FINITE ELEMENT ANALYSIS OF THE LANDAU-DE GENNES MINIMIZATION PROBLEM FOR LIQUID CRYSTALS*

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Abstract. This paper describes the Landau-de Gennes free-energy minimization problem for computing equilibrium configurations of the tensor order parameter field that characterizes the molecular orientational properties of liquid crystal materials. Analytical and numerical issues are addressed. Conditions guaranteeing well posedness (existence, regularity) of the problem are given, as is a nonlinear finite element convergence analysis.

Key words. Liquid crystals, finite elements, nonlinear convergence analysis, Landau-de Gennes free energy

AMS subject classifications. primary 65N30; secondary 35J50, 82D30

1. Introduction.

Liquid crystal materials have generated a great deal of interest in recent years. In addition to their practical uses in display, diagnostic, and other devices, they are a source of interesting problems in applied mathematics and numerical analysis. Some general references include [10, 17, 43, 48].

We are concerned primarily with using continuum models to determine the equilibrium structure (orientational order) of the rod-like molecules in confined liquid-crystal systems. Our interest in these problems is driven by applications in the Liquid Crystal Institute and NSF Science and Technology Center on "Advanced Liquid Crystalline Optical Materials" (ALCOM) at Kent State University. For these applications, the typical confining geometry is microscopic: pixels in active-matrix displays, spherical droplets in polymer-dispersed liquid crystals (PDLC's), cylindrical pores in films, filters, and gels, etc.

The models we consider here can be posed as minimization problems for integral functionals of an unknown tensor field. The functionals depend on a number of parameters and are not convex, in general; they are known as "Landau-de Gennes free-energy functionals." The tensor field, which is to be determined, is known as the "tensor order parameter." We give some background.

For a particular substance, the transition between phases of different symmetry (e.g., crystal to liquid) can be described in terms of an *order parameter*. The order parameter quantifies the difference between the configuration of the less symmetric phase and that of the more symmetric phase [28, 46]. In general, an order parameter is zero in the more symmetric (less ordered) phase and is non-zero in the less symmetric (more ordered) phase. Depending upon the physical system being studied and the underlying assumptions used, an order parameter can be a scalar, a vector, or a tensor quantity. A familiar example is the complex scalar order parameter in the Ginzburg-Landau model for super-conductivity [18].

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Over certain temperature ranges, many materials exhibit a *nematic liquid crystal* phase. This is a *mesophase*, a phase that exhibits orientational order (like a crystal) but no positional order (like an isotropic liquid). Generally, the orientational properties of liquid crystals are described by an order parameter, Q, which is a rank-two, symmetric, traceless tensor [16, 37, 48]. That is, $Q = Q_{\alpha\beta}$ ($\alpha, \beta = 1, 2, 3$), with

$$Q_{\beta\alpha} = Q_{\alpha\beta} \quad \text{and} \quad \mathrm{tr}(Q) = Q_{\alpha\alpha} = 0\,.$$

Here and below, we utilize the summation convention, where summation over repeated indices is implied, and $\mathrm{tr}(\cdot)$ denotes the usual trace of a matrix.

More specifically, the tensor order parameter contains information about the degree of order and the anisotropy of the liquid crystal at a point in space. The eigenvectors of Q give the directions of preferred orientation of the molecules, and the eigenvalues give the degree of order about these directions. These ideas are expressed more rigorously in [31].

One advantage of such a general order parameter is that it admits orientations for which the thermal vibrations of the molecule about its preferred axis of orientation are not rotationally symmetric about this axis (*biaxiality*). Biaxiality is known to occur in a number of circumstances (e.g., in the neighborhood of certain defects), and not all models of liquid crystal behavior can account for it [28].

Confined liquid crystal materials proceed to a configuration (ground state) that minimizes the thermodynamic *free energy*, which involves both internal (strain) energy and entropy. The free-energy minimization requires the determination of minimizers (or, more generally, stationary points) of a nonlinear functional of the state variable, which in our case is a tensor field. Other widely used continuum models utilize vector fields. For the vector models, the free-energy functionals are given by the theories of Oseen [42], Zöcher [49], and Frank [22], and the generalization due to Ericksen [19]. For the tensor models, the Landau-de Gennes theory is used.

The Oseen-Zöcher-Frank models have generally received more analytical and computational attention [13, 32, 36]. This theory is applicable and useful over a wide range of physical situations but is limited by its inability to represent certain known physical phenomena: spatially varying degree of orientational order (in the original formulations) and biaxiality (in both the original and generalized versions). The Landau-de Gennes models have been studied computationally [8, 24, 25, 44] but to a lesser extent, because of their increased complexity.

The Landau-de Gennes free-energy functionals grow out of the Landau theory of phase transitions [35]. To generalize the continuum model of Oseen, Zöcher, and Frank, P.G. de Gennes proposed a Ginzburg-Landau expansion for the free energy, $\mathcal{F}$, of a liquid crystal near the point of its nematic-isotropic phase transition [16, 17]. The expansion involves the order parameter Q and its spatial derivatives [17, 37]. For the liquid crystal systems we consider, the free energy provides a criterion for equilibrium: $\mathcal{F}$ will be a minimum when the system is in equilibrium [4]. We are thus led to the problem of numerically computing order parameter tensor fields Q that minimize $\mathcal{F}$.

The densities for the integral Landau-de Gennes functionals are constructed using truncated expansions involving powers of the components of the tensor order parameter, Q, and its gradient, ∂Q, subject to symmetry and invariance principles. They have a certain general structure, but the form of the individual terms may vary. We have developed a numerical package to compute equilibrium configurations using a particular Landau-de Gennes free energy in the geometry of a circular cylinder [15]. We present an analysis for a more general form of functional; it applies to that in our code as well as to other free-energy densities of which we are aware.

These functionals all contain several material-dependent parameters and typically admit multiple local minimizers and undergo structural phase transitions and bifurcations at critical values of these constants. This is an important aspect of these problems, and these points and the behavior in the vicinity of them are often the issues of greatest interest. This is emphasized in the formulation of our problems; although the present convergence analysis applies only to regular solution branches.

An outline of the paper is as follows. In the next section, a statement of the general minimization problem and notation are given. Analytical background (function spaces, embeddings, etc.) is given in §3. Existence of solutions of the general minimization problem is established in §4. The variational formulation of the problem is discussed in §5; regularity in §6; and the finite element convergence analysis is given in the final section, §7.

2. Statement of the minimization problem. Let Ω be a bounded, open, connected subset of $\mathbf{R}^3$ with boundary Γ. We always assume that Γ is sufficiently regular for the Sobolev embedding and trace theorems to hold—for example, Lipschitz continuous is sufficient [1]. Further restrictions on Ω are introduced as required in the analyses that follow.

Let $x := (x_1, x_2, x_3) \in \Omega$, and let $Q = Q(x)$ be a symmetric, rank-two tensor field having zero trace. We define the *Landau-de Gennes free energy functional*

$$\begin{aligned} \mathcal{F}(Q) &:= \mathcal{F}_E(Q) + \mathcal{F}_B(Q) + \mathcal{F}_S(Q) - \mathcal{F}_L(Q) \\ &= \int_\Omega \{f_E(\partial Q) + f_B(Q)\} + \int_\Gamma \{f_S(Q)\} - \mathcal{F}_L(Q)\,. \end{aligned} \tag{2.1}$$

Here, the terms $f_E(\partial Q)$ and $f_B(Q)$ are the volumetric free-energy densities due to *elastic* and *bulk* contributions; the term $f_S(Q)$ is the *surface* free-energy density; and $\mathcal{F}_L(Q)$ is a *linear* functional. The problem is to find minimizers of $\mathcal{F}(Q)$ over sets of admissible tensor fields Q.

The elastic term consists of the three independent forms that are quadratic in the first partial derivatives of the components of Q and which are invariant under rigid rotations. They give the strain energy density due to spatial variations in the tensor order parameter. Specifically,

$$f_E(\partial Q) := \frac{1}{2}L_1\, Q_{\alpha\beta,\gamma}Q_{\alpha\beta,\gamma} + \frac{1}{2}L_2\, Q_{\alpha\beta,\beta}Q_{\alpha\gamma,\gamma} + \frac{1}{2}L_3\, Q_{\alpha\beta,\gamma}Q_{\alpha\gamma,\beta}\,, \tag{2.2}$$

where L_1, L_2, and L_3 are the material *elastic constants* and $Q_{\alpha\beta,\gamma}$ denotes $\partial Q_{\alpha\beta}/\partial x_\gamma$. Summation over repeated indices is always assumed.

The bulk free energy density is typically a truncated expansion in the scalar invariants of the tensor Q. The form that we use in the code is

$$\begin{aligned} f_B(Q) := {}& \frac{1}{2}A\,\mathrm{tr}(Q^2) - \frac{1}{3}B\,\mathrm{tr}(Q^3) + \frac{1}{4}C\,\mathrm{tr}(Q^2)^2 \\ &+ \frac{1}{5}D\,\mathrm{tr}(Q^2)\mathrm{tr}(Q^3) + \frac{1}{6}E\,\mathrm{tr}(Q^2)^3 + \frac{1}{6}E'\,\mathrm{tr}(Q^3)^2\,, \end{aligned} \tag{2.3}$$

where A, B, C, D, E, and E' are the material *bulk constants* [17]. More general bulk densities can be obtained by including higher order terms. The factors $\mathrm{tr}(Q^2)$ and

$\mathrm{tr}(Q^3)$ are homogeneous polynomials of degrees two and three, respectively, in the components of Q.

This bulk term embodies the ordering/disordering (entropic) effects, which drive the nematic-isotropic phase transition. Meaningful simulations can be performed using an expansion truncated at the fourth order. One needs to go at least out to this order to have a potential with multiple stable local minima. The sixth-order terms are needed if one wishes to have a stable biaxial phase "in the bulk" (no boundaries, no spatial variation) [28]. At a minimum, we will require that f_B is a continuous function and that it is bounded from below.

In general, the surface free-energy density f_S is a truncated expansion much like the bulk density f_B. However the appropriate form seems to be less well settled. The difficulty is that one doesn't have in general the same frame invariance, as the geometry of the boundary can break some of the symmetries. The form that we have employed in our finite element code is

$$f_S(Q) := \frac{1}{2} W \,\mathrm{tr}\left((Q - Q_0)^2 \right) , \tag{2.4}$$

where W is the *surface anchoring strength/constant* and Q_0 is a prescribed tensor field on the boundary Γ.

In this form, the surface integral imposes a free-energy penalty (for $W > 0$) on those configurations that fail to align at the boundary with the field Q_0. Indeed, (2.4) is the tensorial analog of the surface integrand that arises in the variational formulation of the inhomogeneous mixed problem for the scalar Laplacian. Conceivably, the boundary could be subdivided into a finite number of pieces with W then being piecewise constant (constant on each sub-piece), or W could be an essentially bounded function of x on the boundary. We require that f_S satisfy the same minimal conditions as f_B, namely continuity and boundedness from below.

The linear functional $\mathcal{F}_L$ will be continuous in the topology introduced in the next section. It contains effects that couple linearly to Q, e.g., the free-energy density due to an externally applied magnetic field (of low intensity), the linear part of a surface potential, etc. A typical form would be

$$\mathcal{F}_L(Q) = \int_\Omega \mathrm{tr}(FQ) + \int_\Gamma \mathrm{tr}(GQ) , \tag{2.5}$$

where the components of the F and G tensors are square integrable. More general linear forms can occur, e.g., $\int_\Omega F_{\alpha\beta\gamma} Q_{\alpha\beta,\gamma}$; however these do not appear to be common.

