



Nematic–Isotropic Phase Transition in Liquid Crystals: A Variational Derivation of Effective Geometric Motions

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Abstract

In this work, we study the nematic–isotropic phase transition based on the dynamics of the Landau–De Gennes theory of liquid crystals. At the critical temperature, the Landau–De Gennes bulk potential favors the isotropic phase and nematic phase equally. When the elastic coefficient is much smaller than that of the bulk potential, a scaling limit can be derived by formal asymptotic expansions: the solution gradient concentrates on a closed surface evolving by mean curvature flow. Moreover, on one side of the surface the solution tends to the nematic phase which is governed by the harmonic map heat flow into the sphere while on the other side, it tends to the isotropic phase. To rigorously justify such a scaling limit, we prove a convergence result by combining weak convergence methods and the modulated energy method. Our proof applies as long as the limiting mean curvature flow remains smooth.

1. Introduction

Nematic liquid crystals react to shear stress like a conventional liquid while the molecules are oriented in a crystal-like way. One of the successful continuum theories modeling nematic liquid crystals is the Q -tensor theory, also referred to as Landau–De Gennes theory, which uses a 3×3 traceless and symmetric matrix-valued function $Q(x)$ as order parameter to characterize the orientation of molecules near a material point x (cf. [8]). The matrix Q , also called Q -tensor, can be interpreted as the second moment of a number density function

$$Q(x) = \int_{\mathbb{S}^2} (p \otimes p - \frac{1}{3}I_3) f(x, p) dp, \quad (1.1)$$

where $f(x, p)$ corresponds to the number density of liquid crystal molecules which orient along the direction $p \in \mathbb{S}^2$ near the material point x (cf. [5]). The configura-

tion space of the Q -tensor is the 5-dimensional linear space

$$Q = \{Q \in \mathbb{R}^{3 \times 3} \mid Q = Q^T, \operatorname{tr} Q = 0\}. \tag{1.2}$$

By elementary linear algebra, each such Q can be written as

$$Q = s \left(u \otimes u - \frac{1}{3} I_3 \right) + t \left(v \otimes v - \frac{1}{3} I_3 \right) \tag{1.3}$$

for some $s, t \in \mathbb{R}$ and $u, v \in \mathbb{S}^2$ which are perpendicular. In the physics literature, for instance De Gennes–Prost [8], such a representation is called the biaxial nematic configurations, cf. [23]. In case Q has repeated eigenvalues, it is called uniaxial. These Q 's form a 3-dimensional manifold in \mathcal{Q} , denoted by

$$\mathcal{U} := \left\{ Q \in \mathcal{Q} \mid Q = s \left(u \otimes u - \frac{1}{3} I_3 \right) \text{ for some } s \in \mathbb{R} \text{ and } u \in \mathbb{S}^2 \right\}, \tag{1.4}$$

with a conical singularity at $s = 0$. Here the parameter s is called the degree of orientation. To study static configurations of the liquid crystal material in a physical domain Ω , a natural approach is to consider the Ginzburg–Landau type energy

$$E_\varepsilon(Q) = \int_\Omega \left(\frac{\varepsilon}{2} |\nabla Q|^2 + \frac{1}{\varepsilon} F(Q) \right) dx, \tag{1.5}$$

where $\Omega \subset \mathbb{R}^d$ is a bounded domain with smooth boundary, $|\nabla Q| = \sqrt{\sum_{ijk} |\partial_k Q_{ij}|^2}$, and $F(Q)$ is the bulk energy density

$$F(Q) = \frac{a}{2} \operatorname{tr}(Q^2) - \frac{b}{3} \operatorname{tr}(Q^3) + \frac{c}{4} \left(\operatorname{tr}(Q^2) \right)^2. \tag{1.6}$$

Here $a, b, c \in \mathbb{R}^+$ are material and temperature dependent constants, and ε denotes the relative intensity of elastic and bulk energy, which is usually quite small. It can be proved that all critical points of $F(Q)$ are uniaxial (1.4), (cf. [23]), and thus

$$F(Q) = \frac{s^2}{27} (9a - 2bs + 3cs^2) =: f(s), \text{ if } Q \text{ is uniaxial(1.4)}. \tag{1.7}$$

Moreover, $F(Q)$ has two families of stable local minimizers corresponding to the following choices of $s = s_\pm$:

$$s_- = 0, \quad s_+ = \frac{b + \sqrt{b^2 - 24ac}}{4c}. \tag{1.8}$$

In this work we shall consider the bistable case when

$$b^2 = 27ac, \quad \text{and } a, c > 0. \tag{1.9}$$

By rescaling, one can choose $a = 3, b = 9, c = 1$. From the physics view point, such choices of the coefficients correspond to the critical temperature at which the system favors the nematic phase and the isotropic phase equally [8, Section

2.3]. Analytically, it can be shown that, in this case, the two families of minimizers corresponding to (1.8) are the only global minimizers of $F(Q)$:

$$F(Q) \geq 0 \text{ and the equality holds if and only if } Q \in \{0\} \cup \mathcal{N}, \tag{1.10}$$

where

$$\begin{aligned} \mathcal{N} &:= \left\{ Q \in \mathcal{Q} \mid Q = s_+ \left(u \otimes u - \frac{1}{3} I_3 \right) \text{ for some } u \in \mathbb{S}^2 \right\}, \\ \text{with } s_+ &= \sqrt{\frac{3a}{c}}. \end{aligned} \tag{1.11}$$

At this point we digress to mention that the Landau–De Gennes model (1.5) is closely related to Ericksen’s model, where the energy is

$$e_E(s, u) := \int_{\Omega} \left(\kappa |\nabla s|^2 + s^2 |\nabla u|^2 + \psi(s) \right) dx. \tag{1.12}$$

This model was introduced by Ericksen [9] for the purpose of studying line defects. It can be formally obtained by plugging the uniaxial Ansatz (1.4) into (1.5). In contrast to (1.5) which uses $Q \in \mathcal{Q}$ as order parameter, Ericksen’s model uses $(s, u) \in \mathbb{R} \times \mathbb{S}^2$ and is very useful to describe liquid crystal defects. The analysis of this model is very challenging, mainly due to the reason that the geometry of the uniaxial configuration (1.4) corresponds to a double-cone, and the energy (1.12) is highly degenerate when $s = 0$. The analytical aspects of such a model have been investigated by many authors, for instance, by Lin [18], Hardt–Lin–Poon [20], Bedford [7], Alper–Hardt–Lin [2], and Alper [1].

To model nematic–isotropic phase transitions in the framework of Landau–De Gennes theory, we shall investigate the small- ε limit of the natural gradient flow dynamics of (1.5) with initial data undergoing a sharp transition near a smooth interface. To be more precise, we consider the system

$$\partial_t Q_\varepsilon = \Delta Q_\varepsilon - \frac{1}{\varepsilon^2} \nabla_q F(Q_\varepsilon), \quad \text{in } \Omega \times (0, T), \tag{1.13a}$$

$$Q_\varepsilon(x, 0) = Q_\varepsilon^{in}(x), \quad \text{in } \Omega, \tag{1.13b}$$

$$Q_\varepsilon(x, t) = 0, \quad \text{on } \partial\Omega \times (0, T), \tag{1.13c}$$

where $\nabla_q F(Q)$ is the variation of $F(Q)$ in space \mathcal{Q} :

$$(\nabla_q F(Q))_{ij} = a Q_{ij} - b \sum_{k=1}^3 Q_{ik} Q_{kj} + c |Q|^2 Q_{ij} + \frac{b}{3} |Q|^2 \delta_{ij}. \tag{1.14}$$

The system (1.13a) is the L^2 -gradient flow of energy (1.5) on the slow time scale ε .

Our main result, Theorem 2.1, states that starting from initial conditions with a reasonable nematic–isotropic phase transition from a nematic region $\Omega^+(0)$ into an isotropic region $\Omega^-(0)$, before the occurrence of topological changes, the solution Q_ε of (1.13) converges to the isotropic phase $Q \equiv 0$ in $\Omega^-(t)$ and to a field $Q \in \mathcal{N}$

taking values in the nematic phase in $\Omega^+(t)$, where the interface between $\Omega^+(t)$ and $\Omega^-(t)$ moves by mean curvature flow. Furthermore, we show that the limit Q is a harmonic map heat flow from $\Omega^+(t)$ into the closed manifold \mathcal{N} . Finally, if the region $\Omega^+(t)$ is simply-connected, there exists a director field u such that $Q = s_+(u \otimes u - \frac{1}{3}I_3)$, u is a harmonic map heat flow from $\Omega^+(t)$ into \mathbb{S}^2 , and satisfies homogenous Neumann boundary conditions on the evolving boundary $\partial\Omega^+(t)$.

The proof consists of two key steps: (i) an adaptation of the modulated energy inequality in [12] to the vector-valued case to control the leading-order energy contribution, which is of order $O(1)$ and comes from the phase transition across $\partial\Omega^+(t)$. (ii) A version of Chen–Shatah’s wedge-product trick in the sense that (1.13) implies

$$[\partial_t Q_\varepsilon, Q_\varepsilon] = \nabla \cdot [\nabla Q_\varepsilon, Q_\varepsilon], \tag{1.15}$$

where $[\cdot, \cdot]$ denotes the commutator.

In (i) we basically follow [12] but need to carefully regularize the metric d^F on Q induced by the conformal structure $F(Q)$ in order to exploit the fine properties of its derivative $\nabla_q d_\varepsilon^F$. In particular, we will use the crucial commutator relation $[\nabla_q d_\varepsilon^F(Q_\varepsilon), Q_\varepsilon] = 0$ for a.e. (x, t) . This seems to lie beyond the realm of generalized chain rules as in [3], which was employed in the work of Simon and one of the authors in [17]. Regarding (ii), we emphasize that the Neumann boundary condition along the free boundary $\partial\Omega^+(t)$ can be naturally encoded in the distributional formulation of (1.15) by enlarging the space of test functions. This however, requires uniform L^2 -estimates on the commutators $[\partial_t Q_\varepsilon, Q_\varepsilon]$ and $[\nabla Q_\varepsilon, Q_\varepsilon]$, which are one order of ε better than the a priori estimates suggest. We show that these estimates are guaranteed by our bounds on the modulated energy.

2. Main Results

To state the main result of this work, we assume that

$$I = \bigcup_{t \in [0, T]} (I_t \times \{t\}) \text{ is a smoothly evolving closed surface in } \Omega, \tag{2.1}$$

starting from a closed smooth surface $I_0 \subset \Omega$. Let $\Omega^+(t)$ be the domain enclosed by I_t , and $d(x, I_t)$ be the signed-distance from x to I_t which takes positive values in $\Omega^+(t)$, and negative values in $\Omega^-(t) = \Omega \setminus \overline{\Omega^+(t)}$, where

$$\Omega^\pm(t) := \{x \in \Omega \mid d(x, I_t) \gtrless 0\}. \tag{2.2}$$

Moreover, for each $T > 0$ we shall denote the ‘distorted’ parabolic cylinder by

$$\Omega_T^\pm := \bigcup_{t \in (0, T)} (\Omega^\pm(t) \times \{t\}). \tag{2.3}$$

For $\delta > 0$, the δ -neighborhood of I_t is denoted by

$$I_t(\delta) := \{x \in \Omega : |d(x, I_t)| < \delta\}. \tag{2.4}$$

Thus there exists a sufficiently small number $\delta_I \in (0, 1)$ such that the nearest point projection $P_I(\cdot, t) : I_t(\delta_I) \rightarrow I_t$ is smooth for any $t \in [0, T]$, and the interface (2.1) stays at least δ_I distance away from the boundary of the domain $\partial\Omega$.

