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Local Stability and a Renormalized Newton Method for Equilibrium Liquid Crystal Director Modeling

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Abstract

We consider the nonlinear systems of equations that result from discretizations of a prototype variational model for the equilibrium director field characterizing the orientational properties of a liquid crystal material. In the presence of pointwise unit-vector constraints and coupled electric fields, the numerical solution of such equations by Lagrange-Newton methods leads to problems with a double saddle-point form, for which we have previously proposed a preconditioned nullspace method as an effective solver [A. Ramage and E. C. Gartland, Jr., submitted]. The characterization of local stability of solutions is complicated by the double saddle-point structure, and here we develop efficiently computable criteria in terms of minimum eigenvalues of certain projected Schur complements. We also propose a modified outer iteration ("Renormalized Newton Method") in which the orientation variables are normalized onto the constraint manifold at each iterative step. This scheme takes advantage of the special structure of these problems, and we prove that it is locally quadratically convergent. The Renormalized Newton Method bears some resemblance to the Truncated Newton Method of computational micromagnetics, and we compare and contrast the two.

Keywords: liquid crystals, director models, unit-vector constraints, saddle-point problems, reduced Hessian method, local stability, Renormalized Newton Method

AMS classifications: 49K35, 49K40, 49M15, 65H10, 65K10, 65N22

1 Introduction

Many continuum models for the orientational properties of liquid crystals at equilibrium involve one or more state variables that are vector fields of *unit length*. The pointwise unit-vector constraints associated with discretizations of such models give rise to indefinite linear systems of saddle-point form when these constraints are imposed via Lagrange multipliers. In problems such as these, indefiniteness also frequently manifests itself due to another influence (coupling with applied electric fields), and this leads to a *double* saddle-point structure. Models with some similar features arise also in the area of computational micromagnetics.

In [18] we analyzed a model problem of this type and proposed a nullspace method using MINRES with diagonal block preconditioning as a natural approach. The main ideas are briefly summarized below. These models are nonlinear and depend on multiple physical and geometric parameters, and it is typical for the equilibrium solutions (phases) to undergo transitions at critical values of certain of these parameters. The context we imagine is the numerical bifurcation and phase analysis of a discretization of a model for a realistic device or experiment in the large scale regime. In such a setting, parameter continuation leads to the repeated solution of systems of the type we are studying. Good initial guesses are available, however, and global Newton methods are generally employed.

At each computed equilibrium point along a branch of solutions, one performs auxiliary calculations of the *free energy* and the *local stability* of the solution. For parameter ranges in which multiple equilibrium solutions exist, the solution of *least free energy* gives the globally stable phase of the system. Local stability is characterized by certain eigenvalue calculations and identifies equilibria that have the potential of being globally stable. The objectives of this paper are twofold: first, to derive appropriate stability characterizations for the nullspace-method equations in several cases of interest, and second, to introduce an alternative

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outer iteration ("Renormalized Newton Method"), which is a slight variation of Newton's method that takes greater advantage of the special structure of such problems and which we prove retains the local quadratic convergence properties of Newton's method.

2 Liquid crystal director models

Many experiments and devices involving liquid crystal materials can be effectively modeled using a macroscopic continuum framework in which the orientational state of the system is described by a *director field* (a unit-length vector field denoting the average orientation of the molecules in a fluid element at a point), traditionally denoted by $\boldsymbol{n}$:

$$\boldsymbol{n} = n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2 + n_3\boldsymbol{e}_3, \quad |\boldsymbol{n}|^2 = n_1^2 + n_2^2 + n_3^2 = 1.$$

One of the main difficulties in dealing with models such as these numerically is the *unit-vector constraint* on $\boldsymbol{n}$, which must be satisfied at each point in the region occupied by the liquid crystal material. In the simplest cases, this can be managed by representing $\boldsymbol{n}$ in terms of orientation angles (e.g., $\boldsymbol{n} = \cos\theta\,\boldsymbol{e}_1 + \sin\theta\,\boldsymbol{e}_2$, in a 2-D setting), which recasts the problem as an *unconstrained* problem for the scalar fields associated with these angles. When an angle representation can't be employed, it is common to enforce the constraint $|\boldsymbol{n}| = 1$ via Lagrange multipliers. Several other liquid crystal models involve unit-length vector fields and constraints—see [18] for more discussion. Standard references on liquid crystals include [3, 6, 20, 21]. Unit-vector constraints arise in other areas as well, including the modeling of ferromagnetic materials—see [9] or [13].

Most devices and many experiments involve the interaction between a liquid crystal material and an applied electric field (which is used to control the liquid crystal orientational properties). The electric fields are usually created by sandwiching a liquid crystal film between electrodes to which a voltage is applied. This is a coupled interaction, with the electric field influencing the orientations of the liquid crystal molecules and the molecular orientational properties in turn influencing the local electric fields through their effect on the dielectric tensor. The *free energy* (expressed as an integral functional of the field variables) is the thermodynamic potential that determines equilibrium states of systems such as these. For a uniaxial nematic liquid crystal material in equilibrium with a coupled electric field (at constant potential), it has the generic form

$$\mathcal{F} = \int_\Omega \Big[W(\boldsymbol{n}, \nabla\boldsymbol{n}) - \frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E} \Big], \quad \boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n})\boldsymbol{E}, \quad \boldsymbol{E} = -\nabla U.$$

Here Ω is the region occupied by the liquid crystal, W is the distortional elastic energy density, $\boldsymbol{D}$ is the electric displacement, $\boldsymbol{E}$ is the local electric field, $\boldsymbol{\varepsilon}$ is the dielectric tensor, and U is the electrostatic potential.

The simplest approximation to the distortional elasticity is given by the "equal elastic constant" Oseen-Frank model:

$$W = \frac{K}{2}|\nabla\boldsymbol{n}|^2, \quad |\nabla\boldsymbol{n}|^2 = \sum_{i,j=1}^{3} \left(\frac{\partial n_i}{\partial x_j}\right)^2,$$

where K is a positive material-dependent "elastic constant" (which depends on temperature). The anisotropy of the medium is reflected in the tensorial nature of the "dielectric constant," which here corresponds to the real, symmetric, positive-definite tensor field $\boldsymbol{\varepsilon}$ (which is a function of $\boldsymbol{n}$). At a point in a uniaxial nematic liquid crystal, the $\boldsymbol{\varepsilon}$ tensor is transversely isotropic with respect to the local director $\boldsymbol{n}$, that is, it has a distinguished eigenvector parallel to $\boldsymbol{n}$ and a degenerate eigenspace perpendicular to $\boldsymbol{n}$:

$$\boldsymbol{\varepsilon}(\boldsymbol{n}) = \varepsilon_0\big(\varepsilon_\perp \mathbf{I} + \varepsilon_{\mathrm{a}}\boldsymbol{n}\otimes\boldsymbol{n}\big) \quad\leftrightarrow\quad \varepsilon_{ij} = \varepsilon_0(\varepsilon_\perp\delta_{ij} + \varepsilon_{\mathrm{a}}n_in_j), \quad \varepsilon_{\mathrm{a}} = \varepsilon_\parallel - \varepsilon_\perp. \tag{1}$$

In an eigenframe with third eigenvector $\boldsymbol{n}$, the $\boldsymbol{\varepsilon}$ tensor has Cartesian components

$$\boldsymbol{\varepsilon} = \varepsilon_0 \begin{bmatrix} \varepsilon_\perp & & \\ & \varepsilon_\perp & \\ & & \varepsilon_\parallel \end{bmatrix}.$$

Here ε_0 is a positive constant, and $\varepsilon_\parallel$ and $\varepsilon_\perp$ are positive, material-dependent, relative dielectric permittivities. The dielectric anisotropy ε_{a} can be positive or negative.

The total free energy then takes the form

$$\mathcal{F}[\boldsymbol{n}, U] = \frac{1}{2}\int_\Omega \big[K|\nabla \boldsymbol{n}|^2 - \boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U \cdot \nabla U\big]. \tag{2}$$

This is the simplest prototype model that contains the essential features of importance to us. One can see the intrinsic saddle-point nature of the electric-field coupling: equilibria are *minimizing* with respect to $\boldsymbol{n}$ but *maximizing* with respect to U. In a generic sense, the variational problem has the form

$$\min_{|\boldsymbol{n}|=1}\ \max_{U} \mathcal{F}[\boldsymbol{n}, U],$$

where the extremals are found over sufficiently regular fields that conform to any essential boundary conditions. The strong form of the constrained equilibrium equations for (2) (with $\boldsymbol{\varepsilon}$ of the form (1)) is

$$-\Delta \boldsymbol{n} = \lambda \boldsymbol{n} + \varepsilon_0 \varepsilon_{\mathrm{a}}\big(\nabla U \cdot \boldsymbol{n}\big)\nabla U, \quad \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = 0, \quad |\boldsymbol{n}| = 1, \tag{3}$$

which is to be solved in Ω subject to appropriate boundary conditions on $\boldsymbol{n}$ and U. The Lagrange multiplier field λ is associated with the pointwise unit-vector constraint. In terms of Cartesian components, the electrostatics equation takes the form

$$\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = \sum_{i,j} \frac{\partial}{\partial x_i}\left(\varepsilon_{ij}\frac{\partial U}{\partial x_j}\right) = 0. \tag{4}$$

Here one again sees the coupled nature of the problem, the electric field influencing the director equilibrium solution via the ∇U terms in the first equation of (3), and the director field influencing the electric potential through $\boldsymbol{\varepsilon}(\boldsymbol{n})$ in the second equation. Modeling a realistic system of interest can bring in multiple additional complications: more distortional elastic terms and constants, chirality, polarization, weak boundary conditions, periodic solutions with a-priori unknown periodicity, extended electric fields (if the region Ω is not completely enclosed by electrodes), etc.—see [10], for a recent example.

2.1 Comparison with ferromagnetics

The Landau-Lifshitz free energy provides a phenomenological model for equilibrium states of magnetization in ferromagnetic materials and is similar to the Oseen-Frank model for liquid crystals [9, 13]. The free-energy density is expressed in terms of a unit-length vector field $\boldsymbol{m}$, which corresponds to a normalized (saturated) magnetization vector $\boldsymbol{M}$, analogous to the liquid crystal director $\boldsymbol{n}$ but differing from it in the sense that $\boldsymbol{m}$ is a *proper* vector ($\boldsymbol{m}$ and $-\boldsymbol{m}$ are *not* equivalent). The density contains terms proportional to $|\nabla \boldsymbol{m}|^2$, penalizing spatial variations in $\boldsymbol{m}$ (as does $|\nabla \boldsymbol{n}|^2$ to $\boldsymbol{n}$). The magnetic stray field is given in terms of a magnetostatic potential via $\boldsymbol{H} = -\nabla U$ (as with the electric field and electrostatic potential in liquid crystals, $\boldsymbol{E} = -\nabla U$). The magnetic medium can be regarded as isotropic and homogeneous, however, so that the magnetic potential solves $\Delta U = \operatorname{div} \boldsymbol{M}$ (in the material domain); whereas the electric potential for liquid crystals satisfies $\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = 0$. This last equation would become $\operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = \operatorname{div} \boldsymbol{P}$ in a ferroelectric liquid crystal with polarization $\boldsymbol{P}$.

The contribution of the (spontaneous) stray field to the magnetic free-energy density is *positive* ($\frac{1}{2}\boldsymbol{B}\cdot\boldsymbol{H},\ \boldsymbol{B} = \mu_0(\boldsymbol{H}+\boldsymbol{M})$); whereas in a liquid crystal system at constant voltage, the coupling (to an applied electric field) is *negative* ($-\frac{1}{2}\boldsymbol{D}\cdot\boldsymbol{E},\ \boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n})\boldsymbol{E}$). Any externally applied magnetic field is treated as uniform throughout the sample and acts as a fixed force (or torque) on the magnetization in much the same way that external magnetic fields influence liquid crystals. Thus ferromagnetic systems do not have to cope with the indefiniteness that the U variables cause in liquid crystal systems. The combination of inhomogeneity, anisotropy, and negative-definiteness of the coupling between $\boldsymbol{n}$ and U add to the challenge of numerical modeling of liquid crystal systems.

