

Landau-de Gennes Model with Sextic Potentials: Asymptotic Behavior of Minimizers

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Liquid Crystals

Liquid crystals (LCs) are **anisotropic fluids**. The anisotropy arises from the directional nature of the **molecular geometry**, **physical**, or **chemical** properties. They are **intermediate** between:

- **Crystalline solids**: highly ordered.
- **Isotropic liquids**: fully disordered.

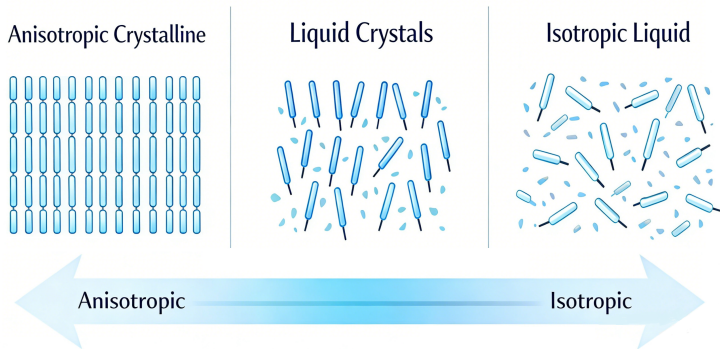


Figure: Order vs. Disorder

Three Phases of Liquid Crystals

- **Nematic:** long-range orientational order (the molecules tend to align parallel to each other); no long-range positional/order correlation of the centers of mass.
- **Cholesteric:** On a larger scale, the director of cholesteric molecules twists in space, forming a helix with a characteristic spatial period.
- **Smectic:** The phase has one-dimensional translational order, resulting in a layered structure.

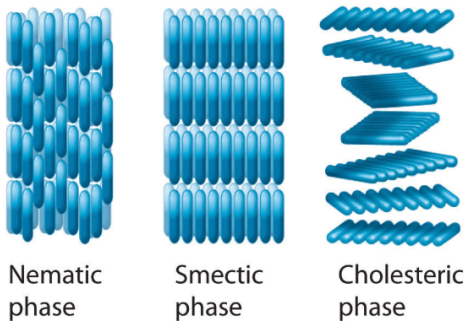


Figure: The Arrangement of Molecules in different Liquid Crystal Phases.

Different Liquid Crystals' Models

- **Vector model:** $\mathbf{n}(x) \in \mathbb{S}^2$ at each material point x .
 - It is **simple** and useful in many cases.
 - It cannot reflect the **head-to-tail symmetry** of **rod-like** molecules with $-\mathbf{n} \sim \mathbf{n}$.
- **Molecular model:** a **distribution function** $f(x, \mathbf{m})$, which is the **number density** of molecules with orientation $\mathbf{m} \in \mathbb{S}^2$ at material point x .
 - It provides a more accurate description.
 - The computation is complex.
- **Q-tensor model:** a symmetric, traceless 3×3 matrix $\mathbf{Q}(x)$ for $x \in \mathbb{R}^3$.
 - In this model, one does not assume a **preferred direction**. It can describe **biaxiality**.
 - The analysis is also complicated.

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Q-tensor: the Landau-de Gennes Model

The state of a liquid crystal is described by a symmetric, traceless 3×3 matrix:

$$\mathbb{S}_0 := \{\mathbf{Q} \in \mathbb{M}^{3 \times 3} : \mathbf{Q} = \mathbf{Q}^T, \operatorname{tr} \mathbf{Q} = 0\}.$$

Eigendecomposition & representation: For orthonormal eigenvectors \mathbf{n} and \mathbf{m} , we can express \mathbf{Q} as:

$$\mathbf{Q} = s \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) + r \left(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3} \mathbf{I} \right).$$

Three different cases:

