to the limit in space and time separately, convergence towards weak solutions of the original model (*cf.* [8] and [6]).

A first existence result for the two-phase flow model (1.5) was already established by Grün and Metzger in [18]. In this paper, we suggest a stable numerical scheme for (1.5) and establish the convergence of discrete solutions for the case of equal fluid mass densities. It turns out, that the resulting existence result is comparable to the one established in [18].

The outline of the paper is as follows. In Section 2, we introduce the discrete function spaces and operators used in the discrete scheme. In Section 3, we introduce the fully discrete finite element scheme for the case of different mass densities and prove a first stability result which suffices to establish the existence of discrete solutions. Restricting ourselves to the case of equal mass densities, we use Section 4 to establish regularity results for discrete solutions, which are independent of the discretization parameters. In Section 5, we pass to the limit as the spatial discretization parameter h and the time step parameter τ tend to zero.

Based on the regularity results of Section 4, we are able to identify subsequences of discrete solutions converging towards weak solutions of (1.5).

As a proof of concept, we present simulations of oscillating non-Newtonian droplets in two and three spatial dimensions in the last section.

Notation 1.1. In this paper, Ω denotes the spatial domain of the flow, and D stands for the configuration space, both sets being contained in $\mathbb{R}^d$ with $d \in \{2,3\}$. By "$\cdot$", we denote the Euclidean scalar product on $\mathbb{R}^d$. Sometimes, we write Ω_T for the space-time cylinder $\Omega \times (0,T)$. By $W^{k,p}(\Omega)$, we denote the space of k-times weakly differentiable functions with weak derivatives in $L^p(\Omega)$. The symbol $W_0^{k,p}(\Omega)$ stands for the closure of $C_0^\infty(\Omega)$ in $W^{k,p}(\Omega)$. For $p = 2$, we will denote $W^{k,2}(\Omega)$ by $H^k(\Omega)$ and $W_0^{k,2}(\Omega)$ by $H_0^k(\Omega)$. Corresponding spaces of vector- and matrix-valued functions are denoted in boldface. A similar notation is used for function spaces defined on D or $\Omega \times D$. The space of solenoidal functions with homogeneous Dirichlet boundary data will be denoted by $\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega) := \{\mathbf{w} \in \boldsymbol{H}_0^1 : \operatorname{div}_{\mathbf{x}} \mathbf{w} = 0\}$, its dual space by $(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'$, and the duality pairing between $(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'$ and $\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$ by $\langle .,. \rangle$. To describe the regularity properties of the scaled configurational density $\hat{\psi}$, we introduce the Maxwellian-weighted Lebesgue and Sobolev spaces

$$L^2(\Omega \times D; M) := \Big\{\theta \in L^1_{\mathrm{loc}}(\Omega \times D) \,:\, \|\theta\|_{L^2(\Omega\times D;M)} < \infty\Big\}, \tag{1.10a}$$

$$\hat{X} := H^1(\Omega \times D; M) := \Big\{\theta \in L^1_{\mathrm{loc}}(\Omega \times D) \,:\, \|\theta\|_{H^1(\Omega\times D;M)} < \infty\Big\}, \tag{1.10b}$$

$$\hat{X}_+ := \Big\{\theta \in \hat{X} \,:\, \theta(\mathbf{x},\mathbf{q}) \geq 0 \text{ for a.e. } (\mathbf{x},\mathbf{q}) \in \Omega \times D\Big\}, \tag{1.10c}$$

with the associated norms

$$\|\theta\|_{L^2(\Omega\times D;M)} := \left(\int_{\Omega\times D} M\,|\theta|^2\right)^{1/2}, \tag{1.11a}$$

$$\|\theta\|_{H^1(\Omega\times D;M)} := \left(\int_{\Omega\times D} M\Big[|\theta|^2 + |\nabla_{\mathbf{x}}\theta|^2 + |\nabla_{\mathbf{q}}\theta|^2\Big]\right)^{1/2}. \tag{1.11b}$$

For a Banach space Y and a time interval I, the symbol $L^p(I;Y)$ stands for the parabolic space of L^p-integrable functions on I with values in Y.

2. Technical preliminaries

This section addresses the discretization techniques used in the presented scheme. We introduce discrete function spaces, list the essential estimates for the used approximation, interpolation, and projection operators, and introduce a discrete version of the mollifier $\mathcal{J}_\varepsilon$.

2.1. Discretization in space and time

Concerning the discretization with respect to time, we assume that

(T) the time interval $I := [0,T)$ is subdivided in intervals $I_k := [t_k, t_{k+1})$ with $t_{k+1} = t_k + \tau_k$ for time increments $\tau_k > 0$ and $k = 0,\dots,N-1$ with $t_N = T$. For simplicity, we take $\tau_k \equiv \tau = \frac{T}{N}$ for $k = 0,\dots,N-1$.

From now on, we consider the two-phase problem on a bounded, convex polygonal (or polyhedral, respectively) spatial domain $\Omega \subset \mathbb{R}^d$ in spatial dimensions $d \in \{2,3\}$. As the mollifier $\mathcal{J}_\varepsilon$ includes a convolution on $\mathbb{R}^d$, we also consider a likewise bounded, convex polygonal (or polyhedral, respectively) superset Ω^* of Ω such that $\operatorname{dist}(\partial\Omega^*, \Omega) \geq \varepsilon$, *i.e.* $\operatorname{supp}\zeta_\varepsilon(\mathbf{x} - .) \subset \Omega^*$ for all $\mathbf{x} \in \Omega$. We introduce partitions $\mathcal{T}_h^{\mathbf{x}}$ and $\mathcal{T}_h^{\mathbf{x}*}$ of Ω and Ω^* depending on a spatial discretization parameter $h > 0$ satisfying the following assumptions:

(S1) Let $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ be a quasiuniform family (in the sense of [9]) of partitions of Ω^* into disjoint, open, nonobtuse simplices $\kappa_{\mathbf{x}}$, so that

$$\overline{\Omega^*} \equiv \bigcup_{\kappa_{\mathbf{x}}\in\mathcal{T}_h^{\mathbf{x}*}} \overline{\kappa_{\mathbf{x}}} \quad \text{with} \quad h_{\mathbf{x}} := \max_{\kappa_{\mathbf{x}}\in\mathcal{T}_h^{\mathbf{x}*}} \operatorname{diam}(\kappa_{\mathbf{x}}) \leq \operatorname{diam}(\Omega^*)h.$$

(S2) Let $\{\mathcal{T}_h^{\mathbf{x}}\}_{h>0}$ be a quasiuniform family of partitions of Ω into disjoint, open, nonobtuse simplices with $\mathcal{T}_h^{\mathbf{x}} \subset \mathcal{T}_h^{\mathbf{x}*}$, so that $\overline{\Omega} \equiv \bigcup_{\kappa_{\mathbf{x}}\in\mathcal{T}_h^{\mathbf{x}}} \overline{\kappa_{\mathbf{x}}}$.

Instead of working with the configurational space $D := B_{Q_{\max}} \subset \mathbb{R}^d$ and simplices with curved edges or faces (see *e.g.* [7]), we use a bounded polygonal (or polyhedral, respectively) domain $\mathfrak{D} \supset D$. A suitable choice for $\mathfrak{D}$ might be *e.g.* the cube of side length $2Q_{\max}$ which includes D. We make the following assumptions on the partitions of $\mathcal{T}_h^{\mathbf{q}}$ of $\mathfrak{D}$.

(S3) Let $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ be a quasiuniform family (in the sense of [9]) of partitions of $\mathfrak{D}$ into disjoint open nonobtuse simplices $\kappa_{\mathbf{q}}$, so that

$$\overline{\mathfrak{D}} \equiv \bigcup_{\kappa_{\mathbf{q}}\in\mathcal{T}_h^{\mathbf{q}}} \overline{\kappa_{\mathbf{q}}} \quad \text{with} \quad h_{\mathbf{q}} := \max_{\kappa_{\mathbf{q}}\in\mathcal{T}_h^{\mathbf{q}}} \operatorname{diam}(\kappa_{\mathbf{q}}) \leq \operatorname{diam}(\mathfrak{D})h.$$

Combining (S1) and (S3), we immediately obtain

$$c_1 h \leq h_{\mathbf{x}} \leq c_2 h, \qquad c_3 h \leq h_{\mathbf{q}} \leq c_4 h, \qquad \frac{h_{\mathbf{x}}}{h_{\mathbf{q}}} + \frac{h_{\mathbf{q}}}{h_{\mathbf{x}}} \leq c_5 \tag{2.1}$$

as $h \searrow 0$ with c_i $(i = 1, \ldots, 5)$ independent of h. For both, $\mathcal{T}_h^{\mathbf{x}*}$ and $\mathcal{T}_h^{\mathbf{q}}$, we use the same standard reference simplex $\tilde{\kappa}$ with vertices $\{\tilde{\mathbf{P}}_i\}_{i=0,\ldots,d}$, where $\tilde{\mathbf{P}}_0$ is the origin and the $\tilde{\mathbf{P}}_i$ are such that the jth component of $\tilde{\mathbf{P}}_i$ is δ_{ij} for $i, j = 1, \ldots, d$.

We denote the vertices of an element $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}*}$ by $\{\mathbf{P}_{\kappa_{\mathbf{x}},i}\}_{i=0,\ldots,d}$ and define $\mathbf{B}_{\kappa_{\mathbf{x}}} \in \mathbb{R}^{d\times d}$ such that the mapping $\mathcal{B}_{\kappa_{\mathbf{x}}} : \mathbb{R}^d \ni y \mapsto \mathbf{P}_{\kappa_{\mathbf{x}},0} + \mathbf{B}_{\kappa_{\mathbf{x}}} y$ maps the vertex $\tilde{\mathbf{P}}_i$ to $\mathbf{P}_{\kappa_{\mathbf{x}},i}$ $(i = 0, \ldots, d)$ and hence $\tilde{\kappa}$ to $\kappa_{\mathbf{x}}$. The quantities $\{\mathbf{P}_{\kappa_{\mathbf{q}},i}\}_{i=0,\ldots,d}$, $\mathcal{B}_{\kappa_{\mathbf{q}}}$, and $\mathbf{B}_{\kappa_{\mathbf{q}}}$ are defined analogously.

2.2. Discrete function spaces and interpolation operators

For the approximation of the phase-field parameter ϕ and its chemical potential μ_ϕ, we introduce the space $U_h^{\mathbf{x}}$ of continuous, piecewise linear finite element functions on $\mathcal{T}_h^{\mathbf{x}}$. The extension of $U_h^{\mathbf{x}}$ to $\mathcal{T}_h^{\mathbf{x}*}$ is denoted by $U_h^{\mathbf{x}*}$. Pressure and velocity field are approximated with the lowest order Taylor–Hood elements, *i.e.* we define the space $\boldsymbol{W}_h \subset \boldsymbol{H}_0^1(\Omega)$ of continuous, piecewise quadratic finite element functions on $\mathcal{T}_h^{\mathbf{x}}$ together with the spaces

$$S_h := \left\{\theta_h^{\mathbf{x}} \in U_h^{\mathbf{x}} \,:\, \int_\Omega \theta_h^{\mathbf{x}} \,\mathrm{d}\mathbf{x} = 0\right\}, \tag{2.2}$$

$$\boldsymbol{W}_{h,\mathrm{div}} := \left\{\mathbf{w}_h \in \boldsymbol{W}_h \,:\, \int_\Omega \mathrm{div}_{\mathbf{x}}\, \mathbf{w}_h \theta_h^{\mathbf{x}} = 0 \quad \forall \theta_h^{\mathbf{x}} \in S_h\right\}. \tag{2.3}$$

Those spaces enjoy the following properties (see [14] and [21] in combination with the regularity results of [12]):

(TH1) The Babuška–Brezzi condition is satisfied, *i.e.* a positive constant C exists such that

$$\sup_{\mathbf{w}_h \in \boldsymbol{W}_h} \frac{(q_h, \mathrm{div}_{\mathbf{x}}\, \mathbf{w}_h)}{\|\mathbf{w}_h\|_{\boldsymbol{H}_0^1(\Omega)}} \geq C \|q_h\|_{L^2(\Omega)} \tag{2.4}$$

for all $q_h \in S_h$.

(TH2) The L^2-projector $\mathcal{Q}_h : \boldsymbol{H}_{0,\mathrm{div}}^1(\Omega) \to \boldsymbol{W}_{h,\mathrm{div}}$ defined by

$$\int_\Omega (\mathbf{v} - \mathcal{Q}_h[\mathbf{v}]) \cdot \mathbf{w}_h = 0 \qquad \forall \mathbf{w}_h \in \boldsymbol{W}_{h,\mathrm{div}},\ \mathbf{v} \in \boldsymbol{H}_{0,\mathrm{div}}^1(\Omega)$$

is uniformly $H^1(\Omega)$-stable, *i.e.*

$$\|\mathcal{Q}_h[\mathbf{v}]\|_{H^1(\Omega)} \leq C \|\mathbf{v}\|_{H^1(\Omega)},$$

and satisfies

$$\|\mathbf{v} - \mathcal{Q}_h[\mathbf{v}]\|_{L^2(\Omega)} + h_{\mathbf{x}} \|\nabla_{\mathbf{x}}(\mathbf{v} - \mathcal{Q}_h[\mathbf{v}])\|_{L^2(\Omega)} \leq C h_{\mathbf{x}}^2 \|\mathbf{v}\|_{H^2(\Omega)}$$

for all $\mathbf{v} \in \boldsymbol{H}_{0,\mathrm{div}}^1(\Omega) \cap \boldsymbol{H}^2(\Omega)$.

Similarly to $U_h^{\mathbf{x}*}$ and $U_h^{\mathbf{x}}$, we denote the space of continuous, piecewise linear finite element functions on $\mathcal{T}_h^{\mathbf{q}}$ by $U_h^{\mathbf{q}}$. To approximate $\hat{\psi}$ on $\Omega \times \mathfrak{D}$, we introduce the space $\hat{X}_h := U_h^{\mathbf{x}} \times U_h^{\mathbf{q}}$. That is for a given basis $\{\chi_{h,i}^{\mathbf{x}}\}_{i=1,\ldots,\dim U_h^{\mathbf{x}}}$ of $U_h^{\mathbf{x}}$ and a given basis $\{\chi_{h,j}^{\mathbf{q}}\}_{j=1,\ldots,\dim U_h^{\mathbf{q}}}$ of $U_h^{\mathbf{q}}$, $\hat{X}_h$ is defined as the span of $\left\{\chi_{h,i}^{\mathbf{x}} \chi_{h,j}^{\mathbf{q}}\right\}_{i=1,\ldots,\dim U_h^{\mathbf{x}}}^{j=1,\ldots,\dim U_h^{\mathbf{q}}}$.

We define the nodal interpolation operator $\mathcal{I}_h^{\mathbf{x}}$ from $C^0(\overline{\Omega^*})$ to $U_h^{\mathbf{x}*}$ by

$$\mathcal{I}_h^{\mathbf{x}}\{a\} := \sum_{i=1}^{\dim U_h^{\mathbf{x}*}} a(\mathbf{x}_i) \chi_{h,i}^{\mathbf{x}}, \tag{2.5}$$

where the functions $\{\chi^{\mathbf{x}}_{h,i}\}_{i=1,\dots,\dim U_h^{\mathbf{x}*}}$ form a dual basis to the vertices $\{\mathbf{x}_i\}_{i=1,\dots,\dim U_h^{\mathbf{x}*}}$ of $\mathcal{T}_h^{\mathbf{x}*}$, *i.e.* $\chi^{\mathbf{x}}_{h,i}(\mathbf{x}_j) = \delta_{ij}$ for $i, j = 1, \dots, \dim U_h^{\mathbf{x}*}$. In a slight misuse of notation, we also denote the nodal interpolation from $C^0(\overline{\Omega})$ to $U_h^{\mathbf{x}}$ by $\mathcal{I}_h^{\mathbf{x}}$. In the context of the discrete mollifier (see (2.38)), we will introduce a second spatial variable $\mathbf{y}$ and the corresponding operator $\mathcal{I}_h^{\mathbf{y}}$ which is defined analogously to $\mathcal{I}_h^{\mathbf{x}}$.

Similarly, we define

$$\mathcal{I}_h^{\mathbf{q}} : C^0\big(\overline{\mathfrak{D}}\big) \to U_h^{\mathbf{q}}, \qquad a \mapsto \mathcal{I}_h^{\mathbf{q}}\{a\} := \sum_{i=1}^{\dim U_h^{\mathbf{q}}} a(\mathbf{q}_i)\chi^{\mathbf{q}}_{h,i}, \tag{2.6}$$

where the functions $\{\chi^{\mathbf{q}}_{h,i}\}_{i=1,\dots,\dim U_h^{\mathbf{q}}}$ form a dual basis to the vertices $\{\mathbf{q}_i\}_{i=1,\dots,\dim U_h^{\mathbf{q}}}$ of $\mathcal{T}_h^{\mathbf{q}}$. Combining these operators defines the nodal interpolation operator

$$\mathcal{I}_h^{\mathbf{xq}} : C^0\big(\overline{\Omega \times \mathfrak{D}}\big) \to \hat{X}_h, \quad a \mapsto \mathcal{I}_h^{\mathbf{xq}}\{a\} := \mathcal{I}_h^{\mathbf{x}}\{\mathcal{I}_h^{\mathbf{q}}\{a\}\} = \mathcal{I}_h^{\mathbf{q}}\{\mathcal{I}_h^{\mathbf{x}}\{a\}\}. \tag{2.7}$$

Sometimes, we write $\mathcal{I}_h^{\mathbf{x}}\{\mathbf{a}\}$ (or $\mathcal{I}_h^{\mathbf{x}}\{\mathbf{A}\}$) with $\mathbf{a} \in \big(C^0(\overline{\Omega})\big)^d$ (or $\mathbf{A} \in \big(C^0(\overline{\Omega})\big)^{d\times d}$) when we apply $\mathcal{I}_h^{\mathbf{x}}$ to each component of $\mathbf{a}$ (or $\mathbf{A}$, respectively). We also use similar conventions for $\mathcal{I}_h^{\mathbf{q}}$ and $\mathcal{I}_h^{\mathbf{xq}}$.

We define the discrete Laplacian $\Delta_h\phi_h \in S_h$ for all $\phi_h \in U_h^{\mathbf{x}}$ by

$$\int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\Delta_h\phi_h\theta_h^{\mathbf{x}}\} = -\int_\Omega \nabla_{\mathbf{x}}\phi_h \cdot \nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} \quad \forall\theta_h^{\mathbf{x}} \in U_h^{\mathbf{x}}. \tag{2.8}$$

Using the nodal interpolation operator $\mathcal{I}_h^{\mathbf{x}}$, we define the norm $\|.\|_h$ *via*

$$\|\theta^{\mathbf{x}}\|_h^2 := \int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{|\theta^{\mathbf{x}}|^2\Big\}, \qquad \text{for all } \theta^{\mathbf{x}} \in C^0(\overline{\Omega}). \tag{2.9}$$

It is well-known that this norm is equivalent to the $L^2(\Omega)$-norm on $U_h^{\mathbf{x}}$, *i.e.* there exist constants $c, C > 0$ such that

$$c\,\|.\|_h \le \|.\|_{L^2(\Omega)} \le C\,\|.\|_h\,. \tag{2.10}$$

Similarly, the following inequalities for the $L^4(\Omega)$- and $L^6(\Omega)$-norm hold true for all $\theta_h^{\mathbf{x}} \in U_h^{\mathbf{x}}$ (*cf.* [25]).

$$c\int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{|\theta_h^{\mathbf{x}}|^4\Big\} \le \int_\Omega |\theta_h^{\mathbf{x}}|^4 \le C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{|\theta_h^{\mathbf{x}}|^4\Big\}, \tag{2.11a}$$
$$c\int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{|\theta_h^{\mathbf{x}}|^6\Big\} \le \int_\Omega |\theta_h^{\mathbf{x}}|^6 \le C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{|\theta_h^{\mathbf{x}}|^6\Big\}. \tag{2.11b}$$

For future reference, we collect additional useful estimates related to the nodal interpolation operators.

Lemma 2.1. *Let* $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ *and* $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ *satisfy (S1)–(S3). Then the following estimates hold true for all* $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}*}$, $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$, *and* $1 \le p < \infty$.

$$|\mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\}(\mathbf{x})|^p \le \mathcal{I}_h^{\mathbf{x}}\{|\theta^{\mathbf{x}}|^p\}(\mathbf{x}) \qquad \forall\mathbf{x} \in \kappa_{\mathbf{x}} \qquad \forall\theta^{\mathbf{x}} \in C^0(\overline{\kappa_{\mathbf{x}}}), \tag{2.12a}$$
$$|\mathcal{I}_h^{\mathbf{q}}\{\theta^{\mathbf{q}}\}(\mathbf{q})|^p \le \mathcal{I}_h^{\mathbf{q}}\{|\theta^{\mathbf{q}}|^p\}(\mathbf{q}) \qquad \forall\mathbf{q} \in \kappa_{\mathbf{q}} \qquad \forall\theta^{\mathbf{q}} \in C^0(\overline{\kappa_{\mathbf{q}}}), \tag{2.12b}$$
$$|\mathcal{I}_h^{\mathbf{xq}}\{\theta\}(\mathbf{x},\mathbf{q})|^p \le \mathcal{I}_h^{\mathbf{xq}}\{|\theta|^p\}(\mathbf{x},\mathbf{q}) \qquad \forall(\mathbf{x},\mathbf{q}) \in \kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}} \qquad \forall\theta \in C^0(\overline{\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}}). \tag{2.12c}$$

Additionally, we have for affine linear functions $\theta_h^{\mathbf{x}}$ *and* $\theta_h^{\mathbf{q}}$

$$\|\theta_h^{\mathbf{x}}\|_{L^\infty(\kappa_{\mathbf{x}})}^2 \leq C h_{\mathbf{x}}^{-d} \int_{\kappa_{\mathbf{x}}} |\theta_h^{\mathbf{x}}|^2 \, \mathrm{d}\mathbf{x}, \tag{2.13a}$$

$$\|\theta_h^{\mathbf{q}}\|_{L^\infty(\kappa_{\mathbf{q}})}^2 \leq C h_{\mathbf{q}}^{-d} \int_{\kappa_{\mathbf{q}}} |\theta_h^{\mathbf{q}}|^2 \, \mathrm{d}\mathbf{q}, \tag{2.13b}$$

$$\int_{\kappa_{\mathbf{x}}} |\nabla_{\mathbf{x}} \theta_h^{\mathbf{x}}|^2 \, \mathrm{d}\mathbf{x} \leq C h_{\mathbf{x}}^{-2} \int_{\kappa_{\mathbf{x}}} |\theta_h^{\mathbf{x}}|^2 \, \mathrm{d}\mathbf{x} \leq C h_{\mathbf{x}}^{-2} \int_{\kappa_{\mathbf{x}}} \mathcal{I}_h^{\mathbf{x}} \left\{ |\theta_h^{\mathbf{x}}|^2 \right\} \mathrm{d}\mathbf{x}, \tag{2.13c}$$

$$\int_{\kappa_{\mathbf{q}}} |\nabla_{\mathbf{q}} \theta_h^{\mathbf{q}}|^2 \, \mathrm{d}\mathbf{q} \leq C h_{\mathbf{q}}^{-2} \int_{\kappa_{\mathbf{q}}} |\theta_h^{\mathbf{q}}|^2 \, \mathrm{d}\mathbf{q} \leq C h_{\mathbf{q}}^{-2} \int_{\kappa_{\mathbf{q}}} \mathcal{I}_h^{\mathbf{q}} \left\{ |\theta_h^{\mathbf{q}}|^2 \right\} \mathrm{d}\mathbf{q}. \tag{2.13d}$$

Proof. The inequalities (2.12) are a direct consequence of Jensen's inequality. Standard inverse estimates (see *e.g.* [9], Lem. 4.5.3) yield (2.13a) and (2.13b), as well as the first inequalities in (2.13c) and (2.13d). The second inequalities in (2.13c) and (2.13d) are a consequence of (2.12a) and (2.12b). □

Using the nodal interpolation operator $\mathcal{I}_h^{\mathbf{q}}$ mentioned above, we define a discrete version M_h of the Maxwellian M. We start by defining an extension of M on $\mathfrak{D}$ *via*

$$\hat{M}(\mathbf{q}) := \begin{cases} M(\mathbf{q}) & \text{if } \mathbf{q} \in D, \\ 0 & \text{if } \mathbf{q} \in \mathfrak{D} \setminus D, \end{cases} \tag{2.14}$$

and continue with its finite element approximation

$$M_h(\mathbf{q}) := c_{h_{\mathbf{q}}} \mathcal{I}_h^{\mathbf{q}} \left\{ \hat{M} \right\}(\mathbf{q}) \qquad \text{for all } \mathbf{q} \in \mathfrak{D}, \tag{2.15}$$

with $c_{h_{\mathbf{q}}} := \left[\int_{\mathfrak{D}} \mathcal{I}_h^{\mathbf{q}}\{\hat{M}\} \, \mathrm{d}\mathbf{q}\right]^{-1}$. As shown in [25], the following lemma holds true which in particular states that $\hat{M}$ is continuous and therefore that M_h is well-defined.

Lemma 2.2. *Let the spring potential* U *and its associated Maxwellian* M *satisfy the properties (P1)–(P5) with* $\kappa > 1$. *Then the extension* $\hat{M}$ *of the Maxwellian on* $\mathfrak{D}$ *(see* (2.14)*) and its discrete approximation* M_h *defined* via (2.15) *have the following properties:*

- $\hat{M} \in C^1\left(\overline{\mathfrak{D}}\right)$ *with* $\hat{M}\Big|_{\partial\mathfrak{D}} = 0$.
- *The constant* $c_{h_{\mathbf{q}}}$ *is bounded from below by some constant* $c_M > 0$ *independently of* $h_{\mathbf{q}}$.
- *For* $h_{\mathbf{q}}$ *small enough,* $c_{h_{\mathbf{q}}}$ *is bounded from above by some constant and we have* $\left\| M_h - \hat{M} \right\|_{L^\infty(\mathfrak{D})} \leq C h_{\mathbf{q}}$.

The proof of the lemma above can be found in the Appendix A.

For future reference, we state the following Maxwellian-weighted approximation results for the interpolation operators.

Lemma 2.3. *Let* M_h *be the finite element approximation of the Maxwellian* M *defined* via (2.15) *and let* $\{\mathcal{T}_h^{\mathbf{x}}\}_{h>0}$ *and* $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ *satisfy (S1)–(S3). Then the following estimates hold true for all* $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$, $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$ *and for all* $\hat{\theta}_h, \tilde{\theta}_h \in \hat{X}_h$.

$$\int_{\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}} \left| M_h (I - \mathcal{I}_h^{\mathbf{x}}) \left\{ \nabla_{\mathbf{q}} \hat{\theta}_h \cdot \nabla_{\mathbf{q}} \tilde{\theta}_h \right\} \right| \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{x}$$
$$\leq C h_{\mathbf{x}} \left(\int_{\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}} M_h \left| \nabla_{\mathbf{q}} \hat{\theta}_h \right|^2 \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{x} \right)^{1/2} \left(\sum_{i=1}^d \sum_{j=1}^d \int_{\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}} M_h \left| \partial_{\mathbf{x}_i} \partial_{\mathbf{q}_j} \tilde{\theta}_h \right|^2 \, \mathrm{d}\mathbf{q} \, \mathrm{d}\mathbf{x} \right)^{1/2} \tag{2.16a}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \left| M_h (I-\mathcal{I}_h^{\mathbf{q}})\left\{\nabla_{\mathbf{x}}\hat{\theta}_h\cdot\nabla_{\mathbf{x}}\tilde{\theta}_h\right\}\right| \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}$$

$$\leq C h_{\mathbf{q}} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\hat{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \left(\sum_{i=1}^{d}\sum_{j=1}^{d}\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\partial_{\mathbf{x}_i}\partial_{\mathbf{q}_j}\tilde{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \tag{2.16b}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \left| M_h (I-\mathcal{I}_h^{\mathbf{xq}})\left\{\hat{\theta}_h\tilde{\theta}_h\right\}\right| \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}$$

$$\leq C h_{\mathbf{x}}^2 \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{x}}\hat{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{x}}\tilde{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2}$$

$$+ C h_{\mathbf{q}}^2 \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\hat{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\tilde{\theta}\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2}. \tag{2.16c}$$

In Lemma 2.3, we denoted the identity operator mapping scalar-valued functions onto themselves by I. For a Proof of Lemma 2.3 we refer to the Appendix A or to [25] or [7]. In contrast to the proof presented in the latter publication, the Proof of Lemma 2.3 uses (2.1) to obtain $\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h|\nabla_{\mathbf{q}}\hat{\theta}|^2$ on the right hand-side of (2.16b). Similar computations yield the following result.

