A VARIATIONAL METHOD FOR GENERATING $N$-CROSS FIELDS USING HIGHER-ORDER $Q$-TENSORS

DMITRY GOLOVATY†, JOSE ALBERTO MONTERO‡, AND DANIEL SPIRN§

Abstract. An $n$-cross field is a locally-defined orthogonal coordinate system invariant with respect to the cubic symmetry group. Cross fields are finding widespread use in mesh generation, computer graphics, and materials science among many applications. We consider the problem of generating an $n$-cross field using a higher-order $Q$-tensor theory that is constructed out of tensored projection matrices. It is shown that by a Ginzburg-Landau relaxation, one can reliably generate an $n$-cross field on arbitrary Lipschitz domains.

Key words. Hexahedral mesh, frame field, cross field, Ginzburg-Landau relaxation

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1. Introduction. In this paper we use variational methods for tensor-valued functions in order to construct $n$-cross fields in $\mathbb{R}^n$. We begin with the following definitions. Given $k, n \in \mathbb{N}$, a $k$-frame $F^k$ in $\mathbb{R}^n$ is an ordered set of $k$ vectors in $\{a_i\}_{i=1}^k \subset \mathbb{R}^n$. If the vectors $\{a_i\}_{i=1}^k$ are mutually orthonormal, then we say that the $k$-frame is orthonormal. Associated with each orthonormal frame $F^k$, we define a $k$-cross $C^k$ as an unordered set of $k$ equivalence classes corresponding to $\{a_i\}_{i=1}^k$ in $\mathbb{R}^n \setminus \{0\}$ under the equivalence relation $y \sim \lambda x$ for all $\lambda \neq 0$. In other words, a $k$-cross is an unordered set of $k$ elements of $\mathbb{R}^{n-1}$; it can also be thought of as $k$ mutually orthogonal lines $\{l_i\}_{i=1}^k$ in $\mathbb{R}^n$, where $l_i$ is parallel to $a_i$ for each $i = 1, \ldots, k$. Without loss of generality, in what follows we will always assume that $k = n$ and simply refer to $n$-frames and $n$-crosses. We will also drop superscript $k$ in the respective notation for frames and crosses. Note that an orthonormal $n$-frame is also an orthonormal basis of $\mathbb{R}^n$. Note that the notions of a frame and a cross vary between throughout the literature and sometimes these are even used interchangeably. Here we make these notions precise and distinct.

With these definitions in hand, we can consider fields of $n$-frames and $n$-crosses on a domain $\Omega \subset \mathbb{R}^n$. A particular question of interest is whether it is possible to construct a smooth field of $n$-crosses in $\Omega$, assuming certain behavior of that field on $\partial \Omega$. This problem has received considerable attention in computer graphics and mesh generation, see for example the review of the many applications of cross and frame fields in [28]. In two dimensions (or on surfaces in three dimensions) hex meshes can be obtained by finding proper parametrization based on a 2-cross field defined over a triangulated surface [19].

A similar two step procedure in three dimensions has been proposed recently by a number of authors with the aim to generate hexahedral meshes. First, a 3-frame field is constructed by assigning a frame to each cell of a tetrahedral mesh, then a parametrization algorithm is applied to generate a hexahedral mesh [17, 22]. From a mathematical point of view, the first step in this procedure requires one to construct a 3-cross field in $\Omega \subset \mathbb{R}^3$ that is sufficiently smooth and properly fits to $\partial \Omega$, e.g., by requiring that one of the lines of the field is orthogonal to $\partial \Omega$. Generally, a cross field that satisfies this type of the boundary condition has singularities on $\partial \Omega$ and/or in $\Omega$ due to topological constraints (as follows from an appropriate analog of the Hairy Ball Theorem).

A number of approaches have been proposed to construct a 2- or 3-frame and cross fields or their analogs. Some schemes involve identification of the field on the boundary and its subsequent reconstruction in the interior of the domain, for example, by using an optimization procedure [7]. In three dimensions, the first task can be accomplished by looking for the harmonic map on the boundary surface that has one of the 3-frame vectors orthogonal to the boundary [5], by prescribing the 3-frame field on the boundary [19]. The reconstruction of the 3-frame field in the interior is achieved by propagating the frame from the boundary and then optimizing its smoothness by minimizing a function that, e.g., penalizes for frame changes in the neighboring tetrahedra [19, 5]. Other, 2-frame reconstruction algorithms over surfaces rely on solving a

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†Department of Mathematics, The University of Akron, Akron, OH 44325, USA (dmitry@uakron.edu).

‡Facultad de Matemáticas, Pontificia Universidad Católica de Chile, Vicuña Mackenna 4860, San Joaquín, Santiago, Chile (amontero@mat.puc.cl).

§School of Mathematics, University of Minnesota, Minneapolis, MN 55455 (spirn@umn.edu).
Ginzburg-Landau equation [29, 4]. Some authors do not distinguish between the frames in the interior of the domain and on its boundary and simply optimize the frame distribution via energy minimization [17]; here the 3-frame has also been described by using spherical harmonics [15].

The related recent work has been done on singularity-constrained octahedral fields for hexahedral meshing [20], boundary element octahedral fields in volumes [27], smoothness driven frame field generation for hexahedral meshing [18], robust hex-dominant mesh generation using field-guided polyhedral agglomeration [13], symmetric moving frames [9], and all-hex meshing using closed-form induced polycube [11].

What then is an "optimal" way to automatically generate a 3-cross field that satisfies prescribed boundary conditions and is not too singular? A promising direction was identified in [4, 29] where a connection to the Ginzburg-Landau theory was noticed. This connection is transparent in two dimensions where a frame- or a cross-field is fully defined by a single angle. The appropriate descriptor in three dimensions is, however, lacking. Note also that the same problem has clear connections to the problem of modeling of dislocation structures in crystalline materials [6, 10].

Our approach is motivated by the experience with modeling of nematic liquid crystals. In these materials partial orientational order exists within certain temperature ranges so that a nematic sample has a preferred molecular orientation at any given point of the domain it occupies. One possible description of a nematic then utilizes a unit vector field \( \mathbf{n} : \mathbb{R}^3 \rightarrow S^2 \) at every point of the domain \( \Omega \subset \mathbb{R}^3 \); note that this essentially generates a 1-frame field in \( \Omega \).

The physics of the problem, however, dictates the same probability of finding a head or a tail of a nematic molecule pointing in a given direction, hence the appropriate descriptor of the nematic state must be invariant with respect to inversion \( \mathbf{n} \rightarrow -\mathbf{n} \). The oriented object satisfying this symmetry condition is not \( \mathbf{n} \) but rather the projection matrix \( \mathbf{n} \otimes \mathbf{n} \) that can also be identified with an element of the projective space \( \mathbb{RP}^2 \) or a 1-cross. Thus we can interpret a field of projection matrices on \( \Omega \) as a 1-cross field. We will generalize this connection between the projection matrices and 1-cross fields to higher dimensional matrices and \( n \)-cross fields in the remainder of this paper.

The connection, in fact, goes a bit deeper if one is interested in exploring singularities of cross fields. As was already alluded to above, a nematic configuration in \( \Omega \) satisfying certain boundary conditions on \( \partial \Omega \) is generally subject to topological constraints that lead to formation of singularities in \( \Omega \). Within a variational theory for nematic liquid crystals one typically assumes that an equilibrium configuration minimizes some form of elastic energy associated with spatial changes of the preferred orientation. In the simplest approximation, this energy reduces to a Dirichlet integral

\[
\int_{\Omega} |\nabla u|^2 \, dx
\]

of \( u = \mathbf{n} \) or \( u = \mathbf{n} \otimes \mathbf{n} \), depending on the kind of order parameter that one needs. It turns out, however, that for certain types of singularities (e.g., vortices in \( \mathbb{R}^2 \) or disclinations in \( \mathbb{R}^3 \) that are topologically necessary, this energy is infinite. One way around this difficulty is to replace the nonlinear constraints on the order parameter field by adding an appropriate, heavily-penalized potential to the energy that forces the constraint to be almost satisfied a.e. in \( \Omega \) in an appropriate limit. For example, instead of using a field of projection matrices, the relaxed competitors can be assumed to take values in the space of symmetric matrices \( Q \) of trace 1 satisfying the same linear constraints as the projection matrices. Then the property \( P^2 - P = 0 \) of the projection matrices can be enforced by adding the term \( \frac{1}{\varepsilon^2} |Q^2 - Q|^2 \) to the energy and letting \( \varepsilon \to 0 \) (cf. [14]). This results in a prototypical expression

\[
\mathcal{E}(Q) = \frac{1}{2} \int_{\Omega} |\nabla Q|^2 + \frac{1}{\varepsilon^2} |Q^2 - Q|^2 \, dx,
\]

that lies at the core of the Ginzburg-Landau-type theory for nematic liquid crystals (with a minor caveat that, for physical reasons, this theory named after Landau and de Gennes, considers translated and dilated version of \( Q \) [21]). In this paper, we show that exactly the same approach can be undertaken to construct \( n \)-cross fields in \( \mathbb{R}^n \).

In Section 2, we construct a tensor representation of an \( n \)-cross and establish the basic linear algebra properties of this tensor. In Section 3, we introduce the notion of an \( n \)-cross on an \( n - 1 \)-dimensional manifold and then use this notion in Section 4 in order to define natural boundary conditions for \( n \)-cross-valued
Fig. 1.1. Solution of the Ginzburg-Landau PDE subject to the natural boundary conditions in a cube-shaped domain with a cylindrical notch: A disclination in the 3-cross field via level surface plot for $\frac{1}{2}(Q^2 - Q)^2$ (left); Streamlines of the 3-cross solution field with colors representing three different directions followed along the cross field (right).

Fig. 1.2. Solution of the Ginzburg-Landau PDE subject to the natural boundary conditions in a cube-shaped domain with a cylindrical notch: A horizontal cross-section of the 3-cross solution field at the level intersecting the notch.

maps. This allows us to formulate a Ginzburg-Landau-type variational problem for relaxed, tensor-valued maps. Sections 5 and 6 are devoted to 2- and 3-cross fields, respectively, and Section 6 presents several computational examples of 3-cross field reconstructions in three-dimensional domains. Here we give one example of a tensor-valued solution of the Ginzburg-Landau problem that replicates a setup discussed in [30] (cf. [25]). In Figs. 1.1-1.2 we show the 3-cross field distribution in the domain consisting of the cube with a notch in the shape of a cylinder. On the boundary, one of the lines of the 3-cross field is assumed to be perpendicular to the surface of the boundary and the cross field is obtained by solving the system of Ginzburg-Landau PDEs subject to the natural boundary condition. The result reproduces that in [30], where it was computed using a different technique.