3 Lagrange-Newton scheme and nullspace method

One can discretize such a coupled, constrained equilibrium problem in a variety of ways, starting from weak or strong formulations of (3), and utilizing various types of finite elements or finite differences or other

discretization methods. Our preference is to approximate $\mathcal{F}$ directly by some appropriate finite elements and quadrature scheme, obtaining

$$\mathcal{F}[\boldsymbol{n}, U] \approx f(\mathbf{n}, \mathbf{U}), \quad \mathbf{n} = (\mathbf{n}_1, \ldots, \mathbf{n}_n), \quad \mathbf{n}_j \in \mathbb{R}^3, \quad \mathbf{U} = (U_1, \ldots, U_n),$$

where $\mathbf{n}$ and $\mathbf{U}$ contain the discrete director and electric potential degrees of freedom in some ordering. Here n represents the total number of free nodes in the discrete model. The precise details of the discretization, which can be in any number of space dimensions, are not important. The unit-length constraint is imposed at each free node, and the full set of discrete, coupled, equality constrained equilibrium equations derives from a Lagrangian:

$$\nabla L = \mathbf{0}, \quad \text{where} \quad L(\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U}) = f(\mathbf{n}, \mathbf{U}) + \sum_{j=1}^{n} \lambda_j g_j(\mathbf{n}), \quad g_j(\mathbf{n}) := \frac{1}{2}(|\mathbf{n}_j|^2 - 1). \tag{5}$$

Here $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_n)$ is the vector of Lagrange multipliers. In most circumstances, the system (5) can be seen to be a consistent approximation to (3) (in an appropriate scaling)—see [18] for a concrete example.

A global Newton method applied to the system $\nabla L = \mathbf{0}$ in (5) above leads to a linear system for the Newton corrections of the form

$$\begin{bmatrix} A & B & D \\ B^T & O & O \\ D^T & O & -C \end{bmatrix} \begin{bmatrix} \boldsymbol{\delta}\mathbf{n} \\ \boldsymbol{\delta}\boldsymbol{\lambda} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} \nabla_{\mathbf{n}} L \\ \nabla_{\boldsymbol{\lambda}} L \\ \nabla_{\mathbf{U}} L \end{bmatrix}, \tag{6}$$

where

$$A = \nabla^2_{\mathbf{nn}} L, \quad B = \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L, \quad D = \nabla^2_{\mathbf{nU}} L, \quad C = -\nabla^2_{\mathbf{UU}} L,$$

and O denotes a zero matrix of appropriate dimensions. Our main interest is in effective numerical bifurcation and phase exploration of problems of such structure in the large scale regime (typically three space dimensions), where iterative methods are called for. This requires efficient solvers for the the linear system above and for the stability eigenvalue problem developed below, both of which must be solved repeatedly in parameter-continuation mode.

In [18] the structure of the matrix blocks in (6) is described in detail for a concrete model problem discretized via piecewise-linear finite elements. The A matrix is $3n \times 3n$ and has the general form

$$A = A_0 + \Lambda, \quad A_0 = \nabla^2_{\mathbf{nn}} f, \quad \Lambda = \begin{bmatrix} \Lambda_1 & & \\ & \ddots & \\ & & \Lambda_n \end{bmatrix}, \quad \Lambda_j = \begin{bmatrix} \lambda_j & & \\ & \lambda_j & \\ & & \lambda_j \end{bmatrix}. \tag{7}$$

For our model problem (2), the leading terms of A_0 take the form of the coefficient matrix of a discrete vector Laplacian (discretization of $-\Delta\boldsymbol{n}$, in finite-element scaling), although lower-order terms can cause loss of positive definiteness. The B matrix is $3n \times n$, built from the constraint normals. Because of the simplicity of the constraints, B has a very clean structure, which we exploit:

$$B = \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L = [\nabla_{\mathbf{n}} g_1, \ldots, \nabla_{\mathbf{n}} g_n] = [\nabla g_1, \ldots, \nabla g_n] = \begin{bmatrix} \mathbf{n}_1 & & \\ & \ddots & \\ & & \mathbf{n}_n \end{bmatrix}. \tag{8}$$

Under any reasonable discretization, the $n \times n$ matrix C will be real, symmetric, and positive definite, corresponding to the coefficient matrix associated with a discretization of (4). The matrix D is $3n \times n$ and embodies the coupling between $\boldsymbol{\delta}\mathbf{n}$ and $\boldsymbol{\delta}\mathbf{U}$.

At regular solution points (away from bifurcation points and turning points), the coefficient matrix is symmetric, non-singular, and indefinite—that is, it has both positive and negative eigenvalues—and the linear system is in so-called *saddle point form*. Note that when both pointwise unit-vector constraints and coupled electric fields are present, these problems have a *double* saddle-point structure. For a model with no electric field or for one with no unit-vector constraints (for example, if an angle representation were used for $\boldsymbol{n}$), one would obtain instead either of the more common saddle-point forms

$$\begin{bmatrix} A & B \\ B^T & O \end{bmatrix} \quad \text{or} \quad \begin{bmatrix} A & D \\ D^T & -C \end{bmatrix}.$$

Stability characterizations for all of these scenarios are developed below.

The *nullspace method* (or *reduced Hessian method*) is a technique for eliminating constraint blocks in a system such as this by using a matrix, Z say, whose column space is the null space of B^T—see for example [2, §6]. As we have shown in [18], it is trivial to construct such a matrix for problems such as ours, and it takes the form

$$Z = \begin{bmatrix} \mathbf{l}_1 & \mathbf{m}_1 & & & & \\ & & \mathbf{l}_2 & \mathbf{m}_2 & & \\ & & & & \ddots & \\ & & & & \mathbf{l}_n & \mathbf{m}_n \end{bmatrix}.$$

Here $\mathbf{l}_j$ and $\mathbf{m}_j$ are local 3-vectors and are constructed by simple formulas from $\mathbf{n}_j$ such that at each node, $\mathbf{l}_j$, $\mathbf{m}_j$, $\mathbf{n}_j$ form an orthogonal triple.

The solution set of the under-determined, second block equation ($B^T\boldsymbol{\delta}\mathbf{n} = -\nabla_{\boldsymbol{\lambda}} L$) can then be written as

$$\boldsymbol{\delta}\mathbf{n} = \widehat{\boldsymbol{\delta}\mathbf{n}} + Z\mathbf{p}, \quad \widehat{\boldsymbol{\delta}\mathbf{n}} = -B(B^TB)^{-1}\nabla_{\boldsymbol{\lambda}} L. \tag{9}$$

Substituting this into (6) leads to the reduced $3n \times 3n$ system of equations

$$\begin{bmatrix} Z^TAZ & Z^TD \\ D^TZ & -C \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} Z^T\big(\nabla_{\mathbf{n}} L + A\,\widehat{\boldsymbol{\delta}\mathbf{n}}\big) \\ \nabla_{\mathbf{U}} L + D^T\widehat{\boldsymbol{\delta}\mathbf{n}} \end{bmatrix}, \tag{10}$$

from which the full solution to (6) can then be recovered using

$$\boldsymbol{\delta\lambda} = -(B^TB)^{-1}B^T(\nabla_{\mathbf{n}} L + A\,\boldsymbol{\delta}\mathbf{n} + D\,\boldsymbol{\delta}\mathbf{U}). \tag{11}$$

Note that B^TB is a *diagonal matrix*; so the computation of $\widehat{\boldsymbol{\delta}\mathbf{n}}$ and $\boldsymbol{\delta\lambda}$ is quite simple, and this is true in any number of space dimensions. This approach is examined analytically and through numerical experiments in [18] on a specific model problem.

3.1 Geometric interpretation

The particular solution $\widehat{\boldsymbol{\delta}\mathbf{n}}$ in (9) can be seen to be the minimum 2-norm solution of $B^T\boldsymbol{\delta}\mathbf{n} = -\nabla_{\boldsymbol{\lambda}} L$, the second block equation of (6). Pointwise it has the explicit form

$$(\widehat{\boldsymbol{\delta}\mathbf{n}})_j = \frac{1}{2}\left(\frac{1-|\mathbf{n}_j|^2}{|\mathbf{n}_j|^2}\right)\mathbf{n}_j, \quad j = 1, \ldots, n. \tag{12}$$

Thus the representation (9) decomposes the $\boldsymbol{\delta}\mathbf{n}$ increment at each point into a component *parallel* to $\mathbf{n}_j$ ($(\widehat{\boldsymbol{\delta}\mathbf{n}})_j$ above) and a component *perpendicular* to $\mathbf{n}_j$ ($(Z\mathbf{p})_j = p_j\mathbf{l}_j + q_j\mathbf{m}_j$ where $\mathbf{p} = [p_1, q_1, \ldots, p_n, q_n]^T$). The component $(\widehat{\boldsymbol{\delta}\mathbf{n}})_j$ is *local*, completely driven by the pointwise unit-vector constraint, and independent of the liquid crystal distortional elasticity (which is captured by the $Z\mathbf{p}$ components). It can be seen as a linearized correction in the $\mathbf{n}_j$ direction towards satisfying the unit-vector constraint at the j-th grid point: setting

$$g_j(\mathbf{n} + \boldsymbol{\delta}\mathbf{n}) = \frac{1}{2}[(\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j)\cdot(\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j) - 1] \approx \frac{1}{2}(|\mathbf{n}_j|^2 - 1) + \mathbf{n}_j \cdot \boldsymbol{\delta}\mathbf{n}_j = 0$$

together with $\boldsymbol{\delta}\mathbf{n}_j = \eta_j\mathbf{n}_j$ implies

$$\eta_j = \frac{1}{2}\left(\frac{1-|\mathbf{n}_j|^2}{|\mathbf{n}_j|^2}\right),$$

exactly as in (12).

One can compare $(\widehat{\boldsymbol{\delta}\mathbf{n}})_j$ in (12) with the true increment (in the $\mathbf{n}_j$ direction) that would be needed to bring an un-normalized local director $\mathbf{n}_j$ onto the local constraint manifold $|\mathbf{n}_j| = 1$:

$$\mathbf{n}_j \;\mapsto\; \frac{\mathbf{n}_j}{|\mathbf{n}_j|} = \mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j^{\text{true}} \quad\Rightarrow\quad \boldsymbol{\delta}\mathbf{n}_j^{\text{true}} = \frac{1-|\mathbf{n}_j|}{|\mathbf{n}_j|}\mathbf{n}_j = \frac{2|\mathbf{n}_j|}{1+|\mathbf{n}_j|}(\widehat{\boldsymbol{\delta}\mathbf{n}})_j.$$

Since

$$\frac{2|\mathbf{n}_j|}{1+|\mathbf{n}_j|} > 1 \quad\Leftrightarrow\quad |\mathbf{n}_j| > 1 \qquad \text{and} \qquad \frac{2|\mathbf{n}_j|}{1+|\mathbf{n}_j|} < 1 \quad\Leftrightarrow\quad |\mathbf{n}_j| < 1,$$

we see that $(\widehat{\boldsymbol{\delta}\mathbf{n}})_j$ is *too large* if $|\mathbf{n}_j| < 1$ and *too small* if $|\mathbf{n}_j| > 1$. We conclude that the calculated Newton correction $\boldsymbol{\delta}\mathbf{n} = \widehat{\boldsymbol{\delta}\mathbf{n}} + Z\mathbf{p}$ necessarily produces a new local director

$$\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j = \mathbf{n}_j + (\widehat{\boldsymbol{\delta}\mathbf{n}})_j + (Z\mathbf{p})_j, \quad (\widehat{\boldsymbol{\delta}\mathbf{n}})_j \parallel \mathbf{n}_j, \quad (Z\mathbf{p})_j \perp \mathbf{n}_j$$

that satisfies

$$|\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j| \geq 1.$$

Thus successive Newton iterates generally exceed the pointwise unit-vector normalization, approaching it in the limit as the Newton iteration converges. Later we will attempt to take advantage of these observations and accelerate this process in an ad hoc way.