Lemma 2.4. *Let $\{\mathcal{T}_h^{\mathbf{x}}\}_{h>0}$ and $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ satisfy (S1)–(S3). Then, for all $\kappa_{\mathbf{x}}\in\mathcal{T}_h^{\mathbf{x}}$, $\kappa_{\mathbf{q}}\in\mathcal{T}_h^{\mathbf{q}}$, and for all $f_h,\tilde{f}_h\in U_h^{\mathbf{x}}$ and $g_h,\tilde{g}_h\in U_h^{\mathbf{q}}$, we have that*

$$\int_{\kappa_{\mathbf{x}}} \left|(I-\mathcal{I}_h^{\mathbf{x}})\left\{f_h\tilde{f}_h\right\}\right| \,\mathrm{d}\mathbf{x} \leq C h_{\mathbf{x}}^2 \left\|\nabla_{\mathbf{x}} f_h\right\|_{L^2(\kappa_{\mathbf{x}})} \left\|\nabla_{\mathbf{x}}\tilde{f}_h\right\|_{L^2(\kappa_{\mathbf{x}})}. \tag{2.17}$$

$$\int_{\kappa_{\mathbf{x}}} \left|(I-\mathcal{I}_h^{\mathbf{x}})\left\{f_h\tilde{f}_h\right\}\right| \,\mathrm{d}\mathbf{x} \leq C h_{\mathbf{x}} \left\|f_h\right\|_{L^2(\kappa_{\mathbf{x}})} \left\|\nabla_{\mathbf{x}}\tilde{f}_h\right\|_{L^2(\kappa_{\mathbf{x}})}, \tag{2.18}$$

$$\int_{\kappa_{\mathbf{q}}} \left|M_h(I-\mathcal{I}_h^{\mathbf{q}})\{g_h\tilde{g}_h\}\right| \,\mathrm{d}\mathbf{q} \leq C h_{\mathbf{q}}^2 \left(\int_{\kappa_{\mathbf{q}}} M_h\left|\nabla_{\mathbf{q}} g_h\right|^2 \,\mathrm{d}\mathbf{q}\right)^{1/2} \left(\int_{\kappa_{\mathbf{q}}} M_h\left|\nabla_{\mathbf{q}}\tilde{g}_h\right|^2 \,\mathrm{d}\mathbf{q}\right)^{1/2}. \tag{2.19}$$

2.3. Discrete versions of the chain rule

As the regularity results in Section 4 will heavily rely on the validity of the formal identities

$$g''(\hat{\psi})^{-1}\nabla_{\mathbf{q}} g'(\hat{\psi}) = \nabla_{\mathbf{q}}\hat{\psi}, \quad g''(\hat{\psi})^{-1}\nabla_{\mathbf{x}} g'(\hat{\psi}) = \nabla_{\mathbf{x}}\hat{\psi}, \text{ and } \quad \hat{\psi}\nabla_{\mathbf{x}}\hat{\psi} = \tfrac{1}{2}\nabla_{\mathbf{x}}|\hat{\psi}|^2, \tag{2.20}$$

we extend the ideas of G. Grün and M. Rumpf (*cf.* [19]) and J.W. Barrett and E. Süli (*cf.* [7,8]) to establish discrete counterparts of (2.20). As we are not able to guarantee $\hat{\psi}\geq 0$ in the discrete setting, we start by defining a regularized version of the entropic function g *via*

$$g_\nu(s) := \begin{cases} s\log s - s & \text{if } s\geq\nu, \\ \frac{s^2-\nu^2}{2\nu} + (\log\nu - 1)s & \text{if } s<\nu, \end{cases} \tag{2.21a}$$

$$g_\nu'(s) = \begin{cases} \log s & \text{if } s\geq\nu, \\ \frac{s}{\nu} + \log\nu - 1 & \text{if } s<\nu, \end{cases} \tag{2.21b}$$

$$g_\nu''(s) = \max\{\nu,s\}^{-1}, \tag{2.21c}$$

for all $s \in \mathbb{R}$ and some regularization parameter $\nu > 0$. Additionally, we define a function $f_\nu : \mathbb{R} \to \mathbb{R}^+$ with $f_\nu'(s) = (g_\nu''(s))^{-1}$ *via*

$$f_\nu(s) := \begin{cases} \frac{1}{2}s^2 & \text{if } s \geq \nu, \\ \nu s - \frac{1}{2}\nu^2 & \text{if } s < \nu, \end{cases} \tag{2.22a}$$

$$f_\nu'(s) = \max\{\nu, s\}. \tag{2.22b}$$

Using the ideas from [19] and [7], we define for a given function $\theta_h \in \hat{X}_h$ and a given element $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$ a diagonal matrix $\hat{\Xi}_\nu^{\mathbf{x}}[\theta_h]$ by

$$\left[\hat{\Xi}_\nu^{\mathbf{x}}[\theta_h]\right]_{ii}(\mathbf{q}) = \begin{cases} \frac{\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) - \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q})}{g_\nu'(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q})) - g_\nu'(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}))} & \text{if } \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) \neq \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}), \\ \frac{1}{g_\nu''(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}))} & \text{if } \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) = \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}), \end{cases} \tag{2.23a}$$

for any $\mathbf{q} \in \mathfrak{D}$. Incorporating the affine mapping from $\tilde{\kappa}$ to $\kappa_{\mathbf{x}}$, we define the matrix-valued operator $\Xi_\nu^{\mathbf{x}}[.]$ *via*

$$\Xi_\nu^{\mathbf{x}}[\theta_h](\mathbf{q})\big|_{\kappa_{\mathbf{x}}} := \mathbf{B}_{\kappa_{\mathbf{x}}}^{-T} \cdot \hat{\Xi}_\nu^{\mathbf{x}}[\theta_h](\mathbf{q}) \cdot \mathbf{B}_{\kappa_{\mathbf{x}}}^T \tag{2.23b}$$

for $\theta_h \in \hat{X}_h$. Analogously, we define $\Lambda_\nu^{\mathbf{x}}[.]$ *via*

$$\left[\hat{\Lambda}_\nu^{\mathbf{x}}[\theta_h]\right]_{ii}(\mathbf{q}) = \begin{cases} \frac{f_\nu(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q})) - f_\nu(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}))}{\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) - \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q})} & \text{if } \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) \neq \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}), \\ f_\nu'(\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q})) & \text{if } \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q}) = \theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{q}), \end{cases} \tag{2.23c}$$

$$\Lambda_\nu^{\mathbf{x}}[\theta_h](\mathbf{q})\big|_{\kappa_{\mathbf{x}}} := \mathbf{B}_{\kappa_{\mathbf{x}}}^{-T} \cdot \hat{\Lambda}_\nu^{\mathbf{x}}[\theta_h](\mathbf{q}) \cdot \mathbf{B}_{\kappa_{\mathbf{x}}}^T, \tag{2.23d}$$

on every $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$ for $\theta_h \in \hat{X}_h$ and $\mathbf{q} \in \mathfrak{D}$. $\Xi_\nu^{\mathbf{q}}[.]$ is defined *via*

$$\left[\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]\right]_{ii}(\mathbf{x}) = \begin{cases} \frac{\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},i}) - \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},0})}{g_\nu'(\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},i})) - g_\nu'(\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},0}))} & \text{if } \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},i}) \neq \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},0}), \\ \frac{1}{g_\nu''(\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},0}))} & \text{if } \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},i}) = \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},0}), \end{cases} \tag{2.23e}$$

$$\Xi_\nu^{\mathbf{q}}[\theta_h](\mathbf{x})\big|_{\kappa_{\mathbf{q}}} := \mathbf{B}_{\kappa_{\mathbf{q}}}^{-T} \cdot \hat{\Xi}_\nu^{\mathbf{q}}[\theta_h](\mathbf{x}) \cdot \mathbf{B}_{\kappa_{\mathbf{q}}}^T, \tag{2.23f}$$

on every $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$ for $\theta_h \in \hat{X}_h$ and $\mathbf{x} \in \Omega$.

Remark 2.5. For a simplex $\kappa_{\mathbf{x}}$, which has a vertex $\mathbf{P}_{\kappa_{\mathbf{x}},0}$ with the property that any two edges intersecting each other in $\mathbf{P}_{\kappa_{\mathbf{x}},0}$ form a right angle, we may define the mapping $\mathcal{B}_{\kappa_{\mathbf{x}}}$ in a way that $\mathbf{B}_{\kappa_{\mathbf{x}}}$ is orthogonal, *i.e.* $\mathbf{B}_{\kappa_{\mathbf{x}}}^T \cdot \mathbf{B}_{\kappa_{\mathbf{x}}}$ is a diagonal matrix. In this case $\Xi_\nu^{\mathbf{x}}[.](.)\big|_{\kappa_{\mathbf{x}}}$ and $\Lambda_\nu^{\mathbf{x}}[.](.)\big|_{\kappa_{\mathbf{x}}}$ are symmetric matrices with eigenvalues greater than or equal to ν.
As we will only consider nonobtuse simplices, $\Xi_\nu^{\mathbf{x}}[.](.)\big|_{\kappa_{\mathbf{x}}}$ and $\Lambda_\nu^{\mathbf{x}}[.](.)\big|_{\kappa_{\mathbf{x}}}$ may not be assumed to be symmetric. Nevertheless, their eigenvalues are still greater than or equal to ν.

Similar considerations apply to $\Xi_\nu^{\mathbf{q}}[.](.)\big|_{\kappa_{\mathbf{q}}}$ and the shape of $\kappa_{\mathbf{q}}$.

As shown in the following lemma, those operators allow for a discrete version of (2.20).

Lemma 2.6. *Let $\Xi_\nu^{\mathbf{q}}[.]$, $\Xi_\nu^{\mathbf{x}}[.]$, and $\Lambda_\nu^{\mathbf{x}}[.]$ be matrix-valued operators on $\Omega \times \mathfrak{D}$ which are defined* via (2.23). *Then the following identities hold true for $\theta_h \in \hat{X}_h$.*

$$\mathcal{I}_h^{\mathbf{q}}\{\Xi_\nu^{\mathbf{x}}[\theta_h]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\{g_\nu'(\theta_h)\}\} = \nabla_{\mathbf{x}}\theta_h, \tag{2.24a}$$

$$\mathcal{I}_h^{\mathbf{q}}\{\Lambda_\nu^{\mathbf{x}}[\theta_h]\nabla_{\mathbf{x}}\theta_h\} = \nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\{f_\nu(\theta_h)\}, \tag{2.24b}$$

$$\mathcal{I}_h^{\mathbf{x}}\{\Xi_\nu^{\mathbf{q}}[\theta_h]\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\{g_\nu'(\theta_h)\}\} = \nabla_{\mathbf{q}}\theta_h. \tag{2.24c}$$

Proof. Restricting ourselves to $\tilde{\kappa} \times \kappa_{\mathbf{q}}$ with the vertices $\{(\tilde{\mathbf{P}}_i, \mathbf{P}_{\kappa_{\mathbf{q}},j})\}_{i,j=0,\dots d}$, we note that the $\mathbf{x}$-gradient of $\mathcal{I}_h^{\mathbf{xq}}\{g_\nu'(\theta_h(\mathbf{x},\mathbf{q}))\}$ for some $\theta_h \in \hat{X}$ may be written as

$$\nabla_{\mathbf{x}} \mathcal{I}_h^{\mathbf{xq}}\{g_\nu'(\theta_h(\mathbf{x},\mathbf{q}))\} = \sum_{i=1}^{d} [g_\nu'(\theta_h(\tilde{\mathbf{P}}_i,\mathbf{q})) - g_\nu'(\theta_h(\tilde{\mathbf{P}}_0,\mathbf{q}))]\mathbf{e}_i, \tag{2.25}$$

for all $\mathbf{x} \in \tilde{\kappa}$ and $\mathbf{q} \in \kappa_{\mathbf{q}}$. Therefore, we may compute on each $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{x}} \otimes \mathcal{T}_h^{\mathbf{q}}$

$$\begin{aligned} &\Xi_\nu^{\mathbf{x}}[\theta_h]\big(\mathbf{P}_{\kappa_{\mathbf{q}},j}\big)\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\big\{g_\nu'\big(\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j})\big)\big\} \\ &\quad = \mathbf{B}_{\kappa_{\mathbf{x}}}^{-T} \cdot \hat{\Xi}_\nu^{\mathbf{x}}[\theta_h]\big(\mathbf{P}_{\kappa_{\mathbf{q}},j}\big) \cdot \mathbf{B}_{\kappa_{\mathbf{x}}}^{T} \cdot \mathbf{B}_{\kappa_{\mathbf{x}}}^{-T} \sum_{i=1}^{d} \big[g_\nu'\big(\theta_h\big(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{P}_{\kappa_{\mathbf{q}},j}\big)\big) - g_\nu'\big(\theta_h\big(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{P}_{\kappa_{\mathbf{q}},j}\big)\big)\big]\mathbf{e}_i \\ &\quad = \mathbf{B}_{\kappa_{\mathbf{x}}}^{-T} \sum_{i=1}^{d} \big[\theta_h\big(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{P}_{\kappa_{\mathbf{q}},j}\big) - \theta_h\big(\mathbf{P}_{\kappa_{\mathbf{x}},0},\mathbf{P}_{\kappa_{\mathbf{q}},j}\big)\big]\mathbf{e}_i = \nabla_{\mathbf{x}}\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j}), \end{aligned} \tag{2.26}$$

where $\{\mathbf{P}_{\kappa_{\mathbf{q}},j}\}_{j=0,\dots,d}$ denote the vertices of $\kappa_{\mathbf{q}}$, which proves (2.24a). Similar arguments yield (2.24b) and (2.24c). □

By definition, the smallest eigenvalues of $\Xi_\nu^{\mathbf{x}}[.]$, $\Lambda_\nu^{\mathbf{x}}[.]$, and $\Xi_\nu^{\mathbf{q}}[.]$ are bounded from below by ν. As we will also stumble upon the largest eigenvalues of those matrices in Section 4, we define piecewise constant functions $\sigma^{\Xi_\nu^{\mathbf{x}}[.]}(\mathbf{x},\mathbf{q})$, $\sigma^{\Lambda_\nu^{\mathbf{x}}[.]}(\mathbf{x},\mathbf{q})$, and $\sigma^{\Xi_\nu^{\mathbf{q}}[.]}(\mathbf{x},\mathbf{q})$ as the supremum on $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}} \ni (\mathbf{x},\mathbf{q})$ of the largest eigenvalues of $\Xi_\nu^{\mathbf{x}}[.]\big|_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}\ni(\mathbf{x},\mathbf{q})}$, $\Lambda_\nu^{\mathbf{x}}[.]\big|_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}\ni(\mathbf{x},\mathbf{q})}$, and $\Xi_\nu^{\mathbf{q}}[.]\big|_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}\ni(\mathbf{x},\mathbf{q})}$, respectively.

Lemma 2.7. *Let $\Xi_\nu^{\mathbf{q}}[.]$, $\Xi_\nu^{\mathbf{x}}[.]$, and $\Lambda_\nu^{\mathbf{x}}[.]$ be matrix-valued operators on $\Omega \times \mathfrak{D}$ which are defined* via (2.23) *and let $\mathcal{T}_h^{\mathbf{x}}$ and $\mathcal{T}_h^{\mathbf{q}}$ be quasiuniform triangulations. Then, for $\theta_h \in \hat{X}_h$, $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$, $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$, and any nonnegative $M_h \in U_h^{\mathbf{q}}$, the estimates*

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\{\Xi_\nu^{\mathbf{q}}[\theta_h] : \Xi_\nu^{\mathbf{q}}[\theta_h]\} \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\}, \tag{2.27a}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\{\Xi_\nu^{\mathbf{x}}[\theta_h] : \Xi_\nu^{\mathbf{x}}[\theta_h]\} \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\}, \tag{2.27b}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\{\Lambda_\nu^{\mathbf{x}}[\theta_h] : \Lambda_\nu^{\mathbf{x}}[\theta_h]\} \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\}, \tag{2.27c}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\sigma^{\Xi_\nu^{\mathbf{q}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\}, \tag{2.27d}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\sigma^{\Xi_\nu^{\mathbf{x}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\}, \tag{2.27e}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\sigma^{\Lambda_\nu^{\mathbf{x}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 \le C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{|\theta_h|^2\Big\} \tag{2.27f}$$

hold true with some $C > 0$ independent of h, M_h, ν, and θ_h.

Proof. To prove (2.27a)–(2.27c), we will use the well-known estimates

$$\|\mathbf{B}_{\kappa_{\mathbf{x}}}^{-T}\|\,\|\mathbf{B}_{\kappa_{\mathbf{x}}}^{T}\| \le C, \qquad \left\|\mathbf{B}_{\kappa_{\mathbf{q}}}^{-T}\right\|\,\left\|\mathbf{B}_{\kappa_{\mathbf{q}}}^{T}\right\| \le C, \tag{2.28}$$

with the Frobenius matrix norm $\|.\|$, which hold true for quasiuniform triangulations (*cf.* [11]). Denoting the supremum on $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}$ of the largest eigenvalue of $\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]$ by $\sigma^{\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]}$, we compute

$$\begin{aligned}\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\{\Xi_\nu^{\mathbf{q}}[\theta_h] : \Xi_\nu^{\mathbf{q}}[\theta_h]\} &\leq C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \left\|\mathbf{B}_{\kappa_{\mathbf{q}}}^{-T}\right\|^2 \left\|\mathbf{B}_{\kappa_{\mathbf{q}}}^{T}\right\|^2 M_h \mathcal{I}_h^{\mathbf{x}}\left\{\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h] : \hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]\right\} \\ &\leq C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h d \left|\sigma^{\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 = C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h d \left|\sigma^{\Xi_\nu^{\mathbf{q}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2, \end{aligned} \tag{2.29}$$

as $\Xi_\nu^{\mathbf{q}}[\theta_h]$ and $\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]$ share the same eigenvalues. Combining (2.23e) with the mean value theorem yields

$$\left|\sigma^{\Xi_\nu^{\mathbf{q}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 = \left|\sigma^{\hat{\Xi}_\nu^{\mathbf{q}}[\theta_h]}(\mathbf{x},\mathbf{q})\right|^2 \leq \left|\max\left\{\nu, \max_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \theta_h\right\}\right|^2 \leq \nu^2 + \max_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} |\theta_h|^2. \tag{2.30}$$

Due to the structure of $\hat{X}_h$, this maximum is attained in one of the vertices of $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}$. The estimate

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \max_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \{\theta_h\}^2 \leq \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \sum_{i,j=0}^{d} \left|\theta_h\left(\mathbf{P}_{\kappa_{\mathbf{x}},i}, \mathbf{P}_{\kappa_{\mathbf{q}},j}\right)\right|^2 \leq C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{xq}}\left\{|\theta_h|^2\right\} \tag{2.31}$$

finally yields (2.27a) and (2.27d). Analogous arguments show (2.27b), (2.27c), (2.27e), and (2.27f). ☐

As already indicated by their definition, the quantities $\Xi_\nu^{\mathbf{q}}[\theta_h]$, $\Xi_\nu^{\mathbf{x}}[\theta_h]$, and $\Lambda_\nu^{\mathbf{x}}[\theta_h]$ are meant to be local approximations of $\theta_h \in \hat{X}_h$. The following lemma characterizes the quality of the approximation. As $\Xi_\nu^{\mathbf{q}}[\theta_h]$, $\Xi_\nu^{\mathbf{x}}[\theta_h]$, and $\Lambda_\nu^{\mathbf{x}}[\theta_h]$ are positive definite matrices, the quality of the approximation will naturally depend on the negative fraction

$$[.]_- : s \mapsto [s]_- := \min\{0, s\} \tag{2.32}$$

of θ_h.

Lemma 2.8. *Let $\Xi_\nu^{\mathbf{q}}[.]$, $\Xi_\nu^{\mathbf{x}}[.]$, and $\Lambda_\nu^{\mathbf{x}}[.]$ be matrix-valued operators on $\Omega \times \mathfrak{D}$ which are defined* via (2.23) *and let the triangulations $\mathcal{T}_h^{\mathbf{x}}$ and $\mathcal{T}_h^{\mathbf{q}}$ be quasiuniform. Then, for $\theta_h \in \hat{X}_h$, $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$, $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$, and any nonnegative $M_h \in U_h^{\mathbf{q}}$, the following estimates hold true*

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{|\Xi_\nu^{\mathbf{q}}[\theta_h] - \theta_h \mathbb{1}|^2\right\} \leq C\left(h_{\mathbf{q}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{|\nabla_{\mathbf{q}}\theta_h|^2\right\} + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \nu^2 + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{xq}}\left\{[\theta_h]_-^2\right\}\right), \tag{2.33a}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\Xi_\nu^{\mathbf{x}}[\theta_h] - \theta_h \mathbb{1}|^2\right\} \leq C\left(h_{\mathbf{x}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\nabla_{\mathbf{x}}\theta_h|^2\right\} + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \nu^2 + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{xq}}\left\{[\theta_h]_-^2\right\}\right), \tag{2.33b}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\Lambda_\nu^{\mathbf{x}}[\theta_h] - \theta_h \mathbb{1}|^2\right\} \leq C\left(h_{\mathbf{x}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\nabla_{\mathbf{x}}\theta_h|^2\right\} + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \nu^2 + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{xq}}\left\{[\theta_h]_-^2\right\}\right), \tag{2.33c}$$

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\Xi_\nu^{\mathbf{x}}[\theta_h] - \Lambda_\nu^{\mathbf{x}}[\theta_h]|^2\right\} \leq C h_{\mathbf{x}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\nabla_{\mathbf{x}}\theta_h|^2\right\}, \tag{2.33d}$$

where $\mathbb{1}$ denotes the unit matrix in $\mathbb{R}^{d\times d}$.

Proof. We start with the estimate

$$\begin{aligned}&\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{|\Xi_\nu^{\mathbf{q}}[\theta_h] - \theta_h \mathbb{1}|^2\right\} \\ &\qquad \leq C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{\left|\Xi_\nu^{\mathbf{q}}[\theta_h] - g_\nu''(\theta_h)^{-1}\mathbb{1}\right|^2\right\} + C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{\left|g_\nu''(\theta_h)^{-1}\mathbb{1} - \theta_h \mathbb{1}\right|^2\right\} \\ &\qquad =: I + II. \end{aligned} \tag{2.34}$$

Similarly to the proof of Lemma 2.7, we use (2.28) to gain access to the entries of the diagonal matrix $\hat{\Xi}^{\mathbf{q}}_{\nu}[\theta_h]$. Then, we use the affine linearity of θ_h with respect to $\mathbf{q}$ to compute

$$\begin{aligned} I &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left\|\mathbf{B}_{\kappa_{\mathbf{x}}}^T\right\|^2 \left\|\mathbf{B}_{\kappa_{\mathbf{x}}}^{-T}\right\|^2 \mathcal{I}_h^{\mathbf{x}}\left\{\left|\hat{\Xi}^{\mathbf{q}}_{\nu}[\theta_h] - \max\{\nu,\theta_h\}\mathbb{1}\right|^2\right\} \\ &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h d\mathcal{I}_h^{\mathbf{x}}\left\{\left|\max_{j=1,\dots,d} \max\{\nu,\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j})\} - \min_{j=1,\dots,d} \max\{\nu,\theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j})\}\right|^2\right\} \\ &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h d\mathcal{I}_h^{\mathbf{x}}\left\{\left|\max_{j=1,\dots,d} \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j}) - \min_{j=1,\dots,d} \theta_h(\mathbf{x},\mathbf{P}_{\kappa_{\mathbf{q}},j})\right|^2\right\} \\ &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h h_{\mathbf{q}}^2 \left\|\nabla_{\mathbf{q}}\theta_h\right\|^2_{L^\infty(\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}})} \le Ch_{\mathbf{q}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \sum_{i=1}^d \left|\nabla_{\mathbf{q}}\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q})\right|^2 \\ &\le Ch_{\mathbf{q}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{|\nabla_{\mathbf{q}}\theta_h|^2\right\}, \end{aligned} \tag{2.35}$$

where we used that $\nabla_{\mathbf{q}}\theta_h$ is constant with respect to $\mathbf{q}$ on each simplex. Concerning the second term, we use that $g_\nu''(s)^{-1} \equiv s$ for $s \ge \nu$.

$$\begin{aligned} II &\le d \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left\|\nu - [\theta_h]_-\right\|^2_{L^\infty(\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}})} \le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left\|\nu^2 + [\theta_h]_-^2\right\|_{L^\infty(\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}})} \\ &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \sum_{i,j=0}^d [\theta_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{P}_{\kappa_{\mathbf{q}},j})]_-^2 \\ &\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h\nu^2 + C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{xq}}\left\{[\theta_h]_-^2\right\}. \end{aligned} \tag{2.36}$$

Therefore, (2.33a) is proven. Analogous computations yield (2.33b) and (2.33c). Noting $g_\nu''(\theta_h)^{-1} \equiv f_\nu'(\theta_h)$, the last inequality follows from

$$\begin{aligned} &\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|\Xi^{\mathbf{x}}_\nu[\theta_h] - \Lambda^{\mathbf{x}}_\nu[\theta_h]|^2\right\} \\ &\quad\le C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{\left|\Xi^{\mathbf{x}}_\nu[\theta_h] - g_\nu''(\theta_h)^{-1}\mathbb{1}\right|^2\right\} + C \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{|f_\nu'(\theta_h)\mathbb{1} - \Lambda^{\mathbf{x}}_\nu[\theta_h]|^2\right\} \end{aligned} \tag{2.37}$$

with arguments similar to (2.35). □

2.4. A discrete mollifier

In this subsection, we introduce a finite element version of the continuous mollifier $\mathcal{J}_\varepsilon$. It will turn out that a suitable weak formulation (or discrete scheme, respectively) allows to drop the properties (1.9a)–(1.9e). Therefore, we only demand that the discrete mollifier satisfies an inequality similar to (1.9f) and converges towards $\mathcal{J}_\varepsilon$ in a suitable sense (*cf.* Lem. 2.11).

We define a discrete mollification operator $\mathcal{J}_{\varepsilon,h}$ analogously to (1.8). Again, we start with a nonnegative, rotationally symmetric $\zeta \in W^{2,\infty}(\mathbb{R}^d)$ satisfying $\operatorname{supp}\zeta \subset \overline{B(0,1)}$ with mass one. We then define $\zeta_\varepsilon(\mathbf{x}) := \varepsilon^{-d}\zeta(\varepsilon^{-1}\mathbf{x})$ and finally $\mathcal{J}_{\varepsilon,h}$ *via*

$$\mathcal{J}_{\varepsilon,h}\{f\}(\mathbf{x}) := c_{\mathcal{J}}(\mathbf{x}) \int_\Omega \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} f(\mathbf{y})\,\mathrm{d}\mathbf{y}, \tag{2.38}$$

for $f \in L^1(\Omega)$ with the nodal interpolation operator $\mathcal{I}_h^{\mathbf{y}}$ which is equivalent to $\mathcal{I}_h^{\mathbf{x}}$ but works on the spatial variable $\mathbf{y}$. The weight function $c_{\mathcal{J}}(\mathbf{x}) := [\int_{\mathbb{R}^d} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y}]^{-1}$ reduces the impact of the triangulation on $\mathcal{J}_{\varepsilon,h}$ but inhibits a property similar to (1.9c). As we defined Ω^* such that $\operatorname{dist}(\Omega, \partial\Omega^*) \geq \varepsilon$, it suffices to write $c_{\mathcal{J}}$ in a practically more convenient way as

$$c_{\mathcal{J}}(\mathbf{x}) := \left[\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y}\right]^{-1}. \tag{2.39}$$

Lemma 2.9. *Let* $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ *and* $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ *satisfy (S1)–(S3) and let* $c_{\mathcal{J}}$ *be the weight function defined* via (2.39). *Then there exists* $C > 0$ *independent of* $h_{\mathbf{x}}$ *such that*

$$\|c_{\mathcal{J}}\|_{W^{1,\infty}(\Omega)} \leq C(\varepsilon), \tag{2.40}$$

for $h_{\mathbf{x}}$ *small enough.*

Proof. Using $\int_{\Omega^*} \zeta_\varepsilon(\mathbf{x}-\mathbf{y}) \,\mathrm{d}\mathbf{y} \equiv 1$ for all $\mathbf{x} \in \Omega$ and the standard error estimates for the interpolation operator (see *e.g.* Thm. 4.4.4 and Them. 4.4.20 in [9]), we obtain

$$\begin{aligned}\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y} &= \int_{\Omega^*} \zeta_\varepsilon(\mathbf{x}-\mathbf{y}) \,\mathrm{d}\mathbf{y} + \int_{\Omega^*} \left(\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} - \zeta_\varepsilon(\mathbf{x}-\mathbf{y})\right) \mathrm{d}\mathbf{y} \\ &\geq 1 - \sum_{\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}*}} |\kappa_{\mathbf{x}}| \left\|\zeta_\varepsilon(\mathbf{x}-\,.\,) - \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\,.\,)\}\right\|_{L^\infty(\kappa_{\mathbf{x}})} \\ &\geq 1 - \sum_{\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}*}} |\kappa_{\mathbf{x}}| \, C h_{\mathbf{x}}^2 \left|\zeta_\varepsilon(\mathbf{x}-\,.\,)\right|_{W^{2,\infty}(\kappa_{\mathbf{x}})} \\ &\geq 1 - C\,|\Omega^*|\, h_{\mathbf{x}}^2 \,|\zeta_\varepsilon|_{W^{2,\infty}(\mathbb{R}^d)} \geq 1 - C(\varepsilon) h_{\mathbf{x}}^2 \geq \tilde{C}(\varepsilon) > 0,\end{aligned} \tag{2.41}$$

for $h_{\mathbf{x}}$ small enough. Therefore, $\|c_{\mathcal{J}}\|_{L^\infty(\Omega)}$ is bounded from above by $\tilde{C}(\varepsilon)^{-1}$. Combining this result with

$$\begin{aligned}|\partial_{\mathbf{x}_i} c_{\mathcal{J}}(\mathbf{x})| &\leq \left[\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y}\right]^{-2} \left|\partial_{\mathbf{x}_i} \int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y}\right| \\ &= c_{\mathcal{J}}^2(\mathbf{x}) \left|\int_{\Omega^*} \sum_{j=1}^{\dim U_h^{\mathbf{x}*}} \partial_{\mathbf{x}_i} \zeta_\varepsilon(\mathbf{x}-\mathbf{y}_j) \chi_{h,j}^{\mathbf{y}}(\mathbf{y}) \,\mathrm{d}\mathbf{y}\right| \leq c_{\mathcal{J}}^2(\mathbf{x}) \,|\Omega^*|\, \|\partial_{\mathbf{x}_i} \zeta_\varepsilon\|_{L^\infty(\mathbb{R}^d)}\end{aligned} \tag{2.42}$$

for all $i = 1, \ldots, d$, where $\{\chi_{h,j}^{\mathbf{y}}\}_{j=1,\ldots,\dim U_h^{\mathbf{x}*}}$ form a dual basis to the nodes $\{\mathbf{y}_j\}_{j=1,\ldots,\dim U_h^{\mathbf{x}*}}$ with $\sum_{j=1}^{\dim U_h^{\mathbf{x}*}} \chi_{h,j}^{\mathbf{y}}(\mathbf{y}) \equiv 1$, yields the result. □

The mollifier $\mathcal{J}_\varepsilon$ was constructed as convolution with a $W^{2,\infty}(\mathbb{R}^d)$-kernel, which allowed for the estimate (1.9f). In the discrete setting, the interpolation operator $\mathcal{I}_h^{\mathbf{y}}$ decreases the regularity. However, we still have an analog to (1.9f) for the $W^{1,\infty}(\Omega)$-norm of the discrete mollifier.

Lemma 2.10. *Let* $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ *and* $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ *satisfy (S1)–(S3) and let* $c_{\mathcal{J}}$ *be the weight function defined* via (2.39). *Then, the discrete mollifier* $\mathcal{J}_{\varepsilon,h}$ *defined in* (2.38) *satisfies*

$$\|\mathcal{J}_{\varepsilon,h}\{f\}\|_{W^{1,\infty}(\Omega)} \leq C(\varepsilon)\, \|f\|_{L^1(\Omega)} \qquad \textit{for all } f \in L^1(\Omega), \tag{2.43}$$

with some $C(\varepsilon) > 0$ *which is independent of* $h_{\mathbf{x}}$.

Proof. We use the result of Lemma 2.9 and the regularity of ζ_ε to compute

$$\begin{aligned}\|\mathcal{J}_{\varepsilon,h}\{f\}\|_{L^\infty(\Omega)} &\le \sup_{\mathbf{x}\in\Omega}\left(c_{\mathcal{J}}(\mathbf{x})\int_\Omega |\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\}|\,|f(\mathbf{y})|\;\mathrm{d}\mathbf{y}\right)\\ &\le C\,\|\zeta_\varepsilon\|_{L^\infty(\mathbb{R}^d)}\int_\Omega |f(\mathbf{y})|\;\mathrm{d}\mathbf{y} \le C(\varepsilon)\,\|f\|_{L^1(\Omega)}.\end{aligned} \tag{2.44}$$

Applying the product rule on the derivative of $\mathcal{J}_{\varepsilon,h}\{f\}$ yields

$$\begin{aligned}|\partial_{\mathbf{x}_i}\mathcal{J}_{\varepsilon,h}\{f\}| \le{}& |\partial_{\mathbf{x}_i}c_{\mathcal{J}}(\mathbf{x})|\int_\Omega |\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\}|\,|f(\mathbf{y})|\;\mathrm{d}\mathbf{y}\\ &+|c_{\mathcal{J}}(\mathbf{x})|\int_\Omega |\partial_{\mathbf{x}_i}\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\}|\,|f(\mathbf{y})|\;\mathrm{d}\mathbf{y}.\end{aligned} \tag{2.45}$$

The first summand is bounded from above by $C(\varepsilon)\,\|f\|_{L^1(\Omega)}$ due to Lemma 2.9 and the regularity of ζ_ε. Concerning the second summand, we have $\|c_{\mathcal{J}}\|_{L^\infty(\Omega)} \le C(\varepsilon)$ and may apply the mean value theorem to obtain the desired result. ☐

With the following lemma, we prove the convergence of $\mathcal{J}_{\varepsilon,h}\{f\}$ towards $\mathcal{J}_\varepsilon\{f\}$ for $f\in L^1(\Omega)$.