For example, for the case of an external magnetic field, $\boldsymbol{H}$, the free-energy density takes the form

$$\frac{1}{2} \boldsymbol{H} \cdot \boldsymbol{B} = \frac{1}{2} H_\alpha \mu_{\alpha\beta} H_\beta = \frac{1}{2} \chi_a H_\alpha Q_{\alpha\beta} H_\beta + \frac{1}{2} \chi_0 H_\alpha H_\beta ,$$

which can be put in the form (2.5) (modulo an additive constant) with $F_{\alpha\beta} := \chi_a H_\alpha H_\beta / 2$. Here, $\boldsymbol{B}$ is the magnetic flux density (or induction, related to the external field via $B_\alpha = \mu_{\alpha\beta} H_\beta$), and we have used the fact that the anisotropic part of the permeability tensor, μ, is proportional to Q (with proportionality constant χ_a). The last term above comes from the isotropic part of the μ tensor (with χ_0 a scalar); it does not depend on Q and therefore only contributes a constant to the free energy and does not affect the equilibrium configurations. In our code, we use a form similar to (2.5) but with F a constant tensor (to handle the magnetic-field case) and $G = 0$ (effectively absorbed into the surface density (2.4)).

It is important to note that the free-energy functional (2.1) depends explicitly on the elastic and bulk constants, the surface anchoring coefficients, and any parameters that may be present in $\mathcal{F}_L$ (e.g., magnetic field strength). These dependencies lead us to view minimizers Q of (2.1) as implicit functions $Q(\lambda)$, where λ is some physical parameter which can assume a continuous range of values. Frequently, λ is chosen to be (absolute) temperature, T, and the bulk parameter A is assumed to have the form $A = A_0(T - T_0)$, where A_0 and T_0 are constants. In that case, the minimizers Q are functions of T, and it is of interest to perform continuation in the variable T and to study the changes in the equilibrium configuration of the liquid crystal material as T varies. Other choices for the continuation parameter include the surface anchoring strength W, external field strength, and the geometric dimensions of Ω. The elastic constants, L_1, L_2, and L_3, can also vary near certain critical temperatures and such.

This paper addresses both theoretical and computational aspects of the Landau-de Gennes minimization problem. We present a discussion of appropriate function spaces in which to set the problem; existence and regularity results associated with the minimization problem; some analysis regarding a variational formulation of the problem; and a convergence analysis for finite element methods applied to this nonlinear problem.

3. Function spaces, embeddings, and mathematical notation. In this section, we define a number of function spaces and introduce much of the notation to be used in the analysis in the sections that follow. Most definitions conform to those of Ciarlet as given in [11] or [12]. The reader is referred to those sources for additional details.

Let $|\cdot|_{m,\Omega}$ and $\|\cdot\|_{m,\Omega}$ denote the usual semi-norm and norm on the Sobolev space $H^m(\Omega)$. Let $H_0^m(\Omega)$ be the subspace of $H^m(\Omega)$ consisting of those functions whose normal derivatives through order $m-1$ vanish (in the sense of traces) on the boundary of Ω. The dual of $H_0^m(\Omega)$ is denoted $H^{-m}(\Omega)$ and is equipped with the usual dual space norm. The space of bounded, continuous functions on Ω (normed by the maximum norm) is denoted $C(\overline{\Omega})$.

We introduce the following notations for sets of symmetric and symmetric/traceless tensors:

$$\mathbf{S} := \left\{ Q \in \mathbf{R}^{3\times 3} : Q_{\beta\alpha} = Q_{\alpha\beta} \right\}, \qquad \mathbf{S}_0 := \left\{ Q \in \mathbf{S} : \operatorname{tr}(Q) = 0 \right\}.$$

The set $\mathbf{S}$ is a six dimensional subspace of $\mathbf{R}^{3\times 3}$; $\mathbf{S}_0$ is a five dimensional subspace of $\mathbf{S}$; the bilinear form $(Q, P) \in \mathbf{S} \times \mathbf{S} \mapsto \operatorname{tr}(QP)$ is an inner product on $\mathbf{S}$; and $Q \in \mathbf{S} \mapsto |Q| = \sqrt{\operatorname{tr}(Q^2)}$ is a norm.

We write $\mathbf{H}^m(\Omega)$ for the vector-valued function space $H^m(\Omega\,; \mathbf{R}^5)$ and $\mathcal{H}^m(\Omega)$ for the tensor-valued function space $H^m(\Omega\,; \mathbf{S}_0)$. Analogous definitions hold for the spaces $\mathbf{L}^p(\Omega)$, $\mathcal{L}^p(\Omega)$, $\mathbf{C}(\overline{\Omega})$, and $\mathcal{C}(\overline{\Omega})$. The norms in these new spaces are understood to be the usual Cartesian product norms. In particular, $\mathcal{L}^2(\Omega)$ and $\mathcal{H}^1(\Omega)$ are Hilbert spaces with inner products

$$(Q, P)_0 := \int_\Omega Q_{\alpha\beta} P_{\alpha\beta}\,, \qquad (Q, P)_1 := \int_\Omega \left\{ Q_{\alpha\beta} P_{\alpha\beta} + Q_{\alpha\beta,\gamma} P_{\alpha\beta,\gamma} \right\},$$

and norms

$$\|Q\|_{0,\Omega}^2 := (Q, Q)_0\,, \qquad \|Q\|_{1,\Omega}^2 := (Q, Q)_1\,,$$

and semi-norm

$$|Q|_{1,\Omega}^2 := \int_\Omega Q_{\alpha\beta,\gamma} Q_{\alpha\beta,\gamma} = \int_\Omega |\partial Q|^2 .$$

Note that for symmetric tensors, we have $Q_{\alpha\beta} P_{\alpha\beta} = Q_{\alpha\beta} P_{\beta\alpha} = \mathrm{tr}(QP)$; so

$$(Q, P)_0 = \int_\Omega \mathrm{tr}(QP) \qquad \text{and} \qquad \|Q\|_{0,\Omega}^2 = |Q|_{0,\Omega}^2 = \int_\Omega \mathrm{tr}(Q^2) = \int_\Omega |Q|^2 .$$

The same symbols will be used to represent norms in the vector and tensor function spaces as are used in their scalar counterparts. The proper interpretation should be clear from context. In cases where there is ambiguity, the norm symbol will be subscripted by the name of the space in which it is to be taken.

We recall the Sobolev embeddings

$$\begin{aligned} H^1(\Omega) &\hookrightarrow L^q(\Omega) , \quad 1 \le q \le 6 , \\ H^1(\Omega) &\overset{c}{\hookrightarrow} L^q(\Omega) , \quad 1 \le q < 6 , \end{aligned} \tag{3.1}$$

and

$$H^2(\Omega) \overset{c}{\hookrightarrow} H^1(\Omega) , \qquad H^2(\Omega) \overset{c}{\hookrightarrow} C(\overline{\Omega}) , \tag{3.2}$$

and dual embeddings

$$\begin{aligned} L^q(\Omega) &\hookrightarrow H^{-1}(\Omega) , \quad q \ge 6/5 , \\ L^q(\Omega) &\overset{c}{\hookrightarrow} H^{-1}(\Omega) , \quad q > 6/5 , \end{aligned} \tag{3.3}$$

and trace theorems

$$\begin{aligned} H^1(\Omega) &\to L^q(\Gamma) , \quad 1 \le q \le 4 , \\ H^1(\Omega) &\overset{c}{\to} L^q(\Gamma) , \quad 1 \le q < 4 , \end{aligned} \tag{3.4}$$

which hold for sufficiently regular $\Omega \subset \mathbf{R}^3$ and boundary Γ (as we have assumed to be the case for our problem) [1, 29]. Here $\hookrightarrow$ denotes continuous embedding, and $\overset{c}{\hookrightarrow}$ denotes compact embedding. The symbols $\to$ and $\overset{c}{\to}$ denote the continuous and compact actions of the boundary trace operator. These embeddings remain valid for the vector and tensor function spaces previously defined.

By definition, any field Q that is to be admissible for the Landau-de Gennes minimization problem must be symmetric and traceless. This means that it has only five independent components—symmetry removes three, and tracelessness, one. Following Gartland, Palffy-Muhoray, and Varga [25], we introduce a convenient representation for any such tensor Q.

Let $\{E^i\}_{i=1}^5$ be an orthonormal basis for $\mathbf{S}_0$, that is, one which satisfies $\mathrm{tr}(E^i E^j) = \delta_{ij}$. Various such bases can be constructed. In our code, we use the one from [25]. Then any $Q \in \mathbf{S}_0$ has the unique representation

$$Q = q_i E^i , \quad \text{where } q_i = \mathrm{tr}(Q E^i) . \tag{3.5}$$

We refer to $\boldsymbol{q} := (q_1, \dots, q_5)$ as the *scalar coordinates* of Q (with respect to the basis $\{E^i\}_{i=1}^5$). The scalar coordinates have a number of uses. First, they provide a convenient way of defining the nodal variables in a finite element discretization. Second, the mapping $Q \in \mathbf{S}_0 \leftrightarrow \boldsymbol{q} \in \mathbf{R}^5$ implicitly defined by (3.5), establishes an isometric isomorphism between $\mathcal{H}^m$ and $\mathbf{H}^m$, $m \ge 0$ [15]. Consequently, there is no essential difference between analyzing $\mathcal{F}(Q)$ and analyzing $F(\boldsymbol{q}) := \mathcal{F}(q_i E^i)$, and in a given situation, one representation may be more useful than the other.

4. Existence of minimizers. We develop conditions under wich the existence of a minimizer for $\mathcal{F}$ in certain spaces of admissible tensor fields can be established. First we show that the quadratic form associated with the elastic part of the free energy is, under appropriate conditions, equivalent to the $\mathcal{H}^1$-semi-norm, and, as a consequence, is $\mathcal{H}_0^1$-elliptic.

LEMMA 4.1. *Let $a(\cdot,\cdot) : \mathcal{H}^1(\Omega) \times \mathcal{H}^1(\Omega) \to \mathbf{R}$ be defined by*

$$a(Q,P) := \int_\Omega \{L_1 Q_{\alpha\beta,\gamma} P_{\alpha\beta,\gamma} + L_2 Q_{\alpha\beta,\beta} P_{\alpha\gamma,\gamma} + L_3 Q_{\alpha\beta,\gamma} P_{\alpha\gamma,\beta}\}\,. \tag{4.1}$$

Then $a(\cdot,\cdot)$ is symmetric, bilinear, and bounded. If the elastic constants L_1, L_2, and L_3 satisfy

$$0 < L_1\,, \qquad -L_1 < L_3 < 2L_1\,, \qquad -\frac{3}{5}\,L_1 - \frac{1}{10}\,L_3 < L_2\,, \tag{4.2}$$

then there is a real number $\alpha > 0$ such that $a(Q,Q) \geq \alpha\,|Q|^2_{1,\Omega}$ for every Q in $\mathcal{H}^1(\Omega)$. As a consequence, $a(\cdot,\cdot)$ is $\mathcal{H}_0^1$-elliptic, in the sense that there exists $\alpha' > 0$ such that $a(Q,Q) \geq \alpha'\,\|Q\|^2_{1,\Omega}$ for every Q in $\mathcal{H}_0^1(\Omega)$.

Proof. The symmetry and bilinearity of $a(\cdot,\cdot)$ are clear. Boundedness follows by application of the Cauchy-Schwarz inequalities for integrals and for sums.