4 Local stability of computed solutions

The numerical investigation of such models generally involves numerical bifurcation and phase analysis—see [10] for a recent example. Numerical continuation techniques are used to follow paths of equilibrium solutions—see for example [12] or [14]. At each step of such a continuation procedure, in addition to computing the equilibrium solution for that set of parameters, one must also compute the associated discretized *free energy* of the solution and its local *stability* properties. For any given parameter values, the globally stable phase of the system is the equilibrium solution of least free energy. Locally stable solutions (also referred to as "metastable" solutions) are equilibrium solutions that admit the possibility of being globally stable (in a way we make precise below).

Even though locally unstable solutions are in a sense not of physical interest (since they would never be observed in nature in equilibrium), it is still the case that one frequently needs to follow branches of unstable solutions in order to reach branches of stable ones or to determine accurately phase boundary lines and metastability limits of individual phases. The characterizations of the local stability of equilibria involve spectral properties of the Hessian of the Lagrangian. In general, four different situations are of interest, depending upon whether a coupled electric field is present or not and upon whether one uses an angle representation for the directors or one uses vector components (with pointwise unit-vector constraints and Lagrange multipliers). We develop the analysis first for the most general case and then summarize the results for the simpler, specialized sub-cases.

4.1 General model: pointwise unit-vector constraints and coupled electric field

We consider the general problem we have addressed throughout: a discretized free energy with coupled electric field and the liquid-crystal director expressed in terms of vector components, with pointwise unit-vector constraints imposed via Lagrange multipliers. The discrete free energy is denoted by $f(\mathbf{n}, \mathbf{U})$, with $\mathbf{n}$ and $\mathbf{U}$ the degrees of freedom of the director field and the electric-potential field (in some ordering), and the discrete Lagrangian is as given in (5). The problem could be in any number of space dimensions. The characterization of local stability is complicated by the double saddle-point nature of the problem, which arises from both the Lagrange multipliers and the coupling to the electric field. By introducing a *deflated* (or *condensed*) free energy, from which the electric-potential degrees of freedom $\mathbf{U}$ have been removed, we are able to recast the problem as an equivalent equality-constrained minimization problem (instead of a constrained minimax problem) and draw from established results to develop appropriate local stability criteria.

4.1.1 Deflated free energy

The equilibrium equations of the electric-field variables are not directly influenced by the Lagrange multipliers or the constraints:

$$\nabla_{\mathbf{U}} L(\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U}) = \nabla_{\mathbf{U}} f(\mathbf{n}, \mathbf{U}) = \mathbf{0}.$$

Since f is quadratic in $\mathbf{U}$, the above is a linear system in $\mathbf{U}$ (for given discrete director field $\mathbf{n}$), which can be written in matrix-vector form as

$$C(\mathbf{n})\mathbf{U} = \mathbf{b}, \quad C(\mathbf{n}) = -\nabla^2_{\mathbf{U}\mathbf{U}} L(\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U}) = -\nabla^2_{\mathbf{U}\mathbf{U}} f(\mathbf{n}, \mathbf{U}),$$

the vector $\mathbf{b}$ coming from the boundary conditions on U. Here $C(\mathbf{n})$ is the C block of the Hessian (which is independent of $\mathbf{U}$, as f is quadratic in $\mathbf{U}$). In general, the matrix C is expected to be positive definite,

as it arises from a consistent discretization of a part of the free-energy functional $\mathcal{F}[\boldsymbol{n}, U]$ that is uniformly H^1-elliptic:

$$\varepsilon_0 \min\{\varepsilon_\perp, \varepsilon_\parallel\} \int_\Omega |\nabla U|^2 \le \int_\Omega \boldsymbol{\varepsilon}(\boldsymbol{n}) \nabla U \cdot \nabla U \le \varepsilon_0 \max\{\varepsilon_\perp, \varepsilon_\parallel\} \int_\Omega |\nabla U|^2.$$

It follows that $\nabla_{\mathbf{U}} f(\mathbf{n}, \mathbf{U}) = \mathbf{0}$ is uniquely solvable for $\mathbf{U}$ given any discrete director field $\mathbf{n}$ (normalized or not). We denote the solution operator $\boldsymbol{\Phi}$:

$$\nabla_{\mathbf{U}} f(\mathbf{n}, \mathbf{U}) = \mathbf{0} \quad \Rightarrow \quad \mathbf{U} = C(\mathbf{n})^{-1}\mathbf{b} =: \boldsymbol{\Phi}(\mathbf{n}). \tag{13}$$

Given that C and $\mathbf{b}$ depend smoothly on $\mathbf{n}$, and since C remains positive definite uniformly in $\mathbf{n}$, it follows that $\boldsymbol{\Phi}$ is a smooth function of $\mathbf{n}$ as well. In terms of this, we can define the deflated (or condensed) discrete free energy $\tilde{f}$ and the deflated Lagrangian $\widetilde{L}$:

$$\tilde{f}(\mathbf{n}) := f(\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})), \quad \widetilde{L}(\mathbf{n}, \boldsymbol{\lambda}) := \tilde{f}(\mathbf{n}) + \lambda_1 g_1(\mathbf{n}) + \cdots + \lambda_n g_n(\mathbf{n}). \tag{14}$$

In the $\tilde{f}$ formulation, the electric field is slaved to the director field: whatever $\mathbf{n}$ is specified, the equilibrium $\mathbf{U}$ associated with that $\mathbf{n}$ is used in the evaluation of the free energy. It is analogous in the continuous setting to having a PDE constraint or side condition attached to the model.

Since $f(\mathbf{n}, \mathbf{U})$ is a negative definite quadratic function of $\mathbf{U}$ (for each fixed $\mathbf{n}$), $\tilde{f}$ also admits the characterization $\tilde{f}(\mathbf{n}) = \max_{\mathbf{U}} f(\mathbf{n}, \mathbf{U})$. Observe also that

$$\nabla \tilde{f}(\mathbf{n}) = \nabla_{\mathbf{n}}[f(\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n}))] = \nabla_{\mathbf{n}} f(\mathbf{n}, \Phi(\mathbf{n})) + \nabla \boldsymbol{\Phi}(\mathbf{n})^T \nabla_{\mathbf{U}} f(\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})) = \nabla_{\mathbf{n}} f(\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})), \tag{15}$$

because $\nabla_{\mathbf{U}} f(\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})) = \mathbf{0}$ by definition of $\boldsymbol{\Phi}$. Here $\nabla\boldsymbol{\Phi}$ is the Jacobian of the transformation. It is not difficult to see that the critical points of $\widetilde{L}$ and L are in one-to-one correspondence:

Claim 1 *The constrained equilibrium points of $\tilde{f}(\mathbf{n})$ are in one-to-one correspondence with those of $f(\mathbf{n}, \mathbf{U})$.*

Proof 1 *Let $\mathcal{R}$ denote the mapping from discrete director fields $\mathbf{n}$ to pairs $(\mathbf{n}, \mathbf{U})$, with $\mathbf{U} = \boldsymbol{\Phi}(\mathbf{n})$:*

$$\mathcal{R}(\mathbf{n}) := (\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})), \quad \mathbf{n} \in \mathbb{R}^{3n}, \quad (\mathbf{n}, \boldsymbol{\Phi}(\mathbf{n})) \in \mathbb{R}^{3n} \times \mathbb{R}^n.$$

By construction, $\mathcal{R}$ is one-to-one ($\mathcal{R}(\mathbf{n}_1) = \mathcal{R}(\mathbf{n}_2) \Rightarrow (\mathbf{n}_1, \boldsymbol{\Phi}(\mathbf{n}_1)) = (\mathbf{n}_2, \boldsymbol{\Phi}(\mathbf{n}_2)) \Rightarrow \mathbf{n}_1 = \mathbf{n}_2$). Now suppose that $\mathbf{n}^*$ is a constrained equilibrium point of $\tilde{f}$, so that there exist Lagrange multipliers $\boldsymbol{\lambda}^*$ such that $\nabla \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) = \mathbf{0}$, that is

$$\nabla \tilde{f}(\mathbf{n}^*) + \lambda_1^* \nabla g_1(\mathbf{n}^*) + \cdots + \lambda_n^* \nabla g_n(\mathbf{n}^*) = \mathbf{0}, \quad g_1(\mathbf{n}^*) = \cdots = g_n(\mathbf{n}^*) = 0.$$

With $\mathbf{U}^* = \boldsymbol{\Phi}(\mathbf{n}^*)$, so that $\mathcal{R}(\mathbf{n}^*) = (\mathbf{n}^*, \mathbf{U}^*)$, and using (15), we see that $(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*)$ satisfies

$$\begin{gathered} \nabla_{\mathbf{n}} f(\mathbf{n}^*, \mathbf{U}^*) + \lambda_1^* \nabla g_1(\mathbf{n}^*) + \cdots + \lambda_n^* \nabla g_n(\mathbf{n}^*) = \mathbf{0}, \\ g_1(\mathbf{n}^*) = \cdots = g_n(\mathbf{n}^*) = 0, \quad \nabla_{\mathbf{U}} f(\mathbf{n}^*, \mathbf{U}^*) = \mathbf{0}. \end{gathered}$$

Thus $(\mathbf{n}^*, \mathbf{U}^*)$ is a constrained equilibrium point of $f(\mathbf{n}, \mathbf{U})$, in fact with the same Lagrange multipliers and same value of the discrete free energy. We see that if $\mathbf{n}^*$ is a constrained equilibrium point of $\tilde{f}$, then $\mathcal{R}(\mathbf{n}^*)$ is a constrained equilibrium point of f.

We can also see that $\mathcal{R}$ is onto. Given any $(\mathbf{n}^*, \mathbf{U}^*)$ that is a constrained equilibrium point of f, it follows that

$$\nabla_{\mathbf{U}} f(\mathbf{n}^*, \mathbf{U}^*) = \mathbf{0} \quad \Rightarrow \quad \mathbf{U}^* = \boldsymbol{\Phi}(\mathbf{n}^*) \quad \Rightarrow \quad (\mathbf{n}^*, \mathbf{U}^*) = \mathcal{R}(\mathbf{n}^*).$$

The same relations as above can be used to show that $\mathbf{n}^*$ is a constrained equilibrium point of $\tilde{f}$ (again with the same $\boldsymbol{\lambda}^*$ as associated with $(\mathbf{n}^*, \mathbf{U}^*)$). We see that every constrained equilibrium point $(\mathbf{n}^*, \mathbf{U}^*)$ of $f(\mathbf{n}, \mathbf{U})$ is the image under $\mathcal{R}$ of some constrained equilibrium point of $\tilde{f}$ (namely $\mathbf{n}^*$ itself). Thus $\mathcal{R}$ is one-to-one and onto between the sets of constrained equilibrium points of $\tilde{f}$ and f, and they are seen to be in one-to-one correspondence.

Recall that the reason for recasting our problem in terms of the deflated free energy $\tilde{f}$ is that the problem formulated in terms of $\tilde{f}$ is an equality-constrained *minimization* problem, not a constrained minimax problem. Let $\mathcal{N}$ denote the constraint manifold

$$\mathcal{N} := \{\mathbf{n} = (\mathbf{n}_1, \ldots, \mathbf{n}_n) \,|\, \mathbf{n}_j \in \mathbb{R}^3,\ |\mathbf{n}_j| = 1,\ j = 1, \ldots, n\},$$

which can be seen to be a smooth compact manifold without boundary in $\mathbb{R}^{3n}$. The deflated free energy $\tilde{f}(\mathbf{n}) = f(\mathbf{n}, \mathbf{\Phi}(\mathbf{n}))$ is a smooth function of $\mathbf{n}$: under conventional finite-difference or finite-element discretization, $f(\mathbf{n}, \mathbf{U})$ is a multivariate polynomial in the components of $\mathbf{n}$ and $\mathbf{U}$, and $\mathbf{\Phi}(\mathbf{n})$, as given by (13), has derivatives of all orders as well. It follows that $\tilde{f}$ attains its minimum (which is not necessarily unique) on $\mathcal{N}$ at a smooth critical point of $\widetilde{L}$. That is, there exists $\mathbf{n}^* \in \mathcal{N}$ such that

$$\tilde{f}(\mathbf{n}^*) = \min_{\mathbf{n}\in\mathcal{N}} \tilde{f}(\mathbf{n}).$$

Such a point must necessarily be a constrained equilibrium point of f of *least free energy*. Any *local* minimum point of $\tilde{f}$ restricted to $\mathcal{N}$ is a potential candidate for being a global minimum point, and so the key to characterizing the local stability of constrained equilibrium points of $f(\mathbf{n}, \mathbf{U})$ is the second-order conditions for $\tilde{f}$ restricted to $\mathcal{N}$, which we now exploit.