To introduce the modulated energy for (1.13), we extend the inner normal vector field n_I of I_t to a neighborhood of it by

$$\xi(x, t) := \eta(d(x, I_t)) n_I(P_I(x, t), t), \tag{2.5}$$

where η is a cutoff function satisfying

$$\begin{aligned} \eta &\text{ is even in } \mathbb{R} \text{ and decreases in } [0, \infty); \\ \eta(z) &= 1 - z^2, \text{ for } |z| \leq \delta_I/2; \quad \eta(z) = 0 \text{ for } |z| \geq \delta_I. \end{aligned} \tag{2.6}$$

Following [12, 16], we define the modulated energy by

$$E_\varepsilon[Q_\varepsilon|I](t) := \int_\Omega \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon(\cdot, t)|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon(\cdot, t)) - \xi \cdot \nabla \psi_\varepsilon(\cdot, t) \right) dx, \tag{2.7}$$

where

$$F_\varepsilon(q) := F(q) + \varepsilon^{K-1} \text{ with } K = 4, \tag{2.8a}$$

$$\psi_\varepsilon(x, t) := d_\varepsilon^F \circ Q_\varepsilon(x, t), \quad \text{and } d_\varepsilon^F(q) := (\phi_\varepsilon * d^F)(q), \quad \forall q \in \mathcal{Q}, \tag{2.8b}$$

and the convolution is understood in the space $\mathcal{Q} \simeq \mathbb{R}^5$. Moreover, we set

$$\phi_\varepsilon(q) := \varepsilon^{-5K} \phi(\varepsilon^{-K} q), \tag{2.9}$$

a family of mollifiers in the 5-dimensional configuration space (1.2). Here ϕ is smooth, non-negative, having support in $B_1^\mathcal{Q}$ (the unit ball in \mathcal{Q}), and isotropic, i.e. for any orthogonal matrix $R \in O(3)$ and any $q \in \mathcal{Q}$ it holds $\phi(R^T q R) = \phi(q)$. The function d^F in (2.8b) is the quasi-distance function

$$d^F(q) := \inf \left\{ \int_0^1 \sqrt{2F(\gamma(t))} |\gamma'(t)| dt \mid \gamma \in C^{0,1}([0, 1]; \mathcal{Q}), \right. \\ \left. \gamma(0) \in \mathcal{N}, \gamma(1) = q \right\}, \tag{2.10}$$

which was introduced by Sternberg [26] and independently by Tartar-Fonseca [13] for the study of the singular perturbation problem. Some properties of d^F are stated in Lemma 3.1 below, and interested readers can find the proof in [19, 26]. One can refer to Section 3 for more details of these functions. Throughout, we will assume an L^∞ -bound of Q_ε , i.e.

$$\|Q_\varepsilon\|_{L^\infty(\Omega \times (0, T))} \leq c_0 \tag{2.11}$$

for some fixed constant c_0 . Such an estimate can be obtained by assuming a uniform L^∞ -bound of the initial data Q_ε^{in} and then applying maximum principle to (1.13a), see Lemma 3.3 in the sequel. Note that the choice $K = 4$ in (2.8a) is due to a technical reason, and is used in the proof of Lemma 4.1.

The main result of this work is the following:

Theorem 2.1. *Assume the surface I_t (2.1) evolves by mean curvature flow and encloses a simply-connected domain $\Omega^+(t)$. If the initial datum Q_ε^{in} of (1.13) is well-prepared in the sense that*

$$E_\varepsilon[Q_\varepsilon|I](0) \leq c_1\varepsilon, \tag{2.12}$$

for some constant c_1 that does not depend on ε , then for some $\varepsilon_k \downarrow 0$ as $k \uparrow +\infty$,

$$Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} Q = s_\pm (u(x, t) \otimes u(x, t) - \frac{1}{3}I_3),$$

strongly in $C([0, T]; L^2_{loc}(\Omega^\pm(t)))$, (2.13)

where s_\pm are given by (1.8) and

$$u \in H^1(\Omega_T^\pm; \mathbb{S}^2). \tag{2.14}$$

Moreover, u is a harmonic map heat flow into \mathbb{S}^2 with homogenous Neumann boundary conditions in the sense that

$$\int_{\Omega_T^+} \partial_t u \wedge u \cdot \varphi \, dxdt = - \sum_{j=1}^d \int_{\Omega_T^+} \partial_j u \wedge u \cdot \partial_j \varphi \, dxdt$$

$\forall \varphi \in C^1(\bar{\Omega} \times [0, T]; \mathbb{R}^3)$, (2.15)

where \wedge is the wedge product in \mathbb{R}^3 .

Remark 2.2. Note that (2.15) encodes both the harmonic map heat flow into \mathbb{S}^2 and the boundary conditions. Indeed, if $(\partial_t u, \nabla^2 u)$ is continuous up to the boundary of $\Omega^+(t)$, then the weak formulation (2.15) implies that u is a harmonic heat flow into \mathbb{S}^2 with Neumann boundary conditions on I_t :

$$\partial_t u = \Delta u + |\nabla u|^2 u \text{ in } \Omega_T^+, \quad \partial_{n_t} u = 0 \text{ on } \bigcup_{t \in (0, T)} (I_t \times \{t\}). \tag{2.16}$$

If $\Omega^+(t)$ is multi-connected, for instance when $\Omega^+(t)$ is the region outside I_t , then a well-known orientability issue arises and the conclusion (2.14) usually only holds away from defects. See the work of Bedford [7] for more discussions of such issues.

Theorem 2.1 solves a special case of the Keller–Rubinstein–Sternberg problem [25] using the energy method. A similar result has been established previously by Fei et al. [10, 11] using matched asymptotic expansions and spectral gap estimates. Our approach has the superiority that it allows more flexible initial data, as indicated by Proposition 2.3 below. The general case of the Keller–Rubinstein–Sternberg problem is fairly sophisticated and remains open. We refer the interested readers to a recent work of Lin–Wang [21] for the well-posedness of the limiting system. On the other hand, the static problem has been investigated by Lin et al. [19]. It is worthy to mention that recently Golovaty et al. [14, 15] studied a model problem based on highly disparate elastic constants. Most recently, Lin–Wang [22] studied isotropic-nematic transitions based on an anisotropic Ericksen’s model.

Now we turn to the construction of initial data Q_ε^{in} satisfying (2.12). Let $I_0 \subset \Omega$ be a smooth closed surface and let $I_0(\delta_0)$ be a neighborhood in which the signed distance function $d(x, I_0)$ is smooth. Let $\zeta(z)$ be a cut-off function such that

$$\zeta(z) = 0 \text{ for } |z| \geq 1, \text{ and } \zeta(z) = 1 \text{ for } |z| \leq 1/2. \tag{2.17}$$

Then we define

$$\tilde{S}_\varepsilon(x) := \zeta\left(\frac{d(x, I_0)}{\delta_0}\right) S\left(\frac{d(x, I_0)}{\varepsilon}\right) + \left(1 - \zeta\left(\frac{d(x, I_0)}{\delta_0}\right)\right) s_+ \mathbf{1}_{\Omega^+(0)}, \tag{2.18}$$

where $S(z)$ is given by the optimal profile

$$S(z) := \frac{s_+}{2} \left(1 + \tanh\left(\frac{\sqrt{a}}{2}z\right)\right), \quad z \in \mathbb{R}. \tag{2.19}$$

Note that (2.19) is the solution of the ODE

$$-S''(z) + aS(z) - \frac{b}{3}S^2(z) + \frac{2}{3}cS^3(z) = 0, \quad S(-\infty) = 0, \quad S(+\infty) = s_+. \tag{2.20}$$

Proposition 2.3. *For every $u^{in} \in H^1(\Omega; \mathbb{S}^2)$, the initial datum defined by*

$$Q_\varepsilon^{in}(x) := \tilde{S}_\varepsilon(x) \left(u^{in}(x) \otimes u^{in}(x) - \frac{1}{3}I_3\right) \tag{2.21}$$

satisfies $Q_\varepsilon^{in} \in H^1(\Omega; \mathcal{Q}) \cap L^\infty(\Omega; \mathcal{Q})$ and

$$Q_\varepsilon^{in}(x) = \begin{cases} s_+(u^{in} \otimes u^{in} - \frac{1}{3}I_3) & \text{if } x \in \Omega^+(0) \setminus I_0(\delta_0), \\ S\left(\frac{d(x, I_0)}{\varepsilon}\right)(u^{in} \otimes u^{in} - \frac{1}{3}I_3) & \text{if } x \in I_0(\delta_0/2), \\ 0 & \text{if } x \in \Omega^-(0) \setminus I_0(\delta_0). \end{cases} \tag{2.22}$$

Moreover, there exists a constant $c_1 > 0$ which only depends on I_0 and $\|u^{in}\|_{H^1(\Omega)}$ such that Q_ε^{in} is well-prepared in the sense of (2.12).

The rest of this work will be organized as follows: in Section 3 we discuss some properties of the quasi-distance function (2.10) and use them to construct the well-prepared initial data (2.21) and thus prove Proposition 2.3. In Section 4 we establish a relative-entropy type inequality for the parabolic system (1.13). Based on the various estimates given by such an inequality, in Section 5 we study the limit $\varepsilon \downarrow 0$ of (1.13) and give the proof of Theorem 2.1.

3. Preliminaries

We start with a lemma about the quasi-distance function (2.10), which was originally due to [13, 26].

Lemma 3.1. *The function $d^F(q)$ is locally Lipschitz in \mathcal{Q} with point-wise derivative satisfying*

$$|\nabla_q d^F(q)| = \sqrt{2F(q)} \text{ for a.e. } q \in \mathcal{Q}. \tag{3.1}$$

Moreover,

$$d^F(q) = \begin{cases} 0 & \text{if } q \in \mathcal{N}, \\ c^F & \text{if } q = 0, \end{cases} \tag{3.2}$$

where c^F is the 1-d energy of the minimal connection between \mathcal{N} and 0:

$$c^F := \inf \left\{ \int_0^1 \left(\frac{|\gamma'(t)|^2}{2} + F(\gamma(t)) \right) dt \mid \gamma \in C^{0,1}([0, 1]; \mathcal{Q}), \right. \\ \left. \gamma(0) \in \mathcal{N}, \gamma(1) = 0 \right\}. \tag{3.3}$$

By elementary linear algebra, any $Q \in \mathcal{Q}$ can be expressed by $Q = \sum_{i=1}^3 \lambda_i(Q) P_i(Q)$ with $\sum_{i=1}^3 \lambda_i(Q) = 0$, where $P_i(Q) = n_i \otimes n_i$ denotes the projection onto the i -th eigenspace, and $\lambda_1(Q) \leq \lambda_2(Q) \leq \lambda_3(Q)$ are the eigenvalues ordered increasingly. Furthermore using the identities $\sum_{j=1}^3 \lambda_j(Q) = 0$ and $I_3 = \sum_{j=1}^3 P_j(Q)$, we may write

$$Q = \left(s + \frac{r}{3} \right) \left(P_3(Q) - \frac{1}{3} I_3 \right) + \frac{2r}{3} \left(P_2(Q) - \frac{1}{3} I_3 \right), \tag{3.4}$$

$$\text{where } s(Q) = \frac{3}{2} \lambda_3(Q), \quad r(Q) = \frac{3}{2} (\lambda_2(Q) - \lambda_1(Q)). \tag{3.5}$$

The next lemma gives a precise form of d^F for uniaxial Q -tensors.

Lemma 3.2. *If $Q = s_0 (u \otimes u - \frac{1}{3} I_3)$ for some $s_0 \in [0, s_+]$ and $u \in \mathbb{S}^2$, then*

$$d^F(Q) = \frac{2}{\sqrt{3}} \int_{s_0}^{s_+} \sqrt{f(\tau)} \, d\tau =: g(s_0), \tag{3.6}$$

where $f(s)$ is given by (1.7).