Lemma 2.11. *Let be $\mathcal{J}_\varepsilon$ be the mollifier defined in (1.8) and $\mathcal{J}_{\varepsilon,h}$ the finite element version of $\mathcal{J}_\varepsilon$ which is defined in (2.38). Furthermore, let $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ and $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ satisfy (S1)–(S3) and let $c_{\mathcal{J}}$ be the weight function defined* via *(2.39). Then, there exists $C>0$ independent of $h_{\mathbf{x}}$ such that*

$$\|\mathcal{J}_{\varepsilon,h}\{f\}-\mathcal{J}_\varepsilon\{f\}\|_{W^{1,\infty}(\Omega)} \le C(\varepsilon)h_{\mathbf{x}}\,\|f\|_{L^1(\Omega)} \tag{2.46}$$

for $f\in L^1(\Omega)$ and $h_{\mathbf{x}}$ small enough.

Proof. We start with the estimate

$$\begin{aligned}\|\mathcal{J}_{\varepsilon,h}\{f\}-\mathcal{J}_\varepsilon\{f\}\|_{W^{1,\infty}(\Omega)} \le{}& \left\|c_{\mathcal{J}}(.)\int_\Omega (\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\,.\,-\mathbf{y})\}-\zeta_\varepsilon(\,.\,-\mathbf{y}))f(\mathbf{y})\;\mathrm{d}\mathbf{y}\right\|_{W^{1,\infty}(\Omega)}\\ &+\left\|(1-c_{\mathcal{J}}(.))\int_\Omega \zeta_\varepsilon(\,.\,-\mathbf{y})f(\mathbf{y})\;\mathrm{d}\mathbf{y}\right\|_{W^{1,\infty}(\Omega)} =: I+II.\end{aligned} \tag{2.47}$$

Applying the product rule on I yields

$$\begin{aligned}I \le{}& \|c_{\mathcal{J}}\|_{W^{1,\infty}(\Omega)}\left\|\int_\Omega (\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\,.\,-\mathbf{y})\}-\zeta_\varepsilon(\,.\,-\mathbf{y}))f(\mathbf{y})\;\mathrm{d}\mathbf{y}\right\|_{L^\infty(\Omega)}\\ &+\|c_{\mathcal{J}}\|_{L^\infty(\Omega)}\max_{i=1,..,d}\left\|\int_\Omega \partial_{\mathbf{x}_i}(\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\,.\,-\mathbf{y})\}-\zeta_\varepsilon(\,.\,-\mathbf{y}))f(\mathbf{y})\;\mathrm{d}\mathbf{y}\right\|_{L^\infty(\Omega)}.\end{aligned} \tag{2.48}$$

Lemma 2.9 provides $\|c_{\mathcal{J}}\|_{W^{1,\infty}(\Omega)} \le C(\varepsilon)$. To control the second factors in the terms on the right-hand side of (2.48), we denote the dual basis to the nodes $\{\mathbf{y}_j\}_{j=1,\ldots,\dim U_h^{\mathbf{x}*}}$ by $\left\{\chi_{h,j}^{\mathbf{y}}\right\}_{j=1,\ldots,\dim U_h^{\mathbf{x}*}}$. Noting $\sum_{j=1}^{\dim U_h^{\mathbf{x}*}}\chi_{h,j}^{\mathbf{y}}(\mathbf{y})\equiv 1$ for $\mathbf{y}\in\Omega$, we compute for $\mathbf{x}\in\Omega$

$$\begin{aligned}\sup_{\mathbf{y}\in\Omega}|(\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\}-\zeta_\varepsilon(\mathbf{x}-\mathbf{y}))| &= \sup_{\mathbf{y}\in\Omega}\left|\sum_{j=1}^{\dim U_h^{\mathbf{x}}}(\zeta_\varepsilon(\mathbf{x}-\mathbf{y}_j)-\zeta_\varepsilon(\mathbf{x}-\mathbf{y}))\chi_{h,j}^{\mathbf{y}}(\mathbf{y})\right|\\ &\le \sup_{\mathbf{y}\in\Omega}\max_{j\,:\,\mathbf{y}\in\operatorname{supp}\chi_{h,j}^{\mathbf{y}}}|\zeta_\varepsilon(\mathbf{x}-\mathbf{y}_j)-\zeta_\varepsilon(\mathbf{x}-\mathbf{y})| \le C(\varepsilon)h_{\mathbf{x}},\end{aligned} \tag{2.49}$$

where we used $0 \leq \chi_{h,j}^{\mathbf{y}} \leq 1$ for $j = 1, \dots, \dim U_h^{\mathbf{x}}$, $|\zeta_\varepsilon(\tilde{\mathbf{x}}) - \zeta_\varepsilon(\tilde{\mathbf{y}})| \leq C(\varepsilon) |\tilde{\mathbf{x}} - \tilde{\mathbf{y}}|$ for $\tilde{\mathbf{x}}, \tilde{\mathbf{y}} \in \Omega$ (as $\zeta_\varepsilon \in W^{2,\infty}(\mathbb{R}^d)$), and $\max_{j=1,\dots,\dim U_h^{\mathbf{x}}} \operatorname{diam}\left(\operatorname{supp} \chi_{h,j}^{\mathbf{y}}\right) \leq C h_{\mathbf{x}}$. Similarly, we compute for $i = 1, \dots, d$ and $\mathbf{x} \in \Omega$

$$\sup_{\mathbf{y} \in \Omega} |\partial_{\mathbf{x}_i} (\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} - \zeta_\varepsilon(\mathbf{x}-\mathbf{y}))| \leq C(\varepsilon) h_{\mathbf{x}}. \tag{2.50}$$

Combining (2.48) with Lemma 2.9, (2.49), and (2.50) yields

$$I \leq C(\varepsilon) h_{\mathbf{x}} \|f\|_{L^1(\Omega)}. \tag{2.51}$$

To control II, we compute

$$II \leq C \|1 - c_{\mathcal{J}}(.)\|_{W^{1,\infty}(\Omega)} \|\mathcal{J}_\varepsilon\{f\}\|_{W^{1,\infty}(\Omega)}. \tag{2.52}$$

As (1.9f) yields $\|\mathcal{J}_\varepsilon\{f\}\|_{W^{1,\infty}(\Omega)} \leq \|\mathcal{J}_\varepsilon\{f\}\|_{W^{2,\infty}(\Omega)} \leq C(\varepsilon) \|f\|_{L^1(\Omega)}$, it remains to show that $\|1 - c_{\mathcal{J}}(.)\|_{W^{1,\infty}(\Omega)} \leq h_{\mathbf{x}} C(\varepsilon)$. From (2.41), we have $\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y} \geq 1 - C(\varepsilon) h_{\mathbf{x}}^2$ for $\mathbf{x} \in \Omega$. Analogously, we may compute $\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} \,\mathrm{d}\mathbf{y} \leq 1 + C(\varepsilon) h_{\mathbf{x}}^2$. Hence, we have for $h_{\mathbf{x}}$ small enough

$$\|1 - c_{\mathcal{J}}(.)\|_{L^\infty(\Omega)} = \left\| \frac{\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\,.\, - \mathbf{y})\} \,\mathrm{d}\mathbf{y} - 1}{\int_{\Omega^*} \mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\,.\, - \mathbf{y})\} \,\mathrm{d}\mathbf{y}} \right\|_{L^\infty(\Omega)} \leq \frac{C(\varepsilon) h_{\mathbf{x}}^2}{1 - C(\varepsilon) h_{\mathbf{x}}^2} \leq C(\varepsilon) h_{\mathbf{x}}^2. \tag{2.53}$$

Noting $\int_{\Omega^*} \zeta_\varepsilon(\mathbf{x}-\mathbf{y}) \,\mathrm{d}\mathbf{y} = 1$ for all $\mathbf{x} \in \Omega$ and reusing the idea of (2.50), we obtain

$$\begin{aligned} &\|\partial_{\mathbf{x}_i}(1 - c_{\mathcal{J}}(.))\|_{L^\infty(\Omega)} \\ &\quad \leq \|c_{\mathcal{J}}\|_{L^\infty(\Omega)}^2 |\Omega^*| \sup_{\mathbf{y} \in \Omega^*,\, \mathbf{x} \in \Omega} |\partial_{\mathbf{x}_i}(\mathcal{I}_h^{\mathbf{y}}\{\zeta_\varepsilon(\mathbf{x}-\mathbf{y})\} - \zeta_\varepsilon(\mathbf{x}-\mathbf{y}))| \leq C(\varepsilon) h_{\mathbf{x}} \end{aligned} \tag{2.54}$$

for $i = 1, \dots, d$, which completes the proof. □

By applying $\mathcal{J}_{\varepsilon,h}$ on each component of a vector-valued function $\mathbf{f} \in \boldsymbol{L}^1(\Omega)$, we obtain a discrete version of $\boldsymbol{\mathcal{J}}_\varepsilon$ denoted by $\boldsymbol{\mathcal{J}}_{\varepsilon,h}$ which satisfies a vector-valued version of Lemma 2.10 and Lemma 2.11. As we will not consider the limit $\varepsilon \searrow 0$, we suppress the dependence of constants on ε and denote the discrete mollifiers by $\mathcal{J}_h$ and $\boldsymbol{\mathcal{J}}_h$.

3. A stable, discrete scheme

In this section, we introduce a stable, fully discrete finite element scheme allowing to approximate the solutions of (1.5) in the case of different mass densities and establishing an *a priori* stability result for possible solutions. An existence result may easily be deduced using Brouwer's fixed point theorem.

As we show in the subsequent sections, the presented scheme is convergent in the case of equal mass densities.

As the mass density function ρ depends affine linearly on the phase-field parameter ϕ, it is positive as long as ϕ stays in the interval $(-\mathfrak{At}^{-1}, \mathfrak{At}^{-1})$ with $\mathfrak{At} := \left|\frac{\tilde{\rho}_2 - \tilde{\rho}_1}{\tilde{\rho}_2 + \tilde{\rho}_1}\right| < 1$ denoting the Atwood number. Since there is no mechanism guaranteeing that ϕ stays in this region, we introduce a regularized mass density function (*cf.* [15]). Picking some parameter $\overline{\phi} \in (1, \mathfrak{At}^{-1})$, we approximate the mass density of the two-phase flow by a smooth, monotonously increasing (or decreasing, respectively), strictly positive function $\overline{\rho}$ satisfying

$$\overline{\rho}(\phi)\big|_{(-\overline{\phi}, +\overline{\phi})} = \tfrac{\tilde{\rho}_2 + \tilde{\rho}_1}{2} - \tfrac{\tilde{\rho}_2 - \tilde{\rho}_1}{2} \phi, \tag{3.1a}$$

$$\overline{\rho}(\phi)\big|_{(-\infty, -\overline{\phi}]} \equiv \text{const}, \qquad \overline{\rho}(\phi)\big|_{[+\overline{\phi}, +\infty)} \equiv \text{const}. \tag{3.1b}$$

As the original mass density ρ depends affine linearly on the phase-field parameter, we introduce $\frac{\delta \overline{\rho}}{\delta \phi} := \frac{\tilde{\rho}_2 - \tilde{\rho}_1}{2}$ as an approximation of the derivative of $\overline{\rho}$ (*cf.* [15]).

Similarly to [16], we make the following assumption on the general structure of the double-well potential W.

(W1) $W \in C^1(\mathbb{R};\mathbb{R}_0^+)$ with $\left|W(s)s^{-3}\right| \to \infty$ for $|s| \to \infty$ such that W' is piecewise C^1 and that its derivatives have at most quadratic growth for $|s| \to \infty$.

We allow for different discrete approximations of the derivative W' which we denote by $W_h' : \mathbb{R}^2 \to \mathbb{R}_0^+$. Thereby, we will assume that the following conditions hold true.

(W2) There is a positive constant C such that for all $a, b \in \mathbb{R}$

$$|W_h'(a,b)| \leq C\Big(1 + |a|^3 + |b|^3\Big).$$

(W3) $W_h'(a,b)(a-b) \geq W(a) - W(b)$ for all $a, b \in \mathbb{R}$.
(W4) $W_h'(a,a) = W'(a)$ for all $a \in \mathbb{R}$.
(W5) There is a positive constant C, such that for all $a, b, c \in \mathbb{R}$

$$|W_h'(a,b) - W_h'(b,c)| \leq C(a^2 + b^2 + c^2)(|a-b| + |b-c|).$$

Remark 3.1. In the simulations presented in Section 6, we will consider a polynomial double-well potential with penalty terms which reads

$$W(\phi) = \tfrac{1}{4}\left(1-\phi^2\right)^2 + \tfrac{1}{\delta'}\max\left\{|\phi| - 1, 0\right\}^2 \tag{3.2}$$

with some penalty parameter $0 < \delta' \ll 1$. This approach often suffices to confine the phase-field parameter to an interval close to the physical meaningful interval $[-1,+1]$. The double-well potential defined in (3.2) satisfies (W1). Suitable choices for $W_h'(\,.\,,\,.\,)$ satisfying (W2)–(W5) are *e.g.* discretizations using a difference quotient or the classical convex-concave splitting (*cf.* [16]).

For the approximation of β', we use a difference quotient, *i.e.* we define β'_{DQ} by

$$\beta'_{DQ}(a,b) := \begin{cases} \frac{\beta(a)-\beta(b)}{a-b} & \text{if } a \neq b, \\ \beta'(a) & \text{if } a = b, \end{cases} \tag{3.3}$$

for all $a, b \in \mathbb{R}$, which immediately yields $\beta'_{DQ}(a,b)(a-b) = \beta(a) - \beta(b)$ for all $a, b \in \mathbb{R}$.

Denoting the backward difference quotient in time by ∂_τ^- and using the above definitions, we introduce the following discrete scheme. Given $\phi_h^{n-1} \in U_h^{\mathbf{x}}$, $\hat{\psi}_h^{n-1} \in \hat{X}_h$, and $\mathbf{u}_h^{n-1} \in \boldsymbol{W}_{h,\mathrm{div}}$, we compute a quadruple $\left\{\phi_h^n,\, \mu_{\phi,h}^n,\, \hat{\psi}_h^n, \mathbf{u}_h^n\right\} \in U_h^{\mathbf{x}} \times U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$ solving

$$\begin{aligned}
&\int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\partial_\tau^- \phi_h^n \theta_h^{\mathbf{x}}\} - \int_\Omega \phi_h^{n-1}\mathbf{u}_h^{n-1} \cdot \nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} \\
&\quad + \tau \int_\Omega \left(\min \overline{\rho}_h^{n-1}\right)^{-1} \left|\phi_h^{n-1}\right|^2 \nabla_{\mathbf{x}}\mu_{\phi,h}^n \cdot \nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} + \int_\Omega \nabla_{\mathbf{x}}\mu_{\phi,h}^n \cdot \nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} = 0 \qquad \forall \theta_h^{\mathbf{x}} \in U_h^{\mathbf{x}},
\end{aligned} \tag{3.4a}$$

$$\begin{aligned}
\int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\mu_{\phi,h}^n \theta_h^{\mathbf{x}}\} &= \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W_h'(\phi_h^n, \phi_h^{n-1})\theta_h^{\mathbf{x}}\} + \int_\Omega (\vartheta\nabla_{\mathbf{x}}\phi_h^n + (1-\vartheta)\nabla_{\mathbf{x}}\phi_h^{n-1}) \cdot \nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} \\
&\quad + \int_\Omega \mathcal{I}_h^{\mathbf{x}}\left\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta'_{DQ}(\phi_h^n, \phi_h^{n-1})\theta_h^{\mathbf{x}}\}\} \int_{\mathfrak{D}} (M_h + \mathfrak{m})\hat{\psi}_h^{n-1}\right\} \qquad \forall \theta_h^{\mathbf{x}} \in U_h^{\mathbf{x}},
\end{aligned} \tag{3.4b}$$

$$\begin{aligned}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\partial_\tau^-\hat{\psi}_h^n\theta_h\Big\} - \int_{\Omega\times\mathfrak{D}} M_h\mathbf{u}_h^n\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\theta_h\Big\}\\
-\int_{\Omega\times\mathfrak{D}} (\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{u}_h^n\}\}\cdot\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\})\cdot\mathcal{I}_h^{\mathbf{x}}\Big\{\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^n]\nabla_{\mathbf{q}}\theta_h\Big\}\\
+(1-\gamma)\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)+\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\Big\}\Big)\cdot\nabla_{\mathbf{x}}\theta_h\Big\}\\
+\gamma\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)+\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\Big\}\Big)\cdot\nabla_{\mathbf{x}}\theta_h\Big\}\\
+\int_{\Omega\times\mathfrak{D}} c_{\mathbf{q}}M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\nabla_{\mathbf{q}}\hat{\psi}_h^n\cdot\nabla_{\mathbf{q}}\theta_h\Big\} = 0\\
\forall\theta_h\in\hat{X}_h,\end{aligned} \tag{3.4c}$$

$$\begin{aligned}\int_\Omega \tfrac{1}{2}\big(\overline{\rho}_h^n+\overline{\rho}_h^{n-1}\big)\partial_\tau^-\mathbf{u}_h^n\cdot\mathbf{w}_h + \tfrac{1}{2}\int_\Omega \partial_\tau^-\overline{\rho}_h^n\mathbf{u}_h^{n-1}\cdot\mathbf{w}_h\\
+\tfrac{1}{2}\int_\Omega \overline{\rho}_h^n\Big((\nabla_{\mathbf{x}}\mathbf{u}_h^n)^T\cdot\mathbf{w}_h\Big)\cdot\mathbf{u}_h^{n-1} - \tfrac{1}{2}\int_\Omega \overline{\rho}_h^n\Big((\nabla_{\mathbf{x}}\mathbf{w}_h)^T\cdot\mathbf{u}_h^n\Big)\cdot\mathbf{u}_h^{n-1}\\
+\tfrac{1}{2}\int_\Omega \tfrac{\delta\overline{\rho}}{\delta\phi}\Big((\nabla_{\mathbf{x}}\mathbf{u}_h^n)^T\cdot\mathbf{w}_h\Big)\cdot\nabla_{\mathbf{x}}\mu_{\phi,h}^n - \tfrac{1}{2}\int_\Omega \tfrac{\delta\overline{\rho}}{\delta\phi}\Big((\nabla_{\mathbf{x}}\mathbf{w}_h)^T\cdot\mathbf{u}_h^n\Big)\cdot\nabla_{\mathbf{x}}\mu_{\phi,h}^n\\
+\int_\Omega 2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^n)\}\mathbf{D}\mathbf{u}_h^n:\mathbf{D}\mathbf{w}_h = -\int_\Omega \phi_h^{n-1}\nabla_{\mathbf{x}}\mu_{\phi,h}^n\cdot\mathbf{w}_h\\
-\int_{\Omega\times\mathfrak{D}} M_h\mathbf{w}_h\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)+\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\Big\}\Big\}\\
-\int_{\Omega\times\mathfrak{D}} (\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{w}_h\}\}\cdot\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\})\cdot\nabla_{\mathbf{q}}\hat{\psi}_h^n\\
\forall\mathbf{w}_h\in\boldsymbol{W}_{h,\mathrm{div}},\end{aligned} \tag{3.4d}$$

with some fixed $\vartheta\in(0.5,1]$, $\gamma\in(0,1)$ and some regularization parameter $\mathfrak{m}>0$. To simplify the notation, we used the abbreviation $\overline{\rho}_h^n:=\mathcal{I}_h^{\mathbf{x}}\{\overline{\rho}(\phi_h^n)\}$. For better readability, we introduce the discrete version of the chemical potential of the polymer densities as

$$\mu_{\psi,h,\nu}^n := \mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)+\mathcal{J}_h\{\beta(\phi_h^n)\}\Big\}\in\hat{X}_h \tag{3.5}$$

for $n=1,\dots,N$.

Remark 3.2. As (3.4a) and (3.4b) do not depend on $\hat{\psi}_h^n$ and $\mathbf{u}_h^n$, it is possible to compute ϕ_h^n and $\mu_{\phi,h}^n$ separately before advancing to (3.4c) and (3.4d). To maintain stability, the third term in (3.4a) was added. Similar splitting ideas have previously been used in [3], [20], and [26] for a model of magnetohydrodynamics and for diffuse interface models for multi-phase and two-phase flows, respectively. For the case of a pure two-phase flow with different mass densities without any additional species, convergence of this splitting approach has been established in [16].

Remark 3.3. For time-discretizations of $\int_\Omega \nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}}$, we have chosen a compromise between

$$\nabla_{\mathbf{x}}\phi_h^n\cdot\nabla_{\mathbf{x}}\partial_\tau^-\phi_h^n = \tfrac{1}{2\tau}\left|\nabla_{\mathbf{x}}\phi_h^n\right|^2+\tfrac{1}{2\tau}\left|\nabla_{\mathbf{x}}\phi_h^n-\nabla_{\mathbf{x}}\phi_h^{n-1}\right|^2-\tfrac{1}{2\tau}\left|\nabla_{\mathbf{x}}\phi_h^{n-1}\right|^2$$

and

$$\tfrac{1}{2}\big(\nabla_{\mathbf{x}}\phi_h^n+\nabla_{\mathbf{x}}\phi_h^{n-1}\big)\cdot\nabla_{\mathbf{x}}\partial_\tau^-\phi_h^n = \tfrac{1}{2\tau}\left|\nabla_{\mathbf{x}}\phi_h^n\right|^2-\tfrac{1}{2\tau}\left|\nabla_{\mathbf{x}}\phi_h^{n-1}\right|^2,$$

to reduce the numerical dissipation of the scheme (*cf.* Sect. 4.2 in [25]). Although the scheme is still stable for $\vartheta = 0.5$, the presented proof of convergence requires $\vartheta > 0.5$, as we need to control $\tau^{-1}\sum_{k=1}^{n}\int_\Omega \left|\nabla_{\mathbf{x}}\phi_h^k - \nabla_{\mathbf{x}}\phi_h^{k-1}\right|^2$ (*cf.* Lem. 5.1).

Remark 3.4. The choice of $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ as an approximation for $\hat{\psi}$ in the $\mathbf{x}$-convective term in (3.4c) allows to establish improved regularity results for the scaled configurational density $\hat{\psi}$ (*cf.* Lem. 4.5). Unfortunately, this enforces the application of $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ on the right-hand side of (3.4d). As a result, we will need control over

$$\int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big\}$$

to prove compactness in time for the velocity field (*cf.* Lem. 4.8). Therefore, the approximation of $\hat{\psi}$ by $(1-\gamma)\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n] + \gamma\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ in the fourth and fifth term in (3.4c) is necessary.

Replacing $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ by $\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ also results in a stable scheme, but by now there is no technique at hand to improve the regularity of $\hat{\psi}$ and therefore to prove convergence of this version of (3.4).

As M_h vanishes on the majority of $\mathfrak{D}\backslash D$ for $h_{\mathbf{q}}$ small enough, we introduced the regularization parameter $\mathfrak{m}$ to prevent definition gaps in (3.4c).

Remark 3.5. By choosing weakly solenoidal test functions in (3.4d), we eliminated the pressure term, which is more convenient for the analysis of the scheme. As shown in ([14], Chap. 1, Sect. 4), the formulation in (3.4d) is equivalent to the straightforward approach using $\mathbf{w}\in\boldsymbol{W}_h$ and the pressure term $-\int_\Omega p_h^n \operatorname{div}_{\mathbf{x}}\mathbf{w}$, as $\boldsymbol{W}_h$ and S_h satisfy the inf-sup condition (*cf.* (TH1)).

After passing to the limit in Theorem 5.2, one may recover the pressure in a very weak sense following the procedure discussed in [28].

Remark 3.6. In the third term on the left-hand-side of (3.4c) and in the third term on the right-hand side of (3.4d) we used $\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\}$. At this point, the interpolation operator is neither necessary for stability nor for convergence, but it reduces the costs of an exact integration of these terms.

Testing (3.4a) and (3.4c) by 1 shows that solutions to (3.4), if they exists, satisfy the conservation properties

$$\int_\Omega \phi_h^n = \int_\Omega \phi_h^{n-1} \quad\text{and}\quad \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\psi}_h^n = \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\psi}_h^{n-1} \tag{3.6}$$

for all $n\in\{1,\dots,N\}$.

As shown in the following lemma, the scheme presented in (3.4) is consistent with thermodynamics in the sense that the discrete version of the energy

$$\begin{aligned}\mathcal{E}_h(\phi_h^n,\hat{\psi}_h^n,\mathbf{u}_h^n) :=& \tfrac{1}{2}\int_\Omega |\nabla_{\mathbf{x}}\phi_h^n|^2 + \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W(\phi_h^n)\} + \int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}_h^n)\Big\}\\ &+\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{x}}\Big\{\hat{\psi}_h^n\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\Big\} + \tfrac{1}{2}\int_\Omega \overline{\rho}_h^n\,|\mathbf{u}_h^n|^2\end{aligned} \tag{3.7}$$

is not increasing. In particular, testing (3.4a) by $\tau\mu_{\phi,h}^n$, (3.4b) by $\tau\partial_\tau^-\phi_h^n$, (3.4c) by $\tau\mu_{\psi,h,\nu}^n$, and (3.4d) by $\tau\mathbf{u}_h^n$ yields the following result (*cf.* [25]).

Lemma 3.7. *Let W and W_h' satisfy (W1)–(W5). Furthermore, let (T) and (S1)–(S3) hold true. Assuming $\eta\geq c>0$ and $\beta\geq 0$, a solution $(\phi_h^n,\,\mu_{\phi,h}^n,\,\hat{\psi}_h^n,\mathbf{u}_h^n)\in U_h^{\mathbf{x}}\times U_h^{\mathbf{x}}\times\hat{X}_h\times\boldsymbol{W}_{h,\mathrm{div}}$ to (3.4), if exists, satisfies for $n=1,\dots,N$*

$$
\begin{aligned}
\mathcal{E}_h(\phi_h^n, \hat{\psi}_h^n, \mathbf{u}_h^n) &+ \tfrac{2\vartheta-1}{2}\int_\Omega \left|\nabla_{\mathbf{x}}\phi_h^n - \nabla_{\mathbf{x}}\phi_h^{n-1}\right|^2 + \tfrac{1}{4}\int_\Omega \overline{\rho}_h^{n-1}\left|\mathbf{u}_h^n - \mathbf{u}_h^{n-1}\right|^2 \\
&+ \tau\int_\Omega \left|\nabla_{\mathbf{x}}\mu_{\phi,h}^n\right|^2 + \tau\int_\Omega 2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^n)\}\left|\mathbf{D}\mathbf{u}_h^n\right|^2 \\
&+ \tau\int_{\Omega\times\mathfrak{D}} c_{\mathbf{q}} M_h \mathcal{I}_h^{\mathbf{x}}\Big\{\Big(\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^n]\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)\Big\}\Big)\cdot\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^n)\Big\}\Big\} \\
&+ \tau\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Big((1-\gamma)\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n] + \gamma\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big\} \\
&\leq \mathcal{E}_h(\phi_h^{n-1}, \hat{\psi}_h^{n-1}, \mathbf{u}_h^{n-1})
\end{aligned} \tag{3.8}
$$

with given initial data $(\phi_h^0, \hat{\psi}_h^0, \mathbf{u}_h^0) \in U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$.

As we can not guarantee $\hat{\psi}_h^n \geq 0$ for $n \in \{1,\dots,N\}$, the Henry energy, *i.e.* the term $\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{x}}\Big\{\hat{\psi}_h^n\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\Big\}$, may become arbitrarily negative and therefore Lemma 3.7 alone does not provide stability of the scheme. By enhancing the ideas of [7], we refine this result to guarantee stability.

Lemma 3.8. *Let initial data* $(\phi_h^0, \hat{\psi}_h^0, \mathbf{u}_h^0) \in U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$ *be given, let* W *and* W_h' *satisfy (W1)–(W5), let (T) and (S1)–(S3) hold true, and let* $\eta \geq c > 0$ *and* $\beta \geq 0$. *For* $n = 1,\dots,N$, *a solution* $(\phi_h^n, \mu_{\phi,h}^n, \hat{\psi}_h^n, \mathbf{u}_h^n) \in U_h^{\mathbf{x}} \times U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$ *to* (3.4), *if exists, satisfies*

$$
\begin{aligned}
\tfrac{1}{2}\int_\Omega |\nabla_{\mathbf{x}}\phi_h^n|^2 &+ \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W(\phi_h^n)\} + \int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}_h^n)\Big\} \\
&+ \nu^{-1}\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}_h^n]_-^2\Big\} + \tfrac{1}{2}\int_\Omega \overline{\rho}_h^n|\mathbf{u}_h^n|^2 \\
&+ \tfrac{2\vartheta-1}{2}\sum_{k=1}^n\int_\Omega\left|\nabla_{\mathbf{x}}\phi_h^k - \nabla_{\mathbf{x}}\phi_h^{k-1}\right|^2 + \tfrac{1}{4}\sum_{k=1}^n\int_\Omega \overline{\rho}_h^{k-1}\left|\mathbf{u}_h^k - \mathbf{u}_h^{k-1}\right|^2 \\
&+ \tau\sum_{k=1}^n\int_\Omega\left|\nabla_{\mathbf{x}}\mu_\phi^k\right|^2 + \tau\sum_{k=1}^n\int_\Omega 2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^k)\}\left|\mathbf{D}\mathbf{u}_h^k\right|^2 \\
&+ \tau\sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} c_{\mathbf{q}}M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big(\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^k]\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^k)\Big\}\Big)\cdot\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^k)\Big\}\Big\} \\
&+ \tau\sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Big((1-\gamma)\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^k] + \gamma\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^k]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^k\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^k\Big\} \\
&\leq C\mathcal{E}_h(\phi_h^0, \hat{\psi}_h^0, \mathbf{u}_h^0) + C,
\end{aligned} \tag{3.9}
$$

with some constant $C > 0$ *independent of* h, τ, $\mathfrak{m}$, *and* ν.