4.1.2 Stability criteria

The second-order necessary conditions of equality-constrained optimization theory dictate that a point $\mathbf{n}^*$ will be a smooth constrained local minimum point of the deflated free energy $\tilde{f}$ only if the Hessian with respect to $\mathbf{n}$ of the deflated Lagrangian $\widetilde{L}$ is positive semi-definite on the tangent space to the constraint manifold at $\mathbf{n}^*$; positive definiteness of this matrix is a sufficient condition—see for example [8, §9.3] or [11, §3.4.1]. We now interpret this in our setting. Thus let us assume that $\mathbf{n}^*$ is a local minimum point of $\tilde{f}$ on $\mathcal{N}$, that is, there is a relative neighborhood $\mathcal{U} \subset \mathcal{N}$ of $\mathbf{n}^*$ such that

$$\tilde{f}(\mathbf{n}^*) \le \tilde{f}(\mathbf{n}), \quad \forall \mathbf{n} \in \mathcal{U}.$$

By virtue of the non-vanishing of $\mathbf{n}_j$ on $\mathcal{N}$, the constraints satisfy the following *non-degeneracy condition* (see (5) and (8)):

$$\mathbf{n} \in \mathcal{N} \quad \Rightarrow \quad \nabla g_1(\mathbf{n}), \ldots, \nabla g_n(\mathbf{n}) \ \text{ linearly independent.} \tag{16}$$

The manifold $\mathcal{N}$ is smooth and without boundary, and $\tilde{f}$ is smooth. Furthermore, the non-degeneracy conditions above necessarily hold at all points on $\mathcal{N}$. These circumstances guarantee that there exist Lagrange multipliers $\boldsymbol{\lambda}^*$ such that

$$\nabla \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) = \mathbf{0} \quad \Leftrightarrow \quad \nabla_{\mathbf{n}} \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) = \mathbf{0}, \ \nabla_{\boldsymbol{\lambda}} \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) = \mathbf{0} \quad \Leftrightarrow$$
$$\nabla \tilde{f}(\mathbf{n}^*) + \lambda_1^* \nabla g_1(\mathbf{n}^*) + \cdots + \lambda_n^* \nabla g_n(\mathbf{n}^*) = \mathbf{0}, \quad g_1(\mathbf{n}^*) = \cdots = g_n(\mathbf{n}^*) = 0.$$

The point $(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*)$ with $\mathbf{U}^* = \mathbf{\Phi}(\mathbf{n}^*)$ likewise satisfies

$$\nabla L(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) = \mathbf{0} \quad \Leftrightarrow \quad \nabla_{\mathbf{n}} L(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) = \mathbf{0}, \ \nabla_{\boldsymbol{\lambda}} L(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) = \mathbf{0}, \ \nabla_{\mathbf{U}} L(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) = \mathbf{0}. \tag{17}$$

The *tangent space* to the constraint manifold at $\mathbf{n}^*$, denoted here by $\mathcal{T}_{\mathcal{N}}(\mathbf{n}^*)$, is by definition the span of the tangent vectors at $\mathbf{n}^*$ to all paths in $\mathcal{N}$ through $\mathbf{n}^*$. The non-degeneracy conditions (16) guarantee that this is the same as the orthogonal complement of the *normal space* to $\mathcal{N}$ at $\mathbf{n}^*$ (the span of the gradients of the constraint functions at $\mathbf{n}^*$):

$$\mathcal{T}_{\mathcal{N}}(\mathbf{n}^*) = \operatorname{span}\{\nabla g_1(\mathbf{n}^*), \ldots, \nabla g_n(\mathbf{n}^*)\}^{\perp}.$$

Notice that in our setting, $\mathcal{T}_{\mathcal{N}}(\mathbf{n}^*)$ is the column space of Z (null space of B^T), while the normal space is the column space of B (null space of Z^T). The second-order necessary conditions require that

$$\mathbf{u}^T \nabla^2_{\mathbf{nn}} \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) \mathbf{u} \ge 0, \quad \forall \mathbf{u} \in \mathcal{T}_{\mathcal{N}}(\mathbf{n}^*). \tag{18}$$

This relation can be expressed in terms of the matrix blocks of $\nabla^2 L$ using the following.

Claim 2 *In terms of the Hessian blocks defined in* (6)*, we can express*

$$\nabla^2 \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*) = \begin{bmatrix} \nabla^2_{\mathbf{nn}} \widetilde{L} & \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} \widetilde{L} \\ \nabla^2_{\boldsymbol{\lambda}\mathbf{n}} \widetilde{L} & \nabla^2_{\boldsymbol{\lambda}\boldsymbol{\lambda}} \widetilde{L} \end{bmatrix} = \begin{bmatrix} A + DC^{-1}D^T & B \\ B^T & O \end{bmatrix}, \tag{19}$$

where A, B, C, and D are all evaluated at $(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*)$, with $\mathbf{U}^* = \mathbf{\Phi}(\mathbf{n}^*)$.

Proof 2 *By definition of the solution operator* $\mathbf{\Phi}$*,*

$$\nabla_{\mathbf{U}} f(\mathbf{n}, \mathbf{\Phi}(\mathbf{n})) = \mathbf{0}, \quad \forall \mathbf{n}.$$

Differentiating this relationship gives

$$O = \nabla_{\mathbf{n}}[\nabla_{\mathbf{U}} f(\mathbf{n}, \mathbf{\Phi}(\mathbf{n}))] = \nabla^2_{\mathbf{Un}} f + (\nabla^2_{\mathbf{UU}} f)\nabla \mathbf{\Phi} \;\Rightarrow\; \nabla \mathbf{\Phi} = -(\nabla^2_{\mathbf{UU}} f)^{-1} \nabla^2_{\mathbf{Un}} f. \tag{20}$$

The inverse always exists, because $\nabla^2_{\mathbf{UU}} f = -C$ *and* C *is positive definite. We also know from* (15) *that*

$$\nabla \tilde{f}(\mathbf{n}) = \nabla_{\mathbf{n}} f(\mathbf{n}, \mathbf{\Phi}(\mathbf{n})), \quad \forall \mathbf{n}.$$

Differentiating this gives

$$\begin{aligned} \nabla^2 \tilde{f}(\mathbf{n}) &= \nabla_{\mathbf{n}}[\nabla_{\mathbf{n}} f(\mathbf{n}, \mathbf{\Phi}(\mathbf{n}))] \\ &= \nabla^2_{\mathbf{nn}} f + (\nabla^2_{\mathbf{nU}} f)\nabla \mathbf{\Phi} \\ &= \nabla^2_{\mathbf{nn}} f - \nabla^2_{\mathbf{nU}} f (\nabla^2_{\mathbf{UU}} f)^{-1} \nabla^2_{\mathbf{Un}} f \\ &= A_0 + DC^{-1}D^T, \end{aligned}$$

where we have used (20)*, with* A_0*,* C*, and* D *as defined in* (6) *and* (7)*.*

The components of $\nabla^2 \widetilde{L}$ *can now be assembled. Recall that the deflated Lagrangian is defined in* (14) *as*

$$\widetilde{L}(\mathbf{n}, \boldsymbol{\lambda}) = \tilde{f}(\mathbf{n}) + \lambda_1 g_1(\mathbf{n}) + \cdots + \lambda_n g_n(\mathbf{n}).$$

From this we obtain

$$\nabla^2_{\mathbf{nn}} \widetilde{L} = \nabla^2 \tilde{f} + \Lambda = A_0 + DC^{-1}D^T + \Lambda = A + DC^{-1}D^T,$$

where Λ *is as defined in* (7)*. We also readily obtain*

$$\nabla^2_{\mathbf{n}\boldsymbol{\lambda}} \widetilde{L} = B, \quad \nabla^2_{\boldsymbol{\lambda}\mathbf{n}} \widetilde{L} = B^T, \quad \textit{and} \quad \nabla^2_{\boldsymbol{\lambda}\boldsymbol{\lambda}} \widetilde{L} = O.$$

Thus (19) *is established.*

As we have already observed, the tangent space $\mathcal{T}_{\mathcal{N}}(\mathbf{n}^*)$ is precisely the column space of Z. It follows that any $\mathbf{u} \in \mathcal{T}_{\mathcal{N}}(\mathbf{n}^*)$ can be written $\mathbf{u} = Z\mathbf{p}$, for some $\mathbf{p}$. Thus for $\mathbf{u} \in \mathcal{T}_{\mathcal{N}}(\mathbf{n}^*)$,

$$\mathbf{u}^T \nabla^2_{\mathbf{nn}} \widetilde{L}(\mathbf{n}^*, \boldsymbol{\lambda}^*)\mathbf{u} = \mathbf{p}^T Z^T (A + DC^{-1}D^T) Z\mathbf{p},$$

and the necessary condition (18) requires that $Z^T(A + DC^{-1}D^T)Z$ (the reduced Hessian with respect to $\mathbf{n}$ of the deflated Lagrangian) be positive semi-definite. In terms of sufficient conditions, we obtain the local stability criterion

$$Z^T(A + DC^{-1}D^T)Z \text{ positive definite, indefinite} \;\Rightarrow\; (\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) \text{ locally stable, unstable.} \tag{21a}$$

Note that positive definiteness of Z^TAZ is *sufficient* for local stability but *not* necessary. That is, the electric-field coupling can stabilize an otherwise seemingly unstable solution; it cannot, on the other hand, destabilize an otherwise stable solution. Furthermore, on unstable branches, Z^TAZ is necessarily *indefinite.* Note also that the reduced Hessian $\mathcal{H}$ satisfies the congruence relation

$$\mathcal{H} := \begin{bmatrix} Z^TAZ & Z^TD \\ D^TZ & -C \end{bmatrix} = \begin{bmatrix} I & -Z^TDC^{-1} \\ & I \end{bmatrix} \begin{bmatrix} \widetilde{S} & \\ & -C \end{bmatrix} \begin{bmatrix} I & \\ -C^{-1}D^TZ & I \end{bmatrix},$$

where

$$\widetilde{S} := Z^T(A + DC^{-1}D^T)Z,$$

the Schur complement of $-C$ in $\mathcal{H}$. Sylvester's Law guarantees that $\mathcal{H}$ and $\begin{bmatrix} \widetilde{S} & \\ & -C \end{bmatrix}$ have the same inertia, and we know that C is $n \times n$ positive definite. It follows that the local stability criterion (21a), which pertains to the positive definiteness of $\widetilde{S}$, can be expressed in terms of sign patterns of the eigenvalues of the full $\mathcal{H}$:

$$\begin{aligned} 2n \text{ positive, } n \text{ negative eigenvalues} &\;\Rightarrow\; (\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) \text{ locally stable} \\ \text{more than } n \text{ negative eigenvalues} &\;\Rightarrow\; (\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) \text{ locally unstable} \end{aligned} \tag{21b}$$

4.2 Special cases: angle representations of directors, no electric fields

The analysis and results of the previous subsection cover various special cases, in particular those in which no electric field is present or in which the liquid crystal director is represented by orientation angles (or both). Not all liquid crystal systems of interest involve electric fields. It is also the case that numerical modelers will often use angle representations of the director field $\boldsymbol{n}$, when this is possible and convenient. Such representations give unit-length director fields by construction, and so it is not necessary in that setting to impose pointwise unit-vector constraints or to introduce any Lagrange multipliers into the formulations. We now derive local stability criteria for each of these commonly occurring cases.

4.2.1 No electric field, angle representation

In the absence of an electric field, the discretized free energy f will be a function of the discrete director field only, no longer depending on $\mathbf{U}$, and the stable phase of the system will be the global minimizer of f over the constraint manifold $\mathcal{N}$. In this situation, an equilibrium solution is a candidate for being a global minimizing point if and only if it is a local minimum point, and the characterization of local stability follows traditional lines. If one were able to use an angle representation for the director, then one would not have to contend with pointwise unit-vector constraints either, and the problem would simply be an unconstrained minimization problem,

$$f(\mathbf{x}^*) = \min_{\mathbf{x}} f(\mathbf{x}),$$

where $\mathbf{x}$ contains the degrees of freedom associated with the orientation angles in some order. Local stability would be deduced from the Hessian of f at the critical point:

$$\nabla^2 f(\mathbf{x}^*) \text{ positive definite, indefinite} \quad \Rightarrow \quad \mathbf{x}^* \text{ locally stable, unstable.}$$

The Hessian would be singular at any bifurcation or turning points.