Proof. The argument here is similar to that in [24]. Let γ be any curve connecting \mathcal{N} to \mathcal{Q} . When expressed in the form of eigenframe $\gamma(t) = \sum_{i=1}^3 \lambda_i(t) n_i(t) \otimes n_i(t)$, we claim that n_i are constant in t . Actually using the identity

$$\lambda_i^2 |n'_i|^2 = \lambda_i^2 \sum_{j=1}^3 (n_j \cdot n'_i)^2 = \lambda_i^2 \sum_{j \neq i} (n_j \cdot n'_i)^2, \tag{3.7}$$

we calculate

$$\begin{aligned}
 |\gamma'|^2 &= (\lambda'_1)^2 + (\lambda'_2)^2 + (\lambda'_3)^2 + 2 \sum_{i=1}^3 \lambda_i^2 |\mathbf{n}'_i|^2 \\
 &+ \sum_{k=1}^3 \sum_{1 \leq i < j \leq 3} 4\lambda_i \lambda_j (\mathbf{n}_i \cdot \mathbf{n}'_j) (\mathbf{n}_j \cdot \mathbf{n}'_i) \\
 &= (\lambda'_1)^2 + (\lambda'_2)^2 + (\lambda'_3)^2 + \sum_{k=1}^3 \sum_{1 \leq i < j \leq 3} 2 \left(\lambda_i (\mathbf{n}_j \cdot \mathbf{n}'_i) + \lambda_j (\mathbf{n}_i \cdot \mathbf{n}'_j) \right)^2 \\
 &\geq (\lambda'_1)^2 + (\lambda'_2)^2 + (\lambda'_3)^2.
 \end{aligned} \tag{3.8}$$

This implies that the global minimum is achieved by a path $\gamma(t)$ with constant eigenframe. So by (3.4) we may write

$$\begin{aligned}
 \gamma(t) &= \text{diag} \left\{ -\frac{s(t) + r(t)}{3}, -\frac{s(t) - r(t)}{3}, \frac{2s(t)}{3} \right\}, \\
 &\text{with } (s, r)|_{t=0} = (s_+, 0), \quad (s, r)|_{t=1} = (s_0, 0).
 \end{aligned} \tag{3.9}$$

then by (1.6)

$$F(\gamma(t)) = \frac{a}{9}(3s^2 + r^2) + \frac{c}{81}(3s^2 + r^2)^2 - \frac{2b}{27}(s^3 - sr^2) =: \tilde{F}(r, s). \tag{3.10}$$

Writing $\sqrt{3}s + ir =: \rho e^{i\theta}$ with $i = \sqrt{-1}$, we have $3\sqrt{3}(s^3 - sr^2) = \rho^3 \cos 3\theta$, and thus

$$\begin{aligned}
 &\int_0^1 |\gamma'(t)| \sqrt{2F(\gamma(t))} \, dt \\
 &= \frac{2}{3} \int_0^1 \sqrt{3s'^2 + r'^2} \sqrt{\tilde{F}(s, r)} \, dt \\
 &= \frac{2}{3} \int_0^1 \sqrt{\rho'^2 + \rho^2 \theta'^2} \sqrt{\frac{a\rho^2}{9} + \frac{c\rho^4}{81} - \frac{2b\rho^3}{81\sqrt{3}} \cos 3\theta} \, dt.
 \end{aligned}$$

It is clear that this energy is minimized when $\theta \equiv 0$, which corresponds to the uniaxial solution $r(t) \equiv 0$. In view of (1.7)

$$\int_0^1 |\gamma'(t)| \sqrt{2F(\gamma(t))} \, dt \geq \frac{2}{\sqrt{3}} \int_0^1 |s'(t)| \sqrt{f(s(t))} \, dt. \tag{3.11}$$

One can verify that the minimum of the right hand side can be achieved by a monotone function $s(t)$, and thus (3.6) follows from a change of variable. \square

At this point we would like to remark that for the general Keller–Rubinstein–Sternberg problem it is very hard to obtain a precise form of d^F like (3.6) (cf. [26, Part 2, Lemmas 5 and 7]).

Before giving the proof of Proposition 2.3, we digress here and discuss the convolution in (2.8b). The space \mathcal{Q} (1.2) is equipped with the inner product $A : B = \text{tr } A^T B$, and one can easily verify that $\{E_i\}_{i=1}^5$ defined below form an orthonormal basis:

$$\begin{aligned}
 E_1 &= \begin{bmatrix} \frac{\sqrt{3}-3}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}+3}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{bmatrix}, & E_2 &= \begin{bmatrix} \frac{\sqrt{3}+3}{6} & 0 & 0 \\ 0 & \frac{\sqrt{3}-3}{6} & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{3} \end{bmatrix}, \\
 E_3 &= \begin{bmatrix} 0 & \frac{\sqrt{2}}{2} & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & E_4 &= \begin{bmatrix} 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & 0 & 0 \\ \frac{\sqrt{2}}{2} & 0 & 0 \end{bmatrix}, & E_5 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{\sqrt{2}}{2} \\ 0 & \frac{\sqrt{2}}{2} & 0 \end{bmatrix}. \tag{3.12}
 \end{aligned}$$

This establishes an isometry $\mathcal{Q} \simeq \mathbb{R}^5$ and thus the convolution operation in (2.8b) can be interpreted as an integration in \mathbb{R}^5 . Concerning the choice of ϕ in (2.9), one can simply choose $g \in C_c^\infty(\mathbb{R})$ and set $\phi(q) := g(\text{tr}(q^2))$, which is obviously isotropic in q .

Proof of Proposition 2.3. As a consequence of the choice of the cutoff function ζ satisfying (2.17), we deduce that (2.22) is fulfilled and \hat{S}_ε is smooth. To compute the modulated energy (2.7) of the initial data Q_ε^{in} , we write (2.18) by

$$\tilde{S}_\varepsilon(x) = S\left(\frac{d(x, I_0)}{\varepsilon}\right) + \hat{S}_\varepsilon(x), \tag{3.13}$$

where

$$\hat{S}_\varepsilon(x) := \left(1 - \zeta\left(\frac{d(x, I_0)}{\delta_0}\right)\right) \left(s_+ \mathbf{1}_{\Omega^+(0)} - S\left(\frac{d(x, I_0)}{\varepsilon}\right)\right). \tag{3.14}$$

It follows from the exponential decay of (2.19) that

$$\|\hat{S}_\varepsilon\|_{L^\infty(\Omega)} + \|\nabla \hat{S}_\varepsilon\|_{L^\infty(\Omega)} \leq C e^{-\frac{C}{\varepsilon}}, \tag{3.15}$$

for some constant $C > 0$ that only depends on I_0 . So we can write

$$|\nabla Q_\varepsilon^{in}|^2 = \frac{2}{3\varepsilon^2} S'^2 + 2S^2 |\nabla u^{in}|^2 + O(e^{-C/\varepsilon})(|\nabla u^{in}|^2 + 1) \tag{3.16}$$

Recalling the form of the bulk energy (1.7) for uniaxial Q -tensors, in view of (1.9), we have

$$f(s) = \frac{c}{9} s^2 (s - s_+)^2, \quad \sqrt{f(s)} = \frac{\sqrt{c}}{3} s |s - s_+|, \quad \text{for all } s \in [0, s_+], \tag{3.17}$$

and $F(Q_\varepsilon^{in}) = f(S + \hat{S}_\varepsilon)$. Thus the integrand of $E_\varepsilon[Q_\varepsilon|I](0)$ can be written as

$$\begin{aligned}
 & \frac{\varepsilon}{2} |\nabla Q_\varepsilon^{in}|^2 + \frac{1}{\varepsilon} F(Q_\varepsilon^{in}) - \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} \\
 &= \frac{S'^2}{3\varepsilon} + \frac{f(S)}{\varepsilon} - \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} \\
 & \quad + \varepsilon S^2 |\nabla u^{in}|^2 + O(e^{-C/\varepsilon})(|\nabla u^{in}|^2 + 1) + \frac{f(S + \hat{S}_\varepsilon) - f(S)}{\varepsilon}. \tag{3.18}
 \end{aligned}$$

The first line on the right hand side vanishes due to the identity $S'(z) = \sqrt{3f(S(z))}$ as a consequence of (2.19) or equivalently the ODE (2.20):

$$\begin{aligned} & \frac{\varepsilon}{2} \left| \nabla Q_\varepsilon^{in} \right|^2 + \frac{1}{\varepsilon} F(Q_\varepsilon^{in}) - \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} \\ &= \varepsilon S^2 |\nabla u^{in}|^2 + O(e^{-C/\varepsilon})(|\nabla u^{in}|^2 + 1) + \frac{f(S + \hat{S}_\varepsilon) - f(S)}{\varepsilon}. \end{aligned} \tag{3.19}$$

On the other hand, since $0 \leq \tilde{S}_\varepsilon \leq s_+$, by Lemma 3.2,

$$d^F(Q_\varepsilon^{in}(x)) = \frac{2}{\sqrt{3}} \int_{\tilde{S}_\varepsilon(x)}^{s_+} \sqrt{f(\tau)} \, d\tau. \tag{3.20}$$

This together with (2.6) and (3.15) implies

$$\begin{aligned} & -(\xi \cdot \nabla) d^F(Q_\varepsilon^{in}) \\ &= -\eta(d(x, I_0)) \frac{2S'}{\sqrt{3\varepsilon}} \sqrt{f(S)} - \xi \cdot n_I \frac{2S'}{\sqrt{3\varepsilon}} \left(\sqrt{f(S)} - \sqrt{f(S + \hat{S}_\varepsilon)} \right) + O(e^{-C/\varepsilon}). \end{aligned} \tag{3.21}$$

Adding up (3.19) and (3.21) yields

$$\begin{aligned} & \frac{\varepsilon}{2} \left| \nabla Q_\varepsilon^{in} \right|^2 + \frac{1}{\varepsilon} F(Q_\varepsilon^{in}) - (\xi \cdot \nabla) d^F(Q_\varepsilon^{in}) \\ &= \varepsilon S^2 |\nabla u^{in}|^2 + O(e^{-C/\varepsilon})(|\nabla u^{in}|^2 + 1) + \frac{f(S + \hat{S}_\varepsilon) - f(S)}{\varepsilon} \\ & \quad + (1 - \eta(d(x, I_0))) \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} - \xi \cdot n_I \frac{2S'}{\varepsilon} \left(\sqrt{\frac{f(S)}{3}} - \sqrt{\frac{f(S + \hat{S}_\varepsilon)}{3}} \right). \end{aligned} \tag{3.22}$$

By the exponential decay of (2.19) and (3.15),

$$\begin{aligned} & \frac{\varepsilon}{2} \left| \nabla Q_\varepsilon^{in} \right|^2 + \frac{F(Q_\varepsilon^{in})}{\varepsilon} - (\xi \cdot \nabla) d^F(Q_\varepsilon^{in}) \\ & \leq \varepsilon S^2 |\nabla u^{in}|^2 + O(e^{-C/\varepsilon})(|\nabla u^{in}|^2 + 1) + (1 - \eta(d(x, I_0))) \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}}. \end{aligned} \tag{3.23}$$

To treat the last term, we first deduce from the exponential decay of (2.19) that

$$\left\| \left(\frac{d(x, I_0)}{\varepsilon} \right)^2 S' \left(\frac{d(x, I_0)}{\varepsilon} \right) \right\|_{L^\infty(I_0(\delta_0))} \leq C \tag{3.24}$$

for some C that only depends on I_0 . This together with (2.6) implies

$$\begin{aligned} & (1 - \eta(d(x, I_0))) \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} \\ &= \varepsilon^2 \frac{d^2(x, I_0)}{\varepsilon^2} \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} - \eta(d(x, I_0)) \mathbf{1}_{\{d(x, I_0) > \delta_0/2\}} \frac{2S'}{\varepsilon} \sqrt{\frac{f(S)}{3}} \\ &\leq \varepsilon C(I_0) + C e^{-\frac{C}{\varepsilon}}. \end{aligned} \tag{3.25}$$

Substituting the above estimate into (3.23) and use (2.8a), we arrive at

$$\begin{aligned} & \int_{\Omega} \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon^{in}|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon^{in}) - (\xi \cdot \nabla) d^F(Q_\varepsilon^{in}) \right) dx \\ & \leq \left(\varepsilon + O(e^{-C/\varepsilon}) \right) \int_{\Omega} |\nabla u^{in}|^2 dx + \varepsilon^2 |\Omega|. \end{aligned} \tag{3.26}$$

On the other hand, by (2.9) and (3.1), we have

$$|d_\varepsilon^F(q) - d^F(q)| = |(\phi_\varepsilon * d^F)(q) - d^F(q)| \leq \varepsilon L, \text{ if } |q| \leq M, \tag{3.27}$$

where $L = L(M, \phi, F)$. This pointwise estimate implies

$$\begin{aligned} & \left| \int_{\Omega} \left((\xi \cdot \nabla) d^F(Q_\varepsilon^{in}) - (\xi \cdot \nabla) d_\varepsilon^F(Q_\varepsilon^{in}) \right) dx \right| \\ & = \left| \int_{\Omega} (\nabla \cdot \xi) \left(d^F(Q_\varepsilon^{in}) - d_\varepsilon^F(Q_\varepsilon^{in}) \right) dx \right| \leq L\varepsilon, \end{aligned} \tag{3.28}$$

which together with (3.26) implies (2.12). □

The next result is concerned with a maximum modulus estimate of (1.13a).