In [37], Longa, Monselesan, and Trebin use "spherical tensors" (from angular momentum theory) to show that the (pointwise) tensorial expression that forms the integrand of (4.1) is a positive definite function of ∂Q if and only if the constants L_1, L_2, and L_3 satisfy a system of inequalities equivalent to (4.2) [37, (18a), p. 781]. Assuming (4.2) to hold, it then follows that there exists a constant α such that

$$a(Q,Q) \geq \alpha\,|Q|^2_{1,\Omega}\,, \quad \forall Q \in \mathcal{H}^1(\Omega)\,.$$

Finally, for $Q \in \mathcal{H}_0^1(\Omega)$, an application of the Poincaré inequality [11, 29] yields

$$a(Q,Q) \geq \alpha'\,\|Q\|^2_{1,\Omega}\,, \quad \forall Q \in \mathcal{H}_0^1(\Omega)\,,$$

where α' is a positive constant that depends only on Ω and the elastic constants L_1, L_2, and L_3. ◻

4.1. Semi-continuity, coerciveness, existence. Establishing the existence of minimizers for problems such as these requires two ingredients: lower semi-continuity with respect to an appropriate topology (here the weak topology on $\mathcal{H}^1(\Omega)$) plus some form of coerciveness. The classical reference for this material is Morrey [38]. We shall follow the development of Giaquinta [27]. We first address the issue of lower semi-continuity.

LEMMA 4.2. *Let the region Ω be open and bounded with boundary Γ sufficiently regular for the Sobolev embedding and trace theorems to apply. Let the elastic constants L_1, L_2, and L_3 satisfy the inequalities (4.2). Let the Landau-de Gennes free-energy functional $\mathcal{F}$ be of the form (2.1), with the bulk and surface free-energy densities, f_B and f_S, continuous functions of Q on $\mathbf{S}_0$ satisfying*

$$f_B(Q) \geq C_1 > -\infty\,, \qquad f_S(Q) \geq C_2 > -\infty\,,$$

for some absolute constants C_1 and C_2 and for all Q in $\mathbf{S}_0$. Let $\mathcal{F}_L$ in (2.1) be a bounded linear functional on $\mathcal{H}^1(\Omega)$. Then $\mathcal{F}$ is weakly sequentially lower semi-continuous (w.s.l.s.c.) on $\mathcal{H}^1(\Omega)$.

Proof. The linear form $\mathcal{F}_L$ is convex and continuous (in the strong topology on $\mathcal{H}^1(\Omega)$), as is $\mathcal{F}_E$, under the assumed conditions on L_1, L_2, and L_3. Thus both are w.s.l.s.c. The assumptions on f_B and f_S guarantee that both of these integrands satisfy conditions *i), . . . ,iv)* of chapter I, section 2 of Giaquinta [27, p. 17] (modulo an additive constant). So the arguments of that section apply directly, and we conclude (as in [27, Th. 2.5, p. 22]) that $\mathcal{F}_B$ and $\mathcal{F}_S$ are also s.l.s.c. with respect to weak convergence in $\mathcal{H}^1(\Omega)$. □

There are ways in which this theorem can be generalized, but it is questionable as to how relevant these extensions are to problems encountered in practice. One could replace the elastic constants by coefficients in $L^\infty(\Omega)$ that satisfy appropriate inequalities in an almost-everywhere sense. One could also replace the constant lower bounds on f_B and f_S by any functions that are absolutely integrable on Ω. One could add in volumetric and surface densities that are not bounded below, but which are smooth and whose gradients satisfy appropriate growth conditions, as is done in [39]. Lastly, one could allow the potentials f_B and f_S to be extended real valued.

In order to establish the existence of minimizing sequences, some form of coerciveness is required. Here we shall consider two typical types of problems: one for which there are no Dirichlet boundary conditions (in which case, a quadratic growth condition on the bulk density f_B is sufficient to assure coerciveness), and the other for which we will pose Dirichlet conditions on a portion of the boundary of positive surface measure—this requires no additional conditions on the free-energy densities. For the latter problem, we require some additional notation.

Let Γ_0 be a subset of the boundary that has positive surface measure. Let Q_0 be a tensor field defined on Γ_0 and admitting an $\mathcal{H}^1$ extension to all of Ω that has finite free energy. For example, if $\Gamma_0 = \Gamma$ (except possibly for a set of surface measure zero), then possessing an $\mathcal{H}^1$ extension is equivalent to Q_0 being in the fractional order Sobolev space $\mathcal{H}^{1/2}(\Gamma)$ ([1, 7.53–7.56, pp. 216–217] or [39, Th. 2.4.20, p. 31]). We define subsets of $\mathcal{H}^1(\Omega)$ satisfying essential and homogeneous essential boundary conditions determined by Γ_0 and Q_0 as follows:

$$\mathcal{H}^1_E(\Omega) := \left\{ Q \in \mathcal{H}^1(\Omega) \mid Q = Q_0 \text{ on } \Gamma_0 \right\},$$
$$\mathcal{H}^1_{E_0}(\Omega) := \left\{ Q \in \mathcal{H}^1(\Omega) \mid Q = 0 \text{ on } \Gamma_0 \right\},$$

where in both instances, equality is meant in the sense of the boundary trace operator. We are now in a position to state and prove our main existence result for the Landau-de Gennes minimization problem.

THEOREM 4.3. *Let $\mathcal{F}$ be of the form (2.1), and let the conditions of Lemma 4.2 hold. In addition, let either of the following conditions and accompanying definition of admissible fields hold:*

(i) *there exist constants C_1 and $C_2 > 0$ such that $f_B(Q) \geq C_1 + C_2|Q|^2$ for all $Q \in \mathbf{S}_0$, and $\mathcal{Q} := \mathcal{H}^1(\Omega)$; or*

(ii) *Γ_0 and Q_0 are as defined above, and $\mathcal{Q} := \mathcal{H}^1_E(\Omega)$.*

Then the problem $\min_{Q \in \mathcal{Q}} \mathcal{F}(Q)$ admits a solution, that is, there exists at least one $Q^* \in \mathcal{Q}$ satisfying

$$\mathcal{F}(Q^*) = \min_{Q \in \mathcal{Q}} \mathcal{F}(Q).$$

Proof. It is sufficient to show that under either set of hypotheses, the functional $\mathcal{F}$ is coercive, in the sense that $\mathcal{F}(Q)$ grows unbounded as $\|Q\|_{1,\Omega} \to \infty$. In the first case, we use the implied conditions

$$\mathcal{F}_E(Q) = \frac{1}{2}a(Q,Q) \geq \frac{1}{2}\alpha\,|Q|^2_{1,\Omega}\,, \qquad f_S(Q) \geq C_3\,, \qquad |\mathcal{F}_L(Q)| \leq M\,\|Q\|_{1,\Omega}\,,$$

to deduce

$$\begin{aligned}
\mathcal{F}(Q) &= \mathcal{F}_E(Q) + \mathcal{F}_B(Q) + \mathcal{F}_S(Q) - \mathcal{F}_L(Q) \\
&\geq \frac{1}{2}\alpha\,|Q|^2_{1,\Omega} + C_1|\Omega| + C_2|Q|^2_{0,\Omega} + C_3|\Gamma| - M\,\|Q\|_{1,\Omega} \\
&\geq \min\left\{\frac{1}{2}\alpha, C_2\right\}\|Q\|^2_{1,\Omega} + C_4 - M\,\|Q\|_{1,\Omega} \to \infty\,, \quad \text{as } \|Q\|_{1,\Omega} \to \infty\,.
\end{aligned}$$

Consider the second case. By assumption, the prescribed tensor field Q_0 admits an extension (which we shall also denote Q_0) to $\mathcal{H}^1(\Omega)$ that has finite free energy. So Q is in $\mathcal{H}^1_E(\Omega)$ if and only if $Q = Q_0 + P$ with $P \in \mathcal{H}^1_{E_0}(\Omega)$, and $\|Q\|_{1,\Omega} \to \infty$ if and only if $\|P\|_{1,\Omega} \to \infty$. Now the $|\cdot|_{1,\Omega}$ semi-norm is equivalent to the $\|\cdot\|_{1,\Omega}$ norm on $\mathcal{H}^1_{E_0}(\Omega)$ (in the sense that $|Q|^2_{1,\Omega} \geq \gamma\|Q\|^2_{1,\Omega}$, $\gamma > 0$, $\forall Q \in \mathcal{H}^1_{E_0}(\Omega)$, see, for example, [11, Th. 1.2.1, p. 21]). So for any $Q \in \mathcal{H}^1_E(\Omega)$ (using also $f_B(Q) \geq C_1$ and $f_S(Q) \geq C_2$), we have

$$\begin{aligned}
\mathcal{F}(Q) &= \mathcal{F}_E(Q) + \mathcal{F}_B(Q) + \mathcal{F}_S(Q) - \mathcal{F}_L(Q) \\
&\geq \frac{1}{2}\,\alpha\,|Q|^2_{1,\Omega} + C_1\,|\Omega| + C_2\,|\Gamma| - M\,\|Q\|_{1,\Omega} \\
&\geq \frac{1}{2}\,\alpha\left\{\frac{1}{2}|Q-Q_0|^2_{1,\Omega} - |Q_0|^2_{1,\Omega}\right\} + (C_1\,|\Omega| + C_2\,|\Gamma|) - M\,\|Q\|_{1,\Omega} \\
&\geq \frac{1}{4}\,\alpha\,\gamma\|Q-Q_0\|^2_{1,\Omega} + C_3 - M\,\|Q\|_{1,\Omega} \\
&\geq \frac{1}{4}\,\alpha\,\gamma\left\{\frac{1}{2}\|Q\|^2_{1,\Omega} - \|Q_0\|^2_{1,\Omega}\right\} + C_3 - M\,\|Q\|_{1,\Omega} \\
&= \frac{1}{8}\,\alpha\,\gamma\,\|Q\|^2_{1,\Omega} + C_4 - M\,\|Q\|_{1,\Omega} \to \infty\,, \quad \text{as } \|Q\|_{1,\Omega} \to \infty\,.
\end{aligned}$$

In either case, the existence of a minimizer $Q^* \in \mathcal{Q}$ can now proceed along familiar lines (as in [27, Ch. I, §3] or [39, §3.2]). Given a minimizing sequence, coerciveness guarantees that it must be bounded. The tensor field Q^* is taken as the limit of a weakly converging subsequence, and the weak lower semi-continuity of $\mathcal{F}$ assures us that $\mathcal{F}(Q^*)$ achieves the minimum value. ∎

We next consider an application of this theorem to standard types of Landau-de Gennes functionals, as we use in our codes.

4.2. Application. The theorem above can be used to prove the existence of minimizers to the particular forms of Landau-de Gennes functionals we have implemented in our codes, under appropriate conditions on the material expansion coefficients. We have the following.