Proof. We consider a dual basis to the nodes $\{\mathbf{x}_i\}_{i=1,\dots,\dim U_h^{\mathbf{x}}}$ and $\{\mathbf{q}_j\}_{j=1,\dots,\dim U_h^{\mathbf{q}}}$ which is denoted by $\{\chi_{h,i}^{\mathbf{x}}\}_{i=1,\dots,\dim U_h^{\mathbf{x}}}$ and $\{\chi_{h,j}^{\mathbf{q}}\}_{j=1,\dots,\dim U_h^{\mathbf{q}}}$. Furthermore, we denote $\hat{\psi}_h^n(\mathbf{x}_i,\mathbf{q}_j)$ by $\hat{\psi}_{h,i,j}^n$ and define positive weights $\lambda_{ij} := \int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\chi_{h,i}^{\mathbf{x}}\chi_{h,j}^{\mathbf{q}}$ for all $i \in \{1,\dots,\dim U_h^{\mathbf{x}}\}$, $j \in \{1,\dots,\dim U_h^{\mathbf{q}}\}$. We compute

$$
\begin{aligned}
\tfrac{1}{2}\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}_h^n)\Big\} &= \tfrac{1}{2}\sum_{i=1}^{\dim U_h^{\mathbf{x}}}\sum_{j=1}^{\dim U_h^{\mathbf{q}}}\lambda_{ij}g_\nu(\hat{\psi}_{h,i,j}^n) \\
&= \tfrac{1}{2}\sum_{i,j\,:\,\hat{\psi}_{h,i,j}^n\geq 0}\lambda_{ij}g_\nu(\hat{\psi}_{h,i,j}^n) + \tfrac{1}{2}\sum_{i,j\,:\,\hat{\psi}_{h,i,j}^n<0}\lambda_{ij}g_\nu(\hat{\psi}_{h,i,j}^n).
\end{aligned} \tag{3.10}
$$

As there exists a ν-independent lower bound for g_ν, the first summand is bounded from below. From (2.21a), we have for negative $\hat{\psi}^n_{h,i,j}$

$$g_\nu(\hat{\psi}^n_{h,i,j}) = \frac{|\hat{\psi}^n_{h,i,j}|^2}{2\nu} - \frac{\nu}{2} + \hat{\psi}^n_{h,i,j}(\log\nu - 1) \geq \frac{1}{2\nu}[\hat{\psi}^n_{h,i,j}]_-^2 - \frac{\nu}{2}, \tag{3.11}$$

as $[\hat{\psi}^n_{h,i,j}]_-(\log\nu - 1) \geq 0$. Therefore, we have

$$\frac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}^n_h)\Big\} \geq -C + \frac{1}{4\nu}\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}^n_h]_-^2\Big\}. \tag{3.12}$$

On the other hand, we may apply Young's inequality to compute

$$\begin{aligned}\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{x}}\Big\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi^n_h)\}\}\hat{\psi}^n_h\Big\} &\geq \int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi^n_h)\}\}[\hat{\psi}^n_h]_-\Big\}\\ &\geq -\delta\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}^n_h]_-^2\Big\} - C_\delta,\end{aligned} \tag{3.13}$$

with $0 < \delta \ll 1$ independent of ν. Combining (3.12) and (3.13) provides

$$\begin{aligned}\left(\tfrac{1}{4\nu} - \delta\right)\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}^n_h]_-^2\Big\} &\leq \int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{x}}\Big\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi^n_h)\}\}\hat{\psi}^n_h\Big\}\\ &\quad + \tfrac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}^n_h)\Big\} + C.\end{aligned} \tag{3.14}$$

Applying this on a discrete integration in time over the result of Lemma 3.7 provides the result. □

At this point, we want to emphasize that the constants in Lemma 3.8 does not depend on the mollification parameter ε. Combining the *a priori* estimates above with Brouwer's fixed point theorem, we obtain the existence of discrete solutions (*cf.* [25]).

Lemma 3.9. *Let the assumptions (W1)–(W5) hold true. Furthermore, let* $\beta \in C^1(\mathbb{R}_0^+) \cap W^{1,\infty}(\mathbb{R})$ *and* $\eta \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ *with* $\eta \geq c > 0$*, then for given* $\left(\phi^{n-1}_h, \hat{\psi}^{n-1}_h, \mathbf{u}^{n-1}_h\right) \in U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$ *and a given time increment* $\tau > 0$*, there exists at least one quadruple* $\left(\phi^n_h, \mu^n_{\phi,h}, \hat{\psi}^n_h, \mathbf{u}^n_h\right) \in U_h^{\mathbf{x}} \times U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\mathrm{div}}$ *satisfying* (3.4)*.*

4. Compactness in space and time

From now on, we restrict ourselves to the case of equal mass densities. Without loss of generality, we assume $\rho \equiv 1$. Furthermore, we make the following general assumptions

- **(A1)** The spring potential U and its associated Maxwellian M satisfy (P1)–(P5) with some $\kappa > 1$ such that Lemma 2.2 holds true.
- **(A2)** The discretization in time satisfies (T).
- **(A3)** Ω^* and Ω are bounded, convex polygonal (or polyhedral) domains with families of partitions $\{\mathcal{T}_h^{\mathbf{x}*}\}_{h>0}$ and $\{\mathcal{T}_h^{\mathbf{x}}\}_{h>0}$ satisfying (S1)–(S2).
  $\mathfrak{D}$ is a bounded polygonal (or polyhedral) domain with a family of partitions $\{\mathcal{T}_h^{\mathbf{q}}\}_{h>0}$ satisfying (S3).
- **(A4)** Assumptions (W1)–(W5) apply to the double-well potential W and the time-discrete approximations of its derivatives.
- **(A5)** The mollification operators $\mathcal{J}_\varepsilon$ and $\boldsymbol{\mathcal{J}}_\varepsilon$ are defined by (1.8), while their discrete counterparts $\mathcal{J}_h$ and $\boldsymbol{\mathcal{J}}_h$ are obtained *via* (2.38).

(A6) β, $\eta \in C^\infty(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$, and there exist constants c_1, $c_2 > 0$ such that

$$0 \le \beta(s) \le c_2 \qquad c_1 \le \eta(s) \le c_2 \quad \forall s \in \mathbb{R}.$$

(A7) There is a constant $C > 0$ such that $h_{\mathbf{q}}^\kappa \le C\mathfrak{m}$ with the $\kappa > 1$ used in assumption (A1). Furthermore, $h_{\mathbf{x}}$ and ν satisfy the relation $\frac{h_{\mathbf{x}}^2}{\nu} \to 0$, as $h_{\mathbf{x}}, \nu \searrow 0$.

(A8) Let initial data $\Phi^0 \in H^2(\Omega; [-1,1])$ and $\mathbf{U}^0 \in \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$ be given such that we have for discrete initial data $\phi_h^0 = \mathcal{I}_h^{\mathbf{x}}\{\Phi^0\}$ and $\mathbf{u}_h^0 := \mathcal{Q}_h\{\mathbf{U}^0\}$ uniformly in $h > 0$ that

$$\left\|\mathbf{u}_h^0\right\|_{H^1(\Omega)} + \int_\Omega \left|\Delta_h \phi_h^0\right|^2 + \int_\Omega \left|\nabla_{\mathbf{x}} \phi_h^0\right|^2 + \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W(\phi_h^0)\} \le C < \infty.$$

(A9) Let nonnegative initial data for the scaled configurational density be given as $\hat{\Psi}^0 \in L^2(\Omega \times \mathfrak{D})$. We compute discrete initial data $\hat{\psi}_h^0$ *via*

$$\begin{aligned}\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\hat{\psi}_h^0 \theta_h\right\} + \tau \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{\nabla_{\mathbf{x}}\hat{\psi}_h^0 \cdot \nabla_{\mathbf{x}}\theta_h\right\}\\ + \tau \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{\nabla_{\mathbf{q}}\hat{\psi}_h^0 \cdot \nabla_{\mathbf{q}}\theta_h\right\} = \int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\hat{\Psi}^0 \theta_h \qquad \forall \theta_h \in \hat{X}_h. \qquad (4.1)\end{aligned}$$

Remark 4.1. The definition of the discrete initial data is an adaption of the ideas used in [7]. As shown in [25], it is also possible to adapt (4.1) to allow for $\hat{\Psi}^0 \in L^2(\Omega \times \mathfrak{D}; \hat{M})$.

Lemma 4.2. *Under the assumptions (A1), (A3), (A7), and (A9) the discrete initial data $\hat{\psi}_h^0$ satisfies*

$$\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^0\right|^2\right\} + \tau \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{q}}\left\{\left|\nabla_{\mathbf{x}}\hat{\psi}_h^0\right|^2\right\} + \tau \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^0\right|^2\right\} \le C, \qquad (4.2)$$

with some $C > 0$ independent of h, τ, $\mathfrak{m}$, and ν. In addition, we have

$$\hat{\psi}_h^0 \ge 0. \qquad (4.3)$$

To prove this lemma, we need an additional result concerning the Maxwellian $\hat{M}$ and its discrete counterpart M_h.

Lemma 4.3. *Let (A1) and (A7) hold true. Then there is a positive constant c independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\hat{M}(\mathbf{q}) \le c(M_h(\mathbf{q}) + \mathfrak{m})$$

for all $\mathbf{q} \in \mathfrak{D}$.

Proof. Let $\mathcal{T}_{h,\mathrm{inner}}^{\mathbf{q}} \subset \mathcal{T}_h^{\mathbf{q}}$ be the set containing all $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}}$ satisfying $\kappa_{\mathbf{q}} \subset D$ and $\operatorname{dist}(\kappa_{\mathbf{q}}, \partial D) \ge h_{\mathbf{q}}$. Then we have for every $\kappa_{\mathbf{q}} \in \mathcal{T}_{h,\mathrm{inner}}^{\mathbf{q}}$

$$\min_{\mathbf{q}\in\kappa_{\mathbf{q}}} \hat{M}(\mathbf{q}) \ge c_1[\operatorname{dist}(\kappa_{\mathbf{q}}, \partial D)]^\kappa, \qquad (4.4)$$

$$\max_{\mathbf{q}\in\kappa_{\mathbf{q}}} \hat{M}(\mathbf{q}) \le c_2[\operatorname{dist}(\kappa_{\mathbf{q}}, \partial D) + h_{\mathbf{q}}]^\kappa \le c_2 2^\kappa [\operatorname{dist}(\kappa_{\mathbf{q}}, \partial D)]^\kappa \qquad (4.5)$$

with $\kappa > 1$ due to (P3) and therefore

$$\hat{M} \le \max_{\mathbf{q}\in\kappa_{\mathbf{q}}} \hat{M}(\mathbf{q}) \le \tfrac{c_2 2^\kappa}{c_1} \tfrac{c_{h_{\mathbf{q}}}}{c_M} \min_{\mathbf{q}\in\kappa_{\mathbf{q}}} \hat{M}(\mathbf{q}) \le \tfrac{c_2 2^\kappa}{c_1 c_M} M_h, \qquad (4.6)$$

as $c_{h_{\mathbf{q}}} \geq c_M$ (see Lem. 2.2). We use (P3) and $h^{\kappa}_{\mathbf{q}} \leq C\mathfrak{m}$ on every $\kappa_{\mathbf{q}} \in \mathcal{T}_h^{\mathbf{q}} \setminus \mathcal{T}_{h,\text{inner}}^{\mathbf{q}}$ to compute

$$\max_{\mathbf{q}\in\kappa_{\mathbf{q}}} \hat{M}(\mathbf{q}) \leq C h^{\kappa}_{\mathbf{q}} \leq C\mathfrak{m}. \tag{4.7}$$

□

Proof of Lemma 4.2. Testing (4.1) by $\hat{\psi}_h^0 \in \hat{X}$ yields

$$(1-\delta c)\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^0\Big|^2\Big\} + \tau\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^0\Big|^2\Big\} + \tau\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^0\Big|^2\Big\} \leq C \tag{4.8}$$

and therefore (4.2) for δ small enough. The nonnegativity of $\hat{\psi}_h^0$ follows from standard arguments (*cf.* Chap. 11 in [29]). □

Combining Lemma 3.8 with the regularity assumptions on the initial data and noting

$$\left|\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}_h^0)\Big\}\right| \leq \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^0\Big|^2\Big\} + C. \tag{4.9}$$

for $\hat{\psi}_h^0 \geq 0$, we obtain our first regularity result.

Lemma 4.4. *Let the assumptions (A1)–(A9) hold true. Then for $n = 1,\dots,N$ a solution $\{\phi_h^n, \mu_{\phi,h}^n, \hat{\psi}_h^n, \mathbf{u}_h^n\} \in U_h^{\mathbf{x}} \times U_h^{\mathbf{x}} \times \hat{X}_h \times \boldsymbol{W}_{h,\text{div}}$ to the equal density version of (3.4) satisfies*

$$\begin{aligned}
&\int_\Omega |\nabla_{\mathbf{x}}\phi_h^n|^2 + \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W(\phi_h^n)\} + \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu(\hat{\psi}_h^n)\Big\} + \nu^{-1}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}_h^n]_-^2\Big\}\\
&\quad + \int_\Omega |\mathbf{u}_h^n|^2 + \tfrac{2\vartheta-1}{2}\sum_{k=1}^n\int_\Omega \Big|\nabla_{\mathbf{x}}\phi_h^k - \nabla_{\mathbf{x}}\phi_h^{k-1}\Big|^2 + \sum_{k=1}^n\int_\Omega \Big|\mathbf{u}_h^k - \mathbf{u}_h^{k-1}\Big|^2 + \tau\sum_{k=1}^n\int_\Omega \Big|\nabla_{\mathbf{x}}\mu_\phi^k\Big|^2\\
&\quad + \tau\sum_{k=1}^n\int_\Omega 2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^k)\}\Big|\mathbf{D}\mathbf{u}_h^k\Big|^2 + \tau\sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big(\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^k]\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^k)\Big\}\Big)\cdot\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^k)\Big\}\Big\}\\
&\quad + \tau\sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Big((1-\gamma)\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^k] + \gamma\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^k]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^k\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^k\Big\} \leq C,
\end{aligned} \tag{4.10}$$

with some constant $C > 0$ independent of h, τ, $\mathfrak{m}$, and ν.

Starting from this result, we use the specific discretization of the $\mathbf{x}$-convective term in (3.4c) to improve the regularity results for the scaled configurational density. In particular, we establish the following lemma.

Lemma 4.5. *Let the assumptions (A1)–(A9) hold true. Then for τ small enough, there is a positive constant $C > 0$ independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\begin{aligned}
&\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n\Big|^2\Big\} + \sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^k - \hat{\psi}_h^{k-1}\Big|^2\Big\}\\
&\quad + \tau\sum_{k=0}^n\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^k\Big|^2\Big\} + \tau\sum_{k=0}^n\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^k\Big|^2\Big\} \leq C
\end{aligned} \tag{4.11}$$

for all $n \in \{0,\dots,N\}$.

Proof. By testing (3.4c) by $\hat{\psi}_h^n$ for $n \in \{1,\dots,N\}$, we obtain

$$
\begin{aligned}
0 =& \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\partial_\tau^- \hat{\psi}_h^n \hat{\psi}_h^n\Big\} - \int_{\Omega\times\mathfrak{D}} M_h \mathbf{u}_h^n \cdot \mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big\} \\
&- \int_{\Omega\times\mathfrak{D}} (\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{u}_h^n\}\}\cdot\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\})\cdot\mathcal{I}_h^{\mathbf{x}}\Big\{\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^n]\nabla_{\mathbf{q}}\hat{\psi}_h^n\Big\} \\
&+ (1-\gamma)\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big)\cdot\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big\} \\
&+ \gamma\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big)\cdot\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big\} + \int_{\Omega\times\mathfrak{D}} c_{\mathbf{q}} M_h \mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^n\Big|^2\Big\} \\
=:& I + II + III + IV + V + VI.
\end{aligned}
\tag{4.12}
$$

Combining (2.24b) with the weak solenoidality of $\mathbf{u}_h^n$, we obtain

$$
II = -\int_{\Omega\times\mathfrak{D}} M_h\mathbf{u}_h^n \cdot \mathcal{I}_h^{\mathbf{q}}\Big\{\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\Big\{f_\nu(\hat{\psi}_h^n)\Big\}\Big\} = 0. \tag{4.13}
$$

Applying Young's inequality with $0<\delta\ll 1$, Lemma 2.10, Lemma 4.4, and Lemma 2.7, we compute

$$
\begin{aligned}
III + IV \geq& (1-\gamma)(c_{\mathbf{x}}-\delta)\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big|^2\Big\} - \delta\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^n\Big|^2\Big\} \\
&- C_\delta\Big[\int_{\Omega\times\mathfrak{D}} M_h\nu^2 + \int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n\Big|^2\Big\}\Big].
\end{aligned}
\tag{4.14}
$$

Applying similar arguments on the fifth term on the right-hand side of (4.12) yields

$$
\begin{aligned}
V =& \gamma\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\cdot\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n]^{-1}\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big)\cdot\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big\} \\
&+ \gamma\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^n)\}\}\}\Big)\cdot\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big\} \\
\geq& -\gamma\delta\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big|^2\Big\} - \gamma C_\delta\Big[\int_{\Omega\times\mathfrak{D}} M_h\nu^2 + \int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n\Big|^2\Big\}\Big],
\end{aligned}
\tag{4.15}
$$

as $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\cdot\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^n]^{-1}$ is positive definite. Combining the above results and multiplying by τ yields

$$
\begin{aligned}
&\tfrac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n\Big|^2\Big\} + \tfrac{1}{2}\int_{\Omega} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n-\hat{\psi}_h^{n-1}\Big|^2\Big\} \\
&\quad+ \tau(1-\gamma)\int_{\Omega\times\mathfrak{D}} c_{\mathbf{x}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big|^2\Big\} + \tau\int_{\Omega\times\mathfrak{D}} c_{\mathbf{q}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^n\Big|^2\Big\} \\
&\quad- \tau\delta\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^n\Big|^2\Big\} - \tau\delta\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^n\Big|\Big\} \\
&\quad\leq \tfrac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^{n-1}\Big|^2\Big\} + \tau C_0\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^n\Big|^2\Big\} + \tau C\int_{\Omega\times\mathfrak{D}} M_h\nu^2.
\end{aligned}
\tag{4.16}
$$

For δ small enough, we have $(1-\gamma)c_{\mathbf{x}} - \delta \geq c > 0$ and $c_{\mathbf{q}} - \delta \geq c > 0$. Therefore, a summation in time yields

$$\begin{aligned}\tfrac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^n\right|^2\right\} + \tfrac{1}{2}\sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^k-\hat{\psi}_h^{k-1}\right|^2\right\} + c\tau\sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\nabla_{\mathbf{x}}\hat{\psi}_h^k\right|^2\right\} \\ + c\tau\sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^k\right|^2\right\} \leq \tfrac{1}{2}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^0\right|^2\right\} \\ + \tau C_0\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^n\right|^2\right\} + \tau C\sum_{k=1}^{n-1}\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^k\right|^2\right\} + \tau nC. \qquad (4.17)\end{aligned}$$

As the constant C_0 on the right-hand side depends neither on τ nor on the solution itself, we may safely assume $\tau C_0 < \frac{1}{4}$. Absorbing $\tau C_0 \int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^n\right|^2\right\}$ on the left-hand side and applying a discrete version of Gronwall's lemma (see *e.g.* [31]) shows

$$\begin{aligned}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^n\right|^2\right\} + \sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left|\hat{\psi}_h^k-\hat{\psi}_h^{k-1}\right|^2\right\} \\ +\tau\sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\nabla_{\mathbf{x}}\hat{\psi}_h^k\right|^2\right\} + \tau\sum_{k=1}^{n}\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^k\right|^2\right\} \leq C \qquad (4.18)\end{aligned}$$

for $n \in \{1,\ldots,N\}$. Combining (4.18) with Lemma 4.2 completes the proof. □

Following the arguments in [15, 16, 18], we establish the following regularity results for the phase-field parameter.

Lemma 4.6. *Let the assumptions (A1)–(A9) hold true and let τ be small enough. Then there is $C > 0$ independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\left|\int_\Omega \mu_{\phi,h}^n\right| + \sum_{k=0}^{n}\tau\left\|\Delta_h\phi_h^k\right\|_{L^2(\Omega)}^2 + \sum_{k=0}^{n}\tau\left\|\phi_h^k\right\|_{L^\infty(\Omega)}^4 \leq C \qquad (4.19)$$

for all $n \in \{1,\ldots,N\}$.

Lemma 4.7. *Let the assumptions (A1)–(A9) hold true and let τ be small enough. Then there is $C > 0$ independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\tau\sum_{k=0}^{N-l}\left\|\phi_h^{k+l}-\phi_h^k\right\|_{L^2(\Omega)}^2 \leq Cl\tau \qquad (4.20)$$

for all $l \in \{1,\ldots,N\}$.

Proof of Lemma 4.6. A straightforward computation relying in particular on (2.11a), (W2), and the already established regularity results yields $\left|\int_\Omega \mu_{\phi,h}^n\right| \leq C$.
Therefore, the mean value of the chemical potential is bounded which allows to apply Poincaré's inequality.

We continue by testing (3.4b) by $-\Delta_h \phi_h^n$ and use the definition of the discrete Laplacian (2.8) to obtain

$$
\begin{aligned}
\vartheta \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\Delta_h \phi_h^n \Delta_h \phi_h^n\} = &- \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\mu_{\phi,h}^n \Delta_h \phi_h^n\} + \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{W_h'(\phi_h^n, \phi_h^{n-1}) \Delta_h \phi_h^n\} \\
&+ \int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m}) \mathcal{I}_h^{\mathbf{x}}\Big\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta_{DQ}'(\phi_h^n, \phi_h^{n-1}) \Delta_h \phi_h^n\}\} \hat{\psi}_h^{n-1}\Big\} \\
&- (1-\vartheta) \int_\Omega \mathcal{I}_h^{\mathbf{x}}\{\Delta_h \phi_h^{n-1} \Delta_h \phi_h^n\} \\
=:& \, I + II + III + IV.
\end{aligned} \tag{4.21}
$$

Combining Hölder's inequality and Poincaré's inequality provides

$$
|I| \leq \left\|\mu_{\phi,h}^n\right\|_h \|\Delta_h \phi_h^n\|_h \leq C\Big(\left\|\nabla_{\mathbf{x}} \mu_{\phi,h}^n\right\|_{L^2(\Omega)} + 1\Big) \|\Delta_h \phi_h^n\|_h . \tag{4.22}
$$

We infer from Hölder's inequality and (W2) that

$$
II \leq \left\|W_h'(\phi_h^n, \phi_h^{n-1})\right\|_h \|\Delta_h \phi_h^n\|_h \leq C \|\Delta_h \phi_h^n\|_h . \tag{4.23}
$$

To gain control over the third term, we combine Hölder's inequality and (2.10) with the results of Lemma 4.5, the results of Lemma 2.10, and (A6).

$$
\begin{aligned}
III &\leq C \left\|\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta_{DQ}'(\phi_h^n, \phi_h^{n-1}) \Delta_h \phi_h^n\}\}\right\|_{L^2(\Omega)} \left(\int_{\Omega\times\mathfrak{D}} (M_h + \mathfrak{m}) \mathcal{I}_h^{\mathbf{xq}}\Big\{\left|\hat{\psi}_h^{n-1}\right|^2\Big\}\right)^{1/2} \\
&\leq C \int_\Omega \left|\mathcal{I}_h^{\mathbf{x}}\{\beta_{DQ}'(\phi_h^n, \phi_h^{n-1}) \Delta_h \phi_h^n\}\right| \leq C \|\Delta_h \phi_h^n\|_h .
\end{aligned} \tag{4.24}
$$

Concerning the fourth term,

$$
|IV| \leq (1-\vartheta) \|\Delta_h \phi_h^n\|_h \left\|\Delta_h \phi_h^{n-1}\right\|_h \tag{4.25}
$$

holds true. Collecting the previous results, we obtain

$$
\vartheta \|\Delta_h \phi_h^n\|_h \leq C \left\|\nabla_{\mathbf{x}} \mu_{\phi,h}^n\right\|_{L^2(\Omega)} + C + (1-\vartheta) \left\|\Delta_h \phi_h^{n-1}\right\|_h . \tag{4.26}
$$

As Young's inequality implies

$$
(a+b+c)^2 = a^2 + b^2 + c^2 + 2ab + 2ac + 2bc \leq C_\delta(a^2 + b^2) + (1+2\delta)c^2 \tag{4.27}
$$

for $a, b, c \in \mathbb{R}$ with $0 < \delta \ll 1$, a discrete integration with respect to time over (4.26) yields

$$
\vartheta^2 \sum_{k=1}^n \tau \left\|\Delta_h \phi_h^k\right\|_h^2 \leq C_\delta \left(\sum_{k=1}^n \left\|\nabla_{\mathbf{x}} \mu_{\phi,h}^k\right\|_{L^2(\Omega)}^2 + T\right) + (1-\vartheta)^2 (1+2\delta) \sum_{k=1}^n \tau \left\|\Delta_h \phi_h^{k-1}\right\|_h^2 . \tag{4.28}
$$

As we assumed $\vartheta \in (0.5, 1]$, we have $\vartheta^2 > (1-\vartheta)^2$. Therefore, we may choose $\delta > 0$ such that $\vartheta^2 - (1-\vartheta)^2(1+2\delta) =: \tilde{c} > 0$. Noting the regularity assumptions on the initial data (*cf.* (A8)), we infer

$$
\tilde{c} \sum_{k=0}^n \tau \left\|\Delta_h \phi_h^k\right\|_{L^2(\Omega)}^2 \leq C_\delta (1+T) . \tag{4.29}
$$

The last claim of Lemma 4.6 follows from Lemma 4.4 and the interpolation inequality

$$
\|\chi_h\|_{L^\infty(\Omega)} \leq C \|\Delta_h \chi_h\|_{L^2(\Omega)}^{1/2} \|\chi_h\|_{H^1(\Omega)}^{1/2} + \|\chi_h\|_{H^1(\Omega)} \qquad \text{for all } \chi_h \in U_h^{\mathbf{x}}, \tag{4.30}
$$

which was proven in Corollary A.1 in [16]. □

Proof of Lemma 4.7. Following the lines of [18], we test (3.4a) by $\tau(\phi_h^{k+l} - \phi_h^k)$ with $0 \le k \le N-l$ and sum from $n = k+1$ to $k+l$ to obtain

$$\begin{aligned} 0 =& \int_\Omega \mathcal{I}_h^{\mathbf{x}}\left\{\left|\phi_h^{k+l} - \phi_h^k\right|^2\right\} - \tau \sum_{n=k+1}^{k+l} \int_\Omega \phi_h^{n-1}\mathbf{u}_h^{n-1} \cdot \nabla_{\mathbf{x}}(\phi_h^{k+l} - \phi_h^k) \\ &+ \tau^2 \sum_{n=k+1}^{k+l} \int_\Omega \left|\phi_h^{n-1}\right|^2 \nabla_{\mathbf{x}}\mu_{\phi,h}^n \cdot \nabla_{\mathbf{x}}(\phi_h^{k+l} - \phi_h^k) + \tau \sum_{n=k+1}^{k+l} \int_\Omega \nabla_{\mathbf{x}}\mu_{\phi,h}^n \cdot \nabla_{\mathbf{x}}(\phi_h^{k+l} - \phi_h^k) \\ =&: I + II + III + IV\,. \end{aligned} \tag{4.31}$$

Using Hölder's inequality, the well-known Sobolev embedding theorem, and Poincaré's inequality, we compute

$$\begin{aligned} |II| \le& \tau \sum_{n=k+1}^{k+l} \left\|\mathbf{u}_h^{n-1}\right\|_{L^6(\Omega)} \left\|\phi_h^{n-1}\right\|_{L^3(\Omega)} \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)} \\ \le& C \sum_{m=0}^{l-1} \tau^{1/2} \left\|\nabla_{\mathbf{x}}\mathbf{u}_h^{k+m}\right\|_{L^2(\Omega)} \left\|\nabla_{\mathbf{x}}\phi_h^{k+m}\right\|_{L^2(\Omega)} \tau^{1/2} \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}\,. \end{aligned} \tag{4.32}$$

Noting the inequality $\left\|\phi_h^{n-1}\right\|_{L^\infty(\Omega)} \le C(1 + \left\|\Delta_h \phi_h^{n-1}\right\|_{L^2(\Omega)})$, which is a direct consequence of the interpolation inequality (4.30) and Lemma 4.4 (see also [15]), we obtain

$$\begin{aligned} |III| \le& \tau^2 \sum_{n=k+1}^{k+l} \left\|\phi_h^{n-1}\right\|_{L^\infty(\Omega)}^2 \left\|\nabla_{\mathbf{x}}\mu_{\phi,h}^n\right\|_{L^2(\Omega)} \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}^2 \\ \le& C \sum_{m=0}^{l-1} \tau(1 + \left\|\Delta_h\phi_h^{k+m}\right\|_{L^2(\Omega)})^2 \tau^{1/2} \left\|\nabla_{\mathbf{x}}\mu_{\phi,h}^{k+m+1}\right\|_{L^2(\Omega)} \tau^{1/2} \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}\,. \end{aligned} \tag{4.33}$$

We deduce by combining (4.31)–(4.33), multiplying by τ, summing from $k = 0$ to $N - l$, and applying Hölder's inequality that

$$\begin{aligned} \tau \sum_{k=0}^{N-l} \left\|\phi_h^{k+l} - \phi_h^k\right\|_h^2 \le& C\tau \sum_{m=0}^{l-1} \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\mathbf{u}_h^{k+m}\right\|_{L^2(\Omega)}^2\right)^{1/2} \left(\sup_{k=0,\dots,N-l} \left\|\nabla_{\mathbf{x}}\phi_h^{k+m}\right\|_{L^2(\Omega)}^2\right)^{1/2} \\ &\times \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}^2\right)^{1/2} + C\tau \sum_{m=0}^{l-1} \left(\sum_{k=0}^{N-l} \tau\left(1 + \left\|\Delta_h\phi_h^{k+m}\right\|_{L^2(\Omega)}\right)^2\right) \\ &\times \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\mu_{\phi,h}^{k+m+1}\right\|_{L^2(\Omega)}^2\right)^{1/2} \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}^2\right)^{1/2} \\ &+ C\tau \sum_{m=0}^{l-1} \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\mu_{\phi,h}^{k+m+1}\right\|_{L^2(\Omega)}^2\right)^{1/2} \left(\sum_{k=0}^{N-l} \tau \left\|\nabla_{\mathbf{x}}\phi_h^{k+l} - \nabla_{\mathbf{x}}\phi_h^k\right\|_{L^2(\Omega)}^2\right)^{1/2}. \end{aligned} \tag{4.34}$$

Applying the results of Lemma 4.4 and Lemma 4.6 to the right-hand side of (4.34) and using the norm equivalence (2.10) yields the result. ∎

In a final step, we show compactness in time for the velocity field.

For this reason, we introduce the Helmholtz–Stokes operator $\boldsymbol{S} : \big(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\big)' \to \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$, $\mathbf{v} \mapsto \boldsymbol{S}\{\mathbf{v}\}$, which is defined *via*

$$\int_\Omega \boldsymbol{S}\{\mathbf{v}\} \cdot \mathbf{w} \,\mathrm{d}\mathbf{x} + \int_\Omega \nabla_{\mathbf{x}} \boldsymbol{S}\{\mathbf{v}\} : \nabla_{\mathbf{x}} \mathbf{w} \,\mathrm{d}\mathbf{x} = \langle \mathbf{v}, \mathbf{w} \rangle \quad \forall \mathbf{w} \in \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega), \tag{4.35}$$

where $\langle .,. \rangle$ denotes the duality pairing between $\big(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\big)'$ and $\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$. This operator satisfies the following properties (see *e.g.* [5]).