- **Isotropic:** If $s = r = 0$, namely, $\mathbf{Q} = \mathbf{O}$.
- **Biaxial:** If s and r are **different** and **non-zero**.
- **Uniaxial:** \mathbf{Q} has a **single preferred direction**, namely,

$$\mathbf{Q} = t \left(\mathbf{u} \otimes \mathbf{u} - \frac{1}{3} \mathbf{I} \right), \quad \text{for some } t \in \mathbb{R}, \mathbf{u} \in \mathbb{S}^2.$$

Free Energy Functional

The **free energy functional** is defined as

$$F(Q, \Omega) := \int_{\Omega} (\mathcal{F}_e(Q) + \mathcal{F}_b(Q)) \, dx, \quad \Omega \subset \mathbb{R}^d, \quad d = 2, 3.$$

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- **Elastic energy density:** With **elastic constants** $L_i \geq 0$ ($i = 1, 2, 3$),

$$\mathcal{F}_e(\mathbf{Q}) := \underbrace{\frac{L_1}{2} |\nabla \mathbf{Q}|^2}_{\text{Isotropic term}} + \underbrace{\frac{L_2}{2} \partial_j \mathbf{Q}_{ij} \partial_k \mathbf{Q}_{ik} + \frac{L_3}{2} \partial_k \mathbf{Q}_{ij} \partial_j \mathbf{Q}_{ik}}_{\text{Anisotropic contributions}}.$$

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- **Bulk potential density:** It has the **polynomial form** given by

$$\begin{aligned} \mathcal{F}_b(\mathbf{Q}) := & a_1 - \frac{a_2}{2} \operatorname{tr} \mathbf{Q}^2 + \frac{a_3}{3} \operatorname{tr} \mathbf{Q}^3 + \frac{a_4}{4} (\operatorname{tr} \mathbf{Q}^2)^2 \\ & + \frac{a_5}{5} (\operatorname{tr} \mathbf{Q}^2)(\operatorname{tr} \mathbf{Q}^3) + \frac{a_6}{6} (\operatorname{tr} \mathbf{Q}^2)^3 + \frac{a'_6}{6} (\operatorname{tr} \mathbf{Q}^3)^2. \end{aligned}$$

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Stable equilibrium configurations correspond to the **minimizers** of $F(\cdot, \Omega)$.

Vanishing Elasticity Limit: Background

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Question (Vanishing elasticity limit)

The asymptotic behavior of minimizers (or critical points) to the quartic Landau-de Gennes model (qLdG) as $\varepsilon \rightarrow 0^+$.

The Limit $\varepsilon \rightarrow 0^+$: Vacuum Manifold

As $\varepsilon \rightarrow 0^+$, the potential term forces $\mathbf{Q}(x)$ to lie in the set of minimizers of $\mathcal{F}_b^{(4)}$, defining the **vacuum manifold**:

$$\mathcal{N}_u := \left\{ s_* \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right) : \mathbf{n} \in \mathbb{S}^2 \right\} \cong \mathbb{RP}^2.$$

The scalar order parameter s_* is given by

$$s_* := \frac{a_3 + \sqrt{a_3^2 + 24a_2a_4}}{4a_4} \quad (\text{normalized such that } \mathcal{F}_b^{(4)}(s_*(\mathbf{n} \otimes \mathbf{n} - \mathbf{I}/3)) = 0).$$

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Limiting energy functional: The limiting functional is the **Dirichlet energy** for \mathcal{N}_u -valued maps, defined by

$$E_0^{(4)}(\mathbf{Q}, \Omega) := \frac{1}{2} \int_{\Omega} |\nabla \mathbf{Q}|^2 dx, \quad (\text{qDir})$$

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- **Physical link:** This connects the \mathbf{Q} -tensor theory to the classical **Oseen-Frank model** under appropriate boundary conditions.
- **Geometry:** The target manifold \mathcal{N}_u allows for **line defects** due to its **non-trivial fundamental group**.