Corollary 4.4. *Let $\mathcal{F}$ be of the form (2.1). Let f_E be of the form (2.2), with the elastic constants L_1, L_2, and L_3 satisfying the inequalities (4.2). Let f_B be of the form (2.3), with the bulk coefficients satisfying any one of the following three sets of conditions:*

(i) $A > 0,\ B = C = D = E = E' = 0$ *; or*
(ii) $C > 0,\ D = E = E' = 0$ *; or*
(iii) $E > 0,\ E' \geq 0$ *.*

Let f_S *be of the form (2.4), with* $Q_0 \in \mathcal{L}^2(\Gamma)$ *and* $W \geq 0$*. Let* $\mathcal{F}_L$ *be of the form (2.5), with* $F \in \mathcal{L}^2(\Omega)$ *and* $G \in \mathcal{L}^2(\Gamma)$*. Then* $\mathcal{F}$ *attains its minimum on* $\mathcal{H}^1(\Omega)$*.*

If Γ_0 *and* Q_0 *are as defined for Theorem 4.3, then the above conditions also are sufficient to guarantee that* $\mathcal{F}$ *attains its minimum on* $\mathcal{H}^1_E(\Omega)$*. This remains true if to the list above we add*

(iv) $A = B = C = D = E = E' = 0$ *,*

i.e., $\mathcal{F}_B = 0$*.*

Proof. We need only verify that the hypotheses of Theorem 4.3 are met. By assumption, the elastic part of the free energy, $\mathcal{F}_E$, satisfies the same ellipticity conditions, (4.2). The continuity of the linear form $\mathcal{F}_L$ follows from the estimate

$$\begin{aligned} |\mathcal{F}_L(Q)| &= \left| \int_\Omega \mathrm{tr}(FQ) + \int_\Gamma \mathrm{tr}(GQ) \right| \\ &\leq \|F\|_{0,\Omega} \|Q\|_{0,\Omega} + \|G\|_{0,\Gamma} \|Q\|_{0,\Gamma} \end{aligned}$$

and the continuous embeddings of $\mathcal{H}^1(\Omega)$ in $\mathcal{L}^2(\Omega)$ and $\mathcal{L}^2(\Gamma)$, from (3.1) and (3.4). If $W \geq 0$, then the surface free-energy term is non-negative, and hence bounded below.

So the only term requiring attention is the bulk term, $\mathcal{F}_B$. In the case of no Dirichlet boundary conditions (minimization over all of $\mathcal{H}^1(\Omega)$), we need the density f_B to have quadratic growth; whereas in the case where we have Dirichlet conditions on at least part of the boundary, we simply need it to be bounded below. For the case of conditions (i) above, the hypothesis (i) of Theorem 4.3 is satisfied with $C_1 = 0$ and $C_2 = A/2$.

Consider the case of conditions (ii). We then have

$$f_B(Q) = \frac{1}{2} A \,\mathrm{tr}(Q^2) - \frac{1}{3} B \,\mathrm{tr}(Q^3) + \frac{1}{4} C \,\mathrm{tr}(Q^2)^2 \,.$$

Give $0 < \varepsilon < 1$. Let $M_1 \geq 1$ be sufficiently large so that $|Q|^2 \geq M_1$ implies

$$f_B(Q) \geq \frac{1}{4} C \,\mathrm{tr}(Q^2)^2 (1 - \varepsilon) \geq \frac{1}{4} C |Q|^2 (1 - \varepsilon) \,.$$

(Recall that $|Q|^2 = \mathrm{tr}(Q^2) = Q_{\alpha\beta} Q_{\alpha\beta}$). Now define

$$M_2 := \min \left\{ f_B(Q) - \frac{1}{4} C |Q|^2 (1 - \varepsilon) \,:\, |Q|^2 \leq M_1 \,,\ Q \in \mathbf{S}_0 \right\} \,.$$

Then we have

$$f_B(Q) \geq M_2 + \frac{1}{4} C |Q|^2 (1 - \varepsilon) \,, \quad \text{if } |Q|^2 \leq M_1 \,,$$

and

$$f_B(Q) \geq \frac{1}{4} C |Q|^2 (1 - \varepsilon) \,, \quad \text{if } M_1 \leq |Q|^2 \,.$$

It follows that f_B satisfies

$$f_B(Q) \geq C_1 + C_2 |Q|^2 \,, \quad \forall Q \in \mathbf{S}_0 \,,$$

with

$$C_1 := \min\{0, M_2\} \qquad \text{and} \qquad C_2 := \frac{1}{4}C(1-\varepsilon) > 0\,.$$

The E term can be handled similarly, for the case (iii). We note, however, that the E' term, $\operatorname{tr}(Q^3)^2$, is not convex and does not satisfy such a quadratic growth estimate for any values of C_1 and C_2. However, $E' \geq 0$ does guarantee that this contribution is nonnegative.

Thus any one of the conditions (i), (ii), or (iii) is sufficient to guarantee that f_B satisfies condition (i) of Theorem 4.3, and so the existence of a solution is assured for the problem of minimizing over all of $\mathcal{H}^1(\Omega)$. For the case of Dirichlet (or partial Dirichlet) conditions, we only need to know that f_B is bounded from below. But this is again guaranteed by any of these three conditions or in the case (iv), where $f_B = 0$. ∎

5. Variational formulation. It is convenient, from both computational and analytical points of view, to replace the minimization of $\mathcal{F}(Q)$ by the problem of finding fields Q that render it stationary: $D\mathcal{F}(Q) = 0$. Here $D\mathcal{F}(Q)$ is the *Fréchet derivative* of $\mathcal{F}$ evaluated at Q [30]. Such points are referred to as weak solutions of the Euler equations (or associated elliptic system). For differentiable functionals, any minimizer is a stationary point. Moreover, a stationary point Q for which the second Fréchet derivative is positive definite is a local minimizer [26].

Our ultimate goal is to demonstrate that stationary points of Landau-de Gennes free-energy functionals can be well-approximated by finite element methods. Here we address the differentiability of $\mathcal{F}$.

For $Q, P \in \mathcal{H}^1(\Omega)$, the derivative of $\mathcal{F}$ at Q acting on P is given by

$$\begin{aligned} D\mathcal{F}(Q)P &= D\mathcal{F}_E(Q)P + D\mathcal{F}_B(Q)P + D\mathcal{F}_S(Q)P - D\mathcal{F}_L(Q)P \\ &= a(Q,P) + \int_\Omega \left\{ \frac{\partial f_B}{\partial Q_{\alpha\beta}}(Q) P_{\alpha\beta} \right\} + \int_\Gamma \left\{ \frac{\partial f_S}{\partial Q_{\alpha\beta}}(Q) P_{\alpha\beta} \right\} - \mathcal{F}_L(P)\,. \end{aligned}$$

Conditions sufficient to guarantee differentiability in $\mathcal{H}^1(\Omega)$ can be gleaned from this expression and the Sobolev embedding and trace theorems. It is sufficient that the densities f_B and f_S be continuously differentiable and that their gradients satisfy growth conditions

$$|Df_B(Q)| \leq C\left(1 + |Q|^5\right) \qquad \text{and} \qquad |Df_S(Q)| \leq C\left(1 + |Q|^3\right)$$

[27, Ch. I, §5, pp. 35–38]. For later needs, we observe that for differentiability in the subspace $\mathcal{H}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$, it is sufficient that f_B and f_S be in $C^1(\mathbf{S}_0)$. For the functionals that we use in our codes, we have the following.

PROPOSITION 5.1. *Let the Landau-de Gennes free-energy functional $\mathcal{F}$ be of the form (2.1), with elastic, bulk, surface, and linear component parts given by (2.2), (2.3), (2.4), and (2.5), respectively. Then $\mathcal{F}$ is differentiable everywhere on $\mathcal{H}^1(\Omega)$.*

Proof. The free-energy density functions $f_B(Q)$ and $f_S(Q)$ are polynomials of total degrees 6 and 2, respectively, in the components of the Q tensor, and the necessary smoothness and growth conditions on their gradients can be established easily [15]. ∎

For simplicity, we shall focus our analysis on the homogeneous Dirichlet problem. That is, we shall assume homogeneous Dirichlet data on the entire boundary Γ. In that case, the surface free-energy term $\mathcal{F}_S$ in (2.1) is zero, and the space of admissible fields becomes $\mathcal{H}_0^1(\Omega)$. The flavor of the analysis for other boundary conditions is not appreciably different [15].

We define the linear functional $\mathcal{G}(Q)$ through its action on fields $P \in \mathcal{H}_0^1(\Omega)$:

$$\langle \mathcal{G}(Q), P \rangle := D\mathcal{F}_B(Q)P - \mathcal{F}_L(P)\,, \tag{5.1}$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $\mathcal{H}^{-1}(\Omega)$ and $\mathcal{H}_0^1(\Omega)$. In terms of this, the stationarity condition $D\mathcal{F}(Q) = 0$ can be written

$$a(Q, P) + \langle \mathcal{G}(Q), P \rangle = 0\,, \quad \forall P \in \mathcal{H}_0^1(\Omega)\,. \tag{5.2}$$

This is the variational formulation of our problem. It defines a nonlinear variational boundary value problem for the unknown tensor field Q. As in the classical linear problems, (5.2) involves a bilinear form $a(\cdot, \cdot)$ defined on $\mathcal{H}_0^1(\Omega)$ and a linear functional $\mathcal{G}(Q)$ in its dual, $\mathcal{H}^{-1}(\Omega)$. In contrast to linear problems, the functional $\mathcal{G}(Q)$ depends explicitly and *nonlinearly* on the unknown field Q. Consequently, the numerical solution of (5.2) will ultimately require an iterative procedure, such as Newton's method.

With a view towards applying the nonlinear approximation theory found in [9, 14], we recast the problem (5.2) into operational, or fixed-point, form. In Lemma 4.1, we demonstrated that for suitably restricted values of the elastic constants L_1, L_2, and L_3, the bilinear form $a(\cdot, \cdot)$ is an inner product on $\mathcal{H}_0^1(\Omega)$ which is equivalent to the usual $\mathcal{H}^1(\Omega)$ inner product. Let $\mathcal{T}$ be the Riesz mapping which assigns to every ℓ in $\mathcal{H}^{-1}(\Omega)$ its unique representer (with respect to $a(\cdot, \cdot)$) in $\mathcal{H}_0^1(\Omega)$:

$$a(Q, P) = \ell(P)\,, \quad \forall P \in \mathcal{H}_0^1(\Omega) \quad \Longleftrightarrow \quad Q = \mathcal{T}\,\ell\,.$$

It follows that the weak formulation (5.2) is equivalent to

$$Q + \mathcal{T}\,\mathcal{G}(Q) = 0\,. \tag{5.3}$$

This equation has the important consequence that a weak solution of our problem is in the range of the operator $\mathcal{T}$. Thus, certain properties of solution fields Q can be deduced from properties of $\mathcal{T}$. The operator $\mathcal{T}$ gives an isomorphism between $\mathcal{H}^{-1}(\Omega)$ and $\mathcal{H}_0^1(\Omega)$. The regularity properties of $\mathcal{T}$ can be established using the theory of strongly elliptic systems. These properties depend on both the form $a(\cdot, \cdot)$ and on the smoothness of the boundary. We address these issues now.

6. Regularity. We use results from the fundamental papers of Agmon, Douglis, and Nirenberg [2, 3] (following the treatment in Morrey [38]) to deal with the case of sufficiently smooth boundaries. We then follow the analysis of Grisvard [29] to extend these results to non-smooth domains.

We introduce some notation needed to establish contact with the theory of strongly elliptic systems. We consider the solution operator for the variational problem

$$a(Q, P) = (F, P)_0\,, \quad \forall P \in \mathcal{H}_0^1(\Omega) \tag{6.1}$$

under the assumption that $F \in \mathcal{L}^2(\Omega)$. To construct the associated Euler equations, we must take into account the pointwise constraints of symmetry and tracelessness.

This can be done using Lagrange multipliers; however, we find it more convenient to use the scalar coordinate representation introduced in (3.5).