Lemma 3.3. *Assume Q_ε is the solution of (1.13) satisfying $\|Q_\varepsilon^{in}\|_{L^\infty(\Omega)} \leq C_0$ for some fixed constant C_0 . Then there exists an ε -independent constant $c_0 = c_0(a, b, c, C_0) > 0$ such that*

$$\|Q_\varepsilon\|_{L^\infty(\Omega \times (0, T))} \leq c_0. \tag{3.29}$$

Proof. On the one hand, by (1.13a), $|Q_\varepsilon|^2$ fulfills the following identity

$$\partial_t |Q_\varepsilon|^2 - \Delta |Q_\varepsilon|^2 + |\nabla Q_\varepsilon|^2 = -\frac{2}{\varepsilon^2} \left(a |Q_\varepsilon|^2 - b \operatorname{tr} Q_\varepsilon^3 + c |Q_\varepsilon|^4 \right). \tag{3.30}$$

On the other hand, there exists $\mu > 0$ (sufficiently large) such that $|Q| \geq \mu$ implies

$$a|Q|^2 - b \operatorname{tr} Q^3 + c|Q|^4 > 0.$$

Assume $|Q_\varepsilon|(x, t)$ achieves its maximum at $(x_\varepsilon, t_\varepsilon) \in \overline{\Omega} \times (0, T)$. If $|Q_\varepsilon(x_\varepsilon, t_\varepsilon)| \leq \mu$, then we obtain the desired estimate. Otherwise there holds $\partial_t |Q_\varepsilon|^2 - \Delta |Q_\varepsilon|^2 \leq 0$, and the weak maximum principle implies the maximum must be achieved on the parabolic boundary $(\partial\Omega \times (0, T)) \cup (\Omega \times \{0\})$, on which $|Q_\varepsilon|$ is bounded by our assumptions. □

4. The Modulated Energy Inequality

As the gradient flow of (1.5), the system (1.13a) has the following energy dissipation law

$$E_\varepsilon(Q_\varepsilon(\cdot, T)) + \int_0^T \int_\Omega \varepsilon |\partial_t Q_\varepsilon|^2 dx dt = E_\varepsilon(Q_\varepsilon^{in}(\cdot)), \text{ for all } T \geq 0. \quad (4.1)$$

Due to the concentration of ∇Q_ε near the interface I_t , this estimate is not sufficient to derive the convergence of Q_ε . Following a recent work of Fisher et al. [12] we shall develop in this section a calibrated inequality, which modulates the surface energy.

Recall in (2.5) that we extend the normal vector field n_I of the interface I_t to a neighborhood of it. We also extend the mean curvature vector H_I of (2.1) to a neighborhood by

$$\begin{aligned} H_I(x, t) &= \tilde{\eta}(d(x, I_t))H_I(P_I(x, t), t) \\ &= \tilde{\eta}(d(x, I_t))(\nabla \cdot n_I)(P_I(x, t), t)n_I(P_I(x, t), t), \end{aligned} \quad (4.2)$$

where $\tilde{\eta} \in C_c^\infty((-\delta_I, \delta_I))$ is a cut-off which is identically equal to 1 for $s \in (-\delta_I/2, \delta_I/2)$, and $P_I(x, t) = x - \nabla d(x, I_t)d(x, I_t)$ is the projection onto I_t . The definitions (2.5) and (4.2) of ξ and H_I , respectively, imply the following relations:

$$\partial_t \xi = - (H_I \cdot \nabla) \xi - (\nabla H_I)^T \xi + O(d(x, I_t)), \quad (4.3a)$$

$$\partial_t |\xi|^2 = - (H_I \cdot \nabla) |\xi|^2 + O(d^2(x, I_t)), \quad (4.3b)$$

where $\nabla H_I := \{\partial_j (H_I)_i\}_{1 \leq i, j \leq d}$ is a matrix with i being the row index. Actually in $I_t(\delta_I/2)$ there holds $\partial_t d(x, I_t) = -n_I \cdot H_I(P_I(x, t))$ and $\nabla d(x, I_t) = n_I(P_I(x, t))$. So we obtain (4.3) by chain rule. Moreover,

$$-\nabla \cdot \xi = H_I \cdot \xi + O(d(x, I_t)), \quad (4.4)$$

and since H_I is extended constantly in normal direction, we have

$$(\xi \cdot \nabla)H_I = 0 \text{ for all } (x, t) \text{ such that } |d(x, I_t)| < \delta_I/2. \quad (4.5)$$

Moreover, by the choice of δ_I at the beginning of Section 2, we have

$$\xi = 0 \text{ on } \partial\Omega \text{ and } H_I = 0 \text{ on } \partial\Omega. \quad (4.6)$$

Finally, we have the following regularity

$$|\nabla \xi| + |H_I| + |\nabla H_I| \leq C(I_0). \quad (4.7)$$

We denote the phase-field analogs of the mean curvature and normal vectors by

$$H_\varepsilon(x, t) := - \left(\varepsilon \Delta Q_\varepsilon - \frac{\nabla_q F(Q_\varepsilon)}{\varepsilon} \right) : \frac{\nabla Q_\varepsilon}{|\nabla Q_\varepsilon|}, \quad (4.8a)$$

$$n_\varepsilon(x, t) := \frac{\nabla \psi_\varepsilon(x, t)}{|\nabla \psi_\varepsilon(x, t)|}, \quad (4.8b)$$

respectively, where ψ_ε is defined by (2.8b). Here and throughout we use the convention that $:$ denotes the contraction in the indices i, j in three-tensors like $\partial_k Q_{i,j}$, i.e., the scalar product in the state space \mathcal{Q} .

By chain rule and (2.8b)

$$\nabla \psi_\varepsilon(x, t) = \nabla_q d_\varepsilon^F(Q_\varepsilon) : \nabla Q_\varepsilon(x, t) \quad \text{for a.e. } (x, t) \in \Omega \times (0, T). \tag{4.9}$$

This motivates the definition of the following projection of $\partial_i Q_\varepsilon$ onto the span of $\nabla_q d_\varepsilon^F(Q_\varepsilon)$

$$\Pi_{Q_\varepsilon} \partial_i Q_\varepsilon = \begin{cases} \left(\partial_i Q_\varepsilon : \frac{\nabla_q d_\varepsilon^F(Q_\varepsilon)}{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|} \right) \frac{\nabla_q d_\varepsilon^F(Q_\varepsilon)}{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|}, & \text{if } \nabla_q d_\varepsilon^F(Q_\varepsilon) \neq 0, \\ 0, & \text{otherwise.} \end{cases} \tag{4.10}$$

Hence, (4.9) implies

$$|\nabla \psi_\varepsilon| = |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| |\nabla_q d_\varepsilon^F(Q_\varepsilon)| \quad \text{for a.e. } (x, t) \in \Omega \times (0, T), \tag{4.11a}$$

$$\Pi_{Q_\varepsilon} \nabla Q_\varepsilon = \frac{|\nabla \psi_\varepsilon|}{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|^2} \nabla_q d_\varepsilon^F(Q_\varepsilon) \otimes n_\varepsilon \quad \text{for a.e. } (x, t) \in \Omega \times (0, T), \tag{4.11b}$$

The next inequality will be crucial to show the non-negativity of the modulated energy (2.7) and various lower bounds of it. It states that the upper bound for the gradient of the convolution d_ε^F is as good as if d^F was $C^{1,1/2}$ and it simply follows from the fact that the modulus $|\nabla d^F|$ is $C^{1/2}$.

Lemma 4.1. *For each $c_0 > 0$ there exists $\varepsilon_0 \in \mathbb{R}^+$ such that*

$$|\nabla_q d_\varepsilon^F(q)| \leq \sqrt{2F_\varepsilon(q)}, \quad \forall q \in \mathcal{Q}, |q| \leq c_0, \forall \varepsilon \in (0, \varepsilon_0). \tag{4.12}$$

Proof. Recall (2.8a), i.e. $F_\varepsilon(q) = F(q) + \varepsilon^{K-1}$ with $K = 4$. It follows from (2.9), (3.1) and $\int_{\mathbb{R}^5} \phi_\varepsilon(p) dp = 1$ that

$$\begin{aligned} |\nabla_q d_\varepsilon^F(q)| &= \left| \int_{\mathbb{R}^5} \phi_\varepsilon(p) \nabla_q d^F(q-p) dp \right| \\ &\leq \int_{\mathbb{R}^5} \sqrt{\phi_\varepsilon(p)} \sqrt{\phi_\varepsilon(p)} \sqrt{2F(q-p)} dp \\ &\leq \sqrt{\int_{\mathbb{R}^5} \phi_\varepsilon(p) 2F(q-p) dp} \\ &\leq \sqrt{\int_{\mathbb{R}^5} \phi_\varepsilon(p) (2F(q) + C_0|p|) dp} \end{aligned}$$

where in the last step C_0 is a local Lipschitz constant of $F(q)$ for $|q| \leq c_0$. By (2.9) and the assumption that ϕ is supported in the unit ball of \mathcal{Q} , the integral in the last step can be treated as follows

$$|\nabla_q d_\varepsilon^F(q)| \leq \sqrt{2F(q) + C_0 \varepsilon^K \int_{\mathbb{R}^5} \phi_\varepsilon(p) |p| \varepsilon^{-K} dp} \leq \sqrt{2F(q) + C_0 \varepsilon^K}.$$

Finally choosing ε_0 sufficiently small leads to (4.12). □

We shall apply the above lemma with c_0 being the constant in (3.29).