Upon completing this paper, we learned of two different investigations that are relevant to present
work. First, [8] recently proposed the same higher dimensional tensor representation for 3-crosses in $\mathbb{R}^3$
from an algebraic geometry perspective. The same perspective is being further developed in [24] to include a Ginzburg-Landau-type relaxation. While the underlying ideas in this paper are similar to those in [8]
and [24], here we use a much simpler linear-algebra-based approach that we believe is more direct. In
particular, Ginzburg-Landau relaxation of the tensored energy—including the associated natural boundary
conditions—is significantly more transparent in this context.

2. $n$-crosses via higher order $\Omega$-tensors. In the following discuss we distinguish a vector as $a$, a
square matrix as $A$, and a tensor as $A$. Let $A, B$ be two square matrices. We denote the inner product
$\langle A, B \rangle = \text{tr}(B^TA)$ that induces the norm, $|A|^2 = \langle A, A \rangle$. Finally, we will let $[A, B] = AB - BA$ and
$\langle A, B \rangle = AB + BA$.

Consider $n$ mutually orthogonal vectors $a^k \in S^{n-1}$ with components $a^k_i$, where $j, k = 1, \ldots, n$ and the
associated $n$-cross. Our main result in this section is to express the $n$-cross in terms of tensor products of $n$
projection matrices. For $n \in \mathbb{N}$ denote $\mathbb{M}^n$ the set of $n \times n$ symmetric matrices with real entries. Since the
$n$-cross is defined by $n$ orthogonal line fields, we introduce $n$ projection matrices

$$P^k_{ij} = (a^k \otimes a^k)_{ij} = a^k_i a^k_j$$

in $\mathbb{M}^n_{ri} := \{ A \in \mathbb{M}^n : \text{tr} A = 1 \}$ that are invariant with respect to inversions $a^k \rightarrow -a^k$. We have

$$P^i P^j = (a^i \otimes a^i)(a^j \otimes a^j) = \delta_{ij}(a^i \otimes a^j),$$

so that

$$\langle P^i, P^j \rangle = \text{tr} \left( (P^i)^T P^j \right) = \text{tr} \left( P^i P^j \right) = \delta_{ij}.$$

An $n$-cross can equivalently be defined as an unordered $n$-tuple of projection matrices $P^k, k = 1, \ldots, n$. Thus we would like to define a mathematical object that incorporates all
permutations of $P^j$ and $P^k$ for all $j, k = 1, \ldots, n$. Clearly, $\sum_{i=1}^3 P^i$ is one possible candidate, however,

$$\sum_{i=1}^3 P^i = I,$$

where $I \in \mathbb{M}^n$ is an identity matrix, hence this sum contains no information about a particular $n$-cross and a higher-order quantity is thus needed. Similar to how we used tensor products to generate elements of the projective space $\mathbb{R}P^n$ from vectors in $S^{n-1}$, we now use products of projection matrices to obtain higher order tensors in $\mathbb{M}^n_{ri} \otimes \mathbb{M}^n_{rs} \subset \mathbb{M}^{n^2}$. We can think about a tensor of this type in a number of different ways. Here we will interpret it as a matrix of matrices and define the tensor product of two matrices as

$$Q^k_{ij} = (P^k \otimes P^k)_{ij} = a^k_i a^k_j P^k$$

with elements

$$(2.1) \quad Q^k_{ijrs} = (P^k \otimes P^k)_{ijrs} = ((a^k \otimes a^k) \otimes (a^k \otimes a^k))_{ijrs} = a^k_i a^k_j a^k_r a^k_s$$

and the associated product for which the blocks satisfy

$$(\Omega \Omega)_{ij} = \sum_{k=1}^n Q_{ik} \Omega_{kj}.$$

Whenever convenient, we will also think of the same tensor as an element $Q \in \mathbb{M}^{n^2}$:

$$Q^k_{pq} = Q^k_{ijrs} \quad p = i (n - 1) + r \quad \text{and} \quad q = j (n - 1) + s.$$

associated with the standard matrix product in $\mathbb{M}^{n^2}$. 
We now define the object $Q$ representing the $n$-cross as the sum of $Q^k$ over the $n$ directions, that is

\begin{equation}
Q = \sum_{k=1}^{n} Q^k,
\end{equation}

or, equivalently,

\begin{equation}
Q_{ij} = \sum_{k=1}^{n} a^k_i a^k_j P^k,
\end{equation}

or

\begin{equation}
Q_{i j r s} = \sum_{k=1}^{n} a^k_i a^k_j a^k_r a^k_s.
\end{equation}

By construction, $Q$ clearly has the symmetries of the $n$-cross: it is invariant with respect to inversions and permutations of the frame vectors $a_j$.

We can prove several important, albeit simple, results that arise from the construction of the tensor $Q$.

**Lemma 2.1.** $Q^2 = Q$

**Proof.**

\[
(Q_{ij})^2 = \sum_{k=1}^{n} Q_{ik} Q_{kj}
\]

\[
= \sum_{k=1}^{n} \left( \sum_{\ell=1}^{n} a_\ell^k a_\ell^k P^\ell \right) \left( \sum_{m=1}^{n} a_m^k a_m^k P^m \right)
\]

\[
= \sum_{k=1}^{n} \sum_{\ell=1}^{n} \sum_{m=1}^{n} a_\ell^k a_\ell^k a_m^k a_m^k P^\ell P^m
\]

\[
= \sum_{k=1}^{n} \sum_{\ell=1}^{n} \sum_{m=1}^{n} a_\ell^k a_m^k (a_\ell^k \otimes a_m^k) (a_\ell^k \otimes a_m^k)
\]

\[
= \sum_{\ell=1}^{n} \sum_{m=1}^{n} a_\ell^m a_\ell^m \left( \sum_{k=1}^{n} a_k^k a_k^k \right) (a_\ell^m \otimes a_m^m)
\]

\[
= \sum_{\ell=1}^{n} \sum_{m=1}^{n} a_\ell^m a_\ell^m (a_\ell^m \otimes a_m^m) \delta_{\ell m}
\]

\[
= \sum_{m=1}^{n} a_m^m (a_m^m \otimes a_m^m)
\]

\[
= Q_{ij}
\]

where we used $a^k \cdot a^\ell = \delta_{k \ell}$.

The consequence of invariance of crosses under permutations of lines that form a cross is the following

**Lemma 2.2.** $Q$ is a symmetric tensor. In particular, it is invariant with respect to permutations of indices:

\begin{equation}
Q_{ijrs} = Q_{\sigma(ijrs)}
\end{equation}

where $\sigma \in S_4$, the group of permutations on \{1, 2, 3, 4\}.

**Proof.** This follows immediately from the form of (2.4).

The remaining facts deal with submatrices of $Q$. 

Lemma 2.3. Submatrices $Q_{ij}$, $i, j = 1 \ldots, n$ of $Q$ are symmetric and satisfy the following trace condition:

\[(2.6) \quad \text{tr} \, Q_{ij} = \delta_{ij} \]

Proof. The symmetry of $Q_{ij}$ immediately follows from the previous lemma. To find the trace of $Q_{ij}$, first note

\[
\text{tr} \, Q_{ij} = \text{tr} \left( \sum_{\ell=1}^{n} a_{i}^{\ell} a_{j}^{\ell} P^{\ell} \right) = \sum_{\ell=1}^{n} a_{i}^{\ell} a_{j}^{\ell} \text{tr} \, P^{\ell} = \sum_{\ell=1}^{n} a_{i}^{\ell} a_{j}^{\ell}.
\]

Next, we note that $a_{1}, \ldots, a_{n}$ form an orthonormal basis which implies the corresponding matrix $(a_{1} \ldots a_{n})$ forms a unitary matrix. Since the matrix is unitary, the row vectors of this matrix, $b_{k} = (a_{1}^{k}, \ldots, a_{n}^{k})$ are an orthonormal basis. Therefore,

\[
\delta_{ij} = b_{i} \cdot b_{j} = \sum_{\ell=1}^{n} a_{i}^{\ell} a_{j}^{\ell},
\]

which completes the proof. \qed

Finally, we have the following,

Lemma 2.4. Submatrices $Q_{ij}$, $i, j = 1 \ldots, n$ of $Q$ have the common eigenframe $\{a_{k}^{i}\}_{k=1}^{n}$ and, therefore, commute.

Proof. For any $i, j, l = 1 \ldots, n$, we have

\[
Q_{ij} a^{l} = \sum_{k=1}^{n} a_{i}^{k} a_{j}^{k} P^{k} a^{l} = (a_{i}^{l} a_{j}^{l}) a^{l}.
\]

The commutation property of $Q_{ij}$, $i, j = 1 \ldots, n$ immediately follows. \qed

We remind the reader of the following related result that we will use in a sequel.

Lemma 2.5. If $A$ and $B$ are any two symmetric matrices in $M^{n}$ that commute with each other, then $A$ and $B$ have a common eigenframe.

Proof. Suppose $Bv = \lambda v$, then $BAv = ABv = \lambda Av$. Therefore, $Av$ is an eigenvector of $B$ associated with the eigenvalue $\lambda$ and $A : \text{ker}(B - \lambda I) \to \text{ker}(B - \lambda I)$. Because $A$ and $B$ are symmetric, both have associated bases of orthonormal eigenvectors in $\mathbb{R}^{n}$ that we will denote by $\{a_{i}\}$ and $\{b_{i}\}$, respectively. Suppose that $v \in \text{ker}(B - \lambda I)$ and the equation $Ax = v$ has a solution. Then

\[
BAx = ABx = \sum_{i} x_{i} ABb_{i} = \sum_{i} x_{i} \lambda_{i} A b_{i} = \lambda v \in \text{ker}(B - \lambda I),
\]

where $\lambda_{i}$ is an eigenvalue of $B$ corresponding to $b_{i}$. It follows that $x_{i} = 0$ for all $b_{i} \notin \text{ker}(B - \lambda I)$ so that $x \in \text{ker}(B - \lambda I)$. From this, we conclude that the preimage of the set $\text{ker}(B - \lambda I)$ under the map $A : \mathbb{R}^{n} \to \mathbb{R}^{n}$ is $\text{ker}(B - \lambda I)$, hence $\text{ker}(B - \lambda I)$ is spanned by eigenvectors of $A$.