Previous Results: the Energy-Bounded Case

Assumption: Uniform bounds on the energy functional and the L^∞ norm:

$$E_\varepsilon^{(4)}(\mathbf{Q}_\varepsilon, \Omega) + \|\mathbf{Q}_\varepsilon\|_{L^\infty(\Omega)} \leq M, \quad \forall 0 < \varepsilon < 1,$$

where $\{\mathbf{Q}_\varepsilon\}$ is a sequence of minimizers with $\mathbf{Q}_\varepsilon|_{\partial\Omega} = \mathbf{Q}_b$.

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- **Dynamic analysis:** [Wang-Wang-Zhang, *ARMA*, 2017] They analyzed the convergence of the corresponding **gradient flow** system.

Previous Results: The Logarithmic Energy Case

Assumption: The energy grows logarithmically in terms of ε :

$$E_{\varepsilon}^{(4)}(\mathbf{Q}_{\varepsilon}, \Omega) \leq M(\log(1/\varepsilon) + 1), \quad \|\mathbf{Q}_{\varepsilon}\|_{L^{\infty}(\Omega)} \leq M, \quad \forall 0 < \varepsilon < 1,$$

where $\{\mathbf{Q}_{\varepsilon}\}$ is a sequence of minimizers. Define $\mu_{\varepsilon} := \frac{E_{\varepsilon}^{(4)}(\mathbf{Q}_{\varepsilon}, \cdot)}{\log(1/\varepsilon)}$ to be the associated **Radon measure**. Up to a subsequence, $\mu_{\varepsilon} \rightharpoonup^* \mu_0$ **in the sense of Radon measures**.

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- **2D analysis:** [Canevari, *ESAIM: COCV*, 2015] The support $\text{supp } \mu_0$ is discrete in Ω . Moreover, there exists $\mathbf{Q}_0 \in C^\infty(\Omega \setminus \text{supp } \mu_0)$ such that up to a subsequence, $\mathbf{Q}_\varepsilon \rightarrow \mathbf{Q}_0$ uniformly in $\Omega \setminus \text{supp } \mu_0$.

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- **3D concentration:** [Canevari, *ARMA*, 2017] In three dimensions, the energy concentrates on **line segments** $\{\ell_i\}$:

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Assumption: The energy grows logarithmically in terms of ε :

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- The analytical techniques for studying these line defects originate from the **Ginzburg-Landau model** in [Lin-Rivière, *JEMS*, 1999].

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Model Simplification: Following [Huang–Lin, CVPDE, 2022], we set $a_3 = a_5 = 0$ for simplicity of exposition. We define the energy functional

$$E_\varepsilon(\mathbf{Q}, \Omega) := \int_\Omega \left(\frac{1}{2} |\nabla \mathbf{Q}|^2 + \frac{1}{\varepsilon^2} f_b(\mathbf{Q}) \right) dx, \quad (\text{sLDG})$$

where $f_b(\mathbf{Q})$ is the **sextic bulk energy density** given by

$$f_b(\mathbf{Q}) := a_1 - \frac{a_2}{2} \text{tr}(\mathbf{Q}^2) + \frac{a_4}{4} (\text{tr}(\mathbf{Q}^2))^2 + \frac{a_6}{6} (\text{tr}(\mathbf{Q}^2))^3 + \frac{a'_6}{6} (\text{tr}(\mathbf{Q}^3))^2.$$

- **Coefficients:** $a_2, a_4, a_6, a'_6 > 0$.
- **Normalization:** The constant a_1 is chosen such that $\min_{\mathbf{Q} \in \mathbb{S}_0} f_b(\mathbf{Q}) = 0$.

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- **2D analysis:** [Monteil-Rodiac-Van Schaftingen, *ARMA*, 2021; *Math. Ann.*, 2022] investigated the [two-dimensional](#) case for generalized Ginzburg–Landau models, including the [sextic LdG model](#).