4.2.2 No electric field, vector components representation

If one deals with the liquid crystal director in vector form (still in the case of no electric field) and imposes the pointwise unit-vector constraints via Lagrange multipliers, then the numerical modeling proceeds along previously discussed lines, with the exception of there being no degrees of freedom present for an electrostatic potential $\mathbf{U}$. One has a discrete Lagrangian of the form

$$L(\mathbf{n}, \boldsymbol{\lambda}) = f(\mathbf{n}) + \lambda_1 g_1(\mathbf{n}) + \cdots + \lambda_n g_n(\mathbf{n}),$$

with f the discretized free energy and $g_j(\mathbf{n}) = \frac{1}{2}(|\mathbf{n}_j|^2 - 1)$, as before. The Hessian takes the form

$$\nabla^2 L = \begin{bmatrix} \nabla^2_{\mathbf{nn}} L & \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L \\ \nabla^2_{\boldsymbol{\lambda}\mathbf{n}} L & \nabla^2_{\boldsymbol{\lambda}\boldsymbol{\lambda}} L \end{bmatrix} = \begin{bmatrix} A & B \\ B^T & O \end{bmatrix},$$

with A derived as before and B identical to (8). There is no need to introduce a deflated free energy. The conditions for equality-constrained minimization require that the Hessian of the Lagrangian (with respect to $\mathbf{n}$) be positive semi-definite on the tangent space to the constraint manifold at the point, and the local stability criterion (21a) becomes

$$Z^T A Z \text{ positive definite, indefinite} \quad \Rightarrow \quad (\mathbf{n}^*, \boldsymbol{\lambda}^*) \text{ locally stable, unstable.}$$

Again, $Z^T A Z$ (which now is the coefficient matrix for our nullspace-method Newton step) will be singular at bifurcation and turning points.

Unstable branches can still be encountered in these situations in which no electric field is present. This can occur, for example, in the situation in which the liquid crystal orientation is controlled by an applied magnetic field, which is common in experiments but not in devices. The influence of the magnetic field enters the free energy in a way very similar to that of an electric field (as discussed in §2 above). At this level of modeling, however, one can assume that the magnetic field remains *uniform* throughout the material, the effect of the liquid crystal anisotropy upon it being negligibly small.

4.2.3 Coupled electric field, angle representation

If the equilibrium problem for the liquid crystal director field contains a coupled electric field interaction but the director field can be represented in terms of orientation angles, then the problem again has an intrinsic saddle-point (minimax) nature to it. To analyze local stability, one must again introduce a deflated discrete free energy, however the problem no longer has the additional complicating feature of pointwise unit-vector constraints and Lagrange multipliers. Representing the director in terms of orientation angles leads to a discretized free energy of the form

$$f = f(\mathbf{x}, \mathbf{U}), \quad \mathbf{U} = (U_1, \ldots, U_n),$$

where $\mathbf{x}$ again contains the degrees of freedom associated with the orientation angles in some order and $\mathbf{U}$ contains the approximate values of the electric potential on the interior grid points. The coupled discrete equilibrium equations and associated Hessian are given by

$$\nabla f = \begin{bmatrix} \nabla_{\mathbf{x}} f \\ \nabla_{\mathbf{U}} f \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \quad \nabla^2 f = \begin{bmatrix} \nabla^2_{\mathbf{xx}} f & \nabla^2_{\mathbf{xU}} f \\ \nabla^2_{\mathbf{Ux}} f & \nabla^2_{\mathbf{UU}} f \end{bmatrix} = \begin{bmatrix} A & D \\ D^T & -C \end{bmatrix}. \tag{22}$$

The equations $\nabla_{\mathbf{U}} f = \mathbf{0}$ form a linear system in $\mathbf{U}$, which again can be solved uniquely for $\mathbf{U} = \mathbf{U}(\mathbf{x})$ for any $\mathbf{x}$. The critical points of the deflated discrete free energy $f(\mathbf{x}, \mathbf{U}(\mathbf{x}))$ coincide with those of the original $f(\mathbf{x}, \mathbf{U})$, and the Hessian is given by

$$\nabla^2_{\mathbf{xx}}[f(\mathbf{x}, \mathbf{U}(\mathbf{x}))] = A + DC^{-1}D^T.$$

The second-order conditions applied to the deflated free energy in this case give

$$A + DC^{-1}D^T \text{ positive definite, indefinite} \quad \Rightarrow \quad (\mathbf{x}^*, \mathbf{U}^*) \text{ locally stable, unstable.}$$

Here again the positive definiteness of $\nabla^2_{\mathbf{xx}} f(\mathbf{x}^*, \mathbf{U}^*) = A$ is *sufficient* for local stability but *not* necessary, and on unstable branches, A is necessarily *indefinite*. Note also that the Hessian in (22) satisfies the congruence relation

$$\begin{bmatrix} A & D \\ D^T & -C \end{bmatrix} = \begin{bmatrix} I & -DC^{-1} \\ & I \end{bmatrix} \begin{bmatrix} S & \\ & -C \end{bmatrix} \begin{bmatrix} I & \\ -C^{-1}D^T & I \end{bmatrix}, \quad S := A + DC^{-1}D^T,$$

where S is the Schur complement of $-C$ in $\nabla^2 f$. Sylvester's Law guarantees that $\begin{bmatrix} A & D \\ D^T & -C \end{bmatrix}$ and $\begin{bmatrix} S & \\ & -C \end{bmatrix}$ have the same inertia, with C here $n \times n$ positive definite. It follows that the local stability criterion (which pertains to the positive definiteness of S) can be expressed in terms of the sign patterns of the eigenvalues of the full Hessian $\nabla^2 f$:

$$\begin{aligned} 2n \text{ positive, } n \text{ negative eigenvalues} \quad &\Rightarrow \quad (\mathbf{x}^*, \mathbf{U}^*) \text{ locally stable} \\ \text{more than } n \text{ negative eigenvalues} \quad &\Rightarrow \quad (\mathbf{x}^*, \mathbf{U}^*) \text{ locally unstable.} \end{aligned}$$

The main results concerning the characterization of local stability for equilibria of liquid crystal director models then are the criteria (21), which apply to a general model with coupled electric field, unit-vector constraints, and Lagrange multipliers. All the matrices that appear there (A, B, C, D, and Z) are already needed to form the nullspace-method equations. In the large-scale setting, the criterion (21a) (which involves the minimum eigenvalue of the reduced Hessian of the deflated Lagrangian) would appear to be the more attractive for implementation, as it would be amenable to numerical methods of Lanczos type—see for example [5] or [19].

5 Alternative outer iteration: Renormalized Newton Method

While a global Newton iteration is a natural choice for an outer iteration, specific features of problems such as these suggest some simplifications, which lead to a closely related variant. In particular, we have already observed the simplifications that accompany the circumstance in which the current approximate $\mathbf{n}$ is *normalized*: $|\mathbf{n}_j| = 1, \quad j = 1, \ldots, n$. In this situation, $\mathbf{l}_j$, $\mathbf{m}_j$, $\mathbf{n}_j$ form an ortho*normal* triple at each grid

point; so $B^TB = I$. Since $\nabla_{\boldsymbol{\lambda}} L = \mathbf{0}$, $\widehat{\boldsymbol{\delta}\mathbf{n}} = \mathbf{0}$, and $\boldsymbol{\delta}\mathbf{n}_j \perp \mathbf{n}_j$ for all j, the nullspace-method equations (10) and (11) take the simpler form

$$\begin{bmatrix} Z^TAZ & Z^TD \\ D^TZ & -C \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} Z^T\nabla_{\mathbf{n}} f \\ \nabla_{\mathbf{U}} f \end{bmatrix}, \quad \boldsymbol{\delta}\mathbf{n} = Z\mathbf{p},$$
$$\boldsymbol{\delta\lambda} = -B^T(\nabla_{\mathbf{n}} f + A\boldsymbol{\delta}\mathbf{n} + D\boldsymbol{\delta}\mathbf{U}).$$

Here we have used the facts that

$$\nabla_{\mathbf{n}} L = \nabla_{\mathbf{n}} f + B\boldsymbol{\lambda} \quad \Rightarrow \quad Z^T\nabla_{\mathbf{n}} L = Z^T\nabla_{\mathbf{n}} f,$$

since $Z^TB = O$ by construction, and $\nabla_{\mathbf{U}} L = \nabla_{\mathbf{U}} f$. By virtue of the simple, local nature of our constraints, it is quite easy to force them upon any approximate discrete director field $\mathbf{n}$ by simply normalizing each local director. Furthermore, we know from the discussion in §3.1 that the basic Newton iteration produces local directors that are systematically too long ($|\mathbf{n}_j| > 1$).

Also, the Lagrange multipliers occur in a simple way, linearly in the $\nabla_{\mathbf{n}} L = \mathbf{0}$ equations, and in general are not of the same level of physical interest as are $\mathbf{n}$ and $\mathbf{U}$—although they are needed to assess local stability. Given the $\mathbf{n}^*$ and $\mathbf{U}^*$ components of an exact solution of $\nabla L(\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*) = \mathbf{0}$, the Lagrange multipliers can be computed directly (and locally) via

$$\nabla_{\mathbf{n}} L = \nabla_{\mathbf{n}} f + B\boldsymbol{\lambda} = \mathbf{0} \quad \Rightarrow \quad \boldsymbol{\lambda}^* = -B(\mathbf{n}^*)^T\nabla_{\mathbf{n}} f(\mathbf{n}^*, \mathbf{U}^*)$$
$$\Leftrightarrow \quad \lambda_j^* = -\nabla_{\mathbf{n}_j} f(\mathbf{n}^*, \mathbf{U}^*) \cdot \mathbf{n}_j^*, \quad j = 1, \ldots, n.$$

When $\mathbf{n}$ and $\mathbf{U}$ correspond to the components of an approximate (not yet converged) solution of $\nabla L = \mathbf{0}$, the over-determined system $\nabla_{\mathbf{n}} f + B\boldsymbol{\lambda} = \mathbf{0}$ (viewed as $3n$ equations in $\lambda_1, \ldots, \lambda_n$) is not necessarily consistent, and the formulas above give the linear least squares solution:

$$\min_{\boldsymbol{\lambda}} \|\nabla_{\mathbf{n}} f + B\boldsymbol{\lambda}\|_2 \quad \Leftrightarrow \quad \boldsymbol{\lambda} = -(B^TB)^{-1}B^T\nabla_{\mathbf{n}} f = -B^T\nabla_{\mathbf{n}} f.$$

These then are the features we will exploit: renormalizing the discrete director at each outer iterative step and eliminating the Lagrange multipliers by the formulas above. Our algorithm for the "Renormalized Newton Method" takes the following form.