(H1) $\langle \mathbf{v}, \boldsymbol{S}\{\mathbf{v}\} \rangle = \|\boldsymbol{S}\{\mathbf{v}\}\|^2_{H^1(\Omega)} \qquad \forall \mathbf{v} \in \big(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\big)'$,

(H2) $\|\boldsymbol{S}\{.\}\|_{H^1(\Omega)}$ is a norm on $\big(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\big)'$,

(H3) $\|\boldsymbol{S}\{\mathbf{v}\}\|^2_{L^2(\Omega)} + \|\nabla_{\mathbf{x}} \boldsymbol{S}\{\mathbf{v}\}\|^2_{L^2(\Omega)} \le \|\mathbf{v}\|^2_{L^2(\Omega)} \qquad \forall \mathbf{v} \in \boldsymbol{L}^2(\Omega)$,

(H4) $\|(\boldsymbol{I} - \boldsymbol{S})\{\mathbf{v}\}\|^2_{L^2(\Omega)} + \|\nabla_{\mathbf{x}}(\boldsymbol{I} - \boldsymbol{S})\{\mathbf{v}\}\|^2_{L^2(\Omega)} \le \|\nabla_{\mathbf{x}} \mathbf{v}\|^2_{L^2(\Omega)} \quad \forall \mathbf{v} \in \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$,

where $\boldsymbol{I}$ denotes the identity operator on $\mathbb{R}^d$. Following the lines of [13], we also consider the orthogonal Stokes projector $\boldsymbol{R}_h : \boldsymbol{W}_{h,\mathrm{div}} \to \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$ which is defined *via*

$$\int_\Omega \nabla_{\mathbf{x}}(\boldsymbol{R}_h\{\mathbf{v}_h\} - \mathbf{v}_h) : \nabla_{\mathbf{x}} \mathbf{w} = 0, \qquad \forall \mathbf{w} \in \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\,. \tag{4.36}$$

Analogously to [13], where $\boldsymbol{R}_h$ is defined on a different finite element space, one can show that $\boldsymbol{R}_h$ satisfies the properties

$$\|\boldsymbol{R}_h\{\mathbf{v}_h\}\|_{H^1(\Omega)} \le C \|\mathbf{v}_h\|_{H^1(\Omega)}\,, \tag{4.37a}$$

$$\|\boldsymbol{R}_h\{\mathbf{v}_h\} - \mathbf{v}_h\|_{L^2(\Omega)} \le C h_{\mathbf{x}} \|\mathrm{div}_{\mathbf{x}}\, \mathbf{v}_h\|_{L^2(\Omega)}\,, \tag{4.37b}$$

$$\|\boldsymbol{R}_h\{\mathbf{v}_h\}\|_{(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'} \le C\Big(h_{\mathbf{x}} \|\mathrm{div}_{\mathbf{x}}\, \mathbf{v}_h\|_{L^2(\Omega)} + \|\mathbf{v}_h\|_{(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'}\Big) \tag{4.37c}$$

for $\mathbf{v}_h \in \boldsymbol{W}_{h,\mathrm{div}} \subset \boldsymbol{L}^2(\Omega) \subset \big(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\big)'$. To prove compactness in time for the velocity field, we start by establishing a bound, which is independent of h, τ, $\mathfrak{m}$, and ν, on the time derivative of the velocity in the dual space of $\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$. Then we use this result to establish a regularity result for projected velocity field. In particular, we prove the following estimates.

Lemma 4.8. *Let the assumptions (A1)–(A9) hold true, let τ and $h_{\mathbf{x}}$ be small enough (such that Lem. 2.10 and Lem. 4.5 hold true), and let $\boldsymbol{S}$ be the Helmholtz–Stokes operator satisfying (H1)–(H4). Then there is a positive constant C independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\sum_{k=1}^N \tau \left\|\boldsymbol{S}\{\partial_\tau^- \mathbf{u}_h^k\}\right\|^{4/\lambda}_{H^1(\Omega)} \le C \tag{4.38}$$

with $\lambda \in (2,4)$, if $d = 2$, or $\lambda = 3$, if $d = 3$.

Lemma 4.9. *Let the assumptions (A1)–(A9) hold true, let τ and $h_{\mathbf{x}}$ be small enough (such that Lem. 2.10 and Lem. 4.5 hold true), let $\boldsymbol{R}_h$ be the orthogonal Stokes projector satisfying* (4.37)*. Then there is a positive constant C independent of h, τ, $\mathfrak{m}$, and ν such that*

$$\tau \sum_{k=0}^{N-l} \left\|\boldsymbol{R}_h\{\mathbf{u}_h^{k+l} - \mathbf{u}_h^k\}\right\|^2_{(\boldsymbol{H}^1_{0,\mathrm{div}}\Omega)'} \le C\tau l^{\lambda/4} + C h_{\mathbf{x}}^2$$

for all $l \in \{1, \dots, N\}$ with $\lambda \in (2,4)$, if $d = 2$, or $\lambda = 3$, if $d = 3$.

Noting that $\lambda/4 < 1$, these results will enable us to apply a "compactness by pertubation" result by Azérad and Guillén [4] and to identify strongly converging subsequences.

Proof of Lemma 4.8. $\boldsymbol{S}\{\partial_\tau^- \mathbf{u}_h^n\} \in \boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)$ is well-defined as $\partial_\tau^- \mathbf{u}_h^n \in \boldsymbol{W}_{h,\mathrm{div}} \subset \boldsymbol{L}^2(\Omega) \subset (\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'$. Recalling the H^1-stable L^2-projector $\mathcal{Q}_h$ from (TH2), we adapt the proof of a similar regularity result in [7] and test (3.4d) by $\mathcal{Q}_h[\boldsymbol{S}\{\partial_\tau^- \mathbf{u}_h^n\}]$.

$$\begin{aligned}
0 = &\int_\Omega \partial_\tau^- \mathbf{u}_h^n \cdot \mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big] - \tfrac{1}{2}\int_\Omega \Big(\big(\nabla_{\mathbf{x}}\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big)^T \cdot \mathbf{u}_h^n\Big)\cdot \mathbf{u}_h^{n-1} \\
&+ \tfrac{1}{2}\int_\Omega \Big((\nabla_{\mathbf{x}}\mathbf{u}_h^n)^T \cdot \mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\Big)\cdot \mathbf{u}_h^{n-1} + \int_\Omega 2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^n)\}\mathbf{D}\mathbf{u}_h^n : \mathbf{D}\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big] \\
&+ \int_\Omega \phi_h^{n-1}\nabla_{\mathbf{x}}\mu_{\phi,h}^n \cdot \mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big] + \int_{\Omega\times\mathfrak{D}} M_h\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\cdot \mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\Big\} \\
&+ \int_{\Omega\times\mathfrak{D}} \big(\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\big\{\boldsymbol{\mathcal{J}}_h\big\{\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big\}\big\}\cdot \mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\}\big)\cdot \nabla_{\mathbf{q}}\hat{\psi}_h^n \\
=:& I + II + III + IV + V + VI + VII\,.
\end{aligned} \tag{4.39}$$

We obtain from (TH2) and from (H1) that

$$I = \int_\Omega \partial_\tau^- \mathbf{u}_h^n \cdot \mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big] = \big\|\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big\|_{H^1(\Omega)}^2\,. \tag{4.40}$$

Using Young's inequality together with the Gagliardo–Nirenberg inequality and Poincaré's inequality, we compute

$$\begin{aligned}
|II| &\le \delta\int_\Omega \big|\nabla_{\mathbf{x}}\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big|^2 + C_\delta\Big(\|\mathbf{u}_h^n\|_{L^4(\Omega)}^4 + \big\|\mathbf{u}_h^{n-1}\big\|_{L^4(\Omega)}^4\Big) \\
&\le \delta\int_\Omega \big|\nabla_{\mathbf{x}}\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big|^2 + C_\delta\Big(\big\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^d + \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^d\Big)\,.
\end{aligned} \tag{4.41}$$

Young's inequality yields, together with Sobolev's embedding theorem,

$$|III| \le \delta\,\big\|\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big\|_{H^1(\Omega)}^2 + C_\delta\,\big\|\big|\mathbf{u}_h^{n-1}\big|\,|\nabla_{\mathbf{x}}\mathbf{u}_h^n|\big\|_{L^{1+\sigma}(\Omega)}^2 \tag{4.42}$$

with $\sigma \in (0,1)$ in the case $d=2$ and $\sigma = \frac{1}{5}$ in the case $d=3$. Similarly to (4.77) in [7], we compute for $d=2$ and $\sigma = \frac{\lambda-2}{6-\lambda}$ by applying Hölder's inequality, the Gagliardo–Nirenberg inequality, Poincaré's inequality, and Young's inequality

$$\begin{aligned}
\big\|\big|\mathbf{u}_h^{n-1}\big|\,|\nabla_{\mathbf{x}}\mathbf{u}_h^n|\big\|_{L^{1+\sigma}(\Omega)}^2 &\le \big\|\mathbf{u}_h^{n-1}\big\|_{L^{2(1+\sigma)/(1-\sigma)}(\Omega)}^2 \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^2 \\
&\le C\,\big\|\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^{\frac{2(1-\sigma)}{1+\sigma}}\left(\|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^{\frac{2+6\sigma}{1+\sigma}} + \big\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^{\frac{2+6\sigma}{1+\sigma}}\right) \\
&\le C\Big(\big\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^\lambda + \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^\lambda\Big),
\end{aligned} \tag{4.43}$$

where we used $\big\|\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)} \le C$ (*cf.* Lem. 4.4) in the last step. Analogously, we obtain for $d=3$

$$\begin{aligned}
\big\|\big|\mathbf{u}_h^{n-1}\big|\,|\nabla_{\mathbf{x}}\mathbf{u}_h^n|\big\|_{L^{6/5}(\Omega)}^2 &\le C\,\big\|\mathbf{u}_h^{n-1}\big\|_{L^3(\Omega)}^2 \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^2 \\
&\le C\,\big\|\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}\Big(\big\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^3 + \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^3\Big) \\
&\le C\Big(\big\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\big\|_{L^2(\Omega)}^3 + \|\nabla_{\mathbf{x}}\mathbf{u}_h^n\|_{L^2(\Omega)}^3\Big)\,.
\end{aligned} \tag{4.44}$$

Therefore,

$$|III| \leq \delta \left\|\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right\|_{H^1(\Omega)}^2 + C_\delta \Big(\left\|\nabla_{\mathbf{x}} \mathbf{u}_h^{n-1}\right\|_{L^2(\Omega)}^\lambda + \left\|\nabla_{\mathbf{x}} \mathbf{u}_h^n\right\|_{L^2(\Omega)}^\lambda\Big). \tag{4.45}$$

As η is a bounded function, Young's inequality yields

$$|IV| \leq \delta \left\|\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right\|_{H^1(\Omega)}^2 + C_\delta \left\|\nabla_{\mathbf{x}} \mathbf{u}_h^n\right\|_{L^2(\Omega)}^2 . \tag{4.46}$$

Using Hölder's inequality, Sobolev's embedding theorem, Poincaré's inequality, the H^1-stability of $\mathcal{Q}_h$, Young's inequality, and the already established regularity results for ϕ_h^{n-1} (see Lem. 4.4), we compute for the fifth term on the right-hand side of (4.39)

$$\begin{aligned} |V| &\leq C \left\|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right\|_{H^1(\Omega)} \left\|\nabla_{\mathbf{x}} \phi_h^{n-1}\right\|_{L^2(\Omega)} \left\|\nabla_{\mathbf{x}} \mu_{\phi,h}^n\right\|_{L^2(\Omega)} \\ &\leq \delta \left\|\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right\|_{H^1(\Omega)}^2 + C_\delta \left\|\nabla_{\mathbf{x}} \mu_{\phi,h}^n\right\|_{L^2(\Omega)}^2 . \end{aligned} \tag{4.47}$$

In order to deal with the sixth term, we use an analogon of Young's inequality which is applicable in the case of matrix-valued coefficients. In particular, we apply the pointwise inequality

$$\begin{aligned} &\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right] \cdot \left(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n] \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\right) \\ &\qquad \leq \delta \sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]} \left|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right|^2 + \tfrac{1}{4\delta}\left(\sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]}\right)^{-1} \left|\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n] \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\right|^2 \\ &\qquad \leq \delta \sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]} \left|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right|^2 + \tfrac{1}{4\delta}\left(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n] \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\right) \cdot \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n . \end{aligned} \tag{4.48}$$

Applying (4.48) to $|VI|$ yields

$$\begin{aligned} |VI| \leq{}& \tilde{\delta} \int_{\Omega\times\mathfrak{D}} M_h \left|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right|^2 \sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]}(\mathbf{x},\mathbf{q}) \\ &+ C_{\tilde{\delta}} \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\left(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n] \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\right) \cdot \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\Big\}, \end{aligned} \tag{4.49}$$

where $\sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]}(\mathbf{x},\mathbf{q})$ denotes the supremum of the largest eigenvalue of $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]$ on $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}} \ni (\mathbf{x},\mathbf{q})$. Recalling (2.27f), we obtain

$$\begin{aligned} &\int_{\Omega\times\mathfrak{D}} M_h \left|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right|^2 \sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]}(\mathbf{x},\mathbf{q}) \\ &\quad \leq \left(\int_{\Omega\times\mathfrak{D}} M_h \left|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right|^4\right)^{1/2} \left(\int_{\Omega\times\mathfrak{D}} M_h \left|\sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]}(\mathbf{x},\mathbf{q})\right|^2\right)^{1/2} \\ &\quad \leq C \left\|\mathcal{Q}_h\left[\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right]\right\|_{L^4(\Omega)}^2 \left(\int_{\Omega\times\mathfrak{D}} M_h \nu^2 + \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{x}\mathbf{q}}\left\{\left|\hat{\psi}_h^n\right|^2\right\}\right)^{1/2} \\ &\quad \leq C \left\|\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right\|_{H^1(\Omega)}^2 . \end{aligned} \tag{4.50}$$

Therefore, we have

$$|VI| \leq \delta \left\|\boldsymbol{S}\left\{\partial_\tau^- \mathbf{u}_h^n\right\}\right\|_{H^1(\Omega)}^2 + C_\delta \int_{\Omega\times\mathfrak{D}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\left(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n] \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\right) \cdot \nabla_{\mathbf{x}} \mu_{\psi,h,\nu}^n\Big\}, \tag{4.51}$$

with some $0 < \delta \ll 1$. Due to our specific discretization (*cf.* Rem. 3.4), the stability result in Lemma 4.4 enables us to control the L^2-norm with respect to time of the second term.
As $\mathfrak{D}$ is bounded, we use Hölder's inequality to compute

$$|VII| \leq C\left(\int_{\Omega\times\mathfrak{D}} M_h \left|\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\big\{\boldsymbol{\mathcal{J}}_h\big\{\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big\}\big\}\right|^2\right)^{1/2}\left(\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^n\right|^2\right\}\right)^{1/2}. \tag{4.52}$$

Due to the mean value theorem, Lemma 2.10, and the H^1-stability of $\mathcal{Q}_h$, we may compute

$$\begin{aligned}\left(\int_{\Omega\times\mathfrak{D}} M_h \left|\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\big\{\boldsymbol{\mathcal{J}}_h\big\{\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big\}\big\}\right|^2\right)^{1/2} &\leq C\left\|\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_h\big\{\mathcal{Q}_h\big[\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\big]\big\}\right\|_{L^\infty(\Omega)} \\ &\leq C\left\|\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\right\|_{H^1(\Omega)}.\end{aligned} \tag{4.53}$$

Combining (4.52) with (4.53) and applying Young's inequality, we deduce

$$|VII| \leq \delta\left\|\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\right\|_{H^1(\Omega)}^2 + C_\delta\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^n\right|^2\right\}. \tag{4.54}$$

Collecting the above results and taking the $\frac{2}{\lambda}$ power on both sides, we obtain

$$\begin{aligned}\left\|\boldsymbol{S}\big\{\partial_\tau^- \mathbf{u}_h^n\big\}\right\|_{H^1(\Omega)}^{4/\lambda} \leq& C + C\left\|\nabla_{\mathbf{x}}\mathbf{u}_h^{n-1}\right\|_{L^2(\Omega)}^2 + C\left\|\nabla_{\mathbf{x}}\mathbf{u}_h^n\right\|_{L^2(\Omega)}^2 + C\left\|\nabla_{\mathbf{x}}\mu_{\phi,h}^n\right\|_{L^2(\Omega)}^2 \\ &+ C\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^n]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\right)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^n\right\} \\ &+ C\int_{\Omega\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{x}}\left\{\left|\nabla_{\mathbf{q}}\hat{\psi}_h^n\right|^2\right\}.\end{aligned} \tag{4.55}$$

A discrete integration with respect to time, together with (A8) and the results of Lemma 4.4 and Lemma 4.5, finally provides the result. □

Proof of Lemma 4.9. From (4.37c) we obtain

$$\begin{aligned}&\tau\sum_{k=0}^{N-l}\left\|\boldsymbol{R}_h\big\{\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\big\}\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^2 \\ &\quad\leq C\tau\sum_{k=0}^{N-l}\left\|\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^2 + Ch_{\mathbf{x}}^2\tau\sum_{k=0}^{N-l}\left\|\mathrm{div}_{\mathbf{x}}\left\{\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\}\right\|_{L^2(\Omega)}^2.\end{aligned} \tag{4.56}$$

Applying Hölder's inequality and (H3) provides

$$\begin{aligned}&\tau\sum_{k=0}^{N-l}\left\|\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^2 \\ &\quad\leq\left(\tau\sum_{k=0}^{N-l}\left\|\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^{4/\lambda}\right)^{\lambda/4}\left(\tau\sum_{k=0}^{N-l}\left\|\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\|_{L^2(\Omega)}^{4/(4-\lambda)}\right)^{(4-\lambda)/\lambda}.\end{aligned} \tag{4.57}$$

Due to the L^∞-L^2-bound for the velocity field obtained in Lemma 3.8, the second factor is bounded. Concerning the first factor, we use Lemma 4.8 and compute

$$\tau\sum_{k=0}^{N-l}\left\|\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^{4/\lambda} \leq C\tau\sum_{k=0}^{N-l}\sum_{m=1}^{l}\tau^{4/\lambda}\left\|\partial_\tau^-\mathbf{u}_h^{k+m}\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^{4/\lambda} \leq C\tau^{4/\lambda}l. \tag{4.58}$$

Combining Korn's inequality and Lemma 3.8 shows that the second term on the right-hand side of (4.56) is bounded by $Ch_{\mathbf{x}}^2$, which gives the result. □

To conclude this section, we collect the bounds derived so far. In particular, we have

$$\max_{k=1,\dots,n}\int_\Omega \left|\nabla_{\mathbf{x}}\phi_h^k\right|^2 + \max_{k=1,\dots,n}\int_\Omega \left|\mathbf{u}_h^k\right| + \max_{k=1,\dots,n}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\left|\hat{\psi}_h^k\right|^2$$
$$+ \nu^{-1}\max_{k=1,\dots,n}\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{[\hat{\psi}_h^k]_-^2\right\}$$
$$+ \sum_{k=1}^n\int_\Omega \left|\nabla_{\mathbf{x}}\phi_h^k - \nabla_{\mathbf{x}}\phi_h^{k-1}\right|^2 + \sum_{k=1}^n\left|\mathbf{u}_h^k-\mathbf{u}_h^{k-1}\right|^2 + \sum_{k=1}^n\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\left|\hat{\psi}_h^k-\hat{\psi}_h^{k-1}\right|^2$$
$$+ \tau\sum_{k=0}^n\int_\Omega\left|\Delta_h\phi_h^k\right|^2 + \tau\sum_{k=0}^n\left\|\phi_h^k\right\|_{L^\infty(\Omega)}^2 + \tau\sum_{k=1}^n\int_\Omega\left|\nabla_{\mathbf{x}}\mu_{\phi,h}^k\right|^2 + \tau\sum_{k=1}^n\int_\Omega\left|\nabla_{\mathbf{x}}\mathbf{u}_h^k\right|^2$$
$$+ \tau\sum_{k=0}^n\int_{\Omega\times\mathfrak{D}} M_h\left|\nabla_{\mathbf{x}}\hat{\psi}_h^k\right|^2 + \tau\sum_{k=0}^n\int_{\Omega\times\mathfrak{D}} M_h\left|\nabla_{\mathbf{q}}\hat{\psi}_h^k\right|^2 + \tau\sum_{k=1}^n\left\|\boldsymbol{S}\{\partial_\tau^-\mathbf{u}_h^k\}\right\|_{H^1(\Omega)}^{4/\lambda} \leq C \tag{4.59a}$$

and

$$\tau\sum_{k=0}^{N-l}\left\|\phi_h^{k+l}-\phi_h^k\right\|_{L^2(\Omega)}^2 \leq Cl\tau, \quad \tau\sum_{k=0}^{N-l}\left\|\boldsymbol{R}_h\{\mathbf{u}_h^{k+l}-\mathbf{u}_h^k\}\right\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^2 \leq C(l\tau)^{\lambda/4} + Ch_{\mathbf{x}}^2 \tag{4.59b}$$

for all $l\in\{1,\dots,N\}$, as $\lambda/4<1$.

5. Passage to the limit

In this section, we simultaneously pass to the limit $(h,\tau,\mathfrak{m},\nu)\searrow 0$. For this purpose, we define time-interpolants of time-discrete functions a^n, $n=0,\dots,N$, and introduce some time-index-free notation as follows.

$$a^\tau(.,t) := \tfrac{t-t^{n-1}}{\tau}a^n(.) + \tfrac{t^n-t}{\tau}a^{n-1}(.) \qquad t\in[t^{n-1},t^n], n\geq 1, \tag{5.1a}$$
$$a^{\tau,+}(.,t) := a^n(.), \quad a^{\tau,-}(.,t) := a^{n-1}(.) \qquad t\in(t^{n-1},t^n], n\geq 1. \tag{5.1b}$$

We want to point out that the time derivative of a^τ coincides with the difference quotient, *i.e.*

$$\partial_t a^\tau = \partial_t\Big(\tfrac{t-t^{n-1}}{\tau}a^n + \tfrac{t^n-t}{\tau}a^{n-1}\Big) = \tfrac{1}{\tau}a^n - \tfrac{1}{\tau}a^{n-1} = \partial_\tau^- a^n\,. \tag{5.2}$$

If a statement is valid for a^τ, $a^{\tau,+}$, and $a^{\tau,-}$, we will use the abbreviation $a^{\tau,(\pm)}$.

Using these notations and summing (3.4a)–(3.4d) from $n=1$ to N, we restate our set of equations as

$$\int_{\Omega_T}\mathcal{I}_h^{\mathbf{x}}\{\partial_t\phi_h^\tau\theta_h^{\mathbf{x}}\} - \int_{\Omega_T}(\mathbf{u}_h^{\tau,-} - \tau\phi_h^{\tau,-}\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+})\phi_h^{\tau,-}\cdot\nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} + \int_{\Omega_T}\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+}\cdot\nabla_{\mathbf{x}}\theta_h^{\mathbf{x}} = 0$$
$$\forall\theta^{\mathbf{x}}\in L^2(0,T;U_h^{\mathbf{x}}), \tag{5.3a}$$

$$\int_{\Omega_T}\mathcal{I}_h^{\mathbf{x}}\left\{\mu_{\phi,h}^{\tau,+}\theta_h^{\mathbf{x}}\right\} = \int_{\Omega_T}\mathcal{I}_h^{\mathbf{x}}\{W_h'(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta_h^{\mathbf{x}}\} + \int_{\Omega_T}(\vartheta\nabla_{\mathbf{x}}\phi_h^{\tau,+} + (1-\vartheta)\nabla_{\mathbf{x}}\phi_h^{\tau,-})\cdot\nabla_{\mathbf{x}}\theta_h^{\mathbf{x}}$$
$$+ \int_{\Omega_T}\mathcal{I}_h^{\mathbf{x}}\left\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta_{DQ}'(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta_h^{\mathbf{x}}\}\}\int_{\mathfrak{D}}(M_h+\mathfrak{m})\hat{\psi}_h^{\tau,-}\right\} \qquad \forall\theta_h^{\mathbf{x}}\in L^2(0,T;U_h^{\mathbf{x}}), \tag{5.3b}$$

$$
\begin{aligned}
&\int_{\Omega_T\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\partial_t\hat{\psi}_h^\tau\theta_h\Big\}-\int_{\Omega_T\times\mathfrak{D}}M_h\mathbf{u}_h^{\tau,+}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\theta_h\Big\}\\
&\quad-\int_{\Omega_T\times\mathfrak{D}}\big(\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{u}_h^{\tau,+}\}\}\cdot\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\}\big)\cdot\mathcal{I}_h^{\mathbf{x}}\Big\{\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{q}}\theta_h\Big\}\\
&+\int_{\Omega_T\times\mathfrak{D}}c_{\mathbf{x}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Big((1-\gamma)\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]+\gamma\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\theta_h\Big\}\\
&\qquad+\int_{\Omega_T\times\mathfrak{D}}c_{\mathbf{q}}M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,+}\cdot\nabla_{\mathbf{q}}\theta_h\Big\}=0\\
&\qquad\qquad\forall\theta_h\in L^2(0,T;\hat{X}_h),
\end{aligned}\tag{5.3c}
$$

$$
\begin{aligned}
&\int_{\Omega_T}\partial_t\mathbf{u}_h^\tau\cdot\mathbf{w}_h-\tfrac{1}{2}\int_{\Omega_T}\Big((\nabla_{\mathbf{x}}\mathbf{w}_h)^T\cdot\mathbf{u}_h^{\tau,+}\Big)\cdot\mathbf{u}_h^{\tau,-}+\tfrac{1}{2}\int_{\Omega_T}\Big((\nabla_{\mathbf{x}}\mathbf{u}_h^{\tau,+})^T\cdot\mathbf{w}_h\Big)\cdot\mathbf{u}_h^{\tau,-}\\
&\quad+\int_{\Omega_T}2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^{\tau,+})\}\mathbf{D}\mathbf{u}_h^{\tau,+}:\mathbf{D}\mathbf{w}_h=-\int_{\Omega_T}\phi_h^{\tau,-}\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+}\cdot\mathbf{w}_h\\
&-\int_{\Omega_T\times\mathfrak{D}}M_h\mathbf{w}_h\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}-\int_{\Omega_T\times\mathfrak{D}}(\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{w}_h\}\}\cdot\mathcal{I}_h^{\mathbf{q}}\{\mathbf{q}M_h\})\cdot\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,+}\\
&\qquad\forall\mathbf{w}_h\in L^{4/(4-\lambda)}(0,T;\boldsymbol{W}_{h,\mathrm{div}}),
\end{aligned}\tag{5.3d}
$$

where we again used the abbreviation

$$
\mu_{\psi,h,\nu}^{\tau,+}:=\mathcal{I}_h^{\mathbf{xq}}\Big\{g_\nu'(\hat{\psi}_h^{\tau,+})+\mathcal{J}_\varepsilon\{\beta(\phi_h^{\tau,+})\}\Big\}.\tag{5.4}
$$

Similarly, we rewrite the bounds from (4.59) as

$$
\int_0^{T-l\tau}\big\|\phi_h^{\tau,+}(\cdot+l\tau)-\phi_h^{\tau,+}(\cdot)\big\|_{L^2(\Omega)}^2\le C(l\tau)\quad\forall l\in\{1,\dots,N\},\tag{5.5a}
$$

$$
\int_0^{T-l\tau}\big\|\boldsymbol{R}_h\{\mathbf{u}_h^{\tau,+}(\cdot+l\tau)\}-\boldsymbol{R}_h\{\mathbf{u}_h^{\tau,+}(\cdot)\}\big\|_{(\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))'}^2\le C(l\tau)^{\lambda/4}+Ch_{\mathbf{x}}^2\quad\forall l\in\{1,\dots,N\},\tag{5.5b}
$$

$$
\begin{aligned}
&\sup_{t\in[0,T]}\int_\Omega\Big|\nabla_{\mathbf{x}}\phi_h^{\tau,(\pm)}\Big|^2+\tau^{-1}\int_{\Omega_T}\big|\nabla_{\mathbf{x}}\phi_h^{\tau,+}-\nabla_{\mathbf{x}}\phi_h^{\tau,-}\big|^2+\int_{\Omega_T}\Big|\Delta_h\phi_h^{\tau,(\pm)}\Big|^2\\
&\quad+\int_0^T\Big\|\phi_h^{\tau,(\pm)}\Big\|_{L^\infty(\Omega)}^4+\int_{\Omega_T}\Big|\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+}\Big|^2\\
&\quad+\sup_{t\in[0,T]}\int_{\Omega_T\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^{\tau,(\pm)}\Big|^2\Big\}+\nu^{-1}\sup_{t\in[0,T]}\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{[\hat{\psi}_h^{\tau,(\pm)}]_-^2\Big\}\\
&\quad+\tau^{-1}\int_{\Omega_T\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\Big|\hat{\psi}_h^{\tau,+}-\hat{\psi}_h^{\tau,-}\Big|^2\Big\}+\int_{\Omega_T\times\mathfrak{D}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,(\pm)}\Big|^2\Big\}\\
&\quad+\int_{\Omega_T\times\mathfrak{D}}M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\Big|\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\Big|^2\Big\}+\int_{\Omega_T\times\mathfrak{D}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\\
&\quad+\int_{\Omega_T\times\mathfrak{D}}M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}
\end{aligned}
$$

$$+\sup_{t\in[0,T]}\int_\Omega \left|\mathbf{u}_h^{\tau,(\pm)}\right|^2+\tau^{-1}\int_{\Omega_T}\left|\mathbf{u}_h^{\tau,+}-\mathbf{u}_h^{\tau,-}\right|^2+\int_{\Omega_T}\left|\mathbf{D}\mathbf{u}_h^{\tau,(\pm)}\right|^2+\int_0^T\|\boldsymbol{S}\{\partial_t\mathbf{u}_h^\tau\}\|_{H^1(\Omega)}^{4/\lambda}$$
$$\leq C\,. \tag{5.5c}$$

Applying (2.12a)–(2.12c) and noting the results of Lemma 4.3, we additionally obtain

$$\sup_{t\in[0,T]}\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\left|\hat{\psi}_h^{\tau,(\pm)}\right|^2+\tau^{-1}\int_{\Omega_T\times\mathfrak{D}}(M_h+\mathfrak{m})\left|\hat{\psi}_h^{\tau,+}-\hat{\psi}_h^{\tau,-}\right|^2$$
$$+\int_{\Omega_T\times\mathfrak{D}}M_h\left|\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,(\pm)}\right|^2+\int_{\Omega_T\times\mathfrak{D}}M_h\left|\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\right|^2$$
$$+\sup_{t\in[0,T]}\int_{\Omega\times\mathfrak{D}}\hat{M}\left|\hat{\psi}_h^{\tau,(\pm)}\right|^2+\tau^{-1}\int_{\Omega_T\times\mathfrak{D}}\hat{M}\left|\hat{\psi}_h^{\tau,+}-\hat{\psi}_h^{\tau,-}\right|^2\leq C\,. \tag{5.5d}$$

We use the bounds in (5.5) to show the existence of a subsequence, which is again denoted by $(\phi_h^{\tau,(\pm)},\mu_{\phi,h}^{\tau,(\pm)},\hat{\psi}_h^{\tau,(\pm)},\mathbf{u}_h^{\tau,(\pm)})_{(h,\tau,\mathfrak{m},\nu)}$, converging towards limit functions in an appropriate sense. As we only have Maxwellian-weighted bounds for the scaled configurational density function $\hat{\psi}_h^{\tau,(\pm)}$, we may not expect to obtain any information on the limit function outside of D. As we will show in Theorem 5.2, the values of the limit functions on $\Omega_T\times\mathfrak{D}\setminus D$ are negligible, as the integrals over this part of the domain do not contribute to the weak formulation. Therefore, we concentrate on identifying its limit functions on $\Omega_T\times D$. Analogously to the notation $a^{\tau,(\pm)}$, we denote the triple of limit functions $(a,\,a^+,\,a^-)$ by $a^{(\pm)}$.