Main Results: Bounded Energy

Theorem (W.-Zhang, *arXiv:2404.00677*)

Let $\Omega \subset \mathbb{R}^3$ be a bounded domain, and let $\{\mathbf{Q}_\varepsilon\}_{0 < \varepsilon < 1}$ be *local minimizers* of (sLDG) satisfying

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- (2) \mathbf{Q}_0 is *locally energy-minimizing harmonic* in Ω . Moreover, \mathbf{Q}_0 is a *weak solution* of

$$\Delta \mathbf{Q}_0 = -\frac{1}{2r_*^2} |\nabla \mathbf{Q}_0|^2 \mathbf{Q}_0 - \frac{3}{r_*^4} \text{tr}(\nabla \mathbf{Q}_0 \nabla \mathbf{Q}_0 \mathbf{Q}_0) \left(\mathbf{Q}_0^2 - \frac{2r_*^2}{3} \mathbf{I} \right).$$

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- (3) There exists a *locally finite singular set* $\mathcal{S}_{\text{pts}} \subset \Omega$ such that $\mathbf{Q}_0 \in C^\infty(\Omega \setminus \mathcal{S}_{\text{pts}}, \mathcal{N})$.

Main Results: Bounded Energy (continued)

- (4) For all $j \in \mathbb{Z}_{\geq 0}$, $\mathbf{Q}_{\varepsilon_n} \rightarrow \mathbf{Q}_0$ in $C_{\text{loc}}^j(\Omega \setminus \mathcal{S}_{\text{pts}})$. Moreover, for every $\overline{B}_r(x) \subset \Omega \setminus \mathcal{S}_{\text{pts}}$, $\mathbf{Q}_{\varepsilon_n}$ is a smooth solution of

$$\begin{aligned} \Delta \mathbf{Q}_{\varepsilon_n} = & -\frac{1}{2r_*^2} |\nabla \mathbf{Q}_{\varepsilon_n}|^2 \mathbf{Q}_{\varepsilon_n} \\ & - \frac{3}{r_*^4} \text{tr}(\nabla \mathbf{Q}_{\varepsilon_n} \nabla \mathbf{Q}_{\varepsilon_n} \mathbf{Q}_{\varepsilon_n}) \left(\mathbf{Q}_{\varepsilon_n}^2 - \frac{2r_*^2}{3} \mathbf{I} \right) + \mathbf{R}_n, \end{aligned}$$

in $B_{r/2}(x)$, where the remainder \mathbf{R}_n satisfies

$$\|D^j \mathbf{R}_n\|_{L^\infty(B_{r/2}(x))} \leq C \varepsilon_n^2 r^{-j-2},$$

with $C = C(f_b, j, M) > 0$.

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- (1) $\text{supp}(\mu_0) = \mathcal{S}_{\text{line}}$.
- (2) $\Omega \cap \mathcal{S}_{\text{line}}$ is countably \mathcal{H}^1 -rectifiable with $\mathcal{H}^1(\Omega \cap \mathcal{S}_{\text{line}}) < +\infty$.

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(3) For each subdomain $U \subset\subset \Omega \setminus \mathcal{S}_{\text{line}}$, we have

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- (6b) If $x \in K$ is an **endpoint** of q segments $\ell_{i_1}, \dots, \ell_{i_q}$, let \mathbf{v}_j be the unit **direction vector** of ℓ_{i_j} pointing **outward** from x . Then $q \geq 2$, $\sum_{j=1}^q \theta_j \mathbf{v}_j = 0$, and the number of j with $\theta_j = \kappa_*$ is **even**.

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- **Energy bounds:** By selecting appropriate **boundary conditions**, both the **bounded** and **logarithmic** energy regimes are physically realizable for global minimizers $\{\mathbf{Q}_\varepsilon\}_{0 < \varepsilon < 1}$.
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- **Open problem:** While our results focus on **minimizers**, it remains **unknown** if these properties hold for general critical points (solutions to Euler-Lagrange equations), similar to the **Ginzburg-Landau** results in [Bethuel-Brezis-Orlandi, *JFA*, 2001].