Algorithm 1 (Renormalized Newton Method)

1. *in:* $\mathbf{n}$, $\mathbf{U}$ *satisfying* $|\mathbf{n}_j| = 1$, $j = 1, \ldots, n$
2. *set*
$$\boldsymbol{\lambda} = -B(\mathbf{n})^T\nabla_{\mathbf{n}} f(\mathbf{n}, \mathbf{U}) \tag{23}$$
3. *solve*
$$\begin{bmatrix} Z^TAZ & Z^TD \\ D^TZ & -C \end{bmatrix} \begin{bmatrix} \mathbf{p} \\ \boldsymbol{\delta}\mathbf{U} \end{bmatrix} = - \begin{bmatrix} Z^T\nabla_{\mathbf{n}} f \\ \nabla_{\mathbf{U}} f \end{bmatrix}$$
4. *update and normalize:*
$$\boldsymbol{\delta}\mathbf{n} = Z\mathbf{p}, \quad \mathbf{n}_j^{\mathrm{RN}} = \frac{\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j}{|\mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j|}, \quad j = 1, \ldots, n, \quad \mathbf{U}^{\mathrm{RN}} = \mathbf{U} + \boldsymbol{\delta}\mathbf{U}$$
5. *out:* $\mathbf{n}^{\mathrm{RN}}$, $\mathbf{U}^{\mathrm{RN}}$ *satisfying* $|\mathbf{n}_j^{\mathrm{RN}}| = 1$, $j = 1, \ldots, n$

We note that the gradient $\nabla_{\mathbf{n}} f(\mathbf{n}, \mathbf{U})$ used to calculate $\boldsymbol{\lambda}$ above is already needed and that the calculation is simply done componentwise: $\lambda_j = -\nabla_{\mathbf{n}_j} f \cdot \mathbf{n}_j$, $j = 1, \ldots, n$. The other matrix and vector components above are computed exactly as before, the Lagrange multipliers entering only in A. If we compare this modified step with the basic Newton step $(\mathbf{n}^{\mathrm{N}}, \boldsymbol{\lambda}^{\mathrm{N}}, \mathbf{U}^{\mathrm{N}})$ from $(\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U})$, with the same input $\mathbf{n}$ and $\mathbf{U}$ and with $\boldsymbol{\lambda}$ computed as above, we see that $\mathbf{n}^{\mathrm{RN}}$ is simply a renormalized version of $\mathbf{n}^{\mathrm{N}} = \mathbf{n} + \boldsymbol{\delta}\mathbf{n}$, $\boldsymbol{\lambda}$ is treated as an intermediary (and computed differently than $\boldsymbol{\lambda}^{\mathrm{N}} = \boldsymbol{\lambda} + \boldsymbol{\delta\lambda}$, only when needed at the next step), and $\mathbf{U}^{\mathrm{RN}} = \mathbf{U}^{\mathrm{N}} = \mathbf{U} + \boldsymbol{\delta}\mathbf{U}$.

Besides the analytical simplifications gained by this scheme, it is physically intuitive and somewhat analogous to other numerical approaches that have been applied to related problems. The numerical device of renormalizing after each step has been used by computational physicists in this area for a long time (in the context of the pseudo-time-relaxation approach to computing constrained equilibria) and has also been employed by numerical analysts in the context of both relaxation and gradient methods [1, 4, 15]. Analogous ideas have been used in the area of micromagnetics, where the magnetization is computed in a normalized form as a unit vector field—see [9, §4] or [13, §2.2.1]. In §5.2 below, we explore the relationship of the Renormalized Newton Method to the Truncated Newton Method of computational micromagnetics.

5.1 Local quadratic convergence analysis of the Renormalized Newton Algorithm

In spite of the attractive features discussed above, one would not contemplate using such an alternative outer iteration if it did not preserve the quadratic local convergence properties of Newton. In fact it does, which we will now prove. The analysis relies upon the following two facts: first, that the error in $\boldsymbol{\lambda}$ computed by (23) as an approximation to the Lagrange multipliers $\boldsymbol{\lambda}^*$ of the exact solution $(\mathbf{n}^*, \mathbf{U}^*)$ is of the same order as the errors in $\mathbf{n}-\mathbf{n}^*$ and $\mathbf{U}-\mathbf{U}^*$, and second, that the renormalization step is *second order* in the Newton correction $\boldsymbol{\delta}\mathbf{n}$. We establish these preliminary results in two lemmas, after first introducing some notation and recalling what the local convergence results for the basic global Newton iteration give us.

Let $\mathbf{x}^* = (\mathbf{n}^*, \boldsymbol{\lambda}^*, \mathbf{U}^*)$ be a *regular* discrete constrained equilibrium solution, that is,

$$\nabla L(\mathbf{x}^*) = \mathbf{0}, \quad \nabla^2 L(\mathbf{x}^*) \text{ non-singular.}$$

We note that this can include locally unstable solutions as well as locally stable solutions. The only situation excluded is that of *singular* equilibrium solutions, at which $\nabla L(\mathbf{x}^*) = \mathbf{0}$ but the Hessian $\nabla^2 L(\mathbf{x}^*)$ is singular. In a typical parameter study, such situations would occur at bifurcation and turning points, for example.

For convenience, we work with vector and matrix 2-norms, and adopt the notation

$$\begin{aligned}
\mathcal{B}_\varepsilon(\mathbf{x}^*) &= \big\{\mathbf{x} \,|\, \|\mathbf{x}-\mathbf{x}^*\|_2 \le \varepsilon\big\} \\
&= \big\{(\mathbf{n},\boldsymbol{\lambda},\mathbf{U}) \,|\, \|\mathbf{n}-\mathbf{n}^*\|_2^2 + \|\boldsymbol{\lambda}-\boldsymbol{\lambda}^*\|_2^2 + \|\mathbf{U}-\mathbf{U}^*\|_2^2 \le \varepsilon^2\big\}, \\
\mathcal{B}'_\varepsilon(\mathbf{x}^*) &= \big\{(\mathbf{n},\mathbf{U}) \,|\, \|\mathbf{n}-\mathbf{n}^*\|_2^2 + \|\mathbf{U}-\mathbf{U}^*\|_2^2 \le \varepsilon^2\big\}, \\
\mathcal{B}''_\varepsilon(\mathbf{x}^*) &= \big\{(\mathbf{n},\mathbf{U}) \in \mathcal{B}'_\varepsilon(\mathbf{x}^*) \,|\, |\mathbf{n}_j| = 1,\ j = 1,\dots,n\big\}.
\end{aligned}$$

We note that $\mathcal{B}'_\varepsilon(\mathbf{x}^*)$ corresponds to the $\boldsymbol{\lambda} = \boldsymbol{\lambda}^*$ section of $\mathcal{B}_\varepsilon(\mathbf{x}^*)$ and that $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U}) \in \mathcal{B}_\varepsilon(\mathbf{x}^*) \Rightarrow (\mathbf{n},\mathbf{U}) \in \mathcal{B}'_\varepsilon(\mathbf{x}^*)$, while $\mathcal{B}''_\varepsilon(\mathbf{x}^*)$ is a subset of $\mathcal{B}'_\varepsilon(\mathbf{x}^*)$, adding only the requirement that $\mathbf{n}$ be normalized. Our Lagrangian L is an algebraic function (a multivariate polynomial in the components of $\mathbf{x}$, for conventional discretizations) and is therefore infinitely continuously differentiable. As such it satisfies any needed regularity hypotheses, and standard results on the local convergence of Newton's Method hold—see for example [7, §5.2] or [17, §10.2.2].

Theorem 1 (Local Newton Convergence) *For any regular point $\mathbf{x}^*$, there exist positive constants C_N and ε_N satisfying $C_N\varepsilon_N < 1$, such that for any $\mathbf{x} \in \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*)$, the Newton step $\mathbf{x}^N$ is well defined and satisfies*

$$\|\mathbf{x}^N - \mathbf{x}^*\|_2 \le C_N \|\mathbf{x}-\mathbf{x}^*\|_2^2. \tag{24}$$

We recall that from this basic estimate it follows that the Newton iteration is quadratically convergent from any initial guess $\mathbf{x}^{(0)} \in \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*)$ by arguing as follows:

$$\|\mathbf{x}^{(1)} - \mathbf{x}^*\|_2 \le C_N \|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2^2 \le C_N\varepsilon_N \|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2,$$

which implies $\{\mathbf{x}^{(k)}\}_{k=0}^\infty \subset \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*)$ (since $C_N\varepsilon_N < 1$),

$$\|\mathbf{x}^{(k)} - \mathbf{x}^*\|_2 \le (C_N\varepsilon_N)^k \|\mathbf{x}^{(0)} - \mathbf{x}^*\|_2 \to 0, \text{ as } k \to \infty,$$

and

$$\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\|_2 \le C_N \|\mathbf{x}^{(k)} - \mathbf{x}^*\|_2^2, \quad k = 0, 1, \dots\ .$$

We aim to establish an analogous result for the Renormalized Newton scheme. The following lemma shows that if $(\mathbf{n},\mathbf{U})$ is sufficiently close to $(\mathbf{n}^*,\mathbf{U}^*)$, then $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$ (with $\boldsymbol{\lambda}$ calculated using (23)) is guaranteed to be within the region of attraction of the basic Newton iteration.

Lemma 1 *For any regular point $\mathbf{x}^*$, there exist positive constants C_1 and ε_1 such that*

$$(\mathbf{n},\mathbf{U}) \in \mathcal{B}'_{\varepsilon_N}(\mathbf{x}^*) \quad \Rightarrow \quad \|\lambda-\lambda^*\|_2 \le C_1\sqrt{\|\mathbf{n}-\mathbf{n}^*\|_2^2+\|\mathbf{U}-\mathbf{U}^*\|_2^2}$$

and

$$(\mathbf{n},\mathbf{U}) \in \mathcal{B}'_{\varepsilon_1}(\mathbf{x}^*) \quad \Rightarrow \quad (\mathbf{n},\boldsymbol{\lambda},\mathbf{U}) \in \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*),$$

with λ computed from $(\mathbf{n},\mathbf{U})$ using (23). Here ε_N is the local Newton radius of Theorem 1.

Proof 3 *Let $(\mathbf{n},\mathbf{U})$ be in $\mathcal{B}'_{\varepsilon_N}(\mathbf{x}^*)$. The approximate $\boldsymbol{\lambda}$ computed using (23) and exact Lagrange multipliers $\boldsymbol{\lambda}^*$ satisfy*

$$\boldsymbol{\lambda} = -B(\mathbf{n})^T\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U}), \quad \boldsymbol{\lambda}^* = -B(\mathbf{n}^*)^T\nabla_{\mathbf{n}}f(\mathbf{n}^*,\mathbf{U}^*).$$

Subtracting these and using the fact that the matrix function B is linear in its argument ($B(\mathbf{n}) = B(\mathbf{n}-\mathbf{n}^*)+B(\mathbf{n}^*)$), we obtain

$$\boldsymbol{\lambda}^*-\boldsymbol{\lambda} = B(\mathbf{n}^*)^T\big[\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U})-\nabla_{\mathbf{n}}f(\mathbf{n}^*,\mathbf{U}^*)\big]+B(\mathbf{n}-\mathbf{n}^*)^T\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U}),$$

which implies

$$\|\boldsymbol{\lambda}-\boldsymbol{\lambda}^*\|_2 \le \|B(\mathbf{n}^*)^T\|_2\|\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U})-\nabla_{\mathbf{n}}f(\mathbf{n}^*,\mathbf{U}^*)\|_2+\|B(\mathbf{n}-\mathbf{n}^*)^T\|_2\|\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U})\|_2. \tag{25}$$

The difference of the gradients above can be estimated using remainder formulas, such as in [7, §4.1] or [17, §3.2]:

$$\begin{aligned}\|\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U})-\nabla_{\mathbf{n}}f(\mathbf{n}^*,\mathbf{U}^*)\|_2 &\le \max_{0\le t\le 1}\|\nabla^2_{\mathbf{nn}}f(\mathbf{n}^*+t(\mathbf{n}-\mathbf{n}^*),\mathbf{U}^*+t(\mathbf{U}-\mathbf{U}^*))\|_2\|\mathbf{n}-\mathbf{n}^*\|_2\\ &+ \max_{0\le t\le 1}\|\nabla^2_{\mathbf{nU}}f(\mathbf{n}^*+t(\mathbf{n}-\mathbf{n}^*),\mathbf{U}^*+t(\mathbf{U}-\mathbf{U}^*))\|_2\|\mathbf{U}-\mathbf{U}^*\|_2\\ &\le M_1\|\mathbf{n}-\mathbf{n}^*\|_2+M_2\|\mathbf{U}-\mathbf{U}^*\|_2,\end{aligned}$$

with

$$M_1 := \max_{(\mathbf{n},\mathbf{U})\in\mathcal{B}'_{\varepsilon_N}(\mathbf{x}^*)}\|\nabla^2_{\mathbf{nn}}f(\mathbf{n},\mathbf{U})\|_2, \quad M_2 := \max_{(\mathbf{n},\mathbf{U})\in\mathcal{B}'_{\varepsilon_N}(\mathbf{x}^*)}\|\nabla^2_{\mathbf{nU}}f(\mathbf{n},\mathbf{U})\|_2.$$