Using the representations $Q = q_i E^i$ and $P = p_j E^j$ (where $\{E^i\}_{i=1}^5$ is an orthonormal basis for the set of symmetric traceless tensors $\mathbf{S}_0$), the bilinear form $a(Q, P)$ becomes

$$a(Q, P) = \int_\Omega q_{i,\alpha} A^{ij}_{\alpha\beta} p_{j,\beta} \,,$$

where the constant coefficient tensor A is given by

$$A^{ij}_{\alpha\beta} = L_1 L^{ij}_{\alpha\beta} + L_2 M^{ij}_{\alpha\beta} + L_3 N^{ij}_{\alpha\beta} \,,$$

with

$$L^{ij}_{\alpha\beta} = \delta_{ij}\delta_{\alpha\beta} \,, \qquad M^{ij}_{\alpha\beta} = \left(E^i E^j\right)_{\alpha\beta} \,, \qquad \text{and} \qquad N^{ij}_{\alpha\beta} = \left(E^j E^i\right)_{\alpha\beta} \,.$$

(Recall that these indices have the ranges $i, j = 1, \ldots, 5$ and $\alpha, \beta = 1, 2, 3$.) Similarly, the right-hand side of (6.1) becomes

$$(F, P)_0 = \int_\Omega f_i p_i \,,$$

where $(f_1, \ldots, f_5)$ are the scalar coordinates of F. Note that the source tensor F can be taken to be symmetric and traceless as well, since this is the only part of it that contributes to the expression $\mathrm{tr}(FQ)$.

Thus, using the scalar coordinate representation, the variational problem (6.1) is transformed into the unconstrained problem

$$\int_\Omega q_{i,\alpha} A^{ij}_{\alpha\beta} p_{j,\beta} = \int_\Omega f_i p_i \,, \quad \forall \boldsymbol{p} \in \mathbf{H}^1_0(\Omega) \,.$$

The associated Euler equations are now given by

$$\begin{aligned} -\frac{\partial}{\partial x_\beta}\left(A^{ij}_{\alpha\beta}\frac{\partial q_i}{\partial x_\alpha}\right) &= f_j \,, \quad \text{in } \Omega \,, \quad j = 1, \ldots, 5 \\ q_i &= 0 \,, \quad \text{on } \Gamma \,, \quad i = 1, \ldots, 5 \,. \end{aligned} \tag{6.2}$$

The tensor A is symmetric ($A^{ji}_{\beta\alpha} = A^{ij}_{\alpha\beta}$), and if the elastic constants satisfy the ellipticity conditions (4.2), then it is also positive definite, in the sense that there exists $\nu > 0$ such that

$$A^{ij}_{\alpha\beta}\lambda^i_\alpha\lambda^j_\beta \geq \nu|\lambda|^2 \,,$$

for all vectors λ. Thus the system is (uniformly) strongly elliptic [27, 38, 39].

We are now in a position to establish the regularity of solutions of (6.1) for smooth boundaries. We conform to the notation of Morrey [38, p. 4] and Giaquinta [27, p. 5] for a boundary of class $C^{2s-1,1}$, which is one that can be parameterized locally by functions whose derivatives of order $2s - 1$ or less are Lipschitz continuous. We have the following.

THEOREM 6.1. *Let the bilinear form $a(\cdot, \cdot)$ be as defined in (4.1), with L_1, L_2, and L_3 satisfying (4.2). Let s be a positive integer. Let the region Ω be of class $C^{2s-1,1}$*

(as described above). Let F be in $\mathcal{H}^{s-1}(\Omega)$. Then the variational problem (6.1) has a unique solution $Q \in \mathcal{H}^{s+1}(\Omega) \cap \mathcal{H}^1_0(\Omega)$.

Proof. This results as a direct consequence of Theorem 6.5.4 of [38, p. 255]. The system (6.2) is strongly elliptic; the coefficient functions are sufficiently smooth (constant, analytic in our case); and zero is not an eigenvalue. The result follows. □

It follows readily that $\mathcal{T}$ is bounded on $\mathcal{H}^{s-1}(\Omega)$ to $\mathcal{H}^{s+1}(\Omega) \cap \mathcal{H}^1_0(\Omega)$ [7, Ch. 6, §2-8 & Ch. 7, §1-9]. The case $s = 1$ of the above result guarantees $\mathcal{H}^2$ regularity for $\mathcal{L}^2$ source and $C^{1,1}$ boundary. We can extend this result to arbitrary convex regions by using the analysis of Grisvard [29]. Convex (open, bounded, connected) regions can be approximated from inside (and from outside) arbitrarily closely by $C^{1,1}$ regions. This is used in [29] in the analysis of scalar elliptic partial differential equations to extend H^2 regularity for homogeneous Dirichlet problems on $C^{1,1}$ regions to convex regions [29, Th. 3.2.1.2, pp. 147–149]. The argument is based on approximating the convex region Ω from the inside by a converging sequence of $C^{1,1}$ regions, extending by zero the solution of the homogeneous Dirichlet problems on the inner regions, and developing the necessary limiting arguments. The proof goes through identically for systems—applied on a component by component basis. We obtain the following.

COROLLARY 6.2. *Let the bilinear form $a(\cdot, \cdot)$ be as defined in (4.1), with L_1, L_2, and L_3 satisfying (4.2). Let the region Ω be open, connected, bounded, and convex. Let F be in $\mathcal{L}^2(\Omega)$. Then the variational problem (6.1) has a unique solution $Q \in \mathcal{H}^2(\Omega) \cap \mathcal{H}^1_0(\Omega)$.*

These regularity properties of $\mathcal{T}$ combined with the properties of the linear functional $\mathcal{G}(Q)$ and the fixed-point equation (5.3) can lead to conclusions about the regularity of solutions Q of the full (nonlinear) variational problem (5.2). For instance, if for all Q in $\mathcal{H}^1_0(\Omega)$, the functional $\mathcal{G}(Q)$ were guaranteed to be bounded on $\mathcal{L}^2(\Omega)$, then we could conclude that the solution of (5.2) would be in $\mathcal{H}^2(\Omega) \cap \mathcal{H}^1_0(\Omega)$ whenever the region Ω was either convex or of class $C^{1,1}$. This is the case under certain conditions. We have the following.

THEOREM 6.3. *Let the bilinear form $a(\cdot, \cdot)$ be as defined in (4.1), with L_1, L_2, and L_3 satisfying (4.2). Let the linear functional $\mathcal{G}(Q)$ be defined as in (5.1). Let f_B be in $C^1(\mathbf{S}_0)$ and satisfy*

$$|Df_B(Q)| \leq C\left(1 + |Q|^3\right), \quad \forall Q \in \mathbf{S}_0 .$$

Let the linear functional $\mathcal{F}_L$ be bounded on $\mathcal{L}^2(\Omega)$. Let the region Ω be open, bounded, connected and either convex or of class $C^{1,1}$. Then any solution of the variational problem (5.2) is in $\mathcal{H}^2(\Omega) \cap \mathcal{H}^1_0(\Omega)$.

Proof. It is sufficient to show that under the assumed conditions, $\mathcal{G}(Q)$ is a bounded linear functional on $\mathcal{L}^2(\Omega)$ for any $Q \in \mathcal{H}^1_0(\Omega)$. We have

$$\langle \mathcal{G}(Q), P \rangle = D\mathcal{F}_B(Q)P - \mathcal{F}_L(P) = \int_\Omega \left\{ \frac{\partial f_B}{\partial Q_{\alpha\beta}}(Q) P_{\alpha\beta} \right\} - \mathcal{F}_L(P) .$$

Now $\mathcal{F}_L$ is bounded on $\mathcal{L}^2(\Omega)$ by assumption. We need the components of $Df_B(Q)$ to be square integrable. The hypotheses are sufficient to guarantee this, since $Q \in \mathcal{H}^1(\Omega) \Rightarrow Q \in \mathcal{L}^6(\Omega)$, by (3.1). Thus $\mathcal{G}(Q)$ can be identified with an $\mathcal{L}^2$ function, and the result follows from the regularity results above for the linear problem and the fact that Q is the image under $\mathcal{T}$ of an $\mathcal{L}^2$ tensor field, (5.3). □

We conclude with some observations. Under these conditions, our minimization problem has solutions, and $\mathcal{F}$ is differentiable in $\mathcal{H}^1(\Omega)$. So the minimizers must satisfy (5.2), and thus we are assured of the $\mathcal{H}^2$ regularity of our minimizers. Also, these conditions are satisfied by the common functionals, like those we use in our code, provided the expansion for the bulk density f_B in (2.3) is truncated at the *fourth order*, which is physically relevant and often done.

We are not aware of analyses adequate to prove general $\mathcal{H}^2$ regularity for the full nonlinear problem in the absence of such growth conditions. However, there certainly exist problems that violate such conditions and yet have bounded regular solutions. Consider the simple (though not physically meaningful) problem of minimizing the functional

$$\mathcal{F}(Q) := \int_\Omega \Big\{ |\partial Q|^2 + \lambda \exp\Big(\operatorname{tr}(Q^2)\Big)\Big\}$$

over smooth tensor fields Q satisfying $Q = Q_0$ on Γ. Assume Ω, Γ, and Q_0 are all sufficiently regular. In terms of the scalar coordinates, the functional, stationarity condition, and Euler Equations become

$$\int_\Omega \Big\{ |\nabla \boldsymbol{q}|^2 + \lambda \exp\Big(|\boldsymbol{q}|^2\Big)\Big\}\ ,$$

$$\int_\Omega \Big\{ \nabla q_i \cdot \nabla p_i + \lambda \exp\Big(|\boldsymbol{q}|^2\Big) q_i p_i \Big\} = 0\,, \quad \forall \boldsymbol{p} \in \mathbf{H}^1_0(\Omega)\,,$$

and

$$\begin{aligned} -\Delta q_i + \lambda \exp\Big(|\boldsymbol{q}|^2\Big)\, q_i &= 0\,, \quad \text{in } \Omega\,, \quad i = 1, \ldots, 5\,, \\ q_i &= q_i^0\,, \quad \text{on } \Gamma\,, \quad i = 1, \ldots, 5\,. \end{aligned}$$

Classical techniques (integral-equation formulation, Schauder Fixed-Point Theorem) can be used to prove that this problem has a bounded regular (classical) solution for $\lambda > 0$ sufficiently small.

Compare also, for example, with [14, 1.1.2.Ex. 2, pp. 3–10]. In the finite-element convergence analysis of the next section, we consider (in addition to the previous situations) cases in which minimizers are assumed to be in $\mathcal{H}^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$, in the absence of growth conditions.

7. Finite element approximation of nonsingular solution branches. In the convergence theory that follows, we generally use the standard terminology and notation of Ciarlet, as found in [11, 12], for all matters pertaining to finite elements and the associated approximation theory. The reader is referred to those works for additional details. Other references include [41, 45, 47].

As discussed in §1, we are interested in situations in which the free-energy functionals (and stationary points) depend on parameters. We restrict ourselves to the case where this dependence can be identified with a single real parameter λ taking values in a compact interval. It is of interest, then, to approximate entire *solution branches*. We focus our attention on nonsingular solution branches; that is, situations for which the Banach space version of the Implicit Function Theorem holds [40]. The following definition is from [9].