Remark 2.1. We can now use Lemma 2.2 to calculate the number of unique entries in $Q$. With the help of (2.1) we can see that this number must be the same as the dimension of the space of polynomials of degree four in $n$ variables, or

\[
\binom{n + 3}{n - 1}
\]
Now, accounting for symmetry, there are \( n(n+1)/2 \) distinct \( n \times n \) submatrices comprising \( Q \). It follows that Lemma 2.3 gives \( n(n+1)/2 \) additional linear constraints on the components of \( Q \). We conclude that the number of unique entries in \( Q \) is

\[
\frac{n + 3}{n - 1} - \frac{n(n + 1)}{2} = \frac{n(n^2 - 1)(n + 6)}{24}.
\]

3. \( n \)-crosses conforming to the boundary of an \( n \)-dimensional domain. In this section we discuss the proper way of prescribing an \( n \)-cross field on the boundary of an \( n \)-dimensional domain (or, more generally on an \( n - 1 \)-dimensional Lipschitz manifold). In particular, we will focus on describing what can be thought of as the natural boundary conditions for the Ginzburg-Landau variational problem that we will consider below. Here we require that the \( n \)-cross field at every point on the boundary contain a line that is parallel to the normal to the boundary. This condition can be phrased in a few equivalent ways, which are presented in Proposition 3.1. Cross fields generate singularities on two dimensional boundaries, see for example [12, 23, 26].

Let us start by recalling that we write \( Q \in \mathcal{M}_n \) as

\[
Q = \begin{pmatrix}
Q_{11} & \cdots & Q_{1n} \\
\vdots & \ddots & \vdots \\
Q_{n1} & \cdots & Q_{nn}
\end{pmatrix},
\]

where where each \( Q_{ij} \in \mathbb{M}_n \). By Theorem 4.2, we know that each \( Q \in \mathcal{M}_n \) as above, has an associated \( n \)-cross. Let us recall here that this is the set of unordered rank one, orthogonal projections \( P^k \in \mathcal{M}_n \), defined by an orthonormal basis \( \{a^k\}_{k=1}^3 \), which in turn is determined by \( Q \) up to order. In particular we have

\[
P^j = a^j \otimes a^j,
\]

and

\[
Q_{ij} = \sum_{k=1}^3 a^j_k a^i_k P^k.
\]

Let us also recall that the \( n \)-cross satisfies \( P^j P^k = P^k P^j = \delta_{jk} P^k \) for all \( j, k = 1, \ldots, n \). In particular, the \( P^k \) commute with each other.

Our main boundary requirement will be \( \nu(x) \), the normal at \( x \in \partial \Omega \), be part of the frame associated to \( \Omega(x) \). As this is an issue between a single projection matrix \( P \) and a tensor \( Q \), we drop the dependence on \( x \), and suppose for concreteness that \( \nu \in \mathbb{S}^{n-1} \) and that \( P \) projects onto the subspace generated by \( \nu \). It is easy to see from the discussion above that if \( \Omega \in \mathcal{M}_n \) and \( P \) is an element of the \( n \)-cross of \( \Omega \), then \( \nu = (\nu_1, \ldots, \nu_n) \) is an eigenvector of every \( n \times n \)-block \( Q_{ij} \) with eigenvalue \( \nu_i \nu_j \). In other words,

\[
Q_{ij} \nu = \nu_i \nu_j \nu
\]

for every \( i, j = 1, \ldots, n \) on \( \partial \Omega \). We shall see that this condition is in fact equivalent to the membership of \( P \) to the \( n \)-cross of \( \Omega \), and to a third condition.

**Proposition 3.1.** Let \( \Omega \in \mathcal{M}_n \), let \( P \) be a fixed \( n \times n \), rank 1, orthogonal projection, and let \( \nu \in \mathbb{S}^{n-1} \) be a unit vector in the image of \( P \). Finally, denote

\[
\mathcal{P} = \begin{pmatrix}
P_{11} P & \cdots & P_{1n} P \\
\vdots & \ddots & \vdots \\
P_{n1} P & \cdots & P_{nn} P
\end{pmatrix} = \begin{pmatrix}
\nu_1 \nu_1 P & \cdots & \nu_1 \nu_n P \\
\vdots & \ddots & \vdots \\
\nu_n \nu_1 P & \cdots & \nu_n \nu_n P
\end{pmatrix},
\]

where the \( \nu_i \) are the coordinates of \( \nu \). The following are equivalent:

1. Either \( \nu \) or \( -\nu \) is part of the \( n \)-cross of \( \Omega \).
2. \( [Q, \mathcal{P}] = 0 \).
3. \( Q_{ij} \nu = \nu_i \nu_j \nu \) for each \( i, j = 1, \ldots, n \).
Proof. Let us start by observing that (1) easily implies (2), and that (1) implies (3) by Lemma 2.4. We show now that (2) implies (1). First, a direct multiplication of matrices shows that
\[
(P\Omega)_{ij} = \sum_{k=1}^{n} (PP^k)_{ij} PP^k.
\]
This shows that the condition \([P, Q] = 0\) implies
\[
\sum_{k=1}^{n} (PP^k)_{ij} PP^k = \sum_{k=1}^{n} (P^k P)_{ij} P^k P
\]
for every \(i, j = 1, \ldots, n\). We now take any matrix \(A \in M^n_{\text{tr}}\) with entries \(a_{ij}\), multiply the last identity by \(a_{ij}\) and add in \(i, j\) to obtain
\[
\sum_{k=1}^{n} \langle PP^k, A \rangle PP^k = \sum_{k=1}^{n} \langle P^k P, A \rangle P^k P.
\]
Since \(A, P\) and \(P^k\) are all symmetric, \(\langle PP^k, A \rangle = \langle P^k P, A \rangle\), so we conclude that
\[
\sum_{k=1}^{n} \langle PP^k, A \rangle [P, P^k] = 0
\]
for every \(A \in M^n_{\text{tr}}\). It is easy to see that
\[
\langle PP^k, P^j \rangle = \delta_{k,j} \langle P, P^k \rangle,
\]
so replacing \(A\) by \(P^j\) in the next to last equation we obtain
\[
0 = \langle P, P^j \rangle [P, P^j]
\]
for every \(j = 1, \ldots, n\). Since the \(P^j\) and \(P\) are all orthogonal projections of rank 1, it is easy to conclude from here that \(P\) is indeed one of the \(P^j\).

We show last that condition (3) also implies (1). To do this we observe that clearly (3) implies that
\[
[\Omega_{ij}, P] = 0
\]
for every \(i, j = 1, \ldots, n\), because \(\Omega \in M^n_{\text{cross}}\). Since
\[
\Omega_{ij} = \sum_{k=1}^{n} P_{ij}^k P^k,
\]
this implies that
\[
[P, \Omega_{ij}] = \sum_{k=1}^{n} P_{ij}^k [P, P^k] = 0
\]
for every \(i, j = 1, \ldots, n\). This clearly implies that \([P, P^k] = 0\) for \(k = 1, \ldots, n\), so again, \(P\) is one of the \(P^k\). □

Next, we record a simple relation between topologically trivial maps \(\Omega : \partial \Omega \to M^n_{\text{cross}}\) that always contain \(P_\nu\) as part of their \(n\)-cross, and tangent vector fields on \(\partial \Omega\).

For this we first consider a map \(\Omega\) defined on \(\partial \Omega \setminus V\), where \(V \subset \partial \Omega\) is some finite subset of the boundary, possibly empty. Denoting by \(\pi_1(A)\) the fundamental group of \(A\), by topologically trivial we mean that the image of \(\pi_1(\Omega \setminus V)\) by the map induced by \(u\) on fundamental groups, is the identity element of \(\pi_1(M^n_{\text{cross}})\). For this situation we have the

**Proposition 3.2.** Let \(n \geq 3\), \(\Omega \subset \mathbb{R}^n\), and \(V \subset \partial \Omega\) be a finite subset of isolated points, possibly empty. For every smooth map \(\Omega : \partial \Omega \setminus V \to M^n_{\text{cross}}\) that is topologically trivial in the sense described above, and that always contains \(\nu\) as part of its frame, there are \((n - 1)\) smooth, unit, tangent vector fields
\[
\tau^j : \partial \Omega \setminus V \to S^{n-1}, j = 1, \ldots, n - 1,
\]
that are also part of the \(n\)-frame of \(\Omega\), and that along with \(\nu\) form an orthonormal basis of \(\mathbb{R}^n\). Conversely, given \((n - 1)\) such unit, tangent vector fields \(\tau^j : \Omega \setminus V \to S^{n-1}, j = 1, \ldots, n - 1\), there is a map \(\Omega : \partial \Omega \setminus V \to M^n_{\text{cross}}\) that has \(\nu\) in its \(n\)-cross, as well as the \(\tau^j\).
Proof. The converse part of the proposition is essentially trivial so we concentrate on the direct implication. We first recall that $SO(n)$ is a covering space for $M_{n \text{cross}}^n$, although not the universal cover of $M_{n \text{cross}}^n$. Still, if $P^1_0$, ..., $P^n_0$ are the projections onto the spaces generated by each of the vectors of some fixed canonical basis, then

$$T : SO(n) \rightarrow M_{n \text{cross}}^n$$

$$R \rightarrow T(R) = \sum_{k=1}^{n} X_{RP^k_0 R^T} \otimes X_{RP^k_0 R^T}$$

is a covering map. Here we use notation of Section 8, in particular the isomorphism $X : M_{n \text{all}}^n \rightarrow \mathbb{R}^{n^2}$ between the set of $M_{n \text{all}}^n$ of all $n \times n$ matrices and $\mathbb{R}^{n^2}$ defined in 8.1.

The condition that $Q : \partial \Omega \setminus V \rightarrow M_{n \text{cross}}^n$ be topologically trivial is known to guarantee that $Q$ lifts through

$$R : \partial \Omega \setminus V \rightarrow SO(n).$$

This means

$$Q(x) = T(R(x)) = \sum_{k=1}^{n} X_{R(x)P^k_0 R(x)^T} \otimes X_{R(x)P^k_0 R(x)^T}.$$

Now we assume that $P_r(x)$ is part of the $n$-cross of $Q(x)$ at every $x \in \partial \Omega \setminus V$. The same arguments we used in our previous lemma show that at every $x \in \partial \Omega \setminus V$, $P_r(x)$ is one of the $R(x)P^k_0 R(x)^T$. Since $V$ is a finite set, and $n \geq 3$, $\partial \Omega \setminus V$ is connected. This implies that $P_r(x)$ is one of the $R(x)P^k_0 R(x)^T$ with the same $k$ for every $x \in \partial \Omega \setminus V$. Without loss of generality assume $k = 1$. Calling $e_0^1$, ..., $e_0^n$ the canonical basis behind $P^1_0$, ..., $P^n_0$, clearly $R(x)e_0^k$, ..., $R(x)e_0^n$ are both smooth, unit, tangent vector fields on $\partial \Omega \setminus V$. □

The second aspect we will consider in this section stems from the fact that there are topological obstructions to the existence of smooth maps that satisfy the boundary conditions we describe here. Because of this, in order to build boundary maps that satisfy our boundary conditions, one is forced to introduce singularities on the boundary. We will give a simple criterion that allows us to build boundary maps with a finite number of point singularities.