As we shall not integrate the time variable t throughout this section, we shall abbreviate the spatial integration \int_{Ω} by \int and sometimes we omit the dx . The following lemma shows that the energy $E_{\varepsilon}[Q_{\varepsilon}|I]$ defined by (2.7) controls various quantities:

Lemma 4.2. *There exists a universal constant $C < \infty$ which is independent of $t \in (0, T)$ and ε such that the following estimates hold for every $t \in (0, T)$:*

$$\int \left(\frac{\varepsilon}{2} |\nabla Q_{\varepsilon}|^2 + \frac{1}{\varepsilon} F_{\varepsilon}(Q_{\varepsilon}) - |\nabla \psi_{\varepsilon}| \right) dx \leq E_{\varepsilon}[Q_{\varepsilon}|I](t), \quad (4.13a)$$

$$\begin{aligned} \frac{1}{2} \int \left(\sqrt{\varepsilon} |\Pi_{Q_{\varepsilon}} \nabla Q_{\varepsilon}| - \frac{1}{\sqrt{\varepsilon}} \sqrt{2F_{\varepsilon}(Q_{\varepsilon})} \right)^2 dx \\ + \frac{\varepsilon}{2} \int \left(|\nabla Q_{\varepsilon} - \Pi_{Q_{\varepsilon}} \nabla Q_{\varepsilon}|^2 \right) dx \leq E_{\varepsilon}[Q_{\varepsilon}|I](t), \end{aligned} \quad (4.13b)$$

$$\frac{1}{2} \int \left(\sqrt{\varepsilon} |\Pi_{Q_{\varepsilon}} \nabla Q_{\varepsilon}| - \frac{1}{\sqrt{\varepsilon}} |\nabla_q d_{\varepsilon}^F(Q_{\varepsilon})| \right)^2 dx \leq E_{\varepsilon}[Q_{\varepsilon}|I](t), \quad (4.13c)$$

$$\begin{aligned} \int \left(\sqrt{\varepsilon} |\nabla Q_{\varepsilon}| - \frac{1}{\sqrt{\varepsilon}} |\nabla_q d_{\varepsilon}^F(Q_{\varepsilon})| \right)^2 dx \\ + \int (1 - \xi \cdot \mathbf{n}_{\varepsilon}) \left(\frac{\varepsilon}{2} |\Pi_{Q_{\varepsilon}} \nabla Q_{\varepsilon}|^2 + |\nabla \psi_{\varepsilon}| \right) dx \leq C E_{\varepsilon}[Q_{\varepsilon}|I](t), \end{aligned} \quad (4.13d)$$

$$\int \left(\frac{\varepsilon}{2} |\nabla Q_{\varepsilon}|^2 + \frac{1}{\varepsilon} F_{\varepsilon}(Q_{\varepsilon}) + |\nabla \psi_{\varepsilon}| \right) \min(d^2(x, I_t), 1) dx \leq C E_{\varepsilon}[Q_{\varepsilon}|I](t). \quad (4.13e)$$

Proof of Lemma 4.2. Since $|\xi \cdot \nabla \psi_{\varepsilon}| \leq |\nabla \psi_{\varepsilon}|$, we obtain the first estimate (4.13a). The second estimate (4.13b) follows from the first one by using the chain rule in form of (4.11a) for the term $|\nabla \psi_{\varepsilon}|$, the Lipschitz estimate (4.12) and then completing the square. Similarly, using the Lipschitz estimate (4.12) to the term $\frac{1}{\varepsilon} F_{\varepsilon}(Q_{\varepsilon})$ instead yields (4.13c).

Let us now turn to the estimate (4.13d). Completing the square and using (4.12) yield

$$\begin{aligned} E_{\varepsilon}[Q_{\varepsilon}|I] &\geq \frac{1}{2} \int \left(\sqrt{\varepsilon} |\nabla Q_{\varepsilon}| - \frac{1}{\sqrt{\varepsilon}} |\nabla_q d_{\varepsilon}^F(Q_{\varepsilon})| \right)^2 dx \\ &\quad + \int \left(|\nabla_q d_{\varepsilon}^F(Q_{\varepsilon})| |\nabla Q_{\varepsilon}| - |\nabla \psi_{\varepsilon}| \right) dx \\ &\quad + \int (1 - \xi \cdot \mathbf{n}_{\varepsilon}) |\nabla \psi_{\varepsilon}| dx. \end{aligned} \quad (4.14)$$

By the chain rule in form of (4.11a), the second right-hand side integral is non-negative. Using (4.11b) and Young’s inequality, it holds that

$$\begin{aligned} \varepsilon |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 &= |\nabla \psi_\varepsilon| + \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| \left(\sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| - \frac{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|}{\sqrt{\varepsilon}} \right) \\ &\leq |\nabla \psi_\varepsilon| + \frac{\varepsilon}{2} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 + \frac{1}{2} \left(\sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| - \frac{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|}{\sqrt{\varepsilon}} \right)^2. \end{aligned} \tag{4.15}$$

Hence

$$\frac{\varepsilon}{2} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \leq |\nabla \psi_\varepsilon| + \frac{1}{2} \left(\sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| - \frac{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|}{\sqrt{\varepsilon}} \right)^2. \tag{4.16}$$

This combined with (4.14), (4.13c) and the trivial estimate $1 - \xi \cdot n_\varepsilon \leq 2$ leads to (4.13d). Finally, by (2.6) and $\delta_I \in (0, 1)$ we have

$$1 - \xi \cdot n_\varepsilon \geq 1 - \eta \geq \min \left(d^2(x, I_t), \frac{\delta_I^2}{4} \right) \geq \frac{\delta_I^2}{4} \min(d^2(x, I_t), 1). \tag{4.17}$$

Applying this to the second right-hand side integral of (4.13d) and then using (4.13a) yield (4.13e). □

The following result was first proved in [12] in the case of the Allen-Cahn equation, and can be generalized to the vectorial case:

Proposition 4.3. *There exists a constant $C = C(I_t)$ depending on the interface I_t such that*

$$\begin{aligned} \frac{d}{dt} E_\varepsilon[Q_\varepsilon|I] + \frac{1}{2\varepsilon} \int (\varepsilon^2 |\partial_t Q_\varepsilon|^2 - |H_\varepsilon|^2) dx \\ + \frac{1}{2\varepsilon} \int \left| \varepsilon \partial_t Q_\varepsilon - (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) \right|^2 dx \\ + \frac{1}{2\varepsilon} \int |H_\varepsilon - \varepsilon |\nabla Q_\varepsilon| H_I|^2 dx \leq C E_\varepsilon[Q_\varepsilon|I]. \end{aligned} \tag{4.18}$$

The following lemma, the proof of which will be given at the end of this section, provides the exact computation of the time derivative of the energy $E_\varepsilon[Q_\varepsilon|I]$:

Lemma 4.4. *Under the assumptions of Theorem 2.1, the following identity holds:*

$$\begin{aligned} & \frac{d}{dt} E[Q_\varepsilon|I] + \frac{1}{2\varepsilon} \int \left| \varepsilon \partial_t Q_\varepsilon - (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) \right|^2 dx \\ & + \frac{1}{2\varepsilon} \int |H_\varepsilon - \varepsilon |\nabla Q_\varepsilon| H_I|^2 dx \\ = & \frac{1}{2\varepsilon} \int \left| (\nabla \cdot \xi) |\nabla_q d_\varepsilon^F(Q_\varepsilon)| n_\varepsilon + \varepsilon |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| H_I \right|^2 dx \end{aligned} \quad (4.19a)$$

$$\begin{aligned} & + \frac{\varepsilon}{2} \int |H_I|^2 \left(|\nabla Q_\varepsilon|^2 - |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right) dx - \int \nabla H_I : (\xi - n_\varepsilon)^{\otimes 2} |\nabla \psi_\varepsilon| dx \end{aligned} \quad (4.19b)$$

$$\begin{aligned} & + \int (\nabla \cdot H_I) \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) - |\nabla \psi_\varepsilon| \right) dx \\ & + \int (\nabla \cdot H_I) (1 - \xi \cdot n_\varepsilon) |\nabla \psi_\varepsilon| dx + J_\varepsilon^1 + J_\varepsilon^2, \end{aligned} \quad (4.19c)$$

where we use the notation

$$\begin{aligned} J_\varepsilon^1 := & \int \nabla H_I : n_\varepsilon \otimes n_\varepsilon \left(|\nabla \psi_\varepsilon| - \varepsilon |\nabla Q_\varepsilon|^2 \right) dx \\ & + \varepsilon \int \nabla H_I : (n_\varepsilon \otimes n_\varepsilon) \left(|\nabla Q_\varepsilon|^2 - |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right) dx \\ & - \varepsilon \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \left((\partial_i Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_i Q_\varepsilon) : (\partial_j Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_j Q_\varepsilon) \right) dx, \end{aligned} \quad (4.20)$$

$$\begin{aligned} J_\varepsilon^2 := & - \int \left(\partial_t \xi + (H_I \cdot \nabla) \xi + (\nabla H_I)^T \xi \right) \cdot (n_\varepsilon - \xi) |\nabla \psi_\varepsilon| dx \\ & - \int \left(\partial_t \xi + (H_I \cdot \nabla) \xi \right) \cdot \xi |\nabla \psi_\varepsilon| dx. \end{aligned} \quad (4.21)$$

In order to prove the proposition, we only need to estimate the terms on the RHS of (4.19).

Proof of Proposition 4.3. According to Lemma 4.4, we only need to estimate the RHS of (4.19) by $E_\varepsilon[Q_\varepsilon|I]$ up to a constant that only depends on I_t . We start with (4.19a): it follows from the triangle inequality that

$$\begin{aligned} & \frac{1}{2} \int \left| \frac{1}{\sqrt{\varepsilon}} (\nabla \cdot \xi) |\nabla_q d_\varepsilon^F(Q_\varepsilon)| n_\varepsilon + \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| H_I \right|^2 dx \\ & \leq \int \left| (\nabla \cdot \xi) \left(\sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| - \frac{1}{\sqrt{\varepsilon}} |\nabla_q d_\varepsilon^F(Q_\varepsilon)| \right) n_\varepsilon \right|^2 dx \\ & + \int |(\nabla \cdot \xi) \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| (n_\varepsilon - \xi)|^2 dx \\ & + \int |(H_I + (\nabla \cdot \xi) \xi) \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 dx. \end{aligned}$$

The first integral is controlled by (4.13c). Using (4.4), the second integral is controlled by (4.13d). The third integral can be treated using the relation $H_I = (H_I \cdot \xi)\xi + O(d(x, I_t))$ and (4.4), so it can be controlled by (4.13e).

The integrals in (4.19b) can be controlled using (4.13b) and (4.13d), recalling that

$$|\xi - n_\varepsilon|^2 \leq 2(1 - n_\varepsilon \cdot \xi).$$

The first term in (4.19c) can be controlled using (4.13a), and the second term can be estimated by (4.13d). It remains to estimate (4.20) and (4.21). The last two terms on the RHS of J_ε^1 can be bounded using (4.13b), and the first integral can be rewritten using $n_\varepsilon = n_\varepsilon - \xi + \xi$:

$$\begin{aligned} J_\varepsilon^1 &\leq \int \nabla H_I : (n_\varepsilon \otimes (n_\varepsilon - \xi)) \left(|\nabla \psi_\varepsilon| - \varepsilon |\nabla Q_\varepsilon|^2 \right) dx \\ &\quad + \int \nabla H_I : n_\varepsilon \otimes \xi \left(|\nabla \psi_\varepsilon| - \varepsilon |\nabla Q_\varepsilon|^2 \right) dx + CE_\varepsilon[Q_\varepsilon|I] \\ &\leq \|\nabla H_I\|_{L^\infty} \int |n_\varepsilon - \xi| \left(\varepsilon |\nabla Q_\varepsilon|^2 - \varepsilon |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right. \\ &\quad \left. + \left| \varepsilon |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 - |\nabla \psi_\varepsilon| \right| \right) dx \\ &\quad + C \int \min(d^2(x, I_t), 1) \left(|\nabla \psi_\varepsilon| + \varepsilon |\nabla Q_\varepsilon|^2 \right) dx + CE_\varepsilon[Q_\varepsilon|I]. \end{aligned} \tag{4.22}$$

Note that in the last step we employed

$$\nabla H_I : n_\varepsilon \otimes \xi = (\xi \cdot \nabla H_I) \cdot n_\varepsilon$$

and the fact that $(\xi \cdot \nabla)H_I$ vanishes in the neighborhood $I_t(\frac{\delta I}{2})$ by definition (4.2). Thus we employ (4.13d) and (4.13b), and (4.11a) to get

$$\begin{aligned} J_\varepsilon^1 &\leq C \int |n_\varepsilon - \xi| \left| \varepsilon |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 - |\nabla \psi_\varepsilon| \right| dx + CE_\varepsilon[Q_\varepsilon|I] \\ &= C \int |n_\varepsilon - \xi| \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| \left| \sqrt{\varepsilon} |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon| - \frac{|\nabla_q d_\varepsilon^F(Q_\varepsilon)|}{\sqrt{\varepsilon}} \right| dx \\ &\quad + CE_\varepsilon[Q_\varepsilon|I]. \end{aligned} \tag{4.23}$$

Finally applying the Cauchy-Schwarz inequality and then (4.13d) and (4.13b), we obtain

$$J_\varepsilon^1 \leq CE_\varepsilon[Q_\varepsilon|I]. \tag{4.24}$$

As for J_ε^2 (4.21), we employ (4.3a) and (4.3b) and yield

$$J_\varepsilon^2 \leq C \int \left(|n_\varepsilon - \xi|^2 + \min(d^2(x, I_t), 1) \right) |\nabla \psi_\varepsilon| dx \leq CE_\varepsilon[Q_\varepsilon|I], \tag{4.25}$$

after applying (4.13d) and (4.13e). Therefore we have proved that the RHS of (4.19) is bounded by $E_\varepsilon[Q_\varepsilon|I]$ up to a multiplicative constant which only depends on I_t .