DEFINITION 7.1. *Let $\Lambda \subset \mathbf{R}$, and let V be a Banach space. Let $F : \Lambda \times V \mapsto V$ be a nonlinear mapping. The set $\{(\lambda, u(\lambda)) : \lambda \in \Lambda\}$ is a branch of nonsingular solutions of F if:*

(i) $\lambda \mapsto u(\lambda)$ *is a continuous mapping from Λ to V;*

(ii) $F(\lambda, u(\lambda)) = 0, \quad \lambda \in \Lambda$;

(iii) $D_u F(\lambda, u(\lambda))$ *is an isomorphism of V, for all $\lambda \in \Lambda$.*

Here, $D_u F$ is the Fréchet partial derivative of $F(\cdot,\cdot)$ with respect to its second argument.

Suppose that $F(\lambda, u(\lambda))$ is of the special form

$$F(\lambda, u) := u(\lambda) + TG(\lambda, u(\lambda))$$

found in (5.3), for example. If the operator $TD_uG(\lambda, u(\lambda))$ is compact as a member of $\mathcal{B}(V,V)$ (the space of bounded linear operators on V to itself), then one can use the Fredholm-Riesz-Schauder theory for compact operators [23, Theorem 5.2.7] to establish condition (iii) of the definition. That is,

$$D_u F(\lambda, u(\lambda)) = I + TD_uG(\lambda, u(\lambda))$$

is an isomorphism of V if the equation

$$w + TD_uG(\lambda, u)w = 0$$

has only the trivial solution $w = 0$ (for each $\lambda \in \Lambda$).

Using slightly generalized forms of the Implicit Function Theorem, Brezzi, Rappaz, and Raviart establish very general results concerning the approximation of branches of nonsingular solutions of functional equations [9]. Their nonlinear convergence theory has the flavor of the *Krasnoselskii calculus* described in [33] and originally developed in [34]. This theory has been effectively employed in [18] in the finite-element analysis of the Ginzburg-Landau model for superconductivity. It has been generalized in [14]. Similar results are also found in [20, 21].

Prior to stating the result that we shall employ, we introduce some notation. Let Λ be a compact interval of the real line. Let V and W be Banach spaces, T a bounded linear map in $\mathcal{B}(W,V)$, and $G : \Lambda \times V \to W$ a C^2-mapping. The objective is to approximate nonsingular solution branches $\{(\lambda, u(\lambda)) : \lambda \in \Lambda,\ u \in V\}$ which satisfy the equation

$$F(\lambda, u) := u + TG(\lambda, u) = 0\,. \tag{7.1}$$

A natural approach is to introduce finite dimensional subspaces V_h of V and approximating operators $T_h \in \mathcal{B}(W, V_h)$ and to seek solutions of finite dimensional problems

$$F_h(\lambda, u_h) := u_h + T_hG(\lambda, u_h) = 0\,, \qquad \lambda \in \Lambda\,, \quad u_h \in V_h\,. \tag{7.2}$$

There are two main issues to be addressed. First, the existence of nonsingular solution branches of the finite dimensional problem (7.2) must be established. Second, it must be determined how well the finite dimensional solutions approximate the solutions to (7.1). The main results of [9] answer both of these questions.

THEOREM 7.1. *Let Λ, V, W, T, and G be as above. Further assume the following:*

(i) *G is a C^2-mapping from $\Lambda \times V$ to W, and the second Fréchet derivative D^2G is bounded on all bounded subsets of $\Lambda \times V$.*

(ii) *There is an operator* $\pi_h \in \mathcal{B}(V, V_h)$ *such that*

$$\lim_{h\to 0} \|v - \pi_h v\|_V = 0\,, \quad \forall v \in V.$$

(iii) *The approximating operators* T_h *satisfy*

$$\lim_{h\to 0} \|T - T_h\|_{\mathcal{B}(W,V)} = 0\,.$$

Let $\{(\lambda, u(\lambda)) : \lambda \in \Lambda\}$ *be a branch of nonsingular solutions of (7.1). Then there exists a neighborhood* $\mathcal{O}$ *of the origin in* V*, and, for* h *sufficiently small, a unique* C^2*-function* $\lambda \in \Lambda \mapsto u_h(\lambda) \in V_h$ *such that*

$$F_h(\lambda, u_h(\lambda)) = 0 \qquad \text{and} \qquad u_h(\lambda) - u(\lambda) \in \mathcal{O},$$

for every $\lambda \in \Lambda$*. Moreover, there is a constant* $K_0 > 0$*, independent of* h *and* λ*, such that*

$$\|u(\lambda) - u_h(\lambda)\|_V \le K_0 \left\{\|u(\lambda) - \pi_h u(\lambda)\|_V + \|(T_h - T)G(\lambda, u(\lambda))\|_V\right\}. \tag{7.3}$$

Proof. Theorem 6 of [9]. □

Under the assumption that a nonsingular branch of solutions of (7.1) exists, Theorem 7.1 guarantees the existence of nonsingular solution branches of the finite dimensional equation (7.2) (for sufficiently small h). It also asserts that the solution branches of (7.2) converge to the solution branches of (7.1), *uniformly* in λ. In practice, one would have precise information regarding the behavior of the right-hand side of (7.3) with respect to mesh size h. For example, $\pi_h u$ could be the finite-element interpolant of u or the Ritz-Galerkin projection of u, quantities whose approximation properties are well-understood. The operators T_h incorporate all approximations made in the numerical solution of (7.1): quadrature, approximation of the boundary, etc.

In this section, we apply Theorem 7.1 to obtain finite-element error estimates for the variational formulation of the Landau-de Gennes minimization problem as stated in §5. Computational results pertaining to a related problem are found in [25, 44]. The analysis separates into two parts, depending upon whether the problem is regular or not. A convergence result can be established for piecewise-linear finite elements under the minimal knowledge that the solution is in $\mathcal{H}^1_0(\Omega)$, as would be the case if the region were not convex and not of class $C^{1,1}$. The analysis we present requires growth conditions on the derivatives of the bulk free-energy density, f_B, and the rate of convergence can be arbitrarily slow.

The typical confining geometries of practical interest are convex. For convex or $C^{1,1}$ regions, the problem is regular, and we are able to establish convergence results without requiring any growth conditions. In this case, we use a different set of spaces in the analysis and application of Theorem 7.1.

7.1. Convergence in the absence of regularity. For the piecewise-linear convergence result (in the absence of regularity), we make the following assumptions:

1. The set $\Omega \subset \mathbf{R}^3$ is bounded, open, and polyhedral.
2. A homogeneous Dirichlet condition is imposed on the entire boundary.
3. The set Λ is a compact interval of the real line in which the parameter λ is permitted to vary.

4. The elastic constants L_1, L_2, and L_3 satisfy inequalities (4.2) of Lemma 4.1, thus assuring that $a(\cdot,\cdot)$ is bounded and $\mathcal{H}_0^1(\Omega)$-elliptic.

5. The variational formulation of the Landau-de Gennes minimization problem admits a nonsingular branch of solutions $\{(\lambda, Q(\lambda)) : \lambda \in \Lambda\}$.

Recall that under these assumptions, the free energy functional takes the form

$$\begin{aligned}\mathcal{F}(\lambda, Q) &= \mathcal{F}_E(Q) + \mathcal{F}_B(\lambda, Q) - \mathcal{F}_L(\lambda, Q) \\ &= \frac{1}{2} a(Q, Q) + \int_\Omega \{f_B(\lambda, Q)\} - \mathcal{F}_L(\lambda, Q)\,,\end{aligned}$$

where the bilinear form $a(\cdot,\cdot)$ is given by (4.1) and $\mathcal{F}_L$ is in $\mathcal{H}^{-1}(\Omega)$. The stationary points Q satisfy (5.2) with $\mathcal{G} \in \mathcal{B}(\Lambda \times \mathcal{H}_0^1(\Omega), \mathcal{H}^{-1}(\Omega))$ given by

$$\begin{aligned}\langle \mathcal{G}(\lambda, Q), P \rangle &= D_Q \mathcal{F}_B(\lambda, Q) P - \mathcal{F}_L(\lambda, P) \\ &= \int_\Omega \left\{ \frac{\partial f_B}{\partial Q_{\alpha\beta}}(\lambda, Q) P_{\alpha\beta} \right\} - \mathcal{F}_L(\lambda, P)\,.\end{aligned}$$

For this case, we shall cast our analysis with $V = \mathcal{H}_0^1(\Omega)$ and $W = \mathcal{L}^2(\Omega)$. We require conditions on f_B and $\mathcal{F}_L$ sufficient to guarantee condition (i) of Theorem 7.1. Again it is more convenient to use the scalar-coordinate representation. Thus, replacing Q and P by $q_i E^i$ and $p_j E^j$, we obtain

$$\langle G(\lambda, \boldsymbol{q}), \boldsymbol{p} \rangle = \int_\Omega \left\{ \frac{\partial f_B}{\partial q_i}(\lambda, \boldsymbol{q})\, p_i \right\} - F_L(\lambda, \boldsymbol{p})\,. \tag{7.4}$$

We have the following.

LEMMA 7.2. *For $\lambda \in \Lambda$ and $\boldsymbol{q} \in \mathbf{H}_0^1(\Omega)$, let $G(\lambda, \boldsymbol{q})$ be defined as above, and let the linear functional $F_L(\lambda, \cdot)$ be bounded on $\mathbf{L}^2(\Omega)$. Let $\boldsymbol{f}(\lambda)$ denote the representer of $F_L(\lambda, \cdot)$ in $\mathbf{L}^2(\Omega)^*$, so that for every $\lambda \in \Lambda$, $\boldsymbol{f}(\lambda)$ is in $\mathbf{L}^2(\Omega)$, and*

$$F_L(\lambda, \boldsymbol{p}) = (\boldsymbol{f}(\lambda), \boldsymbol{p})_0 = \int_\Omega f_i(\lambda)\, p_i\,, \quad \forall \boldsymbol{p} \in \mathbf{H}_0^1(\Omega)\,.$$

Assume that f_B and $\boldsymbol{f}$ satisfy the following conditions:

(i) *f_B is in $C^3(\Lambda \times \mathbf{R}^5)$ and satisfies*

$$\left|\frac{\partial f_B}{\partial q_i}\right|, \left|\frac{\partial^2 f_B}{\partial \lambda\, \partial q_i}\right|, \left|\frac{\partial^3 f_B}{\partial \lambda^2\, \partial q_i}\right| \le C\left(1 + |\boldsymbol{q}|^3\right), \tag{7.5a}$$

$$\left|\frac{\partial^2 f_B}{\partial q_i\, \partial q_j}\right|, \left|\frac{\partial^3 f_B}{\partial \lambda\, \partial q_i\, \partial q_j}\right| \le C\left(1 + |\boldsymbol{q}|^2\right), \tag{7.5b}$$

$$\left|\frac{\partial^3 f_B}{\partial q_i\, \partial q_j\, \partial q_k}\right| \le C\left(1 + |\boldsymbol{q}|\right), \tag{7.5c}$$

for all $\lambda \in \Lambda$ and $\boldsymbol{q} \in \mathbf{R}^5$.

(ii) *$\boldsymbol{f}$ is in $C^2(\Lambda; \mathbf{L}^2(\Omega))$ with $\boldsymbol{f}(\lambda)$, $\boldsymbol{f}'(\lambda)$, and $\boldsymbol{f}''(\lambda)$ uniformly bounded (in $\mathbf{L}^2(\Omega)$) for $\lambda \in \Lambda$.*

Then G is in $C^2\left(\Lambda \times \mathbf{H}_0^1(\Omega); \mathbf{L}^2(\Omega)\right)$, and $D^2 G$ is bounded on bounded subsets of $\Lambda \times \mathbf{H}_0^1(\Omega)$.