Lemma 5.1. *Let the assumptions (A1)–(A9) hold true. Then there exists a subsequence (again denoted by $(\phi_h^{\tau,(\pm)},\mu_{\phi,h}^{\tau,(\pm)},\hat{\psi}_h^{\tau,(\pm)},\mathbf{u}_h^{\tau,(\pm)})_{(h,\tau,\mathfrak{m},\nu)}$) and functions ϕ, μ_ϕ, and $\mathbf{u}$ satisfying*

$$\phi\in L^\infty(0,T;H^1(\Omega))\cap L^2(0,T;H^2(\Omega))\cap L^4(0,T;L^\infty(\Omega)), \tag{5.6a}$$
$$\mu_\phi\in L^2(0,T;H^1(\Omega)), \tag{5.6b}$$
$$\mathbf{u}\in L^\infty(0,T;\boldsymbol{L}^2(\Omega))\cap L^2(0,T;\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))\cap W^{1,4/\lambda}(0,T;(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'), \tag{5.6c}$$

with $\lambda\in(2,4)$, if $d=2$, and $\lambda=3$, if $d=3$, as well as functions $\hat{\psi}$, P_1, P_2, P_3, $\boldsymbol{P}_4^{(\pm)}$, $\boldsymbol{P}_5^{(\pm)}$ satisfying

$$\hat{\psi}\in L^2(0,T;\hat{X}_+)\cap L^\infty(0,T;L^2(\Omega\times D;M)), \tag{5.6d}$$
$$P_1,P_2,P_3\in L^\infty(0,T;L^2(\Omega\times\mathfrak{D})), \tag{5.6e}$$
$$\boldsymbol{P}_4^{(\pm)},\boldsymbol{P}_5^{(\pm)}\in L^2(0,T;\boldsymbol{L}^2(\Omega\times\mathfrak{D})), \tag{5.6f}$$

with

$$P_1\big|_{\Omega_T\times D}=P_2\big|_{\Omega_T\times D}=P_3\big|_{\Omega_T\times D}=\sqrt{M}\hat{\psi}, \tag{5.7a}$$
$$\boldsymbol{P}_4^{(\pm)}\Big|_{\Omega_T\times D}=\sqrt{M}\nabla_{\mathbf{x}}\hat{\psi}, \tag{5.7b}$$
$$\boldsymbol{P}_5^{(\pm)}\Big|_{\Omega_T\times D}=\sqrt{M}\nabla_{\mathbf{q}}\hat{\psi}, \tag{5.7c}$$

such that, as $(h,\tau,\mathfrak{m},\nu)\searrow 0$*,*

$$\phi_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} \phi \quad \text{in } L^\infty(0,T;H^1(\Omega)), \tag{5.8a}$$
$$\phi_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} \phi \quad \text{in } L^4(0,T;L^\infty(\Omega)), \tag{5.8b}$$
$$\phi_h^{\tau,(\pm)} \to \phi \quad \text{in } L^p(0,T;L^s(\Omega)), \quad \forall p<\infty,\ s\in[1,\tfrac{2d}{d-2}), \tag{5.8c}$$
$$\Delta_h\phi_h^{\tau,(\pm)} \rightharpoonup \Delta\phi \quad \text{in } L^2(0,T;L^2(\Omega)), \tag{5.8d}$$
$$\mu_{\phi,h}^{\tau,+} \rightharpoonup \mu_\phi \quad \text{in } L^2(0,T;H^1(\Omega)), \tag{5.8e}$$

$$M_h \to \hat{M} \quad \text{in } L^\infty(\mathfrak{D}), \tag{5.9a}$$
$$\sqrt{\hat{M}}\hat{\psi}_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} P_1 \quad \text{in } L^\infty(0,T;L^2(\Omega\times\mathfrak{D})), \tag{5.9b}$$
$$\sqrt{M_h+\mathfrak{m}}\hat{\psi}_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} P_2 \quad \text{in } L^\infty(0,T;L^2(\Omega\times\mathfrak{D})), \tag{5.9c}$$
$$\sqrt{M_h}\hat{\psi}_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} P_3 \quad \text{in } L^\infty(0,T;L^2(\Omega\times\mathfrak{D})), \tag{5.9d}$$
$$\sqrt{M_h}\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,(\pm)} \rightharpoonup \boldsymbol{P}_4^{(\pm)} \quad \text{in } L^2(0,T;\boldsymbol{L}^2(\Omega\times\mathfrak{D})), \tag{5.9e}$$
$$\sqrt{M_h}\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)} \rightharpoonup \boldsymbol{P}_5^{(\pm)} \quad \text{in } L^2(0,T;\boldsymbol{L}^2(\Omega\times\mathfrak{D})), \tag{5.9f}$$

$$\mathbf{u}_h^{\tau,(\pm)} \overset{*}{\rightharpoonup} \mathbf{u} \quad \text{in } L^\infty(0,T;\boldsymbol{L}^2(\Omega)), \tag{5.10a}$$
$$\mathbf{u}_h^{\tau,(\pm)} \rightharpoonup \mathbf{u} \quad \text{in } L^2(0,T;\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)), \tag{5.10b}$$
$$\boldsymbol{S}\{\partial_t\mathbf{u}_h^\tau\} \rightharpoonup \boldsymbol{S}\{\partial_t\mathbf{u}\} \quad \text{in } L^{4/\lambda}(0,T;\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)), \tag{5.10c}$$
$$\mathbf{u}_h^{\tau,(\pm)} \to \mathbf{u} \quad \text{in } L^2(0,T;\boldsymbol{L}^s(\Omega)),\ s\in[1,\tfrac{2d}{d-2})\,. \tag{5.10d}$$

In addition, we have

$$\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\}\}\} \to \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\} \quad \text{in } L^2(0,T;W^{1,\infty}(\Omega)), \quad \text{for } \theta^{\mathbf{x}}\in C^\infty(0,T;C^\infty(\overline{\Omega})), \tag{5.11a}$$
$$\mathcal{I}_h^{\mathbf{x}}\Big\{\mathcal{J}_h\Big\{\mathcal{I}_h^{\mathbf{x}}\Big\{\beta(\phi_h^{\tau,(\pm)})\Big\}\Big\}\Big\} \to \mathcal{J}_\varepsilon\{\beta(\phi)\} \quad \text{in } L^2(0,T;W^{1,\infty}(\Omega)), \tag{5.11b}$$
$$\mathcal{I}_h^{\mathbf{x}}\Big\{\boldsymbol{\mathcal{J}}_h\Big\{\mathbf{u}_h^{\tau,(\pm)}\Big\}\Big\} \to \boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\} \quad \text{in } L^2(0,T;\boldsymbol{W}^{1,\infty}(\Omega))\,. \tag{5.11c}$$

Proof. The convergence results stated in (5.8a), (5.8b), (5.8d), and (5.8e) are direct consequences of the bounds in (5.5c). As we can control $\tau^{-1}\int_{\Omega_T}\left|\nabla_{\mathbf{x}}\phi_h^{\tau,+}-\nabla_{\mathbf{x}}\phi_h^{\tau,-}\right|^2$ (*cf.* (5.5c)), it is possible to show that appropriate subsequences of $\phi_h^{\tau,+}$, $\phi_h^{\tau,-}$, and ϕ_h^τ converge towards the same limit function. The strong convergence in (5.8c) follows from Simon's compactness theorem (*cf.* [27]) and the bound in (5.5a).

As proving the convergence expressed in (5.9) and (5.7) is more technical, we provide additional details on this part of the proof. (5.9a) is a direct consequence of Lemma 2.2. The convergence implied by (5.9b) follows from (5.5d). Using

$$\int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}\hat{\psi}_h^{\tau,+}\theta = \int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}\hat{\psi}_h^{\tau,-}\theta + \int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}\Big(\hat{\psi}_h^{\tau,+}-\hat{\psi}_h^{\tau,-}\Big)\theta, \tag{5.12}$$

for all $\theta \in L^1(0,T;L^2(\Omega\times\mathfrak{D}))$, we show that $\sqrt{\hat{M}}\hat{\psi}_h^{\tau,+}$, $\sqrt{\hat{M}}\hat{\psi}_h^{\tau,-}$, and $\sqrt{\hat{M}}\hat{\psi}_h^{\tau}$ converge towards the same limit function P_1 which we use to define the limit function $\hat{\psi}$ on $\Omega_T\times D$. Analogously, we obtain that $\sqrt{M_h+\mathfrak{m}}\hat{\psi}_h^{\tau,(\pm)}$ converge towards the same limit function denoted by P_2. Using the strong convergence of the discrete Maxwellian from (5.9a), we choose a test function $\tilde{\theta} := \sqrt{\hat{M}}\theta$ with $\theta \in L^1(0,T;L^2(\Omega\times\mathfrak{D}))$ and deduce

$$\begin{aligned}\int_{\Omega_T\times\mathfrak{D}} P_2\tilde{\theta} \leftarrow \int_{\Omega_T\times\mathfrak{D}} \sqrt{M_h+\mathfrak{m}}\hat{\psi}_h^{\tau,(\pm)}\tilde{\theta} &= \int_{\Omega_T\times\mathfrak{D}} \sqrt{M_h+\mathfrak{m}}\hat{\psi}_h^{\tau,(\pm)}\sqrt{\hat{M}}\theta \\ &\to \int_{\Omega_T\times\mathfrak{D}} \sqrt{\hat{M}}P_1\theta = \int_{\Omega_T\times\mathfrak{D}} P_1\tilde{\theta},\end{aligned} \tag{5.13}$$

which shows that P_1 and P_2 coincide on $\Omega_T\times D$. Similar arguments yield (5.9d). Choosing a test function $\boldsymbol{\eta}\in L^2(0,T;\boldsymbol{C}_0^\infty(\Omega\times D))$, we obtain

$$\begin{aligned}\int_{\Omega_T\times D} \boldsymbol{P}_4^{(\pm)}\cdot\boldsymbol{\eta} \leftarrow \int_{\Omega_T\times D} \sqrt{M_h}\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,(\pm)}\cdot\boldsymbol{\eta} &= \int_{\Omega_T\times D} \nabla_{\mathbf{x}}(\sqrt{M_h}\hat{\psi}_h^{\tau,(\pm)})\cdot\boldsymbol{\eta} \\ = -\int_{\Omega_T\times D} \sqrt{M_h}\hat{\psi}_h^{\tau,(\pm)}\operatorname{div}_{\mathbf{x}}\{\boldsymbol{\eta}\} &\to -\int_{\Omega_T\times D} P_3\operatorname{div}_{\mathbf{x}}\{\boldsymbol{\eta}\} = \int_{\Omega_T\times D}\sqrt{M}\nabla_{\mathbf{x}}\hat{\psi}\cdot\boldsymbol{\eta},\end{aligned} \tag{5.14}$$

which yields (5.9e). Concerning the proof of (5.9f), we infer from the bounds in (5.5d) that the subsequences converge towards limit functions which we denote by $\boldsymbol{P}_5^{(\pm)}$. We prove that $\boldsymbol{P}_5^{(\pm)}$ coincide with $\sqrt{M}\nabla_{\mathbf{q}}\hat{\psi}$ on every compact subset of D. In a first step, we restrict ourselves to subsets $D_\delta := \{\mathbf{q}\in D : \operatorname{dist}(\mathbf{q},\partial D)\geq\delta\}$ of D with $\delta > 2h_{\mathbf{q}}$. From (4.6), we have $\hat{M}\leq CM_h$ on D_δ, which implies $\int_{\Omega_T\times D_\delta}\hat{M}\left|\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\right|^2\leq C$ and therefore the existence of subsequences converging weakly towards some limit function. Following the approach in [7] (see also [5] and [18]), we choose a test function $\boldsymbol{\eta}\in L^2(0,T;\boldsymbol{C}_0^\infty(\Omega\times D_\delta))$ and compute

$$\begin{aligned}\int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\cdot\boldsymbol{\eta} &= -\int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\hat{\psi}_h^{\tau,(\pm)}\frac{\operatorname{div}_{\mathbf{q}}\left\{\sqrt{\hat{M}}\boldsymbol{\eta}\right\}}{\sqrt{\hat{M}}} \to -\int_{\Omega_T\times D_\delta}P_1\frac{\operatorname{div}_{\mathbf{q}}\left\{\sqrt{\hat{M}}\boldsymbol{\eta}\right\}}{\sqrt{\hat{M}}} \\ &= -\int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\hat{\psi}\frac{\operatorname{div}_{\mathbf{q}}\left\{\sqrt{\hat{M}}\boldsymbol{\eta}\right\}}{\sqrt{\hat{M}}} = \int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\nabla_{\mathbf{q}}\hat{\psi}\cdot\boldsymbol{\eta}.\end{aligned} \tag{5.15}$$

In the next step, we choose some test function $\tilde{\boldsymbol{\eta}}\in L^1(0,T;\boldsymbol{C}_0^\infty(\Omega\times D))$. Hence, there exists $\delta>0$ such that $\operatorname{supp}\tilde{\boldsymbol{\eta}}\subset\Omega\times D_\delta$, which implies

$$\begin{aligned}\int_{\Omega_T\times\mathfrak{D}}\sqrt{M_h}\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\cdot\left(\sqrt{\hat{M}}\tilde{\boldsymbol{\eta}}\right) &= \int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,(\pm)}\cdot\left(\sqrt{M_h}\tilde{\boldsymbol{\eta}}\right) \\ &\to \int_{\Omega_T\times D_\delta}\sqrt{\hat{M}}\nabla_{\mathbf{q}}\hat{\psi}\cdot\left(\sqrt{\hat{M}}\tilde{\boldsymbol{\eta}}\right),\end{aligned} \tag{5.16}$$

and therefore yields the result.

The nonnegativity of $\hat{\psi}$ on $\Omega_T\times D$ follows from $\sup_{t\in[0,T]}\int_{\Omega\times\mathfrak{D}}(M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\left\{\left[\hat{\psi}_h^{\tau,(\pm)}\right]_-^2\right\}\leq\nu C$ (*cf.* (5.5c)).

(5.10a) and (5.10b) follow directly from the bounds in (5.5c). Due to the denseness of $\bigcup_{h>0}U_h^{\mathbf{x}}$ in $L^2(\Omega)$, we have $\mathbf{u}\in L^2(0,T;\boldsymbol{H}_{0,\operatorname{div}}^1(\Omega))$. Noting that $\boldsymbol{S}$ denotes the inverse Riesz-isomorphism on $\boldsymbol{H}_{0,\operatorname{div}}^1(\Omega)$ (*cf.* [5], [18]), we obtain (5.10c), which also implies weak* convergence of $\partial_t\mathbf{u}_h^\tau$ towards $\partial_t\mathbf{u}$. To prove the strong convergence postulated in (5.10d), we show that $\|\mathbf{u}_h^{\tau,(\pm)}-\mathbf{u}\|_{L^2(0,T;L^s(\Omega))}$, which is bounded by

$$\|\mathbf{u}_h^{\tau,(\pm)}-\mathbf{u}_h^{\tau,+}\|_{L^2(0,T;L^s(\Omega))} + \|\mathbf{u}_h^{\tau,+}-\boldsymbol{R}_h\{\mathbf{u}_h^{\tau,+}\}\|_{L^2(0,T;L^s(\Omega))} + \|\boldsymbol{R}_h\{\mathbf{u}_h^{\tau,+}\}-\mathbf{u}\|_{L^2(0,T;L^s(\Omega))}, \tag{5.17}$$

tends to zero. The first two terms vanish due to (5.5c), (4.37b), and the Gagliardo–Nirenberg inequality. The convergence of the third term is a direct consequence of the bound in (5.5b) and the bounds in (5.5c) and a "compactness by pertubation" result by Azérad and Guillén [4] which we cited in Lemma B.2.

To prove (5.11a), we apply the decomposition

$$\begin{aligned}
&\big\|\mathcal{I}_h^{\mathbf{x}}\big\{\mathcal{J}_h\big\{\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\}\big\}\big\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\big\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\quad\le \big\|\mathcal{I}_h^{\mathbf{x}}\big\{\mathcal{J}_h\big\{\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\} - \beta'(\phi)\theta^{\mathbf{x}}\big\}\big\}\big\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\qquad + \|\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_h\{\beta'(\phi)\theta^{\mathbf{x}}\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\}\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\qquad + \|\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\|_{L^2(0,T;W^{1,\infty}(\Omega))}
\end{aligned} \tag{5.18}$$

and show that the terms on the right-hand side vanish. Using Lemma 2.10, we compute

$$\begin{aligned}
&\big\|\mathcal{I}_h^{\mathbf{x}}\big\{\mathcal{J}_h\big\{\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\} - \beta'(\phi)\theta^{\mathbf{x}}\big\}\big\}\big\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\quad\le C(\varepsilon)\,\big\|\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\} - \beta'(\phi)\theta^{\mathbf{x}}\big\|_{L^2(0,T;L^1(\Omega))}\,.
\end{aligned} \tag{5.19}$$

Therefore, the first term vanishes, if $\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\}$ converges strongly towards $\beta'(\phi)\theta^{\mathbf{x}}$ in $L^2(0,T;L^1(\Omega))$. To prove this convergence, we start with the estimate

$$\begin{aligned}
\int_\Omega \big|\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}}\big\} - \beta'(\phi)\theta^{\mathbf{x}}\big| &\le \int_\Omega \big|\mathcal{I}_h^{\mathbf{x}}\big\{\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-})\theta^{\mathbf{x}} - \beta'(\phi)\theta^{\mathbf{x}}\big\}\big| \\
&\quad + \int_\Omega |\mathcal{I}_h^{\mathbf{x}}\{\beta'(\phi)\theta^{\mathbf{x}}\} - \beta'(\phi)\theta^{\mathbf{x}}| =: I + II\,.
\end{aligned} \tag{5.20}$$

As we have $\theta^{\mathbf{x}} \in C^\infty(0,T;C^\infty(\overline{\Omega}))$ and $\phi_h^{\tau,+},\phi_h^{\tau,-} \in U_h^{\mathbf{x}}$, we use the mean value theorem to compute

$$\begin{aligned}
I &\le \max_{\mathbf{x}\in\Omega}|\theta^{\mathbf{x}}|\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\beta'_{DQ}(\phi_h^{\tau,+},\phi_h^{\tau,-}) - \beta'(\phi)\big|\big\} \\
&\le C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,+} - \phi\big|\big\} + C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,-} - \phi\big|\big\} \\
&= C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,+} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big|\big\} + C\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,-} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big|\big\}\,.
\end{aligned} \tag{5.21}$$

To deduce the last equality in (5.21), we used in particular that the integrals depend only on the values in the vertices of the simplices. Therefore, it is possible to interchange ϕ and $\mathcal{I}_h^{\mathbf{x}}\{\phi\}$. Combining a discrete version of Hölder's inequality and (2.10) shows

$$\begin{aligned}
\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,+} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big|\big\} &\le C\bigg(\int_\Omega \mathcal{I}_h^{\mathbf{x}}\Big\{\big(\phi_h^{\tau,+} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big)^2\Big\}\bigg)^{1/2} \\
&\le C\,\big\|\phi_h^{\tau,+} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big\|_{L^2(\Omega)} \le C\,\big\|\phi_h^{\tau,+} - \phi\big\|_{L^2(\Omega)} + C\,\|\mathcal{I}_h^{\mathbf{x}}\{\phi\} - \phi\|_{L^2(\Omega)} \to 0
\end{aligned} \tag{5.22}$$

due to (5.8c), $\phi \in L^2(0,T;H^2(\Omega))$, and standard error estimates for the nodal interpolation operator (*cf.* [9]). Similar arguments imply

$$\int_\Omega \mathcal{I}_h^{\mathbf{x}}\big\{\big|\phi_h^{\tau,-} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\big|\big\} \to 0\,. \tag{5.23}$$

From (5.8c), we also infer $II \to 0$. The second term on the right hand side of (5.18) vanishes as we have

$$\begin{aligned}
&\|\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_h\{\beta'(\phi)\theta^{\mathbf{x}}\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\}\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\quad\le \|\mathcal{J}_h\{\beta'(\phi)\theta^{\mathbf{x}}\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\|_{L^2(0,T;W^{1,\infty}(\Omega))} \\
&\quad\le Ch_{\mathbf{x}}\,\|\beta'(\phi)\theta^{\mathbf{x}}\|_{L^2(0,T;L^1(\Omega))} \le Ch_{\mathbf{x}}\,.
\end{aligned} \tag{5.24}$$

Combining standard error estimates for the nodal interpolation operator with (1.9f), we compute for the last term on the right hand side of (5.18)

$$\begin{aligned}\|\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\} - \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\|_{L^2(0,T;W^{1,\infty}(\Omega))} &\leq Ch_{\mathbf{x}}\,\|\mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\|_{L^2(0,T;W^{2,\infty}(\Omega))}\\ &\leq Ch_{\mathbf{x}}\,\|\beta'(\phi)\theta^{\mathbf{x}}\|_{L^2(0,T;L^1(\Omega))} \leq Ch_{\mathbf{x}} \to 0\,. \end{aligned} \tag{5.25}$$

Similar arguments provide (5.11b) and (5.11c). □

Using the above mentioned convergence results, we pass to the limit $(h,\tau,\mathfrak{m},\nu)\searrow(0,0,0,0)$ in (5.3) and obtain the following result.

Theorem 5.2. *Let $d\in\{2,3\}$. Under the assumptions (A1)–(A9), there is a quadruple $(\phi,\mu_\phi,\hat{\psi},\mathbf{u})$ which can be obtained from discrete solutions of (5.3) by passing to the limit $(h,\tau,\mathfrak{m},\nu)\searrow(0,0,0,0)$ and which solves the equal-density version of (1.5) in the following weak sense.*

$$\int_{\Omega_T}(\Phi^0-\phi)\partial_t\theta^{\mathbf{x}} - \int_{\Omega_T}\phi\mathbf{u}\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}} + \int_{\Omega_T}\nabla_{\mathbf{x}}\mu_\phi\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}} = 0 \qquad \forall\theta^{\mathbf{x}}\in C^1([0,T];H^1(\Omega)) \text{ with } \theta^{\mathbf{x}}(.,T)\equiv 0, \tag{5.26a}$$

$$\int_{\Omega_T}\mu_\phi\theta^{\mathbf{x}} = \int_{\Omega_T}\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}} + \int_{\Omega_T}W'(\phi)\theta^{\mathbf{x}} + \int_{\Omega_T}\beta'(\phi)\mathcal{J}_\varepsilon\left\{\int_D M\hat{\psi}\right\}\theta^{\mathbf{x}} \qquad \forall\theta^{\mathbf{x}}\in L^2(0,T;H^1(\Omega)), \tag{5.26b}$$

$$\begin{aligned}&\int_{\Omega_T\times D}(\hat{\Psi}^0-\hat{\psi})\partial_t\theta - \int_{\Omega_T\times D}M\hat{\psi}\mathbf{u}\cdot\nabla_{\mathbf{x}}\theta - \int_{\Omega_T\times D}M\hat{\psi}(\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}\theta\\ &\quad + c_{\mathbf{q}}\int_{\Omega_T\times D}M\nabla_{\mathbf{q}}\hat{\psi}\cdot\nabla_{\mathbf{q}}\theta + c_{\mathbf{x}}\int_{\Omega_T\times D}M\nabla_{\mathbf{x}}\hat{\psi}\cdot\nabla_{\mathbf{x}}\theta\\ &\quad + c_{\mathbf{x}}\int_{\Omega_T\times D}M\hat{\psi}\nabla_{\mathbf{x}}\mathcal{J}_\varepsilon\{\beta(\phi)\}\cdot\nabla_{\mathbf{x}}\theta = 0 \quad \forall\theta\in C^1([0,T],\hat{X}) \text{ with } \theta(.,T)\equiv 0,\end{aligned} \tag{5.26c}$$

$$\begin{aligned}&\int_0^T\langle\partial_t\mathbf{u},\mathbf{w}\rangle + \int_{\Omega_T}(\mathbf{u}\cdot\nabla_{\mathbf{x}})\mathbf{u}\cdot\mathbf{w} + \int_{\Omega_T}2\eta(\phi)\mathbf{D}\mathbf{u}:\mathbf{D}\mathbf{w}\\ &\quad = \int_{\Omega_T}\mu_\phi\nabla_{\mathbf{x}}\phi\cdot\mathbf{w} + \int_{\Omega_T}\operatorname{div}_{\mathbf{x}}\left\{\mathfrak{J}_\varepsilon\left\{\int_D M\nabla_{\mathbf{q}}\hat{\psi}\otimes\mathbf{q}\right\}\right\}\cdot\mathbf{w} + \int_{\Omega_T\times D}\mathcal{J}_\varepsilon\{\beta(\phi)\}M\nabla_{\mathbf{x}}\hat{\psi}\cdot\mathbf{w}\\ &\qquad \forall\mathbf{w}\in L^{4/(4-\lambda)}(0,T;\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)),\end{aligned} \tag{5.26d}$$

with $\lambda\in(2,4)$, if $d=2$, and $\lambda=3$, if $d=3$. Moreover, the solution has the following regularity properties

$$\phi\in L^\infty(0,T;H^1(\Omega))\cap L^2(0,T;H^2(\Omega))\cap L^4(0,T;L^\infty(\Omega)), \tag{5.27a}$$

$$\mu_\phi\in L^2(0,T;H^1(\Omega)), \tag{5.27b}$$

$$\hat{\psi}\in L^2(0,T;\hat{X}_+)\cap L^\infty(0,T;L^2(\Omega\times D;M)), \tag{5.27c}$$

$$\mathbf{u}\in L^\infty(0,T;\boldsymbol{L}^2(\Omega))\cap L^2(0,T;\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))\cap W^{1,4/\lambda}(0,T;(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))'), \tag{5.27d}$$

with $\lambda\in(2,4)$, if $d=2$, and $\lambda=3$, if $d=3$.

Proof. In order to pass to the limit in (5.3a), we choose $\theta_h^{\mathbf{x}} = \mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\}$ with $\theta^{\mathbf{x}} \in C^1([0,T], C^\infty(\overline{\Omega}))$ and $\theta^{\mathbf{x}}(.,T) \equiv 0$. Therefore, the first term in (5.3a) can be rewritten as

$$\int_{\Omega_T} \partial_t \phi_h^\tau \mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\} - \int_\Omega (I - \mathcal{I}_h^{\mathbf{x}})\{\partial_t \phi_h^\tau \mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\}\} =: I_a + I_b \,. \tag{5.28}$$

Partial integration with respect to time, the assumptions on the initial data, (5.8c), and the strong convergence of $\mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\}$ towards $\theta^{\mathbf{x}}$ provided by standard estimates on the interpolation error (*cf.* [9]) yield the convergence of $I_a \to \int_{\Omega_T}(\Phi^0 - \phi)\partial_t\theta^{\mathbf{x}}$. I_b vanishes due to the estimates stated in Lemma 2.4. The convergence of the second term in (5.3a) is a direct consequence of the convergence results obtained in Lemma 5.1 and standard interpolation error estimates (*cf.* Thm. 4.4.4 in [9]). From the bounds in (5.5c), we obtain that the third term is bounded by τC and therefore vanishes when passing to the limit. The last convergence of the last term in (5.3a) follows from the weak convergence of $\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+}$ and the strong convergence of $\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\} \to \nabla_{\mathbf{x}}\theta^{\mathbf{x}}$.

In order to pass to the limit in (5.3b), we choose $\theta_h^{\mathbf{x}} = \mathcal{I}_h^{\mathbf{x}}\{\theta^{\mathbf{x}}\}$ with $\theta^{\mathbf{x}} \in C^\infty([0,T], C^\infty(\overline{\Omega}))$. Then, the convergence of term on the left-hand side of (5.3b) follows from the weak convergence of $\mu_{\phi,h}^{\tau,+}$ stated in (5.8e) and (2.18). The first term on the right-hand side of (5.3b) can be rewritten as

$$\int_{\Omega_T} \mathcal{I}_h^{\mathbf{x}}\big\{(W_h'(\phi_h^{\tau,+},\phi_h^{\tau,-}) - W_h'(\phi_h^{\tau,-},\phi) + W_h'(\phi_h^{\tau,-},\phi) - W_h'(\phi,\phi))\theta^{\mathbf{x}}\big\} + \int_{\Omega_T} \mathcal{I}_h^{\mathbf{x}}\{W_h'(\phi,\phi)\theta^{\mathbf{x}}\}. \tag{5.29}$$

Thereby, the first term vanishes. In particular, (W5) and the bounds on $\|\phi_h^{\tau,(\pm)}\|_{L^4(0,T;L^\infty(\Omega))}$ and $\|\phi\|_{L^4(0,T;L^\infty(\Omega))}$ show that it is bounded by

$$C\left(\int_0^T \left[\int_\Omega \mathcal{I}_h^{\mathbf{x}}\{|\phi_h^{\tau,+} - \phi_h^{\tau,-}| + |\phi_h^{\tau,-} - \phi|\}\right]^2\right)^{1/2}. \tag{5.30}$$

Due to $\left\|\phi_h^{\tau,-} - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\right\|_{L^2(\Omega)} \le \left\|\phi_h^{\tau,-} - \phi\right\|_{L^2(\Omega)} + C\left\|\phi - \mathcal{I}_h^{\mathbf{x}}\{\phi\}\right\|_{L^\infty(\Omega)}$, (5.30) is bounded by

$$C\left\|\phi_h^{\tau,+} - \phi_h^{\tau,-}\right\|_{L^2(\Omega_T)} + C\left\|\phi_h^{\tau,-} - \phi\right\|_{L^2(\Omega_T)} + Ch_{\mathbf{x}}^{1/2}\|\phi\|_{L^2(0,T;H^2(\Omega))} \to 0\,. \tag{5.31}$$

The convergence of the second term in (5.29) towards $\int_{\Omega_T} W'(\phi)\theta^{\mathbf{x}}$ follows from (W4) and the estimate $\|\mathcal{I}_h^{\mathbf{x}}\{f\} - f\|_{L^6(\Omega)} \le Ch_{\mathbf{x}}|f|_{W^{1,6}(\Omega)}$ (*cf.* [9]), as we have

$$|W'(\phi)\theta^{\mathbf{x}}|_{L^1(0,T;W^{1,6}(\Omega))} \le C\Big(\|W'(\phi)\|_{L^1(0,T;L^6(\Omega))} + \|W''(\phi)\nabla_{\mathbf{x}}\phi\|_{L^1(0,T;L^6(\Omega))}\Big)\,. \tag{5.32}$$

Due to (W1), the terms on the right-hand side of (5.32) are bounded. The convergence of the third integral in (5.3b) towards $\int_{\Omega_T}\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}}$ is a direct consequence of (5.8a), while the convergence of the last term follows from the weak* convergence in (5.9c), the strong convergence in (5.11a), and (2.18). Altogether, we have

$$\int_{\Omega_T}\mu_\phi\theta^{\mathbf{x}} = \int_{\Omega_T}\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{x}}\theta^{\mathbf{x}} + \int_{\Omega_T} W'(\phi)\theta^{\mathbf{x}} + \int_{\Omega_T\times\mathfrak{D}} \mathcal{J}_\varepsilon\{\beta'(\phi)\}\sqrt{\hat{M}}P_2\theta^{\mathbf{x}} \qquad \forall\theta^{\mathbf{x}} \in C^\infty([0,T], C^\infty(\overline{\Omega}))\,. \tag{5.33}$$

Noting the estimate

$$\left|\int_{\Omega_T\times(\mathfrak{D}\setminus D)} \mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}\sqrt{\hat{M}}P_2\right| \le \left(\int_{\Omega_T}|\mathcal{J}_\varepsilon\{\beta'(\phi)\theta^{\mathbf{x}}\}|^2\int_{\mathfrak{D}\setminus D}\hat{M}\right)^{1/2}\left(\int_{\Omega_T\times\mathfrak{D}} P_2^2\right)^{1/2} = 0 \tag{5.34}$$

and $P_2\big|_D = \sqrt{M}\hat{\psi}$, shifting the continuous mollifier $\mathcal{J}_\varepsilon$ onto $\int_D M\hat{\psi}$, and recalling the denseness of $C^\infty([0,T], C^\infty(\overline{\Omega}))$ in $L^2(0,T;H^1(\Omega))$, we obtain (5.26b).