Once we have the previous Proposition we can use some classical facts regarding tangent vector fields to draw conclusions relevant to our situation. The first is the following consequence of the Poincaré Hopf theorem:

**Corollary 3.3.** Let $\Omega = B_R(0)$ be the ball of radius $R > 0$ around the origin on $\mathbb{R}^3$. There is no smooth map $Q : \partial \Omega \rightarrow M_{3 \text{frame}}^3$ that contains either $\nu(x)$ or $-\nu(x)$ as part of its frame at every $x \in \partial \Omega$.

Another use of Proposition 3.2 is the following: the Poincaré Hopf Theorem tells us not only that any tangent vector field to $S^2$ must have zeros, but also that the sum of the degrees of the zeros of any tangent vector field to $S^2$ must equal the Euler characteristic of the sphere. For $S^2$ (and also for $S^n$, even $n$), the Euler characteristic is 2. The simplest possible combinations of zeros and degrees under this constraint are one zero with degree two, or two zeros with degree one. We provide next frame fields in $\Omega = B_R(0) \subset \mathbb{R}^3$ that contain $\nu$ in their frame at all but one or two points on $\partial \Omega$ for each of these situations.

For the situation of two zeros on $\partial B_R(0)$, each with degree one, consider cylindrical coordinates $(r, \theta, z)$ in $\mathbb{R}^3$, where, for $x = (x_1, x_2, x_3)$, we use the standard

$$r = \sqrt{x_1^2 + x_2^2} \text{ and } z = x_3.$$

Define $\alpha(r) = \frac{\pi r}{2R}$ and

$$a^1(x) = (\sin(\alpha(r)) \cos(\alpha(r)), 1 - \cos^2(\alpha(r)), \cos(\alpha(r))),$$

$$a^2(x) = (\cos^2(\alpha(r)), \sin(\alpha(r)) \cos(\alpha(r)), -\sin(\alpha(r))) \text{ and }$$

$$a^3(x) = (-\sin(\alpha(r)), \cos(\alpha(r)), 0).$$

It is easy to check that this is indeed an orthonormal frame at every $x \in B_R(0)$, and that $a^1(x) = \nu(x) = \frac{a^1}{|a^1|}$ when $x \in \partial B_R(0)$, except when $x$ is either the north or the south poles.
For the case of a single pole on the boundary with degree 2 we proceed as follows. Denote by $p_s$ the south pole of $\partial B_R(0)$, pick $e \in S^2$ such that $p_s \cdot e = 0$ and let

$$\hat{r}_s(x) = \frac{x - p_s}{|x - p_s|}.$$  

With this define

$$a^1(x) = R^{-1}(p_s - 2(p_s \cdot \hat{r}_s(x))\hat{r}_s(x)),$$

$$a^2(x) = e - 2(e \cdot \hat{r}_s(x))\hat{r}_s(x),$$

and

$$a^3(x) = a^1(x) \times a^2(x).$$

Direct computations show that this is an orthonormal frame at every $x \in \overline{B_R(0)} \setminus \{p_s\}$. Furthermore, whenever $x \in \partial B_R(0) \setminus \{p_s\}$, we have both that $a^1(x) = \frac{x}{|x|} = \nu(x)$, and that the vector field $a^2$ is the image through the (inverse of the) stereographic projection from the south pole of the vector field that differentiates with respect to one of the coordinates on the complex plane.

Remark 3.1. We remark that neither of these examples of the frame fields have interior singularities. Further, for both examples, the energies we consider in (4.5) and (4.6) have finite values independent of $\varepsilon$. More precisely, the energies have finite contributions from the respective gradient terms and zero contributions from the potential and the penalty on the boundary.

4. Ginzburg-Landau relaxation and recovery of the $n$-cross field. We first define our ambient manifold and then define the relaxation procedure to the $n$-cross. Our relaxation will start from the set of symmetric tensors with certain trace conditions on its submatrices. This is a similar definition to one found in [8]:

**Definition 4.1.** Set

$$M^n_{\text{relax}} = \{Q \in M^n_{2} : Q_{ijkl} = Q_{\sigma(ijkl)} \text{ for all } \sigma \in S_4, \ \text{tr}(Q_{ij}) = \delta_{ij}\}.$$

We also describe the subset of elements of this space that are projections:

$$M^n_{\text{cross}} = \{Q \in M^n_{\text{relax}} : Q^2 = Q\}.$$

Our main result in this section is the following theorem which shows that elements of $M^n_{\text{cross}}$ are in fact $n$-cross fields.

**Theorem 4.2.** For every $Q \in M^n_{\text{cross}}$ there are $n$ rank-1, orthogonal projection matrices with pairwise perpendicular images $P^1, \ldots, P^n \in M^n_{\text{tr}}$ such that

$$Q = \sum_{j=1}^{n} P^j \otimes P^j.$$

In other words, for every $Q \in M^n_{\text{cross}}$ there are matrices $P^1, \ldots, P^n \in M^n_{\text{tr}}$ such that

$$I = \sum_{j=1}^{n} P^j$$

where

$$(P^j)^2 = (P^j)^T = P^j, \ \text{tr}(P^j) = 1, P^j P^k = P^k P^j = \delta_{k,j} P^j,$$

for all $j, k = 1, \ldots$, and

$$Q = \sum_{j=1}^{n} P^j \otimes P^j.$$

The proof of Theorem 4.2 is found in the appendix.
4.1. Ginzburg-Landau relaxation to an n-cross field. We will take elements of $M_\text{relax}^n$ and consider relaxations towards $M_\text{cross}^n$ via two different Ginzburg-Landau approximations. As discussed in the introduction, we will relax our symmetric tensors $Q$ by penalizing the potential
\begin{equation}
W(Q) = |Q^2 - Q|^2.
\end{equation}
In the bulk, this can be achieved by the energy,
\begin{equation}
\mathcal{E}(Q) = \frac{1}{2} \int_\Omega |\nabla Q|^2 + \frac{1}{\varepsilon^2} |Q^2 - Q|^2 \, dx.
\end{equation}

By Theorem 4.2 critical points of (4.4) will converge a.e. to a n-cross field as $\varepsilon \to 0$. Following the discussion in Section 3, boundary singularities for n-cross fields are generically possible. To handle these scenarios we relax the condition on the boundary that the tensors are n-crosses; we handle this relaxation in two ways. In the first case we impose boundary condition (3.2) as a hard constraint, and in the second case we penalize our tensor for not aligning with the normal to the boundary.

Let
\begin{align*}
H^1_M &= \{ A \in H^1(\Omega; M_\text{relax}) \} \\
H^1_{M,\nu} &= \{ A \in H^1(\Omega; M_\text{relax}) \text{ such that } A \text{ satisfies (3.2) on } \partial\Omega \}
\end{align*}
then the two Ginzburg-Landau relaxations are:

**Method A** Define the following energy
\begin{equation}
\mathcal{E}(Q) = \frac{1}{2} \int_\Omega |\nabla Q|^2 + \frac{1}{\varepsilon^2} |Q^2 - Q|^2 \, dx + \frac{1}{2\delta^2} \int_{\partial\Omega} |Q^2 - Q|^2 \, ds,
\end{equation}

for $Q \in H^1_{M,\nu}$. In particular, we look for minimizers subject to the tensor constraints in Lemmas 2.2 and 2.3 and subject to boundary condition (3.2) with $\varepsilon \ll 1$ and $\delta \ll 1$. The nonlinear boundary relaxation allows for the formation of boundary vortices.

**Method B** A weak anchoring version of the Ginzburg-Landau relaxation can be similarly defined, see for example [16, 21] in the context of liquid crystals and [3] in the context of Ginzburg-Landau theory. The corresponding weak anchoring version of our energy is
\begin{equation}
\mathcal{E}_{wa}(Q) = \frac{1}{2} \int_\Omega |\nabla Q|^2 + \frac{1}{\varepsilon^2} |Q^2 - Q|^2 \, dx + \frac{1}{2\delta^2} \int_{\partial\Omega} |Q^2 - Q|^2 \, ds + \frac{\lambda}{2} \int_{\partial\Omega} ||Q, P||^2 \, ds
\end{equation}
for $Q \in H^1_M$ where $P = P \otimes P$ with $P = \nu \otimes \nu$ for $\nu$ normal to the boundary. In this case, we take $\varepsilon \ll 1$, $\delta \ll 1$, and $\lambda \gg 1$.

A natural numerical approach to generating an approximate n-cross field is to set up a constrained gradient descent of either (4.5) with data in $H^1_M$ or (4.6) with data in $H^1(\Omega; M_\text{relax})$ and choose $t \gg 1$.

4.2. Removing constraints and the associated gradient descent. A simpler approach avoids dealing with the set of constraints that define our class of symmetric tensors. We first let $q = (q_1, q_2, \ldots, q_k)^T$ be those components of $Q$’s in $M_\text{relax}^n$ that are independent. For example, $Q_{1111} = q_1$, $Q_{1112} = Q_{1121} = q_2$, and so on. Remark 2.1 shows that $k = 2$ for 2-frames and $k = 9$ for 3-frames. We can then redefine our Ginzburg-Landau energies as
\begin{align}
\mathcal{E}(q) &= \frac{1}{2} \int_\Omega |\nabla Q(q)|^2 + \frac{1}{\varepsilon^2} |Q^2(q) - Q(q)|^2 \, dx + \frac{1}{2\delta^2} \int_{\partial\Omega} |Q^2(q) - Q(q)|^2 \, ds \\
\mathcal{E}_{wa}(q) &= \frac{1}{2} \int_\Omega |\nabla Q(q)|^2 + \frac{1}{\varepsilon^2} |Q^2(q) - Q(q)|^2 \, dx + \frac{1}{2\delta^2} \int_{\partial\Omega} |Q^2(q) - Q(q)|^2 \, ds + \frac{\lambda}{2} \int_{\partial\Omega} ||Q(q), P||^2 \, ds.
\end{align}

Our implementation follows the (unconstrained) gradient descent of (4.7),
\begin{equation}
\partial_t q = -\nabla L^2 \mathcal{E}(Q(q)),
\end{equation}
subject to the appropriate natural boundary conditions.

Since the focus of the current work is a practical algorithm for generating n-cross fields on Lipschitz domains, the analysis of these problems will be the subject of a follow-up paper.
5. 2-cross fields. We now apply our theory in two dimensions. One particularly nice feature of the problem in this case is that the boundary conditions are Dirichlet conditions since the normal vector fully defines a 2-cross field.

**Lemma 5.1.** Any \( Q \in M^2_{\text{relax}} \) takes the form

\[
Q = \begin{pmatrix}
q_1 & q_2 \\
q_2 & 1 - q_1 \\
q_1 & 1 - q_2 \\
1 - q_1 & -q_2
\end{pmatrix}
\]

for \( q_1, q_2 \in \mathbb{R} \).