□

The following lemma will be used in the proof of Lemma 4.4:

Lemma 4.5. *Under the assumptions of Theorem 2.1,*

$$\begin{aligned}
 & \int \nabla \mathbf{H}_I : (\xi \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx - \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx \\
 &= \int \nabla \mathbf{H}_I : (\xi - \mathbf{n}_\varepsilon) \otimes \mathbf{n}_\varepsilon |\nabla \psi_\varepsilon| \, dx + \int \mathbf{H}_\varepsilon \cdot \mathbf{H}_I |\nabla Q_\varepsilon| \, dx \\
 &+ \int \nabla \cdot \mathbf{H}_I \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) - |\nabla \psi_\varepsilon| \right) \, dx \\
 &+ \int \nabla \cdot \mathbf{H}_I (|\nabla \psi_\varepsilon| - \xi \cdot \nabla \psi_\varepsilon) \, dx \\
 &- \int \sum_{i,j=1}^3 (\nabla \mathbf{H}_I)_{ij} \varepsilon (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) \, dx + \int \nabla \mathbf{H}_I : (\mathbf{n}_\varepsilon \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx
 \end{aligned} \tag{4.26}$$

Proof. The LHS of (4.26) can be written as

$$\begin{aligned}
 & \int \nabla \mathbf{H}_I : (\xi \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx - \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx \\
 &= \int \nabla \mathbf{H}_I : (\xi - \mathbf{n}_\varepsilon) \otimes \mathbf{n}_\varepsilon |\nabla \psi_\varepsilon| \, dx + \int \nabla \mathbf{H}_I : (\mathbf{n}_\varepsilon \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx \\
 &- \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx.
 \end{aligned} \tag{4.27}$$

To treat the second term on the RHS of (4.26), we introduce the energy stress tensor T_ε

$$(T_\varepsilon)_{ij} = \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) \right) \delta_{ij} - \varepsilon \partial_i Q_\varepsilon : \partial_j Q_\varepsilon. \tag{4.28}$$

In view of (4.8a), we have the identity

$$\nabla \cdot T_\varepsilon = -\varepsilon \nabla Q_\varepsilon : \Delta Q_\varepsilon + \frac{1}{\varepsilon} \nabla_q F_\varepsilon(Q_\varepsilon) : \nabla Q_\varepsilon = \mathbf{H}_\varepsilon |\nabla Q_\varepsilon|. \tag{4.29}$$

Testing this identity by \mathbf{H}_I , integrating by parts and using (4.6), we obtain

$$\begin{aligned}
 \int \mathbf{H}_\varepsilon \cdot \mathbf{H}_I |\nabla Q_\varepsilon| \, dx &= - \int \nabla \mathbf{H}_I : T_\varepsilon \, dx \\
 &= - \int \nabla \cdot \mathbf{H}_I \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) \right) \, dx \\
 &+ \int \sum_{i,j=1}^3 (\nabla \mathbf{H}_I)_{ij} \varepsilon (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) \, dx.
 \end{aligned} \tag{4.30}$$

Adding zero leads to

$$\begin{aligned}
 & \int \nabla H_I : \mathbf{n}_\varepsilon \otimes \mathbf{n}_\varepsilon |\nabla \psi_\varepsilon| \, dx \\
 &= \int \mathbf{H}_\varepsilon \cdot \mathbf{H}_I |\nabla Q_\varepsilon| \, dx + \int \nabla \cdot \mathbf{H}_I \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) - |\nabla \psi_\varepsilon| \right) \, dx \\
 & \quad + \int \nabla \cdot \mathbf{H}_I |\nabla \psi_\varepsilon| \, dx \\
 & \quad - \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \varepsilon (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) \, dx + \int (\nabla H_I) : (\mathbf{n}_\varepsilon \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx.
 \end{aligned} \tag{4.31}$$

Substituting this identity into (4.27) leads to (4.26). □

Proof of Lemma 4.4. Using the energy dissipation law (4.1) and adding zero, we compute the time derivative of the energy (2.7) by

$$\begin{aligned}
 & \frac{d}{dt} E_\varepsilon[Q_\varepsilon|I] + \varepsilon \int |\partial_t Q_\varepsilon|^2 \, dx - \int (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \partial_t Q_\varepsilon \, dx \\
 &= \int (\mathbf{H}_I \cdot \nabla) \xi \cdot \nabla \psi_\varepsilon \, dx + \int (\nabla H_I)^T \xi \cdot \nabla \psi_\varepsilon \, dx \\
 & \quad - \int \left(\partial_t \xi + (\mathbf{H}_I \cdot \nabla) \xi + (\nabla H_I)^T \xi \right) \cdot \nabla \psi_\varepsilon \, dx.
 \end{aligned}$$

Due to the symmetry of the Hessian of ψ_ε and the boundary conditions (4.6), we have

$$\int \nabla \cdot (\xi \otimes \mathbf{H}_I) \cdot \nabla \psi_\varepsilon \, dx = \int \nabla \cdot (\mathbf{H}_I \otimes \xi) \cdot \nabla \psi_\varepsilon \, dx.$$

Hence, the first integral on the RHS above can be rewritten as

$$\begin{aligned}
 \int (\mathbf{H}_I \cdot \nabla) \xi \cdot \nabla \psi_\varepsilon \, dx &= \int \nabla \cdot (\xi \otimes \mathbf{H}_I) \cdot \nabla \psi_\varepsilon \, dx - \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx \\
 &= \int (\nabla \cdot \xi) \mathbf{H}_I \cdot \nabla \psi_\varepsilon \, dx + \int (\xi \cdot \nabla) \mathbf{H}_I \cdot \nabla \psi_\varepsilon \, dx \\
 & \quad - \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx.
 \end{aligned}$$

Therefore

$$\begin{aligned}
 & \frac{d}{dt} E_\varepsilon[Q_\varepsilon|I] + \varepsilon \int |\partial_t Q_\varepsilon|^2 \, dx - \int (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \partial_t Q_\varepsilon \, dx \\
 &= \int (\nabla \cdot \xi) \mathbf{H}_I \cdot \nabla \psi_\varepsilon \, dx + \int (\xi \cdot \nabla) \mathbf{H}_I \cdot \nabla \psi_\varepsilon \, dx - \int (\nabla \cdot \mathbf{H}_I) \xi \cdot \nabla \psi_\varepsilon \, dx \\
 & \quad + \int \nabla H_I : (\xi \otimes \mathbf{n}_\varepsilon) |\nabla \psi_\varepsilon| \, dx - \int \left(\partial_t \xi + (\mathbf{H}_I \cdot \nabla) \xi + (\nabla H_I)^T \xi \right) \cdot \nabla \psi_\varepsilon \, dx.
 \end{aligned}$$

Using (4.26) in Lemma 4.5 to replace the third and fourth integrals on the RHS of the above identity and rewriting the last integral, we arrive at

$$\begin{aligned}
 & \frac{d}{dt} E_\varepsilon[Q_\varepsilon|I] + \varepsilon \int |\partial_t Q_\varepsilon|^2 dx - \int (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \partial_t Q_\varepsilon dx \\
 &= \int (\nabla \cdot \xi) H_I \cdot \nabla \psi_\varepsilon dx + \int (\xi \cdot \nabla) H_I \cdot \nabla \psi_\varepsilon dx \\
 &+ \int \nabla H_I : (\xi - n_\varepsilon) \otimes n_\varepsilon |\nabla \psi_\varepsilon| dx \\
 &+ \int H_\varepsilon \cdot H_I |\nabla Q_\varepsilon| dx + \int \nabla \cdot H_I \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) - |\nabla \psi_\varepsilon| \right) dx \\
 &+ \int \nabla \cdot H_I (|\nabla \psi_\varepsilon| - \xi \cdot \nabla \psi_\varepsilon) dx \tag{4.32} \\
 &- \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \varepsilon (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) dx + \int \nabla H_I : n_\varepsilon \otimes n_\varepsilon |\nabla \psi_\varepsilon| dx \\
 &- \int \left(\partial_t \xi + (H_I \cdot \nabla) \xi + (\nabla H_I)^T \xi \right) \cdot (n_\varepsilon - \xi) |\nabla \psi_\varepsilon| dx \\
 &- \int \left(\partial_t \xi + (H_I \cdot \nabla) \xi \right) \cdot \xi |\nabla \psi_\varepsilon| dx - \int (\nabla H_I)^T : (\xi \otimes \xi) |\nabla \psi_\varepsilon| dx.
 \end{aligned}$$

First, note that the third to last and second to last integrals combine to J_ε^2 . Next, by the property (4.11b) of the orthogonal projection (4.10), we can also find J_ε^1 on the right-hand side. Indeed,

$$\begin{aligned}
 & - \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \varepsilon (\partial_i Q_\varepsilon : \partial_j Q_\varepsilon) dx + \int \nabla H_I : n_\varepsilon \otimes n_\varepsilon |\nabla \psi_\varepsilon| dx \\
 &= \int \nabla H_I : n_\varepsilon \otimes n_\varepsilon |\nabla \psi_\varepsilon| dx - \varepsilon \int (\nabla H_I)_{ij} (\Pi_{Q_\varepsilon} \partial_i Q_\varepsilon : \Pi_{Q_\varepsilon} \partial_j Q_\varepsilon) dx \\
 &- \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \varepsilon \left((\partial_i Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_i Q_\varepsilon) : (\partial_j Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_j Q_\varepsilon) \right) dx \\
 &= \int \nabla H_I : n_\varepsilon \otimes n_\varepsilon \left(|\nabla \psi_\varepsilon| - \varepsilon |\nabla Q_\varepsilon|^2 \right) dx \\
 &+ \varepsilon \int \nabla H_I : (n_\varepsilon \otimes n_\varepsilon) \left(|\nabla Q_\varepsilon|^2 - |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right) dx \\
 &- \int \sum_{i,j=1}^3 (\nabla H_I)_{ij} \varepsilon \left((\partial_i Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_i Q_\varepsilon) : (\partial_j Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_j Q_\varepsilon) \right) dx = J_\varepsilon^1.
 \end{aligned}$$

Using the definition (4.8b) of n_ε , we may merge the second, third, and the last integral on the RHS of (4.32) to obtain

$$\begin{aligned} \frac{d}{dt} E_\varepsilon[Q_\varepsilon|I] &= -\varepsilon \int |\partial_t Q_\varepsilon|^2 dx + \int (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \partial_t Q_\varepsilon dx \\ &\quad + \int (\nabla \cdot \xi) H_I \cdot \nabla \psi_\varepsilon dx + \int H_\varepsilon \cdot H_I |\nabla Q_\varepsilon| dx \\ &\quad - \int \nabla H_I : (\xi - n_\varepsilon)^{\otimes 2} |\nabla \psi_\varepsilon| dx \\ &\quad + J_\varepsilon^1 + \int (\nabla \cdot H_I) \left(\frac{\varepsilon}{2} |\nabla Q_\varepsilon|^2 + \frac{1}{\varepsilon} F_\varepsilon(Q_\varepsilon) - |\nabla \psi_\varepsilon| \right) dx \\ &\quad + \int (\nabla \cdot H_I) (1 - \xi \cdot n_\varepsilon) |\nabla \psi_\varepsilon| dx + J_\varepsilon^2. \end{aligned}$$