To pass to the limit in the Fokker–Planck type equation (5.3c), we again use $\mathcal{I}_h^{\mathbf{xq}}\{\theta\}$ with $\theta \in C^1([0,T];C^\infty(\overline{\Omega \times D}))$ and $\theta(.,T) \equiv 0$ as test function. Applying partial integration with respect to time, we split the first term in (5.3c) into

$$-\int_{\Omega_T\times\mathfrak{D}} M_h\hat{\psi}_h^\tau \partial_t \mathcal{I}_h^{\mathbf{xq}}\{\theta\} + \int_{\Omega_T\times\mathfrak{D}} M_h(I-\mathcal{I}_h^{\mathbf{xq}})\Big\{\hat{\psi}_h^\tau \partial_t \mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\} \\ -\mathfrak{m}\int_{\Omega_T\times\mathfrak{D}} \mathcal{I}_h^{\mathbf{xq}}\Big\{\hat{\psi}_h^\tau \partial_t \mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\} - \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\mathcal{I}_h^{\mathbf{xq}}\Big\{\hat{\psi}_h^0 \mathcal{I}_h^{\mathbf{xq}}\{\theta\big|_{t=0}\}\Big\} \tag{5.35}$$

The results of the previous lemma provide the convergence of the first term towards $-\int_{\Omega_T\times\mathfrak{D}} \sqrt{\hat{M}} P_3 \partial_t\theta$. The second term vanishes due to (2.16c) and the bounds stated in (5.5c). Applying Young's inequality shows that the third term vanishes, too. Recalling the definition of $\hat{\psi}_h^0$ in (4.1), one obtains the convergence of the last term in (5.35) towards $-\int_{\Omega\times\mathfrak{D}} \hat{M}\hat{\Psi}^0\,\theta\big|_{t=0}$.

Concerning the convergence in the second term of (5.3c), we rewrite the term as

$$\int_{\Omega_T\times\mathfrak{D}} M_h \mathbf{u}_h^{\tau,+}\cdot \mathcal{I}_h^{\mathbf{q}}\Big\{\hat{\psi}_h^{\tau,+}\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\} - \int_{\Omega_T\times\mathfrak{D}} M_h \mathbf{u}_h^{\tau,+}\cdot \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\hat{\psi}_h^{\tau,+}\mathbb{1} - \Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\Big)\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\}. \tag{5.36}$$

As $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]$ is an approximation of $\hat{\psi}_h^{\tau,+}$ in the sense of (2.33c), the second term vanishes when passing to the limit, while the first term converges towards $\int_{\Omega_T\times\mathfrak{D}} \sqrt{\hat{M}} P_3 \mathbf{u}\cdot\nabla_{\mathbf{x}}\theta$ due to (5.9a), (5.10d), (5.9d), (2.19), and the standard error estimates for the interpolation error.

Similarly, we obtain from (2.33a) and the convergence results established in Lemma 5.1

$$\int_{\Omega_T\times\mathfrak{D}} \big(\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathbf{u}_h^{\tau,+}\}\}\cdot\mathcal{I}_h^{\mathbf{x}}\{\mathbf{q}M_h\}\big)\cdot\mathcal{I}_h^{\mathbf{x}}\Big\{\Xi_\nu^{\mathbf{q}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\} \\ \to \int_{\Omega_T\times\mathfrak{D}} \sqrt{\hat{M}} P_3 (\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}\theta, \tag{5.37}$$

where we used in particular the high regularity of the mollified velocity field. Recalling (2.24a), we split the fourth term in (5.3c) into

$$\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\theta\}\Big\} = \int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,+}\cdot\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\theta\}\Big\} \\ + \int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}} M_h \mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\mathcal{J}_h\{\mathcal{I}_h^{\mathbf{x}}\{\beta(\phi_h^{\tau,+})\}\}\}\Big)\cdot\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{x}}\{\theta\}\Big\} \\ =: A + B. \tag{5.38}$$

The convergence of A follows from (5.9a), (5.9e), and (2.16b), while the convergence of B can be established using Lemma 2.10, (A6), (2.19), (5.9d), (5.11b), (2.12b), and (2.33b). Therefore, we obtain

$$A + B \to \int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}}\sqrt{\hat{M}}\boldsymbol{P}_4^+\cdot\nabla_{\mathbf{x}}\theta + \int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}}\sqrt{\hat{M}} P_3 \nabla_{\mathbf{x}}\mathcal{J}_\varepsilon\{\beta(\phi)\}\cdot\nabla_{\mathbf{x}}\theta\,. \tag{5.39}$$

As the following computations show, we may substitute $\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]$ by $\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]$ without changing the limit, which provides the convergence in the fifth term (*cf.* (5.38), (5.39)).

$$\begin{aligned}&\left|\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\right|\\ &\quad\leq C\left(\nu^{-1}\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\right|^2\right\}\right)^{1/2}\left(\nu\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\right|^2\right\}\right)^{1/2}.\end{aligned}\tag{5.40}$$

As the eigenvalues of $\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]$ are greater than or equal to ν, we have

$$\nu\int_{\Omega_T\times\mathfrak{D}} M_h\left|\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\right|^2\leq\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\leq C\tag{5.41}$$

due to (5.5c). We obtain from (2.33d) that the first factor on the right-hand side of (5.40) scales with $\frac{h_{\mathbf{x}}^2}{\nu}$. In combination with assumption (A7) and the bounds in (5.5c), we obtain

$$\nu^{-1}\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\right|^2\right\}\leq C\frac{h_{\mathbf{x}}^2}{\nu}\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\left\{\left|\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,+}\right|^2\right\}\to 0\,.\tag{5.42}$$

The convergence

$$\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{q}}M_h\mathcal{I}_h^{\mathbf{x}}\Big\{\nabla_{\mathbf{q}}\hat{\psi}_h^{\tau,+}\cdot\nabla_{\mathbf{q}}\mathcal{I}_h^{\mathbf{xq}}\{\theta\}\Big\}\to\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{q}}\sqrt{\hat{M}}\boldsymbol{P}_5^+\cdot\nabla_{\mathbf{q}}\theta\tag{5.43}$$

follows directly from the results of Lemma 5.1 and (2.16a).

Collecting the above results yields

$$\begin{aligned}\int_{\Omega_T\times\mathfrak{D}}(\hat{M}\hat{\Psi}^0-\sqrt{\hat{M}}P_3)\partial_t\theta-\int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}P_3\mathbf{u}\cdot\nabla_{\mathbf{x}}\theta-\int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}P_3(\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}\theta\\ +\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}}\sqrt{\hat{M}}\boldsymbol{P}_4^+\cdot\nabla_{\mathbf{x}}\theta+\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{x}}\sqrt{\hat{M}}P_3\nabla_{\mathbf{x}}\mathcal{J}_\varepsilon\{\beta(\phi)\}\cdot\nabla_{\mathbf{x}}\theta\\ +\int_{\Omega_T\times\mathfrak{D}} c_{\mathbf{q}}\sqrt{\hat{M}}\boldsymbol{P}_5^+\cdot\nabla_{\mathbf{q}}\theta=0,\end{aligned}\tag{5.44}$$

for all $\theta\in C^1([0,T];C^\infty(\overline{\Omega\times\mathfrak{D}}))$ with $\theta(.,T)\equiv 0$. Arguments similar to (5.34) show that the integrals over $\mathfrak{D}\setminus D$ provide no contribution to (5.44). Recalling (5.7) and $\hat{M}\equiv M$ on D, we obtain (5.26c) as $C^\infty(\overline{\Omega\times D})$ is dense in $\hat{X}$ (*cf.* [30]).

Recalling the strong convergence of $\mathcal{Q}_h[\mathbf{w}]$ towards $\mathbf{w}$ for all $\mathbf{w}\in\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega)\cap\boldsymbol{H}^2(\Omega)$ (see (TH2)), we choose $\mathbf{w}_h=\mathcal{Q}_h[\mathbf{w}]\in\boldsymbol{W}_{h,\mathrm{div}}$ with some $\mathbf{w}\in C^\infty([0,T];C_0^\infty(\Omega)\cap\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))$ and pass to the limit in (5.3d). The convergence in the first term follows immediately from the weak* convergence of $\partial_t\mathbf{u}_h^\tau$ in $L^{4/\lambda}(0,T;(\boldsymbol{H}^1_{0,\mathrm{div}}(\Omega))')$ implied by (5.10c) and the aforementioned strong convergence of $\mathcal{Q}_h[\mathbf{w}]$. The convergence in the next four terms also follows directly from the results of Lemma 5.1 in combination with Hölder's inequality, Young's inequality, Poincaré's inequality and the Gagliardo-Nirenberg inequality. In particular, we have

$$\begin{aligned}\tfrac{1}{2}\int_\Omega\Big(\big(\nabla_{\mathbf{x}}\mathbf{u}_h^{\tau,+}\big)^T\cdot\mathcal{Q}_h[\mathbf{w}]\Big)\cdot\mathbf{u}_h^{\tau,-}-\tfrac{1}{2}\int_{\Omega_T}\Big((\nabla_{\mathbf{x}}\mathcal{Q}_h[\mathbf{w}])^T\cdot\mathbf{u}_h^{\tau,+}\Big)\cdot\mathbf{u}_h^{\tau,-}\to\int_{\Omega_T}(\mathbf{u}\cdot\nabla_{\mathbf{x}})\mathbf{u}\cdot\mathbf{w},\\ \int_{\Omega_T}2\mathcal{I}_h^{\mathbf{x}}\{\eta(\phi_h^{\tau,+})\}\mathbf{D}\mathbf{u}_h^{\tau,+}:\mathbf{D}\mathcal{Q}_h[\mathbf{w}]\to\int_{\Omega_T}2\eta(\phi)\mathbf{D}\mathbf{u}:\mathbf{D}\mathbf{w},\\ -\int_{\Omega_T}\phi_h^{\tau,-}\nabla_{\mathbf{x}}\mu_{\phi,h}^{\tau,+}\cdot\mathcal{Q}_h[\mathbf{w}]\to-\int_{\Omega_T}\phi\nabla_{\mathbf{x}}\mu_\phi\cdot\mathbf{w}\,.\end{aligned}\tag{5.45}$$

Passing to the limit in the sixth term is more technical due to the operator $\Lambda_\nu^{\mathbf{x}}[.]$. Recalling the ideas of the proof of Lemma 4.8 (in particular (4.49)–(4.51)), we dispose the projection operator $\mathcal{Q}_h$ by computing

$$\left|\int_{\Omega_T\times\mathfrak{D}} M_h(\mathcal{Q}_h[\mathbf{w}]-\mathbf{w})\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\right| \leq \left(\int_{\Omega_T\times\mathfrak{D}} M_h\left|\mathcal{Q}_h[\mathbf{w}]-\mathbf{w}\right|^2\sigma^{\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]}(\mathbf{x},\mathbf{q})\right)^{1/2}$$
$$\times\left(\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big)\cdot\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\right)^{1/2} \leq C\left\|\mathcal{Q}_h[\mathbf{w}]-\mathbf{w}\right\|_{L^2(0,T;H^1(\Omega))}\to 0\,. \tag{5.46}$$

Recycling the ideas used to establish convergence in the fifth term of (5.3c), we compute

$$\begin{aligned}&\left|\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Big(\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\Big)\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\right|\\ &\leq C\left(\nu^{-1}\int_{\Omega_T\times\mathfrak{D}} M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\Lambda_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\Big|^2\Big\}\right)^{1/2}\left(\int_{\Omega_T\times\mathfrak{D}}\nu M_h\mathcal{I}_h^{\mathbf{q}}\Big\{\Big|\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big|^2\Big\}\right)^{1/2}\to 0\end{aligned} \tag{5.47}$$

due to (A7). Therefore, replacing replacing $\Lambda_\nu^{\mathbf{x}}[.]$ by $\Xi_\nu^{\mathbf{x}}[.]$ does not change the limit. Using (2.24a) and the convergence implied by Lemma 5.1, we obtain

$$\begin{aligned}&\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mu_{\psi,h,\nu}^{\tau,+}\Big\}\\ &\qquad=\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\nabla_{\mathbf{x}}\hat{\psi}_h^{\tau,+}+\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\big\{\mathcal{J}_h\big\{\beta(\phi_h^{\tau,+})\big\}\big\}\Big\}\\ &\qquad=\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{\hat{\psi}_h^{\tau,+}\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\big\{\mathcal{J}_h\big\{\beta(\phi_h^{\tau,+})\big\}\big\}\Big\}\\ &\qquad\quad+\int_{\Omega_T\times\mathfrak{D}} M_h\mathbf{w}\cdot\mathcal{I}_h^{\mathbf{q}}\Big\{(\Xi_\nu^{\mathbf{x}}[\hat{\psi}_h^{\tau,+}]-\hat{\psi}_h^{\tau,+}\mathbb{1})\nabla_{\mathbf{x}}\mathcal{I}_h^{\mathbf{xq}}\big\{\mathcal{J}_h\big\{\beta(\phi_h^{\tau,+})\big\}\big\}\Big\}\\ &\qquad\to\int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}P_3\mathbf{w}\cdot\nabla_{\mathbf{x}}\mathcal{J}_\varepsilon\{\beta(\phi)\},\end{aligned} \tag{5.48}$$

as $\mathbf{w}$ is solenoidal. Similarly to (5.11c), we obtain the convergence $\mathcal{I}_h^{\mathbf{x}}\{\boldsymbol{\mathcal{J}}_h\{\mathcal{Q}_h[\mathbf{w}]\}\}\to\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{w}\}$ in $L^2(0,T;\boldsymbol{W}^{1,\infty}(\Omega))$ which allows us to show convergence of the last term of (5.3d) towards $\int_{\Omega_T\times\mathfrak{D}}\sqrt{\hat{M}}(\nabla_{\mathbf{x}}\mathcal{J}_h\{\mathbf{w}\}\cdot\mathbf{q})\cdot\boldsymbol{P}_5^+$. As before, we use Young's inequality to justify the restriction to $\Omega_T\times D$. The final result follows from the denseness of $C^\infty([0,T];C_0^\infty(\Omega)\cap\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))$ in $L^{4/(4-\lambda)}(0,T;\boldsymbol{H}_{0,\mathrm{div}}^1(\Omega))$. □

Remark 5.3. In [18], the existence of weak solutions with similar regularity properties was established starting from an only time-discrete scheme. The regularity properties of the marginal $\omega:=\int_D M\hat{\psi}$ established in [18] – namely $\omega\in L^\infty(0,T;L^2(\Omega))\cap L^2(0,T;H^1(\Omega))$ – may be recovered from Theorem 5.2 (*cf.* Rem. 2.2.41 in [25]).

In the presented discrete scheme, the Fokker–Planck type equation was stated on a superset of $\Omega\times D$. While passing to the limit, we restricted ourselves to the original domain $\Omega\times D$. This, however, does not violate the conservation of the number density of the polymer chains.

Corollary 5.4. *Let the assumptions of Theorem 5.2 hold true. Then*

$$\int_{\Omega\times D} M\hat{\psi}(t)=\int_{\Omega\times D} M\hat{\Psi}^0$$

holds true for almost every $t\in(0,T)$.

Proof. Combining (3.6) with the computation of $\hat{\psi}_h^0$ stated in (4.1) in (A9), we obtain

$$\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\psi}_h^{\tau,(\pm)} = \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\psi}_h^0 = \int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\Psi}^0 \tag{5.49}$$

for every $t\in(0,T)$. The strong convergence $(M_h+\mathfrak{m})\to\hat{M}$ in $L^\infty(D)$ (*cf.* Lem. 2.2) implies

$$\int_{\Omega\times\mathfrak{D}} (M_h+\mathfrak{m})\hat{\Psi}^0 \to \int_{\Omega\times\mathfrak{D}} \hat{M}\hat{\Psi}^0 = \int_{\Omega\times D} M\hat{\Psi}^0\,. \tag{5.50}$$

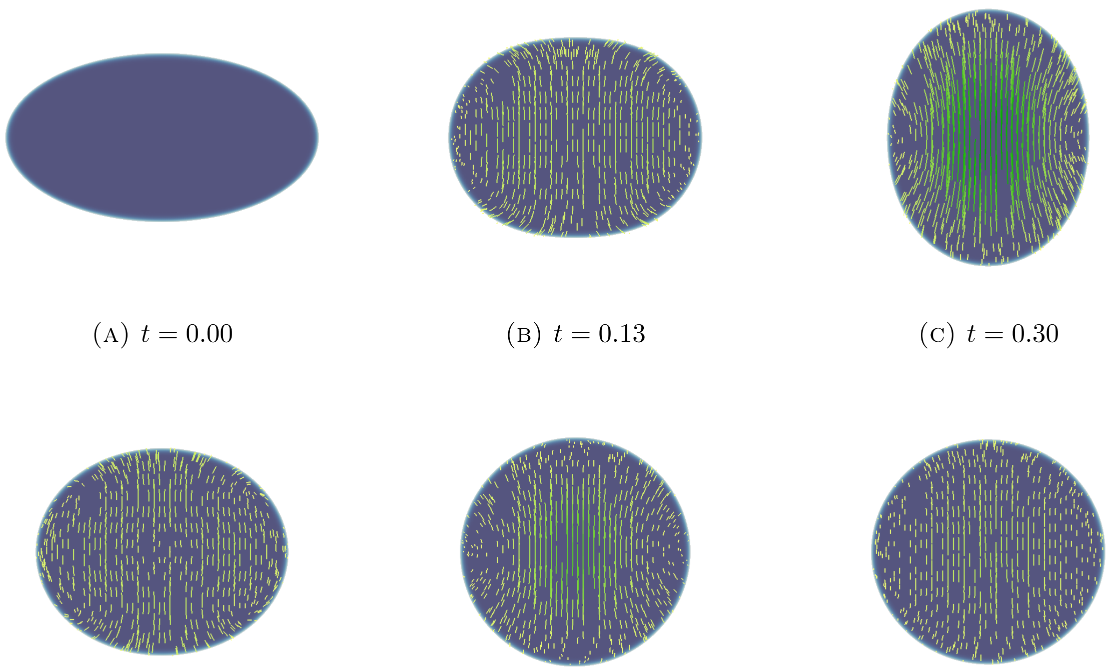
Passing to the limit on the left-hand side of (5.49) then provides the result (*cf.* [25]). □

6. Numerical simulations

For practical computations, the finite element scheme (3.4) is implemented in the framework of the inhouse code `EconDrop` which is written in `C++` (*cf.* [2, 10, 17]). As a proof of concept, we compute the oscillatory

Table 1. Parameters used in the two-dimensional setting.

σ	δ	m	$\rho\ (\pm1)$	$\eta\ (\pm1)$	$c_{\mathbf{x}}$	$c_{\mathbf{q}}$	ν	$\mathfrak{m}$	γ	$\beta\ (-1)$	$\beta\ (+1)$	ε	ϑ
10	0.01	10^{-4}	2	0.005	0.01	0.1	10^{-7}	10^{-23}	10^{-9}	5	1	0.01	1



(A) $t=0.00$ (B) $t=0.13$ (C) $t=0.30$

(D) $t=0.60$ (E) $t=0.90$ (F) $t=2.00$

Figure 1. Oscillating droplet

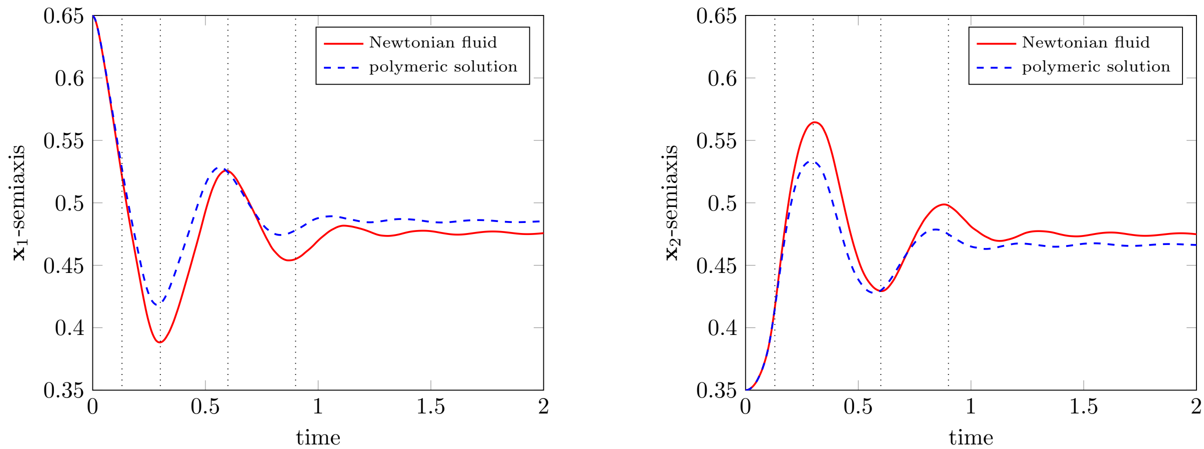


FIGURE 2. Comparison of the length of the semiaxis of oscillating droplets (vertical lines corresponding to shnapshots in Fig. 1).

TABLE 2. Parameters used in the three-dimensional setting.

σ	δ	m	ρ (±1)	η (±1)	$c_{\mathbf{x}}$	$c_{\mathbf{q}}$	ν	$\mathfrak{m}$	γ	β (±1)	τ	ε	ϑ
10	0.02	$2{\cdot}10^{-4}$	2	0.005	0.1	0.2	10^{-7}	10^{-7}	10^{-12}	0	10^{-4}	0.01	1

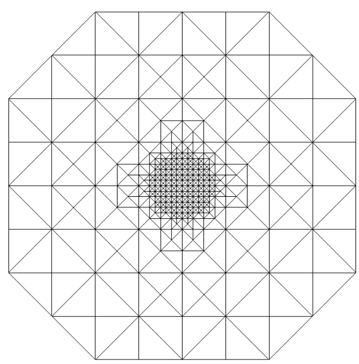


FIGURE 3. Triangulation of $\mathfrak{D}$ ($d = 2$) adapted to values of M_h.

behaviour of non-Newtonian droplets and compare these results to the behaviour of Newtonian ones. Information concerning the implementation of the discrete scheme can be found in [25]. For a more detailed investigation on the influence of the Deborah number

$$De := \frac{\text{relaxation time}}{\text{typical observation time}}, \tag{6.1}$$

which corresponds to $(2c_{\mathbf{q}})^{-1}$, and the polymer concentration, we also refer to [25].

In a first simulation, we consider a non-Newtonian droplet surrounded by a Newtonian fluid in a two-dimensional set-up, *i.e.* $\Omega \times \mathfrak{D} \subset \mathbb{R}^2 \times \mathbb{R}^2$. For this simulation, we use the following general setting. The

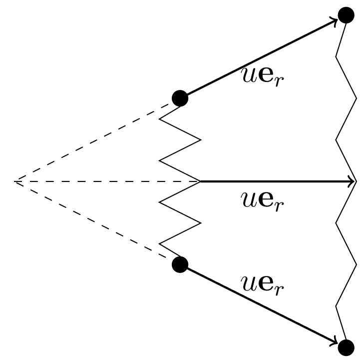


FIGURE 4. Dumbbell subjected to a radial velocity field $u\mathbf{e}_r$.

spatial domain is given as $\Omega = (-1,1)^2$ and discretized using an adaptive triangulation consisting of simplices with diameters between approximately 0.0667 and 0.0083. To evaluate the discrete mollifier which is defined according to (2.38) with $\varepsilon = 0.01$, we choose $\Omega^* = (-1-h_{\mathbf{x}}, 1+h_{\mathbf{x}})^2$ where $h_{\mathbf{x}}$ is the maximal diameter of the simplices (*i.e.* $h_{\mathbf{x}} \approx 0.0667$). Setting $Q_{\max} = 10$, we choose $\mathfrak{D}$ as $\operatorname{supp} M_h \supset D$ on the coarsest triangulation which consists of simplices with a diameter of approximately 3.5355. We refine this triangulation by means of the Maxwellian (*cf.* Fig. 3) such that the smallest simplices have a diamter of approximately 0.3125. Concerning the discretization in time, a fixed time increment $\tau = 10^{-4}$ is used.

Initially, an elliptical shaped droplet (with axes of length 1.3 and 0.7) is placed with its barycenter at $(0,0)$. This droplet, which is indicated by $\phi = 1$, is non-Newtonian and contains polymers with number density $\omega_h^0 = 3$. As the ambient liquid, indicated by $\phi = -1$, is assumed to be Newtonian, we set $\omega_h^0 \equiv 0$ outside of the droplet. Assuming that the polymer chains are in equilibrium at the beginning of the simulations, we set

$$\hat{\psi}_h^0(\mathbf{x},\mathbf{q}) := \omega_h^0(\mathbf{x}) \quad \text{which corresponds to} \quad \psi_h^0(\mathbf{x},\mathbf{q}) := M_h(\mathbf{q})\omega_h^0(\mathbf{x}). \tag{6.2}$$

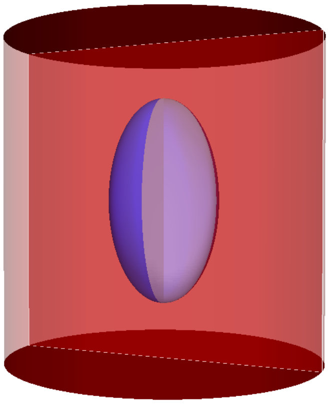
We restrict the polymers to the droplet by an appropriate β-function which interpolates between $\beta(-1) = 5$ and $\beta(1) = 1$. Concerning the double-well potential, we stick to the prototype (3.2) with $\delta' = 4 \cdot 10^{-3}$ and approximate its derivatives using

$$W_h'(a,b) := \tfrac{1}{4}\left(a^3 + a^2 b + a b^2 + b^3\right) - \tfrac{1}{2}(a+b) + \tfrac{1}{\delta'}\,\tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=a} \max\left\{|s|-1, 0\right\}^2. \tag{6.3}$$

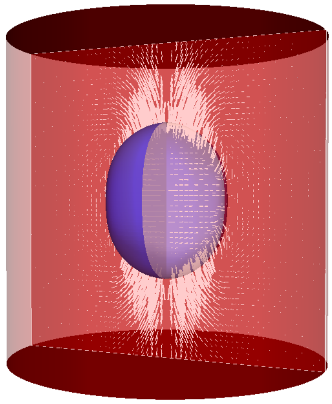
The remaining parameters are chosen according to Table 1.

The elliptical shaped droplet tries to attain its energetically optimal, circular shape and starts to contract giving rise to a velocity field. We are interested in the arising non-Newtonian effects – *i.e.* in the arising changes in the polymer configuration and the resulting additional stresses – and in their impact on the rheological behaviour of the droplet. Figure 1 shows the evolution of the non-Newtonian droplet. To illustrate occuring additional stresses, we computed the Kramers tensor $\int_{\mathfrak{D}} M_h \nabla_{\mathbf{q}} \hat{\psi} \otimes \mathbf{q}$ and, if its eigenvalues are real, its eigenvectors and eigenvalues on each $\kappa_{\mathbf{x}} \in \mathcal{T}_h^{\mathbf{x}}$. The eigenvectors to the largest eigenvalue of these tensors are depicted in Figure 1 as yellow and green lines. While the droplet oscillates, the polymer chains build up stresses in mainly vertical direction. To analyze the impact of those stresses, we measure the $\mathbf{x}_1$- and $\mathbf{x}_2$-semiaxis of the droplet and compare them to the ones of a Newtonian droplet.

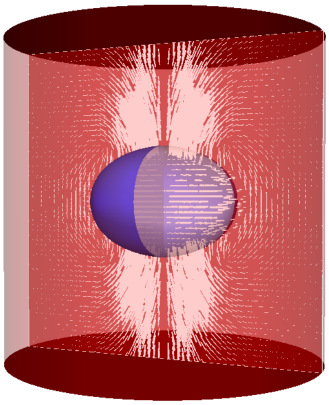
Figure 2 shows that the oscillation is damped in both cases. Comparing the evolution of the length of the semiaxes, we notice that the oscillation of the non-Newtonian droplet is damped asymmetrically: While the elongation of the $\mathbf{x}_2$-axis (and the contraction of the $\mathbf{x}_1$-axis) of the droplet is significantly more damped in the non-Newtonian case, the amplitudes of the second oscillation are almost identical. This phenomenon can be explained as follows. As the polymer chains are initially in equilibrium, *i.e.* the distribution of their



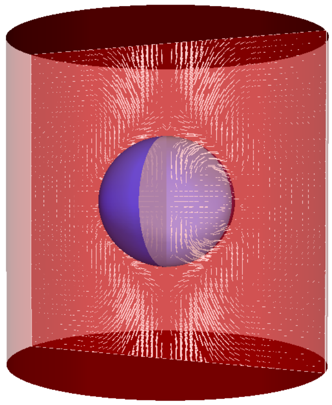
(A) $t = 0.00$



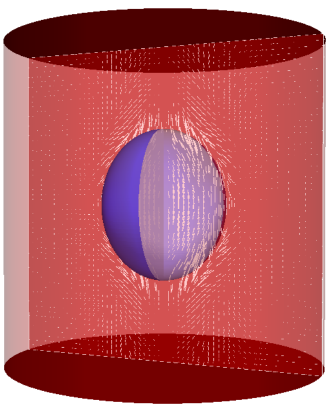
(B) $t = 0.10$



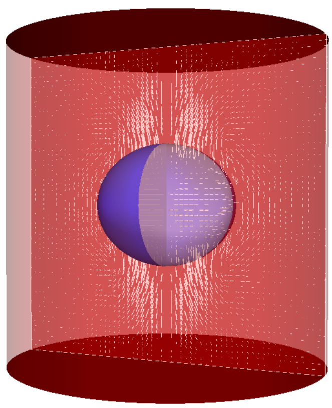
(C) $t = 0.20$



(D) $t = 0.30$



(E) $t = 0.45$



(F) $t = 0.60$

FIGURE 5. Rotationally symmetric, oscillating droplet.