**Proof.** We use Lemmas 2.2 and 2.3 to identify submatrix \( Q_{11} \). These lemmas can be used for the other submatrices. For \( Q_{12} = Q_{21} \), we use \( Q_{1211} = Q_{1112} \) and \( Q_{1212} = Q_{1122} \), along with \( \text{tr} Q_{12} = 0 \), to identify the submatrix entries. Finally, we use \( Q_{2211} = Q_{1122} \), \( Q_{2212} = Q_{1222} \), and \( \text{tr} Q_{22} = 1 \) to identify the last submatrix.

Let \( \Omega \) be a domain in \( \mathbb{R}^2 \) with Lipschitz boundary. For \( Q \in M^2_{\text{relax}} \) we define the associated Ginzburg-Landau energy as

\[
E_\varepsilon(Q(q)) \equiv \frac{1}{2} \int_\Omega |\nabla Q(q)|^2 + \frac{1}{\varepsilon^2} |Q(q) - Q^2(q)|^2 \, dx
\]

with \( q = (q_1, q_2) \). Since

\[
\frac{1}{\varepsilon^2} |Q(q) - Q^2(q)|^2 = \frac{16}{\varepsilon^2} \left( q_1 - \frac{3}{4} \right)^2 + q_2^2 - \frac{1}{16}
\]

the energy becomes

\[
E(Q(q)) = 4 \int_\Omega |\nabla q|^2 + \frac{8}{\varepsilon^2} \left( q_1 - \frac{3}{4} \right)^2 + q_2^2 - \frac{1}{16} \, dx.
\]

Using \( (4.7) \) and \( (5.3) \), we arrive at the parabolic system:

\[
\partial_t q_1 - \Delta q_1 = \frac{16}{\varepsilon^2} \left( q_1 - \frac{3}{4} \right) \left( \left( q_1 - \frac{3}{4} \right)^2 + q_2^2 - \frac{1}{16} \right)
\]

\[
\partial_t q_2 - \Delta q_2 = \frac{16}{\varepsilon^2} q_2 \left( \left( q_1 - \frac{3}{4} \right)^2 + q_2^2 - \frac{1}{16} \right).
\]

We supplement this parabolic system with the following Dirichlet boundary conditions,

**Lemma 5.2.** For \( Q \) satisfying \( (3.2) \) then

\[
\begin{pmatrix}
q_1 \\
q_2
\end{pmatrix} = \begin{pmatrix}
\nu_1^3 + \nu_2^3 \\
\nu_1^3 \nu_2 - \nu_1 \nu_2^2
\end{pmatrix}
\]

on the boundary. If \( \nu = (\cos(\theta(x)), \sin(\theta(x)))^T \) then

\[
\begin{pmatrix}
q_1 \\
q_2
\end{pmatrix} = \frac{1}{4} \begin{pmatrix}
3 + \cos(4\theta(x)) \\
\sin(4\theta(x))
\end{pmatrix}.
\]

**Proof.** From \( Q_{11} \nu = \nu_1 \nu_2 \) and \( \nu_1^2 + \nu_2^2 = 1 \) then

\[
\begin{pmatrix}
\nu_1 & \nu_2 \\
-\nu_2 & \nu_1
\end{pmatrix} \begin{pmatrix}
q_1 \\
q_2
\end{pmatrix} = \begin{pmatrix}
\nu_1^3 \\
-\nu_1^3
\end{pmatrix}.
\]

\( (5.4) \) follows. Equation \( (5.5) \) is a direct calculation.
The form of (5.5) points to the generic formation of degree-$\frac{1}{4}$ vortices in two dimensions. This has been pointed out and studied in [29].

**Remark 5.1.** If $\mathbf{a}^1 = (\cos(\theta), \sin(\theta))$ then a quick calculations show that the corresponding tensor satisfies

$$
\epsilon_\eta = \frac{1}{4} \begin{pmatrix}
\begin{pmatrix}
3 + \cos(4\theta) & \sin(4\theta) \\
\sin(4\theta) & 1 - \cos(4\theta)
\end{pmatrix} & \begin{pmatrix}
\sin(4\theta) & 1 - \cos(4\theta) \\
1 - \cos(4\theta) & -\sin(4\theta)
\end{pmatrix} \\
\begin{pmatrix}
\sin(4\theta) & 1 - \cos(4\theta) \\
1 - \cos(4\theta) & -\sin(4\theta)
\end{pmatrix} & \begin{pmatrix}
1 - \cos(4\theta) & -\sin(4\theta) \\
-\sin(4\theta) & 3 + \cos(4\theta)
\end{pmatrix}
\end{pmatrix}.
$$

Indeed the tensor satisfies symmetries in (5.1). Furthermore, the $4\theta$ in each argument implies a fundamental domain of $[0, \pi/2]$ which corresponds to the symmetry group structure.

**6. 3-cross fields.** We now turn to our primary objective - a practical algorithm for generating 3-cross fields. As in two dimensions, we first identify the higher-order $Q$-tensor.

**Lemma 6.1.** Any $Q \in \mathbb{M}^3_{\text{relax}}$ takes the form

$$
Q = \begin{pmatrix}
Q_{11} & Q_{12} & Q_{13} \\
Q_{12} & Q_{22} & Q_{23} \\
Q_{13} & Q_{23} & Q_{33}
\end{pmatrix}
$$

where

- $Q_{11} = \begin{pmatrix}
q_1 & q_2 & q_3 \\
q_2 & q_4 & q_5 \\
q_3 & q_5 & 1 - q_1 - q_4
\end{pmatrix}$
- $Q_{12} = \begin{pmatrix}
q_2 & q_4 & q_5 \\
q_4 & q_6 & q_7 \\
q_5 & q_7 & -q_2 - q_6
\end{pmatrix}$
- $Q_{13} = \begin{pmatrix}
q_3 & q_5 & 1 - q_1 - q_4 \\
q_5 & q_7 & -q_2 - q_6 \\
1 - q_1 - q_4 & -q_2 - q_6 & -q_3 - q_7
\end{pmatrix}$
- $Q_{22} = \begin{pmatrix}
q_4 & q_6 & q_7 \\
q_6 & q_8 & q_9 \\
q_7 & q_9 & 1 - q_1 - q_4
\end{pmatrix}$
- $Q_{23} = \begin{pmatrix}
q_5 & q_7 & -q_2 - q_6 \\
q_7 & q_9 & 1 - q_4 - q_8 \\
-q_2 - q_6 & 1 - q_4 - q_8 & -q_5 - q_9
\end{pmatrix}$
- $Q_{33} = \begin{pmatrix}
1 - q_1 - q_4 & -q_2 - q_6 & -q_3 - q_7 \\
-q_2 - q_6 & 1 - q_4 - q_8 & -q_5 - q_9 \\
-q_3 - q_7 & -q_5 - q_9 & q_1 + 2q_4 + q_8 - 1
\end{pmatrix}$

**Proof.** We use Lemmas 2.3 and 2.2 to identify all submatrices. $Q_{11}$ follows from symmetry and the trace-one condition. Next for $Q_{12}$ we use $Q_{1212} = Q_{1122}$ and $Q_{1213} = Q_{1123}$, along with the trace-free condition. For $Q_{13}$ we use $Q_{1311} = Q_{1113}$, $Q_{1312} = Q_{1123}$, $Q_{1322} = Q_{1223}$, and $Q_{1323} = Q_{1233}$ with the trace-free condition. For $Q_{22}$ we use $Q_{2211} = Q_{1122}$, $Q_{2212} = Q_{1222}$, $Q_{2213} = Q_{1223}$ and the trace-one condition. For $Q_{23}$ we use $Q_{2311} = Q_{1123}$, $Q_{2312} = Q_{1123}$, $Q_{2313} = Q_{1123}$, $Q_{2322} = Q_{2223}$, $Q_{2323} = Q_{2233}$, along with the trace free condition. Finally, for $Q_{33}$ we use $Q_{3311} = Q_{1133}$, $Q_{3312} = Q_{1233}$, $Q_{3313} = Q_{1333}$, $Q_{3322} = Q_{2233}$, $Q_{3323} = Q_{2333}$ and the trace-one condition.

We now consider relaxations of $Q$ by assuming that $\mathbf{q} := (q_1, \ldots, q_9) \in \mathbb{R}^9$ is arbitrary and imposing the penalty

$$
W(\mathbf{q}) \equiv |Q(\mathbf{q})|^2 - Q(\mathbf{q})|^2.
$$

Following (4.7), the associated Ginzburg-Landau energy becomes

$$
\mathcal{E}(Q(\mathbf{q})) = \frac{1}{2} \int_{\Omega} \left| \nabla Q(\mathbf{q}) \right|^2 + \frac{1}{\varepsilon^2} W(\mathbf{q}) \right| dx + \frac{1}{2\delta^2} \int_{\partial\Omega} W(\mathbf{q}) ds
$$
with $W(q)$ defined above in (6.1).

We now generate the boundary conditions in three dimensions.

**Lemma 6.2.** Let $\nu = (\nu_1, \nu_2, \nu_3)^T$ be an outward normal to the boundary. For $Q = Q(q)$ satisfying (3.2) then $q$ satisfies the following set of constraints on the boundary

$$
(6.3) \begin{pmatrix}
\nu_1 & \nu_2 & \nu_3 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \nu_1 & 0 & \nu_2 & \nu_3 & 0 & 0 & 0 & 0 \\
-\nu_3 & 0 & \nu_1 & -\nu_3 & \nu_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \nu_3 & 0 & \nu_2 & \nu_3 & 0 & 0 \\
0 & -\nu_3 & 0 & 0 & \nu_1 & -\nu_3 & \nu_2 & 0 & 0 \\
0 & 0 & 0 & 0 & \nu_1 & 0 & \nu_2 & \nu_3 & 0 \\
0 & 0 & 0 & -\nu_3 & 0 & 0 & \nu_1 & -\nu_3 & \nu_2 \\
\end{pmatrix}
\begin{pmatrix}
q_1 \\
q_2 \\
q_3 \\
q_4 \\
q_5 \\
q_6 \\
q_7 \\
q_8 \\
q_9
\end{pmatrix}
= \begin{pmatrix}
\nu_1^2 \\
\nu_2^2 \\
\nu_3^2 \\
- (\nu_2^2 + \nu_3^2) \nu_3 \\
\nu_1 \nu_2 \nu_3 \\
\nu_1^2 \nu_3 \\
\nu_2^2 \nu_3 \\
- (\nu_1^2 + \nu_2^2) \nu_3
\end{pmatrix}.
$$

The matrix on the left has rank 7.

**Proof.** Equation (6.3) follows from $Q_{11} \nu = \nu_1^2 \nu$. The matrix rank follows by a direct calculation.

Note that Lemma 6.2 prescribes only seven conditions on the nine variables $q_i$, $i = 1, \ldots, 9$. The remaining two conditions are then the natural boundary conditions for the variational problem associated with the energy (6.2).