The matrix 2-norms of $B(\mathbf{n}^*)^T$ and $B(\mathbf{n}-\mathbf{n}^*)^T$ can be estimated by observing that they both stem from matrices of the general form

$$B(\mathbf{b}) = \begin{bmatrix}\mathbf{b}_1 & & \\ & \ddots & \\ & & \mathbf{b}_n\end{bmatrix}, \quad \mathbf{b}=(\mathbf{b}_1,\dots,\mathbf{b}_n), \quad \mathbf{b}_1,\dots,\mathbf{b}_n\in\mathbb{R}^3,$$

for which

$$B(\mathbf{b})B(\mathbf{b})^T = \begin{bmatrix}\mathbf{b}_1\mathbf{b}_1^T & & \\ & \ddots & \\ & & \mathbf{b}_n\mathbf{b}_n^T\end{bmatrix}.$$

It follows that

$$\|B(\mathbf{b})^T\|_2 = \sqrt{\lambda_{\max}(B(\mathbf{b})B(\mathbf{b})^T)} = \max\big\{|\mathbf{b}_1|,\dots,|\mathbf{b}_n|\big\}.$$

Thus

$$\|B(\mathbf{n}^*)^T\|_2 = \max\big\{|\mathbf{n}_1^*|,\dots,|\mathbf{n}_n^*|\big\} = 1$$

and

$$\|B(\mathbf{n}-\mathbf{n}^*)^T\|_2 = \max\big\{|\mathbf{n}_1-\mathbf{n}_1^*|,\dots,|\mathbf{n}_n-\mathbf{n}_n^*|\big\} \le \|\mathbf{n}-\mathbf{n}^*\|_2.$$

With the help of these estimates, it follows from (25) that

$$\|\boldsymbol{\lambda}-\boldsymbol{\lambda}^*\|_2 \le M_1\|\mathbf{n}-\mathbf{n}^*\|_2+M_2\|\mathbf{U}-\mathbf{U}^*\|_2+M_3\|\mathbf{n}-\mathbf{n}^*\|_2,$$

with

$$M_3 := \max_{(\mathbf{n},\mathbf{U})\in\mathcal{B}'_{\varepsilon_N}(\mathbf{x}^*)}\|\nabla_{\mathbf{n}}f(\mathbf{n},\mathbf{U})\|_2,$$

which in turn implies that

$$\|\boldsymbol{\lambda}-\boldsymbol{\lambda}^*\|_2 \le C_1\sqrt{\|\mathbf{n}-\mathbf{n}^*\|_2^2+\|\mathbf{U}-\mathbf{U}^*\|_2^2}\,, \quad \textit{with } C_1 := \sqrt{(M_1+M_3)^2+M_2^2}\,. \tag{26}$$

If we now take

$$\varepsilon_1 := \frac{\varepsilon_N}{\sqrt{C_1^2+1}},$$

we obtain

$$\begin{array}{rcl} (\mathbf{n},\mathbf{U}) \in \mathcal{B}'_{\varepsilon_1}(\mathbf{x}^*) & \Rightarrow & \\ \|\mathbf{n}-\mathbf{n}^*\|_2^2+\|\boldsymbol{\lambda}-\boldsymbol{\lambda}^*\|_2^2+\|\mathbf{U}-\mathbf{U}^*\|_2^2 & \le & \big(C_1^2+1\big)\big(\|\mathbf{n}-\mathbf{n}^*\|_2^2+\|\mathbf{U}-\mathbf{U}^*\|_2^2\big) \le \big(C_1^2+1\big)\varepsilon_1^2 \le \varepsilon_N^2 \\ & \Rightarrow & (\mathbf{n},\boldsymbol{\lambda},\mathbf{U}) \in \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*). \end{array}$$

The above is consistent with general results for "least squares multipliers"—see for example [11, §6.6] or [16, §18.3]. Thus, for $(\mathbf{n},\mathbf{U}) \in \mathcal{B}'_{\varepsilon_1}(\mathbf{x}^*)$, the Newton step (from $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$, with $\boldsymbol{\lambda}$ as in (23)) is well defined, and hence so is the Renormalized Newton step. Our next preliminary result shows that the renormalization step is second order in $\boldsymbol{\delta}\mathbf{n}$ and therefore preserves the order of accuracy of the basic Newton step.

Lemma 2 *For any regular point $\mathbf{x}^*$, there exists a positive constant C_2 such that*

$$(\mathbf{n},\mathbf{U}) \in \mathcal{B}''_{\varepsilon_1}(\mathbf{x}^*) \quad \Rightarrow \quad \|\mathbf{n}^{RN}-\mathbf{n}^*\|_2 \le C_2\|\mathbf{x}-\mathbf{x}^*\|_2^2,$$

where ε_1 is as in Lemma 1 and $\mathbf{x}=(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$, with λ computed as in (23).

Proof 4 *We know from Lemma 1 that for $(\mathbf{n},\mathbf{U}) \in \mathcal{B}''_{\varepsilon_1}(\mathbf{x}^*) \subset \mathcal{B}'_{\varepsilon_1}(\mathbf{x}^*)$, the point $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$ is in $\mathcal{B}_{\varepsilon_N}(\mathbf{x}^*)$ and that the Newton step from $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$ is well defined and satisfies the inequality* (24). *The Renormalized Newton step is also well defined, and the local geometry relating the two is as follows. For $j=1,\dots,n$,*

$$\mathbf{n}_j^N = \mathbf{n}_j + \boldsymbol{\delta}\mathbf{n}_j, \quad |\mathbf{n}_j|=1, \quad \mathbf{n}_j\cdot\boldsymbol{\delta}\mathbf{n}_j=0, \quad |\mathbf{n}_j^N| \ge 1, \quad \mathbf{n}_j^{RN} = \frac{\mathbf{n}_j^N}{|\mathbf{n}_j^N|},$$

from which follows

$$\mathbf{n}_j^N - \mathbf{n}_j^{RN} = (|\mathbf{n}_j^N|-1)\mathbf{n}_j^{RN}$$

and

$$|\boldsymbol{\delta}\mathbf{n}_j|^2 = |\mathbf{n}_j^N|^2-1 = (|\mathbf{n}_j^N|-1)(|\mathbf{n}_j^N+1) \quad \Rightarrow \quad |\mathbf{n}_j^N|-1 = \frac{|\boldsymbol{\delta}\mathbf{n}_j|^2}{|\mathbf{n}_j^N|+1} \le \frac{1}{2}|\boldsymbol{\delta}\mathbf{n}_j|^2.$$

With this we can estimate

$$\|\mathbf{n}^{RN}-\mathbf{n}^N\|_2 \le \sum_{j=1}^n \|\mathbf{n}_j^{RN}-\mathbf{n}_j^N\|_2 \le \frac{1}{2}\sum_{j=1}^n |\boldsymbol{\delta}\mathbf{n}_j|^2 = \frac{1}{2}\|\boldsymbol{\delta}\mathbf{n}\|_2^2. \tag{27}$$

To proceed, we must relate the Newton correction $\boldsymbol{\delta}\mathbf{n}$ to the errors in the initial vectors $(\mathbf{n},\boldsymbol{\lambda},\mathbf{U})$, which can be done as follows:

$$\begin{array}{rcl} \mathbf{n}^N = \mathbf{n}+\boldsymbol{\delta}\mathbf{n} & \Rightarrow & \mathbf{n}^N-\mathbf{n}^* = \mathbf{n}-\mathbf{n}^*+\boldsymbol{\delta}\mathbf{n} \\ & \Rightarrow & \|\boldsymbol{\delta}\mathbf{n}\|_2 \le \|\mathbf{n}^N-\mathbf{n}^*\|_2+\|\mathbf{n}-\mathbf{n}^*\|_2 \\ & & \qquad \le C_N\|\mathbf{x}-\mathbf{x}^*\|_2^2+\|\mathbf{x}-\mathbf{x}^*\|_2, \quad \textit{using } (24) \\ & & \qquad \le (C_N\varepsilon_N+1)\|\mathbf{x}-\mathbf{x}^*\|_2, \quad \textit{using } \|\mathbf{x}-\mathbf{x}^*\|_2 \le \varepsilon_N, \\ & & \qquad \le 2\|\mathbf{x}-\mathbf{x}^*\|_2, \quad \textit{using } C_N\varepsilon_N < 1 \\ & \Rightarrow & \frac{1}{2}\|\boldsymbol{\delta}\mathbf{n}\|_2^2 \le 2\|\mathbf{x}-\mathbf{x}^*\|_2^2. \end{array} \tag{28}$$

Combining (27) *and* (28) *with* (24), *we obtain*

$$\begin{aligned} \|\mathbf{n}^{RN}-\mathbf{n}^*\|_2 &\le \|\mathbf{n}^{RN}-\mathbf{n}^N\|_2+\|\mathbf{n}^N-\mathbf{n}^*\|_2 \\ &\le \frac{1}{2}\|\boldsymbol{\delta}\mathbf{n}\|_2^2+\|\mathbf{n}^N-\mathbf{n}^*\|_2 \\ &\le (2+C_N)\|\mathbf{x}-\mathbf{x}^*\|_2^2. \end{aligned}$$

Thus the lemma is proved with $C_2 := 2+C_N$.

With the help of these lemmas, we can now prove the basic result that establishes the local quadratic convergence of the Renormalized Newton Method algorithm.

Theorem 2 *For any regular point* $\mathbf{x}^*$*, there exist positive constants* C_{RN} *and* ε_{RN} *satisfying* $C_{RN}\varepsilon_{RN} < 1$*, such that for any* $(\mathbf{n}, \mathbf{U}) \in \mathcal{B}''_{\varepsilon_{RN}}(\mathbf{x}^*)$*, the Renormalized Newton step* $(\mathbf{n}^{RN}, \mathbf{U}^{RN})$*, calculated via Algorithm 1, is well defined and satisfies*

$$\sqrt{\|\mathbf{n}^{RN} - \mathbf{n}^*\|_2^2 + \|\mathbf{U}^{RN} - \mathbf{U}^*\|_2^2} \leq C_{RN}\big(\|\mathbf{n} - \mathbf{n}^*\|_2^2 + \|\mathbf{U} - \mathbf{U}^*\|_2^2\big).$$

Proof 5 *Given any* $(\mathbf{n}, \mathbf{U})$ *in* $\mathcal{B}''_{\varepsilon_1}(\mathbf{x}^*)$*, with* ε_1 *as in Lemma 1, define* $\boldsymbol{\lambda}$ *as in* (23)*. Lemma 1 guarantees that* $\mathbf{x} = (\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U}) \in \mathcal{B}_{\varepsilon_N}(\mathbf{x}^*)$*, and so the Newton and Renormalized Newton steps are well defined. Lemma 2 guarantees that*

$$\|\mathbf{n}^{RN} - \mathbf{n}^*\|_2 \leq C_2\|\mathbf{x} - \mathbf{x}^*\|_2^2,$$

with C_2 *as in Lemma 2, and we also have*

$$\|\mathbf{U}^{RN} - \mathbf{U}^*\|_2 \leq C_N\|\mathbf{x} - \mathbf{x}^*\|_2^2$$

from (24)*, because* $\mathbf{U}^{RN} = \mathbf{U}^N$*. It follows that*

$$\sqrt{\|\mathbf{n}^{RN} - \mathbf{n}^*\|_2^2 + \|\mathbf{U}^{RN} - \mathbf{U}^*\|_2^2} \leq \sqrt{C_2^2 + C_N^2}\,\|\mathbf{x} - \mathbf{x}^*\|_2^2.$$

Now

$$\begin{aligned}\|\mathbf{x} - \mathbf{x}^*\|_2^2 &= \|\mathbf{n} - \mathbf{n}^*\|_2^2 + \|\boldsymbol{\lambda} - \boldsymbol{\lambda}^*\|_2^2 + \|\mathbf{U} - \mathbf{U}^*\|_2^2 \\ &\leq \big(C_1^2 + 1\big)\big(\|\mathbf{n} - \mathbf{n}^*\|_2^2 + \|\mathbf{U} - \mathbf{U}^*\|_2^2\big),\end{aligned}$$

where C_1 *is as in* (26)*. We thus have*

$$\sqrt{\|\mathbf{n}^{RN} - \mathbf{n}^*\|_2^2 + \|\mathbf{U}^{RN} - \mathbf{U}^*\|_2^2} \leq \sqrt{C_2^2 + C_N^2}\,\big(C_1^2 + 1\big)\big(\|\mathbf{n} - \mathbf{n}^*\|_2^2 + \|\mathbf{U} - \mathbf{U}^*\|_2^2\big)$$

and can take

$$C_{RN} := \sqrt{C_2^2 + C_N^2}\,\big(C_1^2 + 1\big)$$

and choose $\varepsilon_{RN} \leq \varepsilon_1$ *such that* $C_{RN}\varepsilon_{RN} < 1$*.*

One can now use exactly the same arguments as in the basic local Newton Convergence Theorem (sketched after the statement of Theorem 1) to show that the Renormalized Newton iteration is well defined and quadratically convergent from any initial point in $\mathcal{B}''_{\varepsilon_{\mathrm{RN}}}(\mathbf{x}^*)$.