Proof. Under these assumptions, the expressions for G and DG are given by

$$\langle G(\lambda,\boldsymbol{q}),\boldsymbol{p}\rangle = \int_\Omega \left\{ \frac{\partial f_B}{\partial q_i}(\lambda,\boldsymbol{q}) - f_i(\lambda) \right\} p_i$$

and

$$\langle DG(\lambda,\boldsymbol{q})(\mu,\boldsymbol{r}),\boldsymbol{p}\rangle = \int_\Omega \left\{ \frac{\partial}{\partial \lambda}\frac{\partial f_B}{\partial q_i}(\lambda,\boldsymbol{q})\,\mu + \frac{\partial}{\partial q_j}\frac{\partial f_B}{\partial q_i}(\lambda,\boldsymbol{q})\,r_j - f_i'(\lambda)\,\mu \right\} p_i\,,$$

with a similar (slightly more complicated) expression for D^2G. (Summations with respect to i and j are implied here).

First, it is necessary to know that for any $\boldsymbol{p},\boldsymbol{q},\boldsymbol{r} \in \mathbf{H}_0^1(\Omega)$ and $\lambda,\mu \in \Lambda$, each individual term in braces is in $L^2(\Omega)$. Now Λ is compact; so $|\lambda|$ and $|\mu|$ are bounded. Also, the components of $\boldsymbol{f}(\lambda)$, $\boldsymbol{f}'(\lambda)$, and $\boldsymbol{f}''(\lambda)$ are square integrable by assumption. The growth conditions (7.5) can be used to control the other terms. Consider, for example, the second term above. We have, from (7.5b),

$$\left| \frac{\partial^2 f_B}{\partial q_i\,\partial q_j}(\lambda,\boldsymbol{q})\,r_j \right|^2 \le C\left(1+|\boldsymbol{q}|^4\right)|\boldsymbol{r}|^2\,,$$

from which follows

$$\int_\Omega \left| \frac{\partial^2 f_B}{\partial q_i\,\partial q_j}(\lambda,\boldsymbol{q})\,r_j \right|^2 \le C\|\boldsymbol{r}\|_{0,2,\Omega}^2 + C'\|\boldsymbol{q}\|_{0,6,\Omega}^4\|\boldsymbol{r}\|_{0,6,\Omega}^2\,.$$

This is finite due to the continuous embedding of $\mathbf{H}^1(\Omega)$ in $\mathbf{L}^6(\Omega)$, (3.1). Other terms can be handled similarly.

Next we need to know that each such term is continuous as a Nemitsky operator on $\Lambda \times \mathbf{H}_0^1(\Omega)$ to $\mathbf{L}^2(\Omega)$. For the terms involving $\boldsymbol{f}$, $\boldsymbol{f}'$, and $\boldsymbol{f}''$, this is a direct consequence of our assumptions. For the terms involving f_B, the growth conditions are again sufficient to verify this. The proofs can be constructed exactly along the lines of Ambrosetti and Prodi [5, §1.2, pp. 15–22] or Nečas [39, §3.1, pp. 37–40], using properties of L^p spaces and the Lebesgue Dominated Convergence Theorem. ◻

We mention that these conditions are satisfied by the densities used in our codes: f_B given by (2.3) (provided $D = E = E' = 0$) and $\mathcal{F}_L$ given by (2.5) (with $G = 0$). We now study the convergence of a piecewise-linear finite-element approximation to this problem.

Let τ_h be a family of exact triangulations of Ω by tetrahedra of type (1), and assume that τ_h satisfies the appropriate regularity hypotheses [11, Theorem 3.1.6]. Let $\mathcal{V}_h$ be the space of symmetric, traceless tensor fields, Q_h, with piecewise linear components, each of which vanishes at the boundary nodes of Ω. We introduce two finite-dimensional operators which are used in the approximation of solutions of (5.3). For any $Q \in \mathcal{H}_0^1(\Omega)$, define the operator Π_h by $\Pi_h Q \in \mathcal{V}_h$ and

$$a(\Pi_h Q - Q, P_h) = 0\,, \quad \forall P_h \in \mathcal{V}_h\,. \tag{7.6}$$

The form $a(\cdot,\cdot)$ is an inner product on the space $\mathcal{H}_0^1(\Omega)$, and the operator Π_h is the a-orthogonal projection (or Ritz-Galerkin projection) of the field Q onto the finite-dimensional space $\mathcal{V}_h$.

For any ℓ belonging to $\mathcal{H}^{-1}(\Omega)$, we define the finite-dimensional operator $\mathcal{T}_h$ by $\mathcal{T}_h \ell \in \mathcal{V}_h$ and

$$a(\mathcal{T}_h \ell, P_h) = \ell(P_h), \quad \forall P_h \in \mathcal{V}_h .$$

The operator $\mathcal{T}_h$ is related to the operator $\mathcal{T}$ through the relation

$$\mathcal{T}_h = \Pi_h \mathcal{T},$$

which shows that $\mathcal{T}_h$ is the composition of a projection and a bounded linear operator. Also note that $\mathcal{V}_h$ inherits the Hilbert space structure of the space $\mathcal{H}_0^1(\Omega)$. Thus, $a(\cdot,\cdot)$ is an inner product on $\mathcal{V}_h$, and the operator $\mathcal{T}_h$ is indeed well defined.

The problem of approximating solutions of (5.3) is now stated: Find $Q_h \in \mathcal{V}_h$ such that

$$Q_h + \mathcal{T}_h \mathcal{G}(\lambda, Q_h) = 0 .$$

We have the following theorem.

THEOREM 7.3. *Under the assumptions and definitions of this subsection and Lemma 7.2, there exists a neighborhood $\mathcal{O}$ of the origin in $\mathcal{H}_0^1(\Omega)$, and, for h sufficiently small, a unique C^2-function $\lambda \in \Lambda \mapsto Q_h(\lambda) \in \mathcal{V}_h$, such that for all $\lambda \in \Lambda$,*

$$Q_h + \mathcal{T}_h \mathcal{G}(\lambda, Q_h) = 0 \qquad \text{and} \qquad Q_h(\lambda) - Q(\lambda) \in \mathcal{O}.$$

Moreover, there is a constant $C > 0$ (independent of h and λ), such that $\forall \lambda \in \Lambda$,

$$\|Q_h(\lambda) - Q(\lambda)\|_{1,\Omega} \le C \|Q(\lambda) - \Pi_h Q(\lambda)\|_{1,\Omega} . \tag{7.7}$$

Thus

$$\lim_{h\to 0} \sup_{\lambda\in\Lambda} \|Q_h(\lambda) - Q(\lambda)\|_{1,\Omega} = 0 . \tag{7.8}$$

If, in addition, the solution branch $Q(\lambda)$ actually belongs to $\mathcal{H}^2(\Omega) \cap \mathcal{H}_0^1(\Omega)$, then

$$\|Q_h(\lambda) - Q(\lambda)\|_{1,\Omega} \le C h |Q(\lambda)|_{2,\Omega} , \quad \forall \lambda \in \Lambda . \tag{7.9}$$

Proof. We proceed by showing that all of the hypotheses of Theorem 7.1 are met with $V = \mathcal{H}_0^1(\Omega)$ and $W = \mathcal{L}^2(\Omega)$. Lemma 7.2 establishes the validity of hypothesis (i) in that theorem. Regarding the operator Π_h, a straightforward extension of [11, Theorem 3.2.3] to the tensor product of H^1 spaces shows that

$$\lim_{h\to 0} \|Q - \Pi_h Q\|_{1,\Omega} = 0 , \quad \forall Q \in \mathcal{H}_0^1(\Omega) .$$

Thus (ii) of Theorem 7.1 is established. Moreover,

$$\lim_{h\to 0} \|\mathcal{T} f - \mathcal{T}_h f\|_{1,\Omega} = \lim_{h\to 0} \|\mathcal{T} f - \Pi_h \mathcal{T} f\|_{1,\Omega} = 0 , \quad \forall f \in \mathcal{H}^{-1}(\Omega) .$$

That is, the operators $\mathcal{T}_h$ converge to $\mathcal{T}$ in the strong operator sense (on $\mathcal{H}^{-1}$). Since the embedding of $\mathcal{L}^2(\Omega)$ into $\mathcal{H}^{-1}(\Omega)$ is compact (by (3.3)), the convergence of $\mathcal{T}_h$

to $\mathcal{T}$ is actually uniform in the space $\mathcal{B}\left(\mathcal{L}^2(\Omega), \mathcal{H}_0^1(\Omega)\right)$ [6]. All of the hypotheses of Theorem 7.1 are satisfied. Hence, the estimate

$$\|Q_h(\lambda) - Q(\lambda)\|_{1,\Omega} \le C\left\{\|Q(\lambda) - \Pi_h Q(\lambda)\|_{1,\Omega} + \|(\mathcal{T}_h - \mathcal{T})\mathcal{G}(\lambda, Q)\|_{1,\Omega}\right\}$$

is valid. The expressions (7.7) and (7.8) follow from this and our definitions of Π_h and $\mathcal{T}_h$, which give

$$(\mathcal{T}_h - \mathcal{T})\mathcal{G}(\lambda, Q) = (\Pi_h \mathcal{T} - \mathcal{T})\mathcal{G}(\lambda, Q) = Q(\lambda) - \Pi_h Q(\lambda)\,.$$

If Q is in fact known to be in $\mathcal{H}^2(\Omega) \cap \mathcal{H}_0^1(\Omega)$, then (7.9) follows from (7.7) and the classical approximation result for piecewise-linear finite elements. ∎

Similar convergence analyses can be constructed which are appropriate for inhomogeneous Dirichlet boundary conditions and natural boundary conditions (see [15]). Again we note that this result applies to the functionals used in our finite-element code, with the expansion of the bulk free-energy density truncated at the fourth order. With higher-order regularity and higher-order finite elements, one can obtain the same classical (higher-order) convergence rates as for linear problems. We next consider regular problems, but with no assumed growth conditions.

7.2. Convergence for regular problems. If the boundary is at least of class $C^{1,1}$ or is convex, then the results of §6 assure us that our problem is regular, in the sense that the Riesz map, $\mathcal{T}$, is bounded on $\mathcal{L}^2(\Omega)$ to $\mathcal{H}^2(\Omega) \cap \mathcal{H}_0^1(\Omega)$. More generally, $\mathcal{T}$ maps $\mathcal{H}^{s-1}(\Omega)$ continuously to $\mathcal{H}^{s+1}(\Omega) \cap \mathcal{H}_0^1(\Omega)$ if the boundary is at least $C^{2s-1,1}$. Thus higher-order elements can be used and higher rates of convergence established.

For this case, we assume that $\Omega \subset \mathbf{R}^3$ is bounded, open, connected, and either convex or of class $C^{2s-1,1}$ for some positive integer s. The other basic assumptions of the previous subsection continue to hold. We now wish to apply Theorem 7.1 with the spaces $V = \mathcal{H}_0^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$ and $W = \mathcal{L}^2(\Omega)$. We again require conditions on f_B and $\mathcal{F}_L$ that are sufficient to guarantee condition (i) of Theorem 7.1. The following is a slight variation of Lemma 7.2 adequate for these new circumstances. The space $\mathbf{H}_0^1(\Omega) \cap \mathbf{C}(\overline{\Omega})$ is normed by $|\cdot|_{1,\Omega} + |\cdot|_{0,\infty,\Omega}$.