**Remark 6.1.** We note that if $\nu = (1, 0, 0)$, then the boundary condition reduces to two dimensions and the boundary conditions in three dimensions. In particular, assume that $(1, 0, 0)$ is an eigenvector of every $3 \times 3$ block $Q_{ij}$ with the eigenvalue $\delta_{i1} \delta_{1,j}$

$$
(6.4) \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & q_8 & q_9 & 0 & 0 & q_9 & 1 - q_8 & 0 \\
0 & 0 & q_9 & 1 - q_8 & 0 & q_9 & 1 - q_8 & -q_9 & 0 \\
0 & 0 & q_9 & 1 - q_8 & 0 & 0 & q_9 & q_8 & 0 \\
0 & 0 & q_9 & 1 - q_8 & 0 & -q_9 & q_8 & 0 & 0 \\
\end{pmatrix}
$$

We note the similarity between (5.1) and (6.4).

7. **Numerical Examples in 3D.** In this section we use the finite elements software package COMSOL [1] to find solutions of the Euler-Lagrange equations for the functional (6.2), subject to the constraints (6.3) on the boundary. In what follows, we refer to this equation as the Ginzburg-Landau PDE. For each domain geometry we ran a gradient flow simulation until the numerical solution reached an equilibrium. The system of PDEs that we solve is given in the Appendix 9. The parameters $\varepsilon$ and $\delta_\varepsilon$ were taken to be small, typically around 10% of the domain size. Note that there is a relationship between $\varepsilon$ and $\delta_\varepsilon$ that determines whether the topological defects of minimizers of (6.2) lie on the boundary or the interior of the domain [2]. We do not investigate this issue further in the present paper.

7.1. **Cube with a cylindrical notch.** The first simulation was run for a domain in the shape of a cube with a cylindrical notch (Figs. 1.1-1.2) and was motivated by an example in [30]. A critical solution of the Ginzburg-Landau PDE recovered via gradient flow shows that the vertical line remains one of directions of the 3-cross everywhere in the domain. The solution has one disclination line depicted in blue in the left inset in Fig. 1.1. The 3-cross distribution in a horizontal cross-section of the domain at the level that includes the notch is shown in Fig. 1.2. The trace of the disclination in this cross-section is circled in red. The right inset in Fig. 1.1 shows three families of streamlines along the lines of the 3-cross field.
7.2. Spherical shell. Here we solve the Ginzburg-Landau PDE in a three-dimensional shell that lies between the spheres of radii 0.495 and 0.5 with $\varepsilon = \delta = 0.02$, subject to the system of constraints (6.3) on both boundaries of the shell. As expected, the solution gives the array of eight vortices shown in Fig. 7.1. These vortices are actually short disclination lines that connect the components of $\partial \Omega$. The distribution of 3-crosses on one eighth of the outer sphere is shown in Fig. 7.2. The vortex of degree 1/4 is indicated by the red ellipse.

7.3. Ball. Simulations in a ball resulted in Figs. 7.3-7.4. One can see a similar pattern of surface vortices as in the case of a spherical shell, now connected by the line singularities that run close to the surface of the ball. The cross-section of the 3-cross field in the ball are depicted in Fig. 7.4. The lengths of the frame vectors inside the disclination cores are scaled to make the intersections between the disclinations and $xy$-plane more visible.

7.4. Toroidal domain with a cylindrical hole. The next example deals with the domain in a shape of a toroid with a cylindrical hole (Fig. 7.5, left), motivated by an example in [30]. One can see in the right inset in Fig. 7.5 that four line singularities are present in the undrilled part of the torus. This is expected since two out of the free line fields that form a 3-cross should have the winding number 1 along the
Fig. 7.3. Singularities in a ball. The contour plot of the potential $W(Q)$ indicates that there are eight surface vortices connected by eight disclination lines.

Fig. 7.4. Cross-section along the xy-plane of the 3-cross field inside a ball.

circumference of the torus and the 3-cross makes four turns along the same path. This suggests that there are four line singularities in this part of the domain as it should be energetically preferable for a degree one singularity to split into four degree 1/4 singularities of the same type. The cross-sections of the 3-cross field in the sphere are depicted in Fig. 7.6.

7.5. Domains with complex geometries. The last set of examples (Fig. 7.7) shows disclinations networks in domains with complex geometries. The common features dictated by the topology of a domain include, for example, disclinations associated with rounded corners, four disclination lines associated with a cylindrical hole in a rectangular cylinder, and the absence of disclinations in a cylindrical region with a
concentric cylindrical hole.

8. Appendix A: Proof of Theorem 4.2. In this appendix we prove Theorem 4.2. To do this we will need to set up our notation, and we do that first. After that we provide the proof of the Theorem.

8.1. Notation. In this section $\mathcal{L}(F)$ denotes the set of linear maps from the vector space $F$ to itself. We will also use the notation $u \otimes v$, for $u \in \mathbb{R}^p$ and $v \in \mathbb{R}^q$, to denote the $p \times q$, rank-1 matrix $uv^T$.

The symbol $\mathbb{M}_{n\text{all}}$ will denote the set of all $n \times n$ matrices with real entries. We will continue to write

$$\langle A, B \rangle = \text{tr}(B^T A)$$

for $A, B \in \mathbb{M}_{n\text{all}}$. The spaces $\mathbb{M}_{n\text{all}}^2$ and $\mathcal{L}(\mathbb{M}_{n\text{all}})$ are isomorphic and we consider an explicit isomorphism identifying $\mathbb{M}_{n\text{all}}$ with $\mathbb{R}^{n^2}$. To this end, if $B \in \mathbb{M}_{n\text{all}}$, we write $B = (b^1|...|b^n)$ where $b^j \in \mathbb{R}^n$, $j = 1, ..., n$, is the $j$-th column of $B$. Then we set

$$X : \mathbb{M}_{n\text{all}} \rightarrow \mathbb{R}^{n^2}$$

$$B \rightarrow X(B) = X_B = \begin{pmatrix} b^1 \\ \vdots \\ b^n \end{pmatrix}$$

(8.1)

In other words, we identify $B$ with the vector in $\mathbb{R}^{n^2}$ that has the columns of $B$ stacked up vertically. We will use the notations $X(B)$ and $X_B$ interchangeably. It is easy to check that we have

$$X_A \cdot X_B = \langle A, B \rangle = \text{tr}(B^T A)$$

for all $A, B \in \mathbb{M}_{n\text{all}}$.

With this particular identification we define

$$\Phi_0 : \mathbb{M}_{n\text{all}}^2 \rightarrow \mathcal{L}(\mathbb{M}_{n\text{all}})$$

by the conditions that (a) $\Phi_0$ be linear and (b) for any $A, B, C \in \mathbb{M}_{n\text{all}}$

$$\Phi_0(X_A \otimes X_B)(C) = \langle B, C \rangle A.$$
Recall that here, for \( \mathbf{X}_A, \mathbf{X}_B \in \mathbb{R}^{n^2} \), \( \mathbf{X}_A \otimes \mathbf{X}_B \) denotes the rank-1, \( n^2 \times n^2 \) matrix \( \mathbf{X}_A \mathbf{X}_B^T \). The well-known properties of tensor products show that this defines \( \Phi_0 \) completely.

The condition that defines \( \Phi_0 \) can be equivalently stated as follows: if \( A, B, C \in \mathbb{M}_{all}^n \), and \( R_{A,B} \in \mathcal{L}(\mathbb{M}_{all}^{n^2}) \) is defined by

\[
(8.3) \quad R_{A,B}(C) = (B, C)A,
\]

then

\[
(8.4) \quad R_{A,B} = \Phi_0(\mathbf{X}_A \otimes \mathbf{X}_B).
\]

For \( A = B \) we will write \( R_A \) instead of \( R_{A,A} \).

Yet a third way to interpret the definitions of \( \Phi_0 \) and \( \mathbf{X} \) is the following: for every \( \Omega \in \mathbb{M}_{all}^{n^2} \) and every \( A \in \mathbb{M}_{all}^n \), if \( \Omega_L = \Phi_0(\Omega) \), then

\[
(8.5) \quad \mathbf{X}_{\Omega_L}(A) = \Omega \mathbf{X}_A.
\]
Here we interpret $\Omega X_A$ as the $n^2 \times n^2$ matrix $\Omega$ multiplying the vector $X_A \in \mathbb{R}^{n^2}$ in a standard fashion, whereas on the left hand side $\Omega_L(A)$ denotes the linear map $\Omega_L$ from $\mathcal{M}^{n}_{\text{all}}$ to itself, acting on the matrix $A \in \mathcal{M}^{n}_{\text{all}}$. This is the standard identification between $\mathcal{M}^{n}_{\text{all}}$ and $\mathcal{L}(\mathcal{M}^{n}_{\text{all}}) \cong \mathcal{L}(\mathbb{R}^{n^2})$ that comes from the identification $\mathcal{M}^{n}_{\text{all}} \cong \mathbb{R}^{n^2}$ provided by the isomorphism $X: \mathcal{M}^{n}_{\text{all}} \to \mathbb{R}^{n^2}$. In particular, this shows that if $A \in \mathcal{M}^{n}_{\text{all}}$, then $X_A$ is an eigenvector of $\Omega$, if and only if $A$ is an eigenvector of $\Omega_L = \Phi_0(\Omega)$ with the same eigenvalue.

For later reference it will be useful to have concrete expressions for the $n^2 \times n^2$ matrices of two maps in $\mathcal{L}(\mathcal{M}^{n}_{\text{all}})$. We record them here. The first one is the matrix of $R_{A,B}$ defined in 8.3. Note that 8.4 already gives us an expression for the matrix of $R_{A,B}$. More precisely, the matrix $\Omega_{A,B}^{R} \in \mathcal{M}^{n^2}_{\text{all}}$ defined by the equation

$$X_{R_{A,B}}(C) = \Omega_{A,B}^{R} \cdot X_C$$

can be expressed as

$$\Omega_{A,B}^{R} = X_A \otimes X_B.$$

The second map from $\mathcal{L}(\mathcal{M}^{n}_{\text{all}})$ we will refer to later is $L_{A,B} \in \mathcal{L}(\mathcal{M}^{n}_{\text{all}})$, for $A, B \in \mathcal{M}^{n}_{\text{all}}$, defined by the equation

$$L_{A,B}(C) = A CB^T$$

(8.6)
for all $C \in \mathbb{M}_n^2$. We write $L_A$ when $A = B$. A direct computation shows that the matrix $Q^L_{A,B} \in \mathbb{M}_n^2$ defined by the equation

$$X_{L_A,B}(C) = Q_{A,B}^L X_C$$

for all $C \in \mathbb{M}_n^2$ can be expressed as

$$Q_{A,B}^L = \begin{pmatrix}
B_{11}A & \cdots & B_{1n}A \\
\vdots & \ddots & \vdots \\
B_{n1}A & \cdots & B_{nn}A
\end{pmatrix}.$$

### 8.2. Permutation Operators.

Recall $S_4$, the group of permutation of the set $\{1, 2, 3, 4\}$. For $\sigma \in S_4$, define (

8.7)

$$T_\sigma : \mathbb{M}_n^2 \rightarrow \mathbb{M}_n^2$$

by the conditions that $T_\sigma$ be linear and

$$T_\sigma(X_{u^1 \otimes u^2} \otimes X_{u^3 \otimes u^4}) = X_{u^{\sigma(1)} \otimes u^{\sigma(2)}} \otimes X_{u^{\sigma(3)} \otimes u^{\sigma(4)}}$$

for every $u^1, u^2, u^3, u^4 \in \mathbb{R}^n$. Again, standard facts about tensor products show that this condition defines $T_\sigma$ completely.