Now we complete squares for the first four terms on the RHS of (4.33): Re-ordering terms, we have

$$\begin{aligned} &-\varepsilon |\partial_t Q_\varepsilon|^2 + (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \partial_t Q_\varepsilon + (\nabla \cdot \xi) H_I \cdot \nabla \psi_\varepsilon + H_\varepsilon \cdot H_I |\nabla Q_\varepsilon| \\ &= -\frac{1}{2\varepsilon} \left(|\varepsilon \partial_t Q_\varepsilon|^2 - 2(\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) : \varepsilon \partial_t Q_\varepsilon + (\nabla \cdot \xi)^2 |\nabla_q d_\varepsilon^F(Q_\varepsilon)|^2 \right) \\ &\quad - \frac{1}{2\varepsilon} |\varepsilon \partial_t Q_\varepsilon|^2 + \frac{1}{2\varepsilon} (\nabla \cdot \xi)^2 |\nabla_q d_\varepsilon^F(Q_\varepsilon)|^2 + (\nabla \cdot \xi) H_I \cdot \nabla \psi_\varepsilon \\ &\quad - \frac{1}{2\varepsilon} \left(|H_\varepsilon|^2 - 2H_\varepsilon \cdot \varepsilon |\nabla Q_\varepsilon| H_I + \varepsilon^2 |\nabla Q_\varepsilon|^2 |H_I|^2 \right) \\ &\quad + \frac{1}{2\varepsilon} \left(|H_\varepsilon|^2 + \varepsilon^2 |\nabla Q_\varepsilon|^2 |H_I|^2 \right) \\ &= -\frac{1}{2\varepsilon} \left| \varepsilon \partial_t Q_\varepsilon - (\nabla \cdot \xi) \nabla_q d_\varepsilon^F(Q_\varepsilon) \right|^2 - \frac{1}{2\varepsilon} \left| H_\varepsilon - \varepsilon |\nabla Q_\varepsilon| H_I \right|^2 \\ &\quad - \frac{1}{2\varepsilon} |\varepsilon \partial_t Q_\varepsilon|^2 + \frac{1}{2\varepsilon} |H_\varepsilon|^2 \\ &\quad + \frac{1}{2\varepsilon} \left((\nabla \cdot \xi)^2 |\nabla_q d_\varepsilon^F(Q_\varepsilon)|^2 + 2\varepsilon (\nabla \cdot \xi) \nabla \psi_\varepsilon \cdot H_I + |\varepsilon \Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 |H_I|^2 \right) \\ &\quad + \frac{\varepsilon}{2} \left(|\nabla Q_\varepsilon|^2 - |\Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right) |H_I|^2. \tag{4.33} \end{aligned}$$

Using the definition (4.8b) of the normal n_ε and the chain rule in form of (4.11a), the terms in (4.33) form the last missing square. Integrating over the domain Ω and substituting into (4.33) we arrive at (4.19). □

5. Convergence to the Harmonic Map Heat Flow

This section is devoted to the proof of Theorem 2.1. We start with a lemma about uniform estimates of Q_ε .

Lemma 5.1. *There exists a universal constant $C = C(I_0)$ such that*

$$\begin{aligned} & \operatorname{ess\,sup}_{t \in [0, T]} \int_{\Omega} \left(|\nabla Q_\varepsilon - \Pi_{Q_\varepsilon} \nabla Q_\varepsilon|^2 \right) dx \\ & + \int_0^T \int_{\Omega} \left(|\partial_t Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon|^2 \right) dx dt \leq e^{(1+T)C(I_0)}. \end{aligned} \quad (5.1)$$

Moreover, for any fixed $\delta \in (0, \delta_I)$, it holds that

$$\operatorname{ess\,sup}_{t \in [0, T]} \int_{\Omega^\pm(t) \setminus I_t(\delta)} \left(|\nabla Q_\varepsilon|^2 + \frac{F(Q_\varepsilon) + \varepsilon^3}{\varepsilon^2} \right) dx \leq \delta^{-2} e^{(1+T)C(I_0)}, \quad (5.2)$$

$$\int_0^T \int_{\Omega^\pm(t) \setminus I_t(\delta)} |\partial_t Q_\varepsilon|^2 dx dt \leq \delta^{-2} e^{(1+T)C(I_0)}. \quad (5.3)$$

Proof. We first establish a priori estimates of the solutions Q_ε which are independent of ε . It follows from (4.18) and the assumption (2.12) that

$$\begin{aligned} & \operatorname{ess\,sup}_{t \in [0, T]} \frac{1}{\varepsilon} E_\varepsilon[Q_\varepsilon | I](t) + \frac{1}{\varepsilon^2} \int_0^T \int_{\Omega} \left| \varepsilon \partial_t Q_\varepsilon - \nabla_q d_\varepsilon^F(Q_\varepsilon)(\nabla \cdot \xi) \right|^2 dx dt \\ & + \frac{1}{\varepsilon^2} \int_0^T \int_{\Omega} \left(\varepsilon^2 |\partial_t Q_\varepsilon|^2 - |H_\varepsilon|^2 + |H_\varepsilon - \varepsilon H_I |\nabla Q_\varepsilon|^2 \right) dx dt \\ & \leq \frac{e^{(1+T)C(I_0)}}{\varepsilon} E_\varepsilon[Q_\varepsilon | I](0) \leq e^{(1+T)C(I_0)}. \end{aligned} \quad (5.4)$$

On the other hand, using the orthogonal projection (4.10), we obtain

$$\begin{aligned} \left| \varepsilon \partial_t Q_\varepsilon - \nabla_q d_\varepsilon^F(Q_\varepsilon)(\nabla \cdot \xi) \right|^2 &= \left| \varepsilon \partial_t Q_\varepsilon - \varepsilon \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon \right|^2 \\ &+ \left| \varepsilon \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon - \nabla_q d_\varepsilon^F(Q_\varepsilon)(\nabla \cdot \xi) \right|^2. \end{aligned}$$

This, together with (5.4), yields

$$\begin{aligned} & \frac{1}{\varepsilon^2} \int_0^T \int_{\Omega} \left| \varepsilon \partial_t Q_\varepsilon - \varepsilon \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon \right|^2 \\ & + \frac{1}{\varepsilon^2} \int_0^T \int_{\Omega} \left| \varepsilon \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon - \nabla_q d_\varepsilon^F(Q_\varepsilon)(\nabla \cdot \xi) \right|^2 \leq e^{(1+T)C(I_0)}. \end{aligned} \quad (5.5)$$

The above two estimates together with (4.13b) implies (5.1). Moreover, (5.2) follows from (5.4) and (4.13e). Now we turn to the time derivative. It follows from (5.4) that

$$\frac{1}{\varepsilon^2} \int_0^T \int_{\Omega} \left(\varepsilon^2 |\partial_t Q_\varepsilon|^2 - |H_\varepsilon|^2 + |H_\varepsilon - \varepsilon H_I |\nabla Q_\varepsilon|^2 \right) dx dt \leq e^{(1+T)C(I_0)}. \quad (5.6)$$

By (1.13a) and (4.8a) we have $H_\varepsilon = -\varepsilon \partial_t Q_\varepsilon : \frac{\nabla Q_\varepsilon}{|\nabla Q_\varepsilon|}$. Using this, we can expand the integrand in the above estimate and apply the Cauchy-Schwarz inequality to obtain

$$\begin{aligned} & \varepsilon^2 |\partial_t Q_\varepsilon|^2 - |H_\varepsilon|^2 + |H_\varepsilon - \varepsilon H_I |\nabla Q_\varepsilon||^2 \\ &= \varepsilon^2 |\partial_t Q_\varepsilon|^2 + \varepsilon^2 |H_I|^2 |\nabla Q_\varepsilon|^2 + 2\varepsilon^2 (H_I \cdot \nabla) Q_\varepsilon : \partial_t Q_\varepsilon \\ &\geq \varepsilon^2 |\partial_t Q_\varepsilon|^2 + \varepsilon^2 |(H_I \cdot \nabla) Q_\varepsilon|^2 + 2\varepsilon^2 (H_I \cdot \nabla) Q_\varepsilon : \partial_t Q_\varepsilon \\ &= \varepsilon^2 |\partial_t Q_\varepsilon + (H_I \cdot \nabla) Q_\varepsilon|^2. \end{aligned}$$

This implies

$$\int_0^T \int_\Omega |\partial_t Q_\varepsilon + (H_I \cdot \nabla) Q_\varepsilon|^2 \, dx dt \leq e^{(1+T)C(I_0)}, \tag{5.7}$$

so combining (5.2) with (5.7) leads us to (5.3). □

With the above uniform estimates, we can prove the following convergence result:

Proposition 5.2. *There exists a subsequence of $\varepsilon_k > 0$ such that*

$$\begin{aligned} [\partial_t Q_{\varepsilon_k}, Q_{\varepsilon_k}] &= [\partial_t Q_{\varepsilon_k} - \Pi_{Q_{\varepsilon_k}} \partial_t Q_{\varepsilon_k}, Q_{\varepsilon_k}] \\ &\xrightarrow{k \rightarrow \infty} \bar{S}_0(x, t) \text{ weakly in } L^2(0, T; L^2(\Omega)), \end{aligned} \tag{5.8a}$$

$$\begin{aligned} [\partial_i Q_{\varepsilon_k}, Q_{\varepsilon_k}] &= [\partial_i Q_{\varepsilon_k} - \Pi_{Q_{\varepsilon_k}} \partial_i Q_{\varepsilon_k}, Q_{\varepsilon_k}] \\ &\xrightarrow{k \rightarrow \infty} \bar{S}_i(x, t) \text{ weakly-star in } L^\infty(0, T; L^2(\Omega)) \end{aligned} \tag{5.8b}$$

for $1 \leq i \leq d$. Moreover,

$$\partial_t Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \partial_t Q, \text{ weakly in } L^2(0, T; L^2_{loc}(\Omega^\pm(t))), \tag{5.9a}$$

$$\nabla Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \nabla Q, \text{ weakly in } L^\infty(0, T; L^2_{loc}(\Omega^\pm(t))), \tag{5.9b}$$

$$Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} Q, \text{ strongly in } C([0, T]; L^2_{loc}(\Omega^\pm(t))), \tag{5.9c}$$

where $Q = Q(x, t)$ is represented as

$$Q(x, t) = s^\pm \left(u(x, t) \otimes u(x, t) - \frac{1}{3} I_3 \right) \text{ a.e. } (x, t) \in \Omega_T^\pm \tag{5.10}$$

for some unit vector field

$$\begin{aligned} u \in L^\infty(0, T; H^1(\Omega^+(t); \mathbb{S}^2)) \cap H^1(0, T; L^2(\Omega^+(t); \mathbb{S}^2)) \\ \cap C([0, T]; L^2(\Omega^+(t); \mathbb{S}^2)). \end{aligned} \tag{5.11}$$

Proof. We first deduce from (1.6) and (2.10) that $d^F(Q)$ is an isotropic function, which only depends on the eigenvalue of $Q \in \mathcal{Q}$. So by (2.8b), the mollified distance function $d_\varepsilon^F(Q)$ is isotropic and smooth in Q . By [4] there exists a smooth symmetric function $g(\lambda_1, \lambda_2, \lambda_3)$ such that $d_\varepsilon^F(Q) = g(\lambda_1(Q), \lambda_2(Q), \lambda_3(Q))$. Let $Q_0 \in \mathcal{Q}$ be a matrix having distinct eigenvalues, then $\lambda_i(Q)$ as well as the eigenvectors $n_i(Q)$ are real-analytic functions of Q near Q_0 , and then by chain rule

$$\frac{\partial d_\varepsilon^F(Q)}{\partial Q} = \sum_{k=1}^3 \frac{\partial g}{\partial \lambda_k} \frac{\partial \lambda_k}{\partial Q} = \sum_{k=1}^3 \frac{\partial g}{\partial \lambda_k} n_k(Q) \otimes n_k(Q),$$

in a neighborhood of Q_0 . (5.12)

In a neighborhood of Q_0 , we also have $Q = \sum_{k=1}^3 \lambda_k(Q) n_k(Q) \otimes n_k(Q)$. So we have

$$\left[\nabla_Q d_\varepsilon^F(Q), Q \right] = 0, \tag{5.13}$$

holds in a neighborhood of Q_0 having distinct eigenvalues, and thus for every $Q \in \mathcal{Q}$ by continuity. Now in view of (4.10), we have

$$\begin{aligned} [\Pi_{Q_\varepsilon} \partial_t Q_\varepsilon(x, t), Q_\varepsilon(x, t)] &= 0, \\ [\Pi_{Q_\varepsilon} \partial_i Q_\varepsilon(x, t), Q_\varepsilon(x, t)] &= 0 \text{ a.e. } (x, t) \in \Omega_T \end{aligned} \tag{5.14}$$

for $1 \leq i \leq d$. This together with (3.29) and (5.1) implies

$$\begin{aligned} &\| [\partial_t Q_\varepsilon, Q_\varepsilon] \|_{L^2(0, T; L^2(\Omega))} + \| [\nabla Q_\varepsilon, Q_\varepsilon] \|_{L^\infty(0, T; L^2(\Omega))} \\ &= \| [\partial_t Q_\varepsilon - \Pi_{Q_\varepsilon} \partial_t Q_\varepsilon, Q_\varepsilon] \|_{L^2(0, T; L^2(\Omega))} \\ &\quad + \| [\nabla Q_\varepsilon - \Pi_{Q_\varepsilon} \nabla Q_\varepsilon, Q_\varepsilon] \|_{L^\infty(0, T; L^2(\Omega))} \leq C \end{aligned} \tag{5.15}$$

for some C independent of ε . Combining this estimate with weak compactness implies (5.8).