5.2 Comparison with Truncated Newton Method of computational micromagnetics

The closest analogue to the Renormalized Newton scheme of which we are aware is the Truncated Newton Method utilized in micromagnetics [9, §4.2], and it is natural and interesting to compare the two. The Truncated Newton Method (as adapted to micromagnetics) is used to minimize a discretization of the Landau-Lifshitz free energy of a ferromagnetic material subject to pointwise unit-length constraints on the normalized magnetization vector field, which is usually denoted by $\boldsymbol{m}$ and is analogous to the liquid crystal director field $\boldsymbol{n}$—see §2.1 above. In our setting, the approach amounts to the following. Let $f = f(\mathbf{n}_1, \ldots, \mathbf{n}_n)$ be a discretized free energy, with $\mathbf{n} = (\mathbf{n}_1, \ldots, \mathbf{n}_n)$, $\mathbf{n}_j \in \mathbb{R}^3$ a current approximate director (or magnetization) field. One develops a constrained local quadratic model using paths of the form

$$\mathbf{n}_j(\varepsilon) = \frac{\mathbf{n}_j + \varepsilon\mathbf{p}_j}{|\mathbf{n}_j + \varepsilon\mathbf{p}_j|}, \quad -\varepsilon_0 < \varepsilon < \varepsilon_0, \quad \text{so that } |\mathbf{n}_j(\varepsilon)| = 1 \text{ and } \mathbf{n}_j(0) = \mathbf{n}_j,$$

where $\mathbf{p}$ is an arbitrary direction

$$\mathbf{p} = \begin{bmatrix}\mathbf{p}_1 \\ \vdots \\ \mathbf{p}_n\end{bmatrix}, \quad \mathbf{p}_1, \ldots, \mathbf{p}_n \in \mathbb{R}^3.$$

We note that this kind of device is commonly used for analytical as well as numerical purposes in both the liquid crystals and micromagnetics areas—see for example [21, 3.5], where it is used systematically to derive constrained equilibrium equations, natural boundary conditions, and the like for the Oseen-Frank elastic model for nematic liquid crystals. The constrained local quadratic model follows by expanding

$$f(\mathbf{n}_1(\varepsilon),\dots,\mathbf{n}_n(\varepsilon)) = f(\mathbf{n}) + \varepsilon\,\mathbf{G}(\mathbf{n})\cdot\mathbf{p} + \frac{\varepsilon^2}{2}H(\mathbf{n})\mathbf{p}\cdot\mathbf{p} + \cdots,$$

where $\mathbf{G}(\mathbf{n})$ and $H(\mathbf{n})$ are the constrained/projected gradient and Hessian evaluated at $\mathbf{n}(0) = \mathbf{n}$. The constrained Newton direction is characterized by

$$H(\mathbf{n})\mathbf{p} = -\mathbf{G}(n)$$

(which corresponds to Eqn. (89) of [9]) and must be appropriately safeguarded to provide a descent direction.

If one performs the necessary calculus, one finds that

$$\mathbf{G} = \begin{bmatrix}\mathbf{G}_1\\ \vdots\\ \mathbf{G}_n\end{bmatrix},\quad \mathbf{G}_j = \nabla_{\mathbf{n}_j} f - (\nabla_{\mathbf{n}_j} f\cdot\mathbf{n}_j)\,\mathbf{n}_j = \Pi_j\nabla_{\mathbf{n}_j} f,\quad \Pi_j := I - \mathbf{n}_j\mathbf{n}_j^T,$$

which is Eqn. (86) of [9]. Here Π_j is the local orthogonal projector transverse to $\mathbf{n}_j$, which is commonly denoted $P(\boldsymbol{n}) = \mathbf{I} - \boldsymbol{n}\otimes\boldsymbol{n}$ in the liquid crystals area (see [21]), and we can write

$$\mathbf{G} = \Pi\,\nabla_{\mathbf{n}} f,\quad \Pi = \begin{bmatrix}\Pi_1 & & \\ & \ddots & \\ & & \Pi_n\end{bmatrix}.$$

Notice that in our Renormalized Newton Method, the approximate Lagrange multipliers are computed via (23) as

$$\boldsymbol{\lambda} = -B(\mathbf{n})^T\nabla_{\mathbf{n}} f(\mathbf{n}) \quad\Leftrightarrow\quad \lambda_j = -\nabla_{\mathbf{n}_j} f\cdot\mathbf{n}_j,\ j = 1,\dots,n.$$

In terms of this, then, we can write

$$\mathbf{G}_j = \nabla_{\mathbf{n}_j} f + \lambda_j\mathbf{n}_j \quad\Leftrightarrow\quad \mathbf{G} = \nabla_{\mathbf{n}} f + B(\mathbf{n})\boldsymbol{\lambda},$$

and we see that our formulas for the λ_j arise naturally in this expansion calculus. The projected Hessian takes the form

$$H = \Pi\,\nabla^2 f\,\Pi + \Lambda\,\Pi - H_2,$$

where the diagonal matrix of approximate Lagrange multipliers Λ is as given in (7), and

$$H_2 := \begin{bmatrix}\mathbf{n}_1\mathbf{G}_1^T + \mathbf{G}_1\mathbf{n}_1^T & & \\ & \ddots & \\ & & \mathbf{n}_n\mathbf{G}_n^T + \mathbf{G}_n\mathbf{n}_n^T\end{bmatrix}.$$

This is equivalent to Eqn. (87) of [9]. The $3n\times 3n$ matrices H and H_2 are real and symmetric.

The projection Π can be seen to be related to the matrices B and Z utilized in our Renormalized Newton algorithm via

$$\Pi = I - BB^T = ZZ^T.$$

Using also the observation that $\Lambda\,\Pi = \Pi\,\Lambda\,\Pi$, one is able to compare directly the Truncated Newton step

$$H(\mathbf{n})\mathbf{p} = -\mathbf{G}(\mathbf{n}),\quad H = ZZ^T(\nabla^2_{\mathbf{nn}} f + \Lambda)ZZ^T - H_2,\quad \mathbf{G} = ZZ^T\nabla_{\mathbf{n}} f \tag{29}$$

with the Renormalized Newton step

$$Z^T(\nabla^2_{\mathbf{nn}} f + \Lambda)Z\mathbf{q} = -Z^T\nabla_{\mathbf{n}} f,\quad \mathbf{p} = Z\mathbf{q}. \tag{30}$$

Observe that $\nabla^2_{\mathbf{nn}} f + \Lambda$ is simply the A block of the Hessian of the Lagrangian L in the notation of §3 here. Also note that at equilibrium, the projected gradient must necessarily vanish ($Z^T\nabla_{\mathbf{n}} f = \mathbf{0} \Rightarrow \mathbf{G} =$

$ZZ^T\nabla_{\mathbf{n}} f = \mathbf{0}$) and so, therefore, must the H_2 part of the projected Hessian matrix H. The convergence analysis of §5.1 here shows that this H_2 term is not needed for local quadratic convergence anyway.

We see that there is a definite relationship between the Truncated Newton Method of computational micromagnetics and the Renormalized Newton Method we have developed here. There are also important differences. The Truncated Newton system (29) is of size $3n$, whereas (30) is of size $2n$. Furthermore, since H_2 is necessarily the zero matrix at any constrained equilibrium point $\mathbf{n}^*$, it follows that at any such point,

$$H(\mathbf{n}^*) = \Pi\,(\nabla^2_{\mathbf{nn}} f + \Lambda)\,\Pi = ZZ^T(\nabla^2_{\mathbf{nn}} f + \Lambda)ZZ^T,$$

which is necessarily *singular*, with a nullity at least n (since Z^T has an n-dimensional null space)—the claim of [9, §4.2] that H becomes positive definite near a local minimum seems not to be true. Thus the coefficient matrix of the linear system (29) is necessarily singular (with a large nullity) at the local minimizers being sought, and the system will be very badly ill-conditioned in neighborhoods of any such points. The coefficient matrix $Z^T(\nabla^2_{\mathbf{nn}} f + \Lambda)Z$ of (30), on the other hand, is guaranteed to be nonsingular at any regular constrained stationary point, that is, at any point at which

$$\nabla^2 L(\mathbf{n}, \boldsymbol{\lambda}) = \begin{bmatrix} \nabla^2_{\mathbf{nn}} L & \nabla^2_{\mathbf{n}\boldsymbol{\lambda}} L \\ \nabla_{\boldsymbol{\lambda}\mathbf{n}} L & \nabla^2_{\boldsymbol{\lambda}\boldsymbol{\lambda}} L \end{bmatrix} = \begin{bmatrix} A & B \\ B^T & O \end{bmatrix}, \quad A = \nabla^2_{\mathbf{nn}} f + \Lambda$$

is nonsingular. This remains valid in the inflated case in which a coupled electric field is present, that is, when $L = L(\mathbf{n}, \boldsymbol{\lambda}, \mathbf{U})$.

6 Summary

We have introduced and studied a prototype director model for the equilibrium orientational configuration in a liquid crystal material, emphasizing the commonly occurring case of a coupled electric-field interaction. The prototype model embodies the essential features of models for realistic experiments and device simulations. It also shares similar features with the Landau-Lifshitz model for the magnetization in a ferromagnetic material, and the relationship between the two has been discussed. The equilibrium equations associated with discretizations of the model have a double saddle-point structure, arising from the pointwise unit-vector constraints on the components of the director field and the nature of the coupling between the director field and the local electric field. This paper complements [18], where we have proposed a preconditioned nullspace method as an effective way to solve the associated Lagrange-Newton equations, and the basic ideas of that paper have been reviewed here. Special attention has been paid to the equations associated with the pointwise unit-vector constraints, in particular to their geometric interpretation. The main results here are the development of efficiently computable criteria to assess the local stability of computed constrained equilibrium solutions and the introduction of a modified version of a global Newton method that takes advantage of the special structure of the problem and which is proven to be locally quadratically convergent.

The characterization of local stability of equilibria is complicated by the double saddle-point nature of the problem. By reformulating the problem as a mathematically equivalent equality-constrained minimization problem for a deflated discrete free-energy functional, we have deduced appropriate local stability criteria phrased in terms of minimum eigenvalues of certain projected Schur complements. The local stability calculation can then be accomplished via Lanczos iteration approaches. The local stability criteria also have implications for preconditioning the reduced Hessian in the nullspace-method equations, as they reveal that the leading diagonal block submatrix can fail to be positive definite on stable (as well as unstable) equilibrium solution branches.

Several aspects of our problem simplify when the local discrete directors are normalized ($|\mathbf{n}_j| = 1$, $\forall j$), however the generic global Newton iteration applied to the Lagrangian only approaches this normalized state in the limit as the outer iteration converges. We have presented here an ad-hoc "Renormalized Newton Method" that overcomes this. The scheme has two key features: eliminating the Lagrange multipliers (by least-squares approximations) and renormalizing the local directors at each iterative step. The resulting outer iteration only involves the director and electrostatic variables and remains on the constraint manifold at each stage. We have analyzed this scheme and rigorously proved that it is locally quadratically convergent whenever the basic global Newton method is. The Renormalized Newton Method bears some resemblance to the Truncated Newton Method as adapted to the area of computational micromagnetics, and so we have carefully contrasted the two. Our analysis suggests that the Renormalized Newton Method could provide a good approach for computational micromagnetics as well.

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