LEMMA 7.4. *For $\lambda \in \Lambda$ and $\boldsymbol{q} \in \mathbf{H}_0^1(\Omega)$, let $G(\lambda, \boldsymbol{q})$ be defined as in (7.4). Let the linear functional $F_L(\lambda, \cdot)$ be bounded on $\mathbf{L}^2(\Omega)$ with representer $\boldsymbol{f}(\lambda)$. Assume that f_B and $\boldsymbol{f}$ satisfy the following conditions:*

(i) *f_B is in $C^3(\Lambda \times \mathbf{R}^5)$.*

(ii) *$\boldsymbol{f}$ is in $C^2(\Lambda\,; \mathbf{L}^2(\Omega))$ with $\boldsymbol{f}(\lambda)$, $\boldsymbol{f}'(\lambda)$, and $\boldsymbol{f}''(\lambda)$ uniformly bounded for $\lambda \in \Lambda$.*

Then G is in $C^2(\Lambda \times \mathbf{H}_0^1(\Omega) \cap \mathbf{C}(\overline{\Omega})\,; \mathbf{L}^2(\Omega))$, and $D^2 G$ is bounded on bounded subsets of $\Lambda \times \mathbf{H}_0^1(\Omega) \cap \mathbf{C}(\overline{\Omega})$.

Proof. The expressions for G, DG, and D^2G are all as before (in (7.4) and the proof of Lemma 7.2). With $\boldsymbol{q}$ in $\mathbf{C}(\overline{\Omega})$ now, the quantities that we require to be in $L^2(\Omega)$ are all in fact continuous and bounded. Moreover, convergence in $\mathbf{H}^1(\Omega) \cap \mathbf{C}(\overline{\Omega})$ implies uniform convergence, from which follows the needed L^2 convergence. The result follows. ∎

We now define finite-element approximations in a standard way, using families of finite-dimensional subspaces $\mathcal{V}_h \subset \mathcal{H}_0^1(\Omega) \cap \mathcal{C}(\overline{\Omega})$. For simplicity, we restrict our attention to affine families of Lagrangian finite elements and assume that they conform exactly to the boundary and that they satisfy the following approximation properties:

$$|Q - \Pi_h Q|_{1,\Omega} + \sqrt{h}\,|Q - \Pi_h Q|_{0,\infty,\Omega} \le Ch|Q|_{2,\Omega}\,, \quad \forall Q \in \mathcal{H}^2(\Omega)\,, \tag{7.10}$$

for the case where Ω is only assumed to be a general convex or $C^{1,1}$ region, and

$$(7.11)\quad |Q-\Pi_h Q|_{1,\Omega}+\sqrt{h}\,|Q-\Pi_h Q|_{0,\infty,\Omega}\le Ch^s|Q|_{s+1,\Omega}\,,\quad \forall Q\in\mathcal{H}^{s+1}(\Omega)\,,$$

when Ω is of class $C^{2s-1,1}$. Here we assume that these hold for both the case when Π_h denotes the Ritz-Galerkin projection, Π_h^G, associated with $a(\cdot,\cdot)$ (as defined in (7.6)), as well as for the case when Π_h denotes the finite-element interpolation operator, Π_h^I, associated with $\mathcal{V}_h$.

These approximations do not capture the optimum uniform convergence rates associated with typical elements (i.e., $O(h^{s+1-\varepsilon})$ for $Q\in\mathcal{W}^{s+1,\infty}(\Omega)$). However, they can be easily established using inverse inequalities, regularity (Aubin-Nitsche lemma, L^2 convergence rates), and finite-element interpolation theory—see [11, ex. 3.3.2, pp. 167–8]. We have the following.

THEOREM 7.5. *Under the assumptions of this subsection and Lemma 7.4, there exists a neighborhood $\mathcal{O}$ of the origin in $\mathcal{H}_0^1(\Omega)\cap\mathcal{C}(\overline{\Omega})$, and for h sufficiently small, a unique C^2-function $\lambda\in\Lambda\mapsto Q_h(\lambda)\in\mathcal{V}_h$, such that for all $\lambda\in\Lambda$,*

$$Q_h+\mathcal{T}_h\mathcal{G}(\lambda,Q_h)=0\qquad\text{and}\qquad Q_h(\lambda)-Q(\lambda)\in\mathcal{O}.$$

Moreover, there is a constant $C>0$ (independent of h and λ), such that for all $\lambda\in\Lambda$,

$$|Q_h(\lambda)-Q(\lambda)|_{1,\Omega}+|Q_h(\lambda)-Q(\lambda)|_{0,\infty,\Omega}\le Ch^{1/2}|Q(\lambda)|_{2,\Omega}\,,$$

in the case where Ω is a general convex or $C^{1,1}$ region, and

$$|Q_h(\lambda)-Q(\lambda)|_{1,\Omega}+|Q_h(\lambda)-Q(\lambda)|_{0,\infty,\Omega}\le Ch^{s-1/2}|Q(\lambda)|_{s+1,\Omega}\,,$$

when Ω is of class $C^{2s-1,1}$.

Proof. Assumption (i) of Theorem 7.1 is satisfied by virtue of Lemma 7.4. Assume Ω is of class $C^{2s-1,1}$, with s a positive integer—the case of a general convex region identically corresponds to this argument with $s=1$.

The Banach space $\mathcal{V}:=\mathcal{H}_0^1(\Omega)\cap\mathcal{C}(\overline{\Omega})$ is normed by

$$\|Q\|_{\mathcal{V}}:=|Q|_{1,\Omega}+|Q|_{0,\infty,\Omega}\,.$$

We require that the finite-element interpolation operator Π_h^I satisfy

$$\lim_{h\to 0}\|Q-\Pi_h^I Q\|_{\mathcal{V}}=0\,,\quad\forall Q\in\mathcal{V}\,.$$

This can be established using the assumed validity of the result for $\mathcal{H}^2$ fields plus a density argument. We first note that Π_h^I is bounded on $\mathcal{V}$ to itself. This is a consequence of being associated with an affine family of Lagrangian elements (and the fact that our norm dominates the maximum norm): letting $(\widehat{K},\widehat{P},\widehat{\Sigma})$ denote the master finite-element triple, and assuming $\widehat{P}\subset H^1(\widehat{K})\cap C(\widehat{K}^-)$, we have

$$\widehat{\Pi}_h^I\widehat{Q}=\sum_i\widehat{Q}(\hat{a}_i)\hat{p}_i\quad\Longrightarrow$$
$$\|\widehat{\Pi}_h^I\widehat{Q}\|_{\mathcal{V},\widehat{K}}\le\|\widehat{Q}\|_{0,\infty,\widehat{K}}\sum_i\|\hat{p}_i\|_{\mathcal{V},\widehat{K}}\le C(\widehat{K},\widehat{P},\widehat{\Sigma})\|\widehat{Q}\|_{\mathcal{V},\widehat{K}}\,,$$

from which follows $\Pi_h^I\in\mathcal{B}(\mathcal{V},\mathcal{V})$.

Now we know from our assumed approximation properties that

$$\|Q - \Pi_h^I Q\|_{\mathcal{V}} \to 0\,, \quad \forall Q \in \mathcal{H}^2(\Omega) \cap \mathcal{V}\,.$$

Also, $\mathcal{H}^2(\Omega)$ is continuously and densely embedded in both $\mathcal{H}_0^1(\Omega)$ and $\mathcal{C}(\overline{\Omega})$, and therefore in $\mathcal{V}$. So, given any $Q \in \mathcal{V}$, we have (for any $Q_\varepsilon \in \mathcal{H}^2(\Omega)$)

$$\begin{aligned}\|Q - \Pi_h^I Q\|_{\mathcal{V}} &\le \|(I - \Pi_h^I)(Q - Q_\varepsilon)\|_{\mathcal{V}} + \|(I - \Pi_h^I)(Q_\varepsilon)\|_{\mathcal{V}} \\ &\le C\|Q - Q_\varepsilon\|_{\mathcal{V}} + \|Q_\varepsilon - \Pi_h^I Q_\varepsilon\|_{\mathcal{V}}\,.\end{aligned}$$

The first term can be made arbitrarily small by choosing $Q_\varepsilon \in \mathcal{H}^2(\Omega) \cap \mathcal{V}$ sufficiently close to Q. Given Q_ε, the second term converges to zero as $h \to 0$. Therefore condition (ii) of Theorem 7.1 holds with π_h the finite-element interpolation operator Π_h^I.

We also require that the solution operator $\mathcal{T}$ satisfy

$$\lim_{h\to 0} \|\mathcal{T} - \mathcal{T}_h\|_{\mathcal{B}(\mathcal{W},\mathcal{V})} = 0$$

with $\mathcal{V}$ as defined above and $\mathcal{W} := \mathcal{L}^2(\Omega)$. This also readily follows, since $\mathcal{T}$ is bounded on $\mathcal{L}^2(\Omega)$ to $\mathcal{H}^2(\Omega)$, which is compactly embedded in both $\mathcal{H}^1(\Omega)$ and $\mathcal{C}(\overline{\Omega})$, (3.2).

The hypotheses of Theorem 7.1 are satisfied, and we are assured of the existence of solutions of the discrete problem (twice continuously differentiable with respect to λ) satisfying $Q_h(\lambda) - Q(\lambda) \in \mathcal{O}$, for all $\lambda \in \Lambda$ and all h sufficiently small. Moreover we have

$$\|Q_h(\lambda) - Q(\lambda)\|_{\mathcal{V}} \le C\left\{\|Q(\lambda) - \Pi_h^I Q(\lambda)\|_{\mathcal{V}} + \|\,(\mathcal{T}_h - \mathcal{T})\,G(\lambda, Q)\|_{\mathcal{V}}\right\}\,.$$

But as before, $(\mathcal{T}_h - \mathcal{T})\,G(\lambda, Q) = Q(\lambda) - \Pi_h^G Q(\lambda)$. So we obtain

$$\|Q_h(\lambda) - Q(\lambda)\|_{\mathcal{V}} \le C\left\{\|Q(\lambda) - \Pi_h^I Q(\lambda)\|_{\mathcal{V}} + \|Q(\lambda) - \Pi_h^G Q(\lambda)\|_{\mathcal{V}}\right\}\,,$$

and our convergence rates follow from this and the assumed approximation properties of Π_h^I and Π_h^G. □

We observe that the established convergence rates are not optimal, with respect to either the $\mathcal{H}^1$ or $\mathcal{L}^\infty$ norms. The reduction in order can be attributed to the factor $\sqrt{h}$ in (7.10) and (7.11). Optimality could be recovered for the $\mathcal{H}^1$ norm, if it were known that the results of [9] were valid with respect to weighted (h-dependent) norms of the form

$$\|\cdot\|_{\mathcal{V}} := |\cdot|_{1,\Omega} + \sqrt{h}\,|\cdot|_{0,\infty,\Omega}\,.$$

We have presented here only illustrative results. Other combinations of norms and finite elements are certainly possible. For example, to capture the optimal uniform convergence rates, one should use the framework of Nitsche [11, §3.3] and interpret $\mathcal{T}$ as an operator on $\mathcal{W}^{s-1,\infty}(\Omega)$ to $\mathcal{W}^{s+1,\infty}(\Omega)$. We also mention that in the present context, the Aubin-Nitsche Lemma yields the higher convergence rates in the $\mathcal{L}^2$-norm:

$$|Q_h(\lambda) - Q(\lambda)|_{0,\Omega} \le Ch^{s+1/2}|Q(\lambda)|_{s+1,\Omega}\,.$$

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