It follows from (5.2), (5.3), (3.29), and the Aubin-Lions lemma that, for any $\delta > 0$, there exists a subsequence $\varepsilon_k = \varepsilon_k(\delta) > 0$ such that

$$\partial_t Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \partial_t \bar{Q}_\delta, \text{ weakly in } L^2(0, T; L^2(\Omega^\pm(t) \setminus I_t(\delta))), \tag{5.16a}$$

$$\nabla Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \nabla \bar{Q}_\delta, \text{ weakly-star in } L^\infty(0, T; L^2(\Omega^\pm(t) \setminus I_t(\delta))), \tag{5.16b}$$

$$Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \bar{Q}_\delta, \text{ weakly-star in } L^\infty(\Omega \times (0, T)), \tag{5.16c}$$

$$Q_{\varepsilon_k} \xrightarrow{k \rightarrow \infty} \bar{Q}_\delta, \text{ strongly in } C([0, T]; L^2(\Omega^\pm(t) \setminus I_t(\delta))). \tag{5.16d}$$

By a diagonal argument, we infer there exists

$$Q \in L^2(0, T; H^1_{loc}(\Omega^\pm(t))) \cap L^\infty(\Omega^\pm), \text{ with } \partial_t Q \in L^2(0, T; L^2_{loc}(\Omega^\pm(t))) \tag{5.17}$$

such that the convergence (5.9) as well as

$$Q(x, t) = \bar{Q}_\delta(x, t) \text{ in } L^\infty(0, T; H^1(\Omega^\pm(t) \setminus I_t(\delta)))$$

hold for every $\delta > 0$ and every $t \in [0, T]$. Moreover, by (5.17), the interpolation theory and (5.16c), we have

$$Q \in C([0, T]; L^2(\Omega^\pm(t)) \cap L^\infty(\Omega \times (0, T))).$$

To prove (5.10), we first deduce that $F(Q)$ has the same regularity as Q in (5.17), and thus by interpolation theory we obtain

$$F(Q) \in C([0, T]; L^2(\Omega^\pm(t))).$$

We use (5.9c), (5.2), and Fatou’s lemma to deduce that

$$F(Q(x, t)) = 0, \quad \forall t \in [0, T] \text{ and a.e. in } x \in \Omega^\pm(t). \tag{5.18}$$

This, together with (1.10), implies

$$|Q|(x, t) \in \{0, s^+ \sqrt{\frac{2}{3}}\}, \quad \forall t \in [0, T] \text{ and a.e. in } x \in \Omega^\pm(t). \tag{5.19}$$

By taking the L^2 -norm, we obtain two continuous functions:

$$f^\pm(t) := \|Q(\cdot, t)\|_{L^2(\Omega^\pm(t))} \in C([0, T]; \{0, s^+ \sqrt{\frac{2}{3}|\Omega^\pm(t)|}\}).$$

On the other hand, by the choice of the initial condition (2.21) and the convergence (5.16d), we deduce that

$$Q(x, 0) = \mathbf{1}_{\Omega^+(0)} s^+ \left(u^{in}(x) \otimes u^{in}(x) - \frac{1}{3} I_3 \right), \quad \text{a.e. in } \Omega^\pm(0) \setminus I_0(\delta)$$

for any $\delta > 0$ and thus for $\delta = 0$. This implies $f^+(0) = s^+ \sqrt{\frac{2}{3}|\Omega^+(0)|}$, $f^-(0) = 0$ and thus

$$f^+(t) = s^+ \sqrt{\frac{2}{3}|\Omega^+(t)|}, \quad f^-(t) = 0, \quad \forall t \in [0, T].$$

This, together with (5.19), implies

$$Q(x, t) = 0, \quad \forall t \in [0, T] \text{ and a.e. in } x \in \Omega^-(t), \tag{5.20}$$

$$Q(x, t) \in \mathcal{N}, \quad \forall t \in [0, T] \text{ and a.e. in } x \in \Omega^+(t), \tag{5.21}$$

and thus (5.10) is proved.

By (5.10), (5.17), and the orientability theorem by Ball–Zarnescu [6, Section 3.2] implies that Q is uniaxial (5.10) for some

$$u \in L^\infty(0, T; H^1_{loc}(\Omega^+(t); \mathbb{S}^2)) \text{ with } \partial_t u \in L^2(0, T; L^2_{loc}(\Omega^+(t); \mathbb{S}^2)). \tag{5.22}$$

It remains to improve the integrability of $\nabla_{x,t} u$. To this end, we choose a sequence

$$\psi_\ell(x, t) \in C^\infty_c(\Omega^+_T) \text{ such that } \psi_\ell(x, t) \xrightarrow{\ell \rightarrow \infty} \mathbf{1}_{\Omega^+_T}(x, t). \tag{5.23}$$

Since $|u| = 1$ a.e., by (5.8a), (5.8b) and (5.9), we deduce that for almost every $(x, t) \in \Omega_T^+$, it holds that

$$\psi_\ell \bar{S}_i = \psi_\ell [\partial_i Q, Q] = s_+^2 \psi_\ell (\partial_i u \otimes u - u \otimes \partial_i u), \quad 0 \leq i \leq d, \quad (5.24)$$

where $\partial_0 := \partial_t$. Note that for each fixed $i \in \{0, \dots, 3\}$,

$$\partial_i u \otimes u - u \otimes \partial_i u = \begin{pmatrix} 0 & (\partial_i u \wedge u)_3 & -(\partial_i u \wedge u)_2 \\ -(\partial_i u \wedge u)_3 & 0 & (\partial_i u \wedge u)_1 \\ (\partial_i u \wedge u)_2 & -(\partial_i u \wedge u)_1 & 0 \end{pmatrix}, \quad (5.25)$$

where $(\partial_i u \wedge u)_k$ denotes the k -th component of the 3-vector $\partial_i u \wedge u$. Since \bar{S}_i are L^2 integrable in Ω_T , sending $\ell \rightarrow \infty$ and applying the dominated convergence theorem to the above identity lead us to

$$\partial_t u \wedge u \in L^\infty(0, T; L^2(\Omega^+(t))), \quad (5.26a)$$

$$\partial_i u \wedge u \in L^2(0, T; L^2(\Omega^+(t))), \quad \text{for } i \in \{1, \dots, d\}. \quad (5.26b)$$

Retaining that u maps into S^2 , we deduce

$$|\partial_t u|^2 = |\partial_t u \wedge u|^2, \quad |\partial_i u|^2 = |\partial_i u \wedge u|^2 \text{ a.e. in } \Omega_T^+, \quad 1 \leq i \leq d,$$

so we improve (5.22) to (5.11). □

Proof of Theorem 2.1. In the course of the proof, we shall adopt the notation $A : B = \text{tr } A^T B$ for any $A, B \in \mathbb{R}^{3 \times 3}$. We associate each testing vector field $\varphi(x, t) = (\varphi_1, \varphi_2, \varphi_3) \in C^1(\bar{\Omega}_T, \mathbb{R}^3)$ a matrix-valued function

$$\Phi(x, t) = \begin{pmatrix} 0 & \varphi_3 & -\varphi_2 \\ -\varphi_3 & 0 & \varphi_1 \\ \varphi_2 & -\varphi_1 & 0 \end{pmatrix} \quad (5.27)$$

Since $[\nabla_q F(Q_{\varepsilon_k}), Q_{\varepsilon_k}] = 0$, applying the anti-symmetric product $[\cdot, Q_{\varepsilon_k}]$ to (1.13a) and integration by parts over Ω_T yields

$$\int_{\Omega_T} [\partial_t Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \Phi \, dxdt + \int_{\Omega_T} \sum_{j=1}^3 [\partial_j Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \partial_j \Phi \, dxdt = 0. \quad (5.28)$$

Note that no boundary integral will occur due to (1.13c). Recall that we denote $I_t(\delta)$ the δ -neighborhood of I_t . Equivalently, we can write the above equation by

$$\begin{aligned} & \sum_{\pm} \int_0^T \int_{\Omega^\pm(t) \setminus I_t(\delta)} \left([\partial_t Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \Phi + \sum_{j=1}^3 [\partial_j Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \partial_j \Phi \right) dxdt \\ & + \int_0^T \int_{I_t(\delta)} \left([\partial_t Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \Phi + \sum_{j=1}^3 [\partial_j Q_{\varepsilon_k}, Q_{\varepsilon_k}] : \partial_j \Phi \right) dxdt = 0. \end{aligned} \quad (5.29)$$

Using (5.9), (5.8) and (5.10), we can pass $k \rightarrow \infty$ and yield

$$\int_0^T \int_{\Omega^+(t) \setminus I_t(\delta)} \left([\partial_t Q, Q] : \Phi + \sum_{j=1}^3 [\partial_j Q, Q] : \partial_j \Phi \right) dxdt + \int_0^T \int_{I_t(\delta)} \left(\bar{S}_0 : \Phi + \sum_{j=1}^3 \bar{S}_j : \partial_j \Phi \right) dxdt = 0. \tag{5.30}$$

By $|u| = 1$ a.e., (5.10), (5.27) and (5.25), we obtain the following identities :

$$[\partial_t Q, Q] : \Phi = s_+^2 (\partial_t u \otimes u - u \otimes \partial_t u) : \Phi = 2s_+^2 \partial_t u \wedge u \cdot \varphi$$

$$[\partial_j Q, Q] : \partial_j \Phi = s_+^2 (\partial_j u \otimes u - u \otimes \partial_j u) : \partial_j \Phi = 2s_+^2 \partial_j u \wedge u \cdot \partial_j \varphi$$

Thus we obtain

$$2s_+^2 \int_0^T \int_{\Omega^+(t) \setminus I_t(\delta)} \left(\partial_t u \wedge u \cdot \varphi + \sum_{j=1}^3 (\partial_j u \wedge u) \cdot \partial_j \varphi \right) dxdt + \int_0^T \int_{I_t(\delta)} \left(\bar{S}_0 : \Phi + \sum_{j=1}^3 \bar{S}_j : \partial_j \Phi \right) dxdt = 0. \tag{5.31}$$

Due to (5.11) we have the absolute continuity of $\partial_t u \wedge u$ and $\nabla u \wedge u$ in Ω_T^+ . Moreover, (5.8) implies the absolute continuity of $\{\bar{S}_i\}_{0 \leq i \leq d}$ in Ω_T . So we can pass to the limit $\delta \rightarrow 0$ in the above identity, which yields

$$\int_0^T \int_{\Omega^+(t)} \partial_t u \wedge u \cdot \varphi dxdt + \int_0^T \int_{\Omega^+(t)} \sum_{j=1}^3 (\partial_j u \wedge u) \cdot \partial_j \varphi dxdt = 0. \tag{5.32}$$

This concludes the proof of Theorem 2.1. □

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