For later reference we record expressions of $T_\sigma$ for the following three permutations:

$$\sigma_1(1, 2, 3, 4) = (3, 4, 1, 2),$$

$$\sigma_2(1, 2, 3, 4) = (2, 1, 3, 4) \quad \text{and} \quad$$

$$\sigma_3(1, 2, 3, 4) = (1, 3, 2, 4),$$

and write $T_j$ instead of $T_{\sigma_j}$. Direct computations starting from $X_{u^1 \otimes u^2} \otimes X_{u^3 \otimes u^4}$ give the

**Proposition 8.1.** We have the identities

(8.9)

$$T_1(Z) = Z^T$$

for all $Z \in \mathbb{M}_n^2(\mathbb{R})$, as well as

(8.10)

$$T_1(X_A \otimes X_B) = X_B \otimes X_A,$$

(8.11)

$$T_2(X_A \otimes X_B) = X_{AT} \otimes X_B$$

and

(8.12)

$$T_3(X_A \otimes X_B) = Q^L_{A,B}$$

for all $A, B \in \mathbb{M}_n$, where $Q^L_{A,B}$ is the matrix of the linear map $L_{A,B}$ defined in 8.6.

**Remark 8.1.** Let $P^1, \ldots, P^n \in \mathbb{M}_n$ satisfy $(P^j)^2 = (P^j)^T = P^j$, $P^j P^k = P^k P^j = \delta_{kj} P^j$, $\text{tr}(P^j) = 1$, and

$$\sum_{j=1}^n P^j = I_n.$$

Define $Q \in \mathbb{M}_n^2$ by

$$Q = \sum_{j=1}^n X_{P^j} \otimes X_{P^j}.$$

It is easy to check that $T_3(Q) = Q$. This plus 8.12 shows that the equation above provides an equivalent definition for $Q$ defined in 2.2.
We now turn to the

*Proof of Theorem 4.2.* For \( \Omega \in M_{\text{all}}^{n^2} \) define

\[
\Omega_L = \Phi_0(\Omega) \in L(M_{\text{all}}^n),
\]

where \( \Phi_0 \) is the isomorphism defined in 8.2. Assume \( \Omega \in M_{\text{cross}}^n \). The proof consists of three main steps: First observe that \( \Omega_L \), as a linear map from \( M_{\text{all}}^n \) to itself, is an orthogonal projection of rank \( n \) in \( M_{\text{all}}^n \). Second, take a basis for the image of \( \Omega_L \) and show that the elements of this basis, which belong to \( M_{\text{all}}^n \), are symmetric and commute with each other. Third, we use this to finish the proof.

To show that \( \Omega_L \) is an orthogonal projection we proceed as follows. First recall that \( T_\sigma(\Omega) = \Omega \) for all \( \sigma \in S_4 \). By 8.9 we conclude that

\[
T_1(\Omega) = \Omega^T = \Omega.
\]

Since by definition of \( \Omega \in M_{\text{cross}}^n \) we have \( \Omega^2 = \Omega \) and \( \text{tr}(\Omega) = n \), we conclude that \( \Omega \) is the matrix of an orthogonal projection of rank \( n \) in \( \mathbb{R}^{n^2} \). Through 8.5, this implies that \( \Omega_L \) is an orthogonal projection of rank \( n \) in \( M_{\text{all}}^n \).

Let now \( Q^1, \ldots, Q^n \in M_{\text{all}}^n \) be an orthonormal basis of the image of \( \Omega_L \). Since \( \Omega_L \) is an orthogonal projection of rank \( n \), for every \( A \in M_{\text{all}}^n \) we have

\[
\Omega_L(A) = \sum_{j=1}^n \langle A, Q^j \rangle Q^j = \sum_{j=1}^n R_{Q^j}(A),
\]

where the notation \( R_B = R_{B,B} \) was defined in 8.3. Let us now recall here that by the comment after equation 8.5 the vectors \( X_{Q^j} \in \mathbb{R}^{n^2} \) are eigenvectors of \( \Omega \) with eigenvalue 1, and \( \langle X_{Q^j}, X_{Q^k} \rangle = \delta_{j,k} \) for each \( j, k = 1, \ldots, n \). Since \( \Omega \) is an \( n^2 \times n^2 \) matrix such that \( \Omega = \Omega^T = \Omega^2 \) and \( \text{tr}(\Omega) = n \), we deduce that

\[
\Omega = \sum_{j=1}^n X_{Q^j} \otimes X_{Q^j}.
\]

Next we show that the \( Q^j \) are symmetric. To do this we appeal to the permutation \( \sigma_2 \) from (8.8), and its operator \( T_2 \). 8.11 gives us

\[
\Omega = T_2(\Omega) = \sum_{j=1}^n X_{Q^j}^T \otimes X_{Q^j}.
\]

It is not hard from here to deduce that in fact \( Q^j = (Q^j)^T \) for \( j = 1, \ldots, n \). So far then we have

\[
\Omega = \sum_{j=1}^n X_{Q^j} \otimes X_{Q^j},
\]

with \( \langle Q^j, Q^k \rangle = \delta_{ij} \) and \( (Q^j)^T = Q^j \).

To show that the \( Q^j \) commute with each other we proceed as follows. Since \( T_3(\Omega) = \Omega \), equation 8.12 gives us

\[
\Omega = T_3(\Omega) = \sum_{j=1}^n T_3(X_{Q^j} \otimes X_{Q^j}) = \sum_{j=1}^n \left( \begin{array}{ccc}
Q_{11}^j Q^j & \cdots & Q_{1n}^j Q^j \\
\vdots & \ddots & \vdots \\
Q_{n1}^j Q^j & \cdots & Q_{nn}^j Q^j
\end{array} \right).
\]

A direct computation shows then that

\[
\Omega^2 = \sum_{i,j=1}^n \left( \begin{array}{ccc}
(Q^i Q^j)^{11} & \cdots & (Q^i Q^j)_{1n} Q^j \\
\vdots & \ddots & \vdots \\
(Q^i Q^j)_{n1} Q^j & \cdots & (Q^i Q^j)_{nn} Q^j
\end{array} \right).
\]

Since \( \Omega^2 = \Omega \), we conclude that

\[
\sum_{j=1}^n \left( \begin{array}{ccc}
Q_{11}^j & \cdots & Q_{1n}^j \\
\vdots & \ddots & \vdots \\
Q_{n1}^j & \cdots & Q_{nn}^j
\end{array} \right) = \sum_{i,j=1}^n \left( \begin{array}{ccc}
(Q^i Q^j)^{11} & \cdots & (Q^i Q^j)_{1n} Q^j \\
\vdots & \ddots & \vdots \\
(Q^i Q^j)_{n1} Q^j & \cdots & (Q^i Q^j)_{nn} Q^j
\end{array} \right).
\]
From here we obtain directly that, for any $A \in M_{all}^n$, we have

$$\Omega_L(A) = \sum_{j=1}^{n} \langle Q^j, A \rangle Q^j = \sum_{j,k=1}^{n} \langle Q^j Q^k, A \rangle Q^j Q^k.$$  

Next recall that

$$(A, B) = AB + BA \quad \text{and} \quad [A, B] = AB - BA.$$  

Since

$$2Q^j Q^k = (Q^j, Q^k) + [Q^j, Q^k],$$  

it is easy to check that

$$\Omega_L(A) = \sum_{j=1}^{n} \langle Q^j, A \rangle Q^j = \frac{1}{4} \sum_{j,k=1}^{n} \langle (Q^j, Q^k), A \rangle (Q^j, Q^k) + \frac{1}{4} \sum_{j,k=1}^{n} \langle [Q^j, Q^k], A \rangle [Q^j, Q^k].$$  

We finally in a position to conclude that the $Q^j$ commute with each other. For this consider an anti-symmetric $A \in M_{all}^n$ in the above equation. The first expression for $\Omega_L$ gives $\Omega_L(A) = 0$ because $(Q^j)^T = Q^j$. Then, since $(Q^j, Q^k)$ is symmetric, we get

$$0 = \frac{1}{4} \sum_{j,k=1}^{n} \langle [Q^j, Q^k], A \rangle [Q^j, Q^k]$$  

for every anti-symmetric $A \in M_{all}^n$. Since $[Q^j, Q^k]$ is anti-symmetric, we deduce

$$[Q^j, Q^k] = 0$$  

for all $j, k = 1, ..., n$. This is of course the statement that the $Q^j$ commute with each other.

From here it is now easy to conclude the proof of the theorem. Indeed, since the $Q^j$ commute with each other and are symmetric, they have a common basis of eigenvectors. If we denote this basis by $a^1, ..., a^n$, and define the associated projections

$$P^j = a^j \otimes a^j = a^j (a^j)^T,$$  

then it is easy to show that $Q = \sum_{j=1}^{n} X_{p_j} \otimes X_{p_j}$, which is the main claim of the theorem.