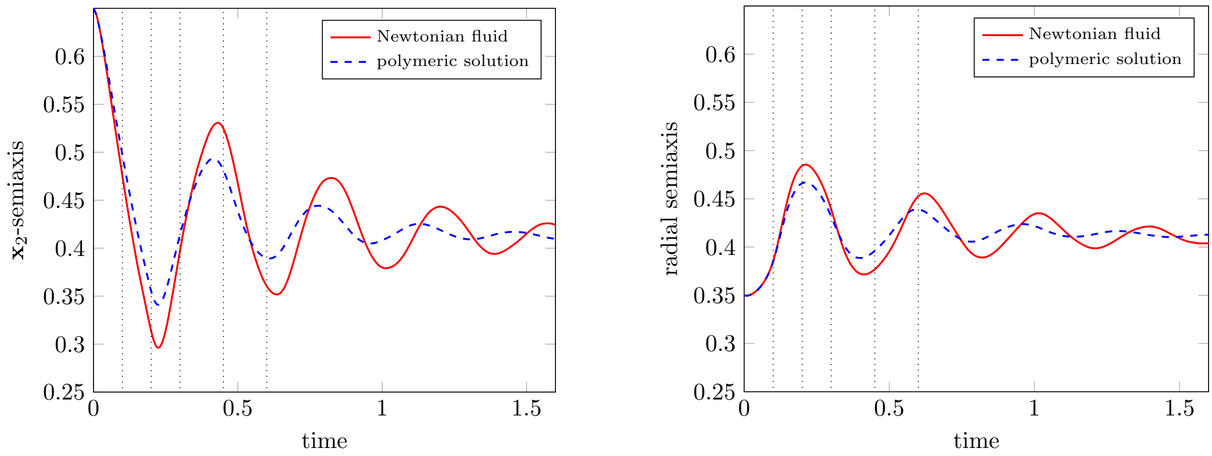


FIGURE 6. Comparison of the length of the semiaxis of oscillating droplets (vertical lines corresponding to shnapshots in Fig. 5).

configurational density is aligned to the Maxwellian, the first oscillation stretches the polymer chains in $\mathbf{x}_2$-direction (*i.e.* vertically). This deflection from equilibrium slows down the oscillation. When swinging back, the oscillation is supported by the polymer chains as it reduces their deviation from their preferred state.

On the long run, both droplets seem to attain a stationary state. Nevertheless, the non-Newtonian one does not attain a perfectly circular shape, but stays slightly elliptical. As Figure 1f shows, there remain still vertical stresses inside of the droplet, which are not dissipated fast enough and therefore still influence the shape of the droplet.

In the second scenario, we consider a non-Newtonian droplet surrounded by an also non-Newtonian fluid. To underline the practicality of the presented scheme, we consider a three-dimensional, rotationally symmetric set-up. We place an ellipsoidal shaped, rotationally symmetric droplet with barycenter at $(0, 0, 0)$ in the rotationally symmetric, cylindrical domain $\Omega := \{\mathbf{x} \in \mathbb{R}^3 : -1 < \mathbf{x}_2 < 1, \mathbf{x}_1^2 + \mathbf{x}_3^2 < 1\}$. The longest principal axis points in $\mathbf{x}_2$-direction and has length 1.3. The other principal axes are of length 0.7. We parameterize the spatial domain using cylindrical coordinates, *i.e.* it suffices to compute the spatial quantities on a two-dimensional domain $(0, 1) \times (-1, 1)$ which we discretize using triangles with diameters between approximately 0.0471 and 0.0118. Specifying $Q_{\max} = 10$, we set $\mathfrak{D} := (-10, 10)^3$. Adapting the triangulation of $\mathfrak{D}$ to the values of the Maxwellian, we end up with tetrahedrons with diameters between approximately 3.536 and 0.442. In contrast to the last scenario, we consider a two-phase flow consisting of two dilute polymeric solutions. Assuming that the polymer chains are equally soluble in both phases and that the polymer chains are initially in equilibrium, we set $\beta \equiv 0$ and $\hat{\psi}_h^0 \equiv 1$. Similarly to the two-dimensional setting, we use the penalized, polynomial double-well potential introduced in (3.2) with $\delta' = 4 \cdot 10^{-3}$ and approximate its derivatives using (6.3). The remaining parameters are specified in Table 2.

Figure 5 shows the evolution of the droplet. Again, the eigenvectors and eigenvalues of the additional stress tensor are computed. For better readability, we depict the eigenvectors to positive eigenvalues (white lines) of the additional stress tensor only in a cross section of Ω. Although we assumed rotational symmetry, the additional stresses still span a three-dimensional space. In particular, stresses perpendicular to the cross section appear in Figures 5b and 5c on the inside of the droplet, as the radial component of the velocity field may induce elongation of polymer chains in azimuthal direction (*cf.* Fig. 4).

Similar to the first scenario, we compare the evolution of the semiaxes for the case of dilute polymeric solutions and pure Newtonian fluids. As depicted in Figure 6, the oscillation is more damped in the non-Newtonian case than in the Newtonian one. As the Deborah number is chosen larger and the polymer concentration is chosen smaller than in the two-dimensional setting, the additional stresses caused by the polymer chains dissipate faster and have less impact on the evolution of the droplet. Consequently, the damping is not as asymmetric as in the first scenario.

Appendix A. Proofs of Section 2

Proof of Lemma 2.2. (P3) provides $c_3[\mathrm{dist}\,(\mathbf{q},\partial D)]^\kappa \leq M(\mathbf{q}) \leq c_4[\mathrm{dist}\,(\mathbf{q},\partial D)]^\kappa$ on D with $\kappa>1$ implying the continuity of $\hat{M}$. Recalling the definition of the Maxwellian (see (1.3)), we compute for $\mathbf{q}$-derivatives on D

$$\begin{aligned}\left|\partial_{\mathbf{q}_i} M\right| &= C\left|\exp\left(-U(\tfrac{1}{2}\left|\mathbf{q}\right|^2)\right)U'(\tfrac{1}{2}\left|\mathbf{q}\right|^2)\mathbf{q}_i\right| \\ &\leq C\left|M(\mathbf{q})U'(\tfrac{1}{2}\left|\mathbf{q}\right|^2)\right| \leq C[\mathrm{dist}\,(\mathbf{q},\partial D)]^{\kappa-1} \to 0 \end{aligned} \tag{A.1}$$

as $\mathbf{q}\to\partial D$, for $i=1,\dots,d$. Noting $\hat{M}\equiv 0$ on $\mathfrak{D}\setminus D$, we have $\hat{M}\in C^1\left(\overline{\mathfrak{D}}\right)$ with $\hat{M}\Big|_{\partial\mathfrak{D}}=0$.
Due to $\int_{\mathfrak{D}}\mathcal{I}_h^{\mathbf{q}}\{\hat{M}\}\,\mathrm{d}\mathbf{q} \leq |\mathfrak{D}|\max_{\mathbf{q}\in\mathfrak{D}}\hat{M}(\mathbf{q}) \leq C$, there is a constant $c_M>0$ independent of $h_{\mathbf{q}}$ such that $c_{h_{\mathbf{q}}}\geq c_M$.
Noting $\hat{M}\in C^1\left(\overline{\mathfrak{D}}\right)$ and applying standard bounds for the interpolation error (*cf.* [9]), we infer

$$\begin{aligned}1-\int_{\mathfrak{D}}\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}\mathrm{d}\mathbf{q} \leq \left|\int_{\mathfrak{D}}\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}\mathrm{d}\mathbf{q}-1\right| &= \left|\int_{\mathfrak{D}}\left(\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right)\mathrm{d}\mathbf{q}\right| \\ &\leq C\left\|\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right\|_{L^\infty(\mathfrak{D})} \leq Ch_{\mathbf{q}}\left|\hat{M}\right|_{W^{1,\infty}(\mathfrak{D})} \leq Ch_{\mathbf{q}}, \end{aligned} \tag{A.2}$$

which implies $c_{h_{\mathbf{q}}} \leq \frac{1}{1-Ch_{\mathbf{q}}} \leq C$ for $h_{\mathbf{q}}$ small enough. Computing

$$\begin{aligned}\left\|M_h-\hat{M}\right\|_{L^\infty(\mathfrak{D})} &= \left\|c_{h_{\mathbf{q}}}\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right\|_{L^\infty(\mathfrak{D})} \\ &\leq c_{h_{\mathbf{q}}}\left\|\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right\|_{L^\infty(\mathfrak{D})} + \left\|\hat{M}\right\|_{L^\infty(\mathfrak{D})} c_{h_{\mathbf{q}}}\left|c_{h_{\mathbf{q}}}^{-1}-1\right| \\ &\leq c_{h_{\mathbf{q}}}\left\|\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right\|_{L^\infty(\mathfrak{D})} + \left\|\hat{M}\right\|_{L^\infty(\mathfrak{D})} c_{h_{\mathbf{q}}}\left|\int_{\mathfrak{D}}\left(\mathcal{I}_h^{\mathbf{q}}\left\{\hat{M}\right\}-\hat{M}\right)\right|. \end{aligned} \tag{A.3}$$

and applying (A.2) completes the proof. □

Proof of Lemma 2.3. As $\hat{\theta}_h,\tilde{\theta}_h\in\hat{X}_h$, $\nabla_{\mathbf{q}}\hat{\theta}_h$ and $\nabla_{\mathbf{q}}\tilde{\theta}_h$ are constant on $\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}$ with respect to $\mathbf{q}$ and $\nabla_{\mathbf{x}}\hat{\theta}_h$ and $\nabla_{\mathbf{x}}\tilde{\theta}_h$ are constant on $\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}$ with respect to $\mathbf{x}$. We use $\|\mathcal{I}_h^{\mathbf{x}}\{g_{\mathbf{x}}\}-g_{\mathbf{x}}\|_{L^\infty(\kappa_{\mathbf{x}})} \leq Ch_{\mathbf{x}}^2\left|g_{\mathbf{x}}\right|_{W^{2,\infty}(\kappa_{\mathbf{x}})}$ for $g_{\mathbf{x}}\in W^{2,\infty}(\kappa_{\mathbf{x}})$ (*cf.* [9]) to compute

$$\begin{aligned}&\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}}\left|M_h(I-\mathcal{I}_h^{\mathbf{x}})\left\{\nabla_{\mathbf{q}}\hat{\theta}_h\cdot\nabla_{\mathbf{q}}\tilde{\theta}_h\right\}\right|\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x} \\ &\leq \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}}M_h\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)\left\|(I-\mathcal{I}_h^{\mathbf{x}})\left\{\nabla_{\mathbf{q}}\hat{\theta}_h\cdot\nabla_{\mathbf{q}}\tilde{\theta}_h\right\}\right\|_{L^\infty(\kappa_{\mathbf{x}})} \\ &\leq Ch_{\mathbf{x}}^2\left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}}M_h\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)\left|\nabla_{\mathbf{q}}\hat{\theta}_h\cdot\nabla_{\mathbf{q}}\tilde{\theta}_h\right|_{W^{2,\infty}(\kappa_{\mathbf{x}})} \\ &\leq Ch_{\mathbf{x}}^2\left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}}M_h\,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)\sum_{i,j,k=1}^{d}\left|\partial_{\mathbf{x}_j}\partial_{\mathbf{q}_i}\hat{\theta}_h\partial_{\mathbf{x}_k}\partial_{\mathbf{q}_i}\tilde{\theta}_h\right| \end{aligned} \tag{A.4}$$

as $\hat{\theta}_h, \tilde{\theta}_h \in \hat{X}_h$and $\partial_{\mathbf{x}_i}\partial_{\mathbf{x}_j}\hat{\theta}_h = \partial_{\mathbf{x}_i}\partial_{\mathbf{x}_j}\tilde{\theta}_h = 0$ $(i, j = 1, \ldots, d)$. Since $\partial_{\mathbf{x}_j}\partial_{\mathbf{q}_i}\hat{\theta}_h$ and $\partial_{\mathbf{x}_j}\partial_{\mathbf{q}_i}\tilde{\theta}_h$ are constant on $\kappa_{\mathbf{x}} \times \kappa_{\mathbf{q}}$ for $i, j = 1, \ldots, d$, we obtain that the right-hand side of (A.4) is bounded by

$$Ch_{\mathbf{x}}^2 \sum_{i,j,k=1}^{d} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\partial_{\mathbf{x}_j}\partial_{\mathbf{q}_i}\hat{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\partial_{\mathbf{x}_k}\partial_{\mathbf{q}_i}\tilde{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2}. \quad \text{(A.5)}$$

We apply (2.13c) to the first integral in (A.5) and obtain

$$\begin{aligned} \sum_{i,j=1}^{d} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\partial_{\mathbf{x}_j}\partial_{\mathbf{q}_i}\hat{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2} &\leq C \sum_{i=1}^{d} \left(\int_{\kappa_{\mathbf{q}}} M_h \int_{\kappa_{\mathbf{x}}} \left|\nabla_{\mathbf{x}}(\partial_{\mathbf{q}_i}\hat{\theta}_h)\right|^2 \, \mathrm{d}\mathbf{x}\, \mathrm{d}\mathbf{q} \right)^{1/2} \\ &\leq Ch_{\mathbf{x}}^{-1} \sum_{i=1}^{d} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\partial_{\mathbf{q}_i}\hat{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2} \leq Ch_{\mathbf{x}}^{-1} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\hat{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2}, \end{aligned} \quad \text{(A.6)}$$

which yields (2.16a). Analogous computations provide a bound similar to (A.5) for the left-hand side of (2.16b) with $h_{\mathbf{x}}$ substituted by $h_{\mathbf{q}}$. We apply (A.6) to the first integral and use $\frac{h_{\mathbf{q}}}{h_{\mathbf{x}}} \leq C$ (*cf.* (2.1)) to complete the proof of (2.16b).

To prove the last inequality, we use that the left-hand side of (2.16c) is bounded by

$$\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \left| M_h (I - \mathcal{I}_h^{\mathbf{x}}) \left\{ \hat{\theta}_h \tilde{\theta}_h \right\} \right| \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} + \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} \left| M_h (I - \mathcal{I}_h^{\mathbf{q}}) \left\{ \mathcal{I}_h^{\mathbf{x}} \left\{ \hat{\theta}_h \tilde{\theta}_h \right\} \right\} \right| \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \quad =: I + II. \quad \text{(A.7)}$$

As before, we use that $\hat{\theta}_h$ and $\tilde{\theta}_h$ are affine linear with respect to $\mathbf{x}$ on $\kappa_{\mathbf{x}}$ and compute

$$\begin{aligned} I &\leq \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left\| (I - \mathcal{I}_h^{\mathbf{x}}) \left\{ \hat{\theta}_h \tilde{\theta}_h \right\} \right\|_{L^\infty(\kappa_{\mathbf{x}})} \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \leq Ch_{\mathbf{x}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left| \hat{\theta}_h \tilde{\theta}_h \right|_{W^{2,\infty}(\kappa_{\mathbf{x}})} \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \\ &\leq Ch_{\mathbf{x}}^2 \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \sum_{i,j=1}^{d} \left| \partial_{\mathbf{x}_i}\hat{\theta}_h \partial_{\mathbf{x}_j}\tilde{\theta}_h \right| \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \\ &\leq Ch_{\mathbf{x}}^2 \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{x}}\hat{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{x}}\tilde{\theta}_h\right|^2 \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right)^{1/2} \end{aligned} \quad \text{(A.8)}$$

and

$$\begin{aligned} II &\leq \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right) \left\| (I - \mathcal{I}_h^{\mathbf{q}}) \left\{ \mathcal{I}_h^{\mathbf{x}} \left\{ \hat{\theta}_h \tilde{\theta}_h \right\} \right\} \right\|_{L^\infty(\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}})} \\ &\leq Ch_{\mathbf{q}}^2 \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \, \mathrm{d}\mathbf{q}\, \mathrm{d}\mathbf{x} \right) \left\| \nabla_{\mathbf{q}}\hat{\theta}_h \right\|_{L^\infty(\kappa_{\mathbf{x}})} \left\| \nabla_{\mathbf{q}}\tilde{\theta}_h \right\|_{L^\infty(\kappa_{\mathbf{x}})}. \end{aligned} \quad \text{(A.9)}$$

As $\nabla_{\mathbf{q}}\hat{\theta}_h$ and $\nabla_{\mathbf{q}}\tilde{\theta}_h$ are affine linear with respect to $\mathbf{x}$, they will attain their maximum in one of the vertices of $\kappa_{\mathbf{x}}$, which are denoted by $\{\mathbf{P}_{\kappa_{\mathbf{x}},i}\}_{i=0,\dots,d}$. Therefore, we may compute

$$\begin{aligned}
&\left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right) \left\|\nabla_{\mathbf{q}}\hat{\theta}_h\right\|_{L^\infty(\kappa_{\mathbf{x}})} \left\|\nabla_{\mathbf{q}}\tilde{\theta}_h\right\|_{L^\infty(\kappa_{\mathbf{x}})} \\
&\leq \int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \sum_{i=0}^{d} \left|\nabla_{\mathbf{q}}\hat{\theta}_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q})\right| \sum_{j=0}^{d} \left|\nabla_{\mathbf{q}}\tilde{\theta}_h(\mathbf{P}_{\kappa_{\mathbf{x}},j},\mathbf{q})\right| \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x} \\
&\leq \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left(\sum_{i=0}^{d} \left|\nabla_{\mathbf{q}}\hat{\theta}_h(\mathbf{P}_{\kappa_{\mathbf{x}},i},\mathbf{q})\right|\right)^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \\
&\leq C\left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\hat{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2} \left(\int_{\kappa_{\mathbf{x}}\times\kappa_{\mathbf{q}}} M_h \left|\nabla_{\mathbf{q}}\tilde{\theta}_h\right|^2 \,\mathrm{d}\mathbf{q}\,\mathrm{d}\mathbf{x}\right)^{1/2}.
\end{aligned} \tag{A.10}$$

Combining (A.7)–(A.10) yields (2.16c). ☐

Appendix B. Miscellaneous

Lemma B.1. *Let ϕ, $\hat{\psi}$, and $\mathbf{u}$ satisfy (1.5) on a formal level. Then the energy $\mathcal{E}$ defined in (1.7) satisfies*

$$\begin{aligned}
&\mathcal{E}(\phi,\hat{\psi},\mathbf{u})\Big|_{t=T} + \int_{\Omega_T\times D} M\hat{\psi}\left|\nabla_{\mathbf{q}} g'(\hat{\psi})\right|^2 + \int_{\Omega_T\times D} M\hat{\psi}\left|\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\right|^2 \\
&\quad + \int_{\Omega_T} |\nabla_{\mathbf{x}}\mu_\phi|^2 + \int_{\Omega_T} 2\eta(\phi)\,|\mathbf{D}\mathbf{u}|^2 = \mathcal{E}(\phi,\hat{\psi},\mathbf{u})\Big|_{t=0},
\end{aligned} \tag{B.1}$$

for all $T \geq 0$ In particular, we have $\mathcal{E}(\phi,\hat{\psi},\mathbf{u})\Big|_{t=T} \leq \mathcal{E}(\phi,\hat{\psi},\mathbf{u})\Big|_{t=0}$.

Proof. Testing (1.5a) by μ_ϕ and (1.5b) by $\partial_t\phi$ and integrating by parts yields

$$\int_\Omega \partial_t\phi\mu_\phi - \int_\Omega \phi\mathbf{u}\cdot\nabla_{\mathbf{x}}\mu_\phi + \int_\Omega |\nabla_{\mathbf{x}}\mu_\phi|^2 = 0, \tag{B.2}$$

$$\int_\Omega \partial_t\phi\mu_\phi = \int_\Omega \tfrac{1}{2}\partial_t\,|\nabla_{\mathbf{x}}\phi|^2 + \int_\Omega \partial_t W(\phi) + \int_{\Omega\times D} \mathcal{J}_\varepsilon\{\partial_t\beta(\phi)\}M\hat{\psi}\,. \tag{B.3}$$

In the next step, we test (1.5c) by the chemical potential $(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\})$. Using the identity $\hat{\psi}\nabla_{\mathbf{q}} g'(\hat{\psi}) = \nabla_{\mathbf{q}}\hat{\psi}$ and the fact that $\mathcal{J}_\varepsilon\{\beta(\phi)\}$ is independent of $\mathbf{q}$, we obtain

$$\begin{aligned}
&\int_{\Omega\times D} M\partial_t g(\hat{\psi}) + \int_{\Omega\times D} \mathcal{J}_\varepsilon\{\beta(\phi)\}\partial_t\hat{\psi} - \int_{\Omega\times D} M\hat{\psi}\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\cdot\mathbf{u} \\
&\quad - \int_{\Omega\times D} M(\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}\hat{\psi} + \int_{\Omega\times D} c_{\mathbf{q}} M\hat{\psi}\left|\nabla_{\mathbf{q}} g'(\hat{\psi})\right|^2 + \int_{\Omega\times D} c_{\mathbf{x}} M\hat{\psi}\left|\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\right|^2 = 0 \\
&.
\end{aligned} \tag{B.4}$$

Testing (1.5d) by $\mathbf{u}$ and integrating by parts with respect to $\mathbf{x}$, we obtain

$$\begin{aligned}
&\int_\Omega \tfrac{1}{2}\rho(\phi)\partial_t\,|\mathbf{u}|^2 + \int_\Omega \tfrac{1}{2}\rho(\phi)\mathbf{u}\cdot\nabla_{\mathbf{x}}\,|\mathbf{u}|^2 - \int_\Omega \tfrac{1}{2}\rho'(\phi)m(\phi)\nabla_{\mathbf{x}}\mu_\phi\cdot\nabla_{\mathbf{x}}\,|\mathbf{u}|^2 + \int_\Omega 2\eta(\phi)\,|\mathbf{D}\mathbf{u}|^2 \\
&= -\int_\Omega \phi\nabla_{\mathbf{x}}\mu_\phi\cdot\mathbf{u} - \int_{\Omega\times D} M\hat{\psi}\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\cdot\mathbf{u} - \int_{\Omega\times D} M(\nabla_{\mathbf{x}}\boldsymbol{\mathcal{J}}_\varepsilon\{\mathbf{u}\}\cdot\mathbf{q})\cdot\nabla_{\mathbf{q}}\hat{\psi}\,.
\end{aligned} \tag{B.5}$$

In order to get rid of the second and third term in (B.5), we additionally test (1.5a) by $\frac{1}{2}\rho'(\phi)\left|\mathbf{u}\right|^2$. Using the fact that ρ' is constant and that the convection terms in (B.2) and (B.4) reappear on the right-hand side of (B.5), we add the equations above and end up with

$$\int_{\Omega\times D} M\partial_t g(\hat{\psi}) + \int_{\Omega\times D} M\partial_t\Big(\mathcal{J}_\varepsilon\{\beta(\phi)\}\hat{\psi}\Big) + \int_\Omega \tfrac{1}{2}\partial_t\left|\nabla_{\mathbf{x}}\phi\right|^2 + \int_\Omega \partial_t W(\phi) + \int_\Omega \tfrac{1}{2}\partial_t\left|\mathbf{u}\right|^2 + \int_{\Omega\times D} M\hat{\psi}\left|\nabla_{\mathbf{q}} g'(\hat{\psi})\right|^2 + \int_{\Omega\times D} M\hat{\psi}\left|\nabla_{\mathbf{x}}\Big(g'(\hat{\psi}) + \mathcal{J}_\varepsilon\{\beta(\phi)\}\Big)\right|^2 + \int_\Omega \left|\nabla_{\mathbf{x}}\mu_\phi\right|^2 + \int_\Omega 2\eta(\phi)\left|\mathbf{D}\mathbf{u}\right|^2 = 0 \quad . \tag{B.6}$$

As M is time-independent an integration with respect to time yields (B.1). □

For the reader's convenience, we cite a compactness result by Azérad and Guillén (*cf.* [4]).

Lemma B.2. *Let $T>0$, and let the Banach spaces $\mathbf{X} \overset{compact}{\hookrightarrow} \mathbf{B} \hookrightarrow \mathbf{Y}$. Let $(f_\epsilon)_{\epsilon>0}$ be a family of functions of $L^p(0,T;\mathbf{X})$, $1\le p\le\infty$, with the extra condition $(f_\epsilon)_{\epsilon>0}\subset C(0,T;\mathbf{Y})$ if $p=\infty$, such that*

- *$(f_\epsilon)_{\epsilon>0}$ is bounded in $L^p(0,T;\mathbf{X})$,*
- *$\|f_\epsilon(\cdot+\tau)-f_\epsilon(\cdot)\|_{L^p(0,T-\tau;\mathbf{Y})}\le\varphi(\tau)+\psi(\epsilon)$ with $\lim_{\tau\to0}\varphi(\tau)=0=\lim_{\epsilon\to0}\psi(\epsilon)$.*

Then the family $(f_\epsilon)_{\epsilon>0}$ posses a cluster point in $L^p(0,T;\mathbf{B})$ and also in $C(0,T;\mathbf{B})$ if $p=\infty$, as $\epsilon\to0$.

Acknowledgements. This research has been supported by Deutsche Forschungsgemeinschaft (German Science Foundation) through the Priority Programme 1506 "Transport processes at fluidic interfaces".

References

[1] H. Abels, H. Garcke and G. Grün, Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Math. Models Methods Appl. Sci.* **22** (2012) 1150013.

[2] S. Aland, S. Boden, A. Hahn, F. Klingbeil, M. Weismann and S. Weller, Quantitative comparison of Taylor flow simulations based on sharp-interface and diffuse-interface models. *Int. J. Numer. Methods Fluids* **73** (2013) 344–361.

[3] F. Armero and J.C. Simo, Formulation of a new class of fractional-step methods for the incompressible MHD equations that retains the long-term dissipativity of the continuum dynamical system. *Fields Inst. Commun.* **10** (1996) 1–24.

[4] P. Azêrad and F. Guilln, Mathematical justification of the hydrostatic approximation in the primitive equations of geophysical fluid dynamics. *SIAM J. Math. Anal.* **33** (2001) 847–859.

[5] J.W. Barrett and E. Süli, Existence of global weak solutions to some regularized kinetic models for dilute polymers. *Multiscale Model. Simul.* **6** (2007) 506–546.

[6] J.W. Barrett and E. Süli, Existence and equilibration of global weak solutions to kinetic models for dilute polymers. I: Finitely extensible nonlinear bead-spring chains. *M3AS* **21** (2011) 1211–1289.

[7] J.W. Barrett and E. Süli, Finite element approximation of kinetic dilute polymer models with microscopic cut-off. *ESAIM: M2AN* **45** (2011) 39–89.

[8] J.W. Barrett and E. Süli, Finite element approximation of finitely extensible nonlinear elastic dumbbell models for dilute polymers. *ESAIM: M2AN* **46** (2012) 949–978.

[9] S.C. Brenner and L.R. Scott, The mathematical theory of finite element methods. Springer (2002).

[10] E. Campillo-Funollet, G. Grün and F. Klingbeil, On modeling and simulation of electrokinetic phenomena in two-phase flow with general mass densities. *SIAM J. App. Math.* **72** (2012) 1899–1925.

[11] Ph.G. Ciarlet, The finite element method for elliptic problems. North-Holland (1978).

[12] M. Dauge, Stationary stokes and Navier–Stokes systems on two- or three-dimensional domains with corners. Part I. Linearized equations. *SIAM J. Math. Anal.* **20** (1989) 74–97.

[13] F.M. Guillén-González and J.V. Gutiérrez-Santacreu, A linear mixed finite element scheme for a nematic ericksenleslie liquid crystal model. *ESAIM: M2AN* **47** (2013) 1433–1464.

[14] V. Girault and P. Raviard, Finite element methods for Navier–Stokes equations. In Vol. 5 of *Springer Series in Computational Mathematics.* Springer (1986).

[15] G. Grün, On convergent schemes for diffuse interface models for two-phase flow of incompressible fluids with general mass densities. *SIAM J. Numer. Anal.* **51** (2013) 3036–3061.

[16] G. Grün, F. Guillén-González and S. Metzger, On fully decoupled, convergent schemes for diffuse interface models for two-phase flow with general mass densities. *CiCP* **19** (2016) 1473–1502.

[17] G. Grün and F. Klingbeil, Two-phase flow with mass density contrast: stable schemes for a thermodynamic consistent and frame-indifferent diffuse-interface model. *J. Comput. Phys.* **257** Part A (2014) 708–725.

[18] G. Grün and S. Metzger, On micro-macro-models for two-phase flow with dilute polymeric solutions – modeling and analysis. *Math. Model. Methods Appl. Sci.* **26** (2016), 823–866.

[19] G. Grün and M. Rumpf, Nonnegativity preserving convergent schemes for the thin film equation. *Numer. Math* **87** (2000) 113–152.

[20] F. Guillén-González and G. Tierra, Splitting schemes for a Navier–Stokes–Cahn–Hilliard model for two fluids with different densities. *J. Comput. Math.* **32** (2014) 643–664.

[21] J.G. Heywood and R. Rannacher, Finite element approximation of the nonstationary Navier–Stokes problem. I. Regularity of solutions and second-order error estimates for spatial discretization. *SIAM J. Numer. Anal.* **19** (1982) 275–311.

[22] C. Le Bris and T. Lelièvre, Multiscale modelling of complex fluids: a mathematical initiation, in Multiscale modeling and simulation in science, edited by B. Engquist, P. Lötstedt and O. Runborg. In Vol. 66 of *Lecture Notes in Computational Science and Engineering.* Springer (2009) 49–137.

[23] N. Masmoudi, Well-posedness for the fene dumbbell model of polymeric flows. *Commun. Pure Appl. Math.* **61** (2008) 1685–1714.

[24] N. Masmoudi, Global existence of weak solutions to the FENE dumbbell model of polymeric flows. *Invent. Math.* **191** (2013) 427–500.

[25] S. Metzger, *Diffuse interface models for complex flow scenarios: modeling, analysis and simulations*. Ph.D. thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg (2017).

[26] S. Minjeaud, An unconditionally stable uncoupled scheme for a triphasic Cahn–Hilliard/Navier-Stokes model. *Numer Methods Partial Differ Equ.* **29** (2013) 584–618.

[27] J. Simon, Compact sets in the space $L^p(0,T;B)$. *Ann. Mat. Pura Appl.* (IV) **146** (1987) 65–96.

[28] R. Temam, Navier–Stokes equations: theory and numerical analysis. Reprint. with corr. AMS Chelsea Publ. (2001).

[29] V. Thomée, Galerkin finite element methods for parabolic problems. Springer (1984).

[30] H. Triebel, Interpolation theory, function spaces, differential operators. North-Holland Publ. (1978).

[31] H. Werner and H. Arndt, Gewöhnliche Differentialgleichungen. Springer Verlag (1991).