9. Appendix B: Evolution equations for 3-cross fields. In this appendix we present the system of partial differential equations that governs the gradient flow evolution of 3-cross fields in our simulations. Taking variational derivatives of the functional in (6.2), we arrive at the following system of equations

$$q_{1t} - \text{div} \left( 4(\nabla q_1 + \nabla q_4) + \frac{1}{2} \nabla q_8 \right) = -\frac{4}{r^2} (32q_2 + 72q_2^2 + 24q_3^2 + 8q_7^2 (4q_2 + 3q_6) + 2q_3(6q_6 q_7) + 8q_5(-1 + 2q_4 + q_8 + 2q_4 q_9) + 2q_3(12q_2(-3 + 4q_4 + q_8) + q_6(-30 + 42q_4 + 13q_8) + q_2(49 + 32q_3^2 + 108q_5^2) + 72q_3^2 + 72q_4(-2 + q_8) + q_2(-51 + 20q_8) + 4(8q_5^2 + 4q_5 q_9 + 5q_9^2) + 3(8q_6^2 + 4q_5 q_7(-3 + 4q_4 + q_8) + 6(-1 + 2q_4) q_7 q_9 + q_6(34q_4^2 + q_4(-47 + 28q_8) + 4(2q_5^2 + 2q_7^2 + q_8(-5 + 2q_8) + q_5 q_9 + 2q_9^2)))},$$

$$q_{2t} - 2 \text{div} \left( 4(\nabla q_2 + 3\nabla q_6) \right) = -\frac{4}{r^2} (32q_2 + 72q_2^2 + 24q_3^2 + 8q_7^2 (4q_2 + 3q_6) + 2q_3(6q_6 q_7) + 8q_5(-1 + 2q_4 + q_8 + 2q_4 q_9) + 2q_3(12q_2(-3 + 4q_4 + q_8) + q_6(-30 + 42q_4 + 13q_8) + q_2(49 + 32q_3^2 + 108q_5^2) + 72q_3^2 + 72q_4(-2 + q_8) + q_2(-51 + 20q_8) + 4(8q_5^2 + 4q_5 q_9 + 5q_9^2) + 3(8q_6^2 + 4q_5 q_7(-3 + 4q_4 + q_8) + 6(-1 + 2q_4) q_7 q_9 + q_6(34q_4^2 + q_4(-47 + 28q_8) + 4(2q_5^2 + 2q_7^2 + q_8(-5 + 2q_8) + q_5 q_9 + 2q_9^2)))),$$
\[ q_{31} - 2 \operatorname{div} (2 \nabla q_3 + \nabla q_7) = -\frac{4}{\varepsilon^2} (16q_3^2 - 18q_5q_6 + 36q_4q_5q_6 + 2(6 + q_1(-7 + 4q_1))q_7 + 24q_3^2q_7 \\
- 29q_{47} + 16q_1q_4q_7 + 14q_7^2q_2 + 32q_7^2q_2 + 8q_7^2q_2 + 8q_7^2 + 20q_5q_6q_8 - 16q_7q_8 + 2q_1q_7q_8 + 20q_4q_7q_8 + 8q_7q_8^2 \\
+ 2q_6q_9 - 4q_4q_9q_9 + 28q_5q_7q_9 + 8q_7q_9^2 + 2q_2(6q_6q_7 \\
+ 8q_5(-1 + 2q_4 + q_8) + q_9 - 2q_9q_9) + q_3(15 + 32q_7^2 - 40q_4 \\
+ 48q_2q_6 + 20q_6^2 + 24q_2^2 - 11q_8 + 4(4q_1^2 + 7q_2^2 + 4q_4q_8 + q_8^2 \\
+ q_1(-7 + 8q_4 + q_8)) + 4(8q_6^2 + 4q_5q_9 + q_8^2)), \]

\[ q_{41} - \operatorname{div} (4\nabla q_1 + 11\nabla q_4 + 4\nabla q_8) = -\frac{2}{\varepsilon^2} (-57 + 32q_1^3 - 40q_3^2 + 221q_4 + 56q_3^2q_4 - 285q_4^2 \\
+ 130q_4^3 - 56q_5^2 + 88q_4q_5^2 + 72q_4q_5q_6 - 144q_6^2 + 216q_4q_6^2 - 58q_4q_7 + 56q_4q_4q_7 \\
+ 96q_5q_6q_7 - 56q_5^2 + 88q_5q_7^2 + 109q_8 + 16q_4^2q_8 - 276q_8q_9 \\
+ 168q_4^2q_8 + 32q_4^2q_8 + 96q_5^2q_8 + 40q_5q_7q_8 + 32q_5^2q_8 - 96q_8^2 \\
+ 120q_4q_9^2 + 32q_4^3 + 72q_4^2(-2 + 3q_4 + q_8) + 24q_4^2(-4 + 5q_4 + q_8) \\
+ 6q_2q_6(-47 + 68q_1 + 28q_8) - 8q_6(q_1 - 8q_4)q_9 + 2q_5(-29 + 28q_4 + 16q_9)q_9 \\
+ (8(-5 + 7q_4 + 4q_8)q_9^2 + 8q_2(8q_3q_5 + 12q_4q_7 - q_5q_9 + 9q_7q_9) \\
+ q_1(109 + 168q_4^2 + 24(q_2 + q_6)(4q_2 + 3q_6)) + 32(q_4^2 + q_3q_7 + q_7^2) \\
+ 3q_8(-27 + 8q_8) + 6q_4(-46 + 17q_8) + 8(4q_5^2 + 5q_5q_9 + 2q_4^3)), \]

\[ q_{51} - 2 \operatorname{div} (4\nabla q_5 + \nabla q_9) = -\frac{4}{\varepsilon^2} (32q_5^3 + 6q_6(q_3(-3 + 6q_4) + 2(-3 + q_1 + 4q_4)q_7) + 4q_5(5q_4 + 8q_7)q_9 \\
+ 24q_5^2q_9 + (12 + 8q_4^2 + 8q_5^2 - 29q_4 + 14q_4^2 + 28q_5q_7 + 32q_7^2 + 2(-7 + 8q_4)q_9 \\
+ 8q_5^2 + 2q_1(-8 + 10q_4 + q_8))q_9 + 8q_5^3 + 8q_5^2(4q_5 + q_9) \\
+ q_5(21 + 32q_4^2 + 32q_5^2 + 44q_7^2 + 36q_6^2 + 64q_3q_7 + 68q_4^2 \\
+ 8q_1(-5 + 4q_4 - q_8) - 19q_8 + 16q_8^2 + 8q_4(-7 + 4q_8) + 24q_5^2 \\
+ 4q_2(8q_1q_7 + 4q_3(-1 + 2q_4 + q_8) + 3q_7(-3 + 4q_4 + q_8) + 3q_6(4q_5 + q_9))), \]

\[ q_{61} - 2 \operatorname{div} (3\nabla q_2 + 4\nabla q_6) = -\frac{4}{\varepsilon^2} (24q_2^3 + (49 + q_1(-51 + 20q_1))q_6 + 72q_2^2q_6 + 20q_3^2q_6 \\
+ 2q_4(8q_6q_7 + q_5(-9 + 18q_4 + 10q_8) + q_9 - 2q_4q_9) + 4(27q_6^2 + q_6^2q_9 + 8q_6^2q_9^2 + 8q_6^2q_9^2 + 2q_4(6q_5q_7 + 3q_6(-6 + 3q_1 + 4q_8) \\
+ 4q_7q_9)) + q_2(24q_5^3 + q_1(-60 + 84q_4 + 26q_8) + 3(8q_3^2 + q_4(-47 + 34q_4) \\
+ 4q_3q_7 + 28q_4q_8 + 8q_5^2 + 4(4 + 2q_6^2 + 6q_6^2 + 2q_6^2 - 5q_8 + 9q_5q_9 + 2q_6^2))), \]

\[ q_{71} - 2 \operatorname{div} (\nabla q_3 + 4\nabla q_7) = -\frac{4}{\varepsilon^2} (8q_3^3 - 36q_2q_5 + 21q_7 + 16q_1^2q_7 + 24q_3^2q_7 + 4(9q_2^2q_7 \\
+ 17q_2^2q_7 + q_5q_6(-9 + 12q_4 + 8q_8) + 3q_2(4q_4q_5 + 4q_6q_7 + q_5q_8) \\
+ q_7(-14 + 11q_4 + q_5(q_1(-14 + 11q_4) + 8(q_5^2 + q_7^2) - 10q_8 + 8q_5q_9 + 8q_8^2)) \\
+ 2((-1 + 2q_4)(9q_2 + 8q_8) + 32q_5q_7q_9 + 32q_7^2q_7 + q_1(q_7(-19 + 32q_4 - 8q_8) \\
+ 4(8q_2q_5 + 3q_5q_6 + 5q_2q_9 + 4q_6q_9)) + q_3(8q_2^2 + 14q_4 \\
+ 2q_1(-7 + 8q_4 + q_8) + q_4(-29 + 20q_8) + 4(-3 + 8q_2^2 \\
+ q_6(3q_4 + 2q_6) + 6q_5^2 + 2(-2 + q_8)q_8 + 7q_5q_9 + 2q_8^2)) \)), \]
\[
q_{st} - \text{div} \left( \frac{1}{2} \nabla q_1 + 4(\nabla q_4 + \nabla q_8) \right) = -\frac{1}{\varepsilon^2}(-57 + 8q_1^3 + 218q_4 - 38q_5 + 158q_9 + 6q_1^2(-6 + 8q_4 + 3q_8) \\
+ 2q_1^2(-51 + 72q_4 + 40q_8) + 16q_2(4q_3q_5 + 3q_5q_7 + 3q_6(-5 + 7q_4 + 4q_8)) \\
+ q_1(61 + 102q_2^2 + 8(3q_2 + 2q_6)(2q_2 + 3q_6) + 8(q_3 - q_7)(q_3 + 2q_7) \\
+ 24(-3 + q_8)q_5 + 6q_4(-27 + 16q_8) + 8(-2q_2^2 + q_5q_9 + q_5^2)) + 2(56q_4^3 \\
+ q_1^2(-11 + 16q_8) + 6q_2^2(-23 + 20q_8) + 8q_3(5q_5q_6 + q_7(-4 + 5q_4 + 4q_8)) \\
+ 32q_4(q_2^2 + 2q_6^2 + q_7^2 + 3(-2 + q_5)q_8 + q_5q_9 + q_2^4 + 4(16q_5q_9 + q_2^6(-9 + 8q_8) \\
+ 2q_2^6(-5 + 8q_8) + q_6(8q_5^2 + q_8(-21 + 8q_8)) + q_5(-7 + 8q_8)q_9 + (-7 + 8q_5)q_2^2)),
\]

\[
q_{st} - 2\text{div} (\nabla q_5 + 2\nabla q_8) = -\frac{4}{\varepsilon^2}(8q_3^3 + 2q_4q_3 - 3q_3q_4 + 8(-1 + q_1 + 2q_4)q_7) + 15q_5 + 24q_5^2g_q \\
+ (4q_1^2 + q_1(-11 + 16q_4 + 4q_8) + 4q_3 + q_4(-10 + 7q_4) + 4q_3q_7 + 8(q_5 + q_7^2) - 7q_8 \\
+ 8q_5q_8 + 4q_5^2)q_9 + 16q_9 + 4q_2^2(2q_5 + 5q_9) + q_5(12 + 8q_1^2 \\
+ 8q_3^2 - 29q_4 + 14q_3^2 + 28q_3q_7 + 32q_4^2 - 14q_5 + 14q_4q_8 + 8q_5^2 + 2q_1(-8 + 10q_1 + 4q_8) \\
+ 24q_5^2) + 2q_2(q_3 - 3q_3q_4 + (-9 + 10q_1 + 18q_4)q_7 + 6q_6(q_5 + 4q_9)).
\]

This system is solved subject to the boundary constraints (6.3) and the natural (Robin) boundary conditions arising in the variational problem for the functional (6.2).

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