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- 1 Brief Introduction of Liquid Crystals
- 2 Motivations and Main Results
- 3 Difficulties and Strategies

Differences Between Uniaxial and Biaxial Vacuum Manifolds

	Uniaxial	Biaxial
Representation	$s_* \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{I}}{3} \right)$	$r_* (\mathbf{n} \otimes \mathbf{n} - \mathbf{m} \otimes \mathbf{m})$
Eigenvalues	$\frac{2s_*}{3}, -\frac{s_*}{3}, -\frac{s_*}{3}$	$r_*, 0, -r_*$
Dimension	2	3
Universal covering	\mathbb{S}^2	\mathbb{S}^3
Fundamental group	\mathbb{Z}_2	$Q_8 := \{\pm 1, \pm i, \pm j, \pm k\}$
Topological structure	$\mathbb{S}^2 / \mathbb{Z}_2 \cong \mathbb{RP}^2$	\mathbb{S}^3 / Q_8
Free homotopy classes	h_0, h_1	$H_0 \leftrightarrow \{1\},$ $H_1 \leftrightarrow \{\pm i\}, \quad H_2 \leftrightarrow \{\pm j\},$ $H_3 \leftrightarrow \{\pm k\}, \quad H_4 \leftrightarrow \{-1\}$

Table: Comparison between uniaxial and biaxial vacuum manifolds.

Multi-valued Product on Free Homotopy Classes

Definition

Let G be a group. We define a **multi-valued product** on the set of its **conjugacy classes** as follows:

Given two conjugacy classes G_1 and G_2 , we define $G_1 \cdot G_2$ to be the **collection of conjugacy classes** containing elements of the form

$$g_1 g_2, \quad g_1 \in G_1, \quad g_2 \in G_2.$$

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	H_0	H_1	H_2	H_3	H_4
H_0	H_0	H_1	H_2	H_3	H_4
H_1	H_1	H_0, H_4	H_3	H_2	H_1
H_2	H_2	H_3	H_0, H_4	H_1	H_2
H_3	H_3	H_2	H_1	H_0, H_4	H_3
H_4	H_4	H_1	H_2	H_3	H_0

Table: Multi-valued product on $[\mathbb{S}^1, \mathcal{N}]$.

Energy of Free Homotopy Classes

Let $\mathcal{X} = \mathcal{N}_u$ or \mathcal{N} . We define the **energy** of a **free homotopy class** $[\alpha]_{\mathcal{X}} \in [\mathbb{S}^1, \mathcal{X}]$ by

$$\mathcal{E}([\alpha]_{\mathcal{X}}) := \inf \left\{ \frac{1}{2} \int_{\mathbb{S}^1} |\beta'(\theta)|^2 d\theta : \beta \in H^1(\mathbb{S}^1, \mathcal{X}), [\beta]_{\mathcal{X}} = [\alpha]_{\mathcal{X}} \right\}.$$

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We further define the **relaxed energy**

$$\mathcal{E}^*([\alpha]_{\mathcal{X}}) := \inf \left\{ \sum_{j=1}^n \mathcal{E}([\alpha_j]_{\mathcal{X}}) : [\alpha]_{\mathcal{X}} \in \prod_{j=1}^n [\alpha_j]_{\mathcal{X}} \right\}.$$

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Free homotopy class	h_0	h_1	H_0	H_1	H_2	H_3	H_4
\mathcal{E}^*	0	$\frac{\pi s_*^2}{2}$	0	$\frac{\pi r_*^2}{2}$	$\frac{\pi r_*^2}{2}$	πr_*^2	πr_*^2

Sketch of the Proof: Bounded Energy

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- Obtain C^j -convergence by iterative elliptic estimates.
- Represent the remainder terms via \mathbf{Y}_ε and h_ε and derive uniform bounds.

Sketch of the Proof: Logarithmic Energy

- (1) **Clearing-out property:** Let $\{\mathbf{Q}_\varepsilon\}_{0 < \varepsilon < 1} \subset H^1(\Omega, \mathbb{S}_0)$ be local minimizers and let $\overline{B}_{2r}(x) \subset \Omega$. Then

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- **Jerrard-Sandier type lower bound:** Let $A := B_1^2 \setminus B_{1/80}^2$. Assume $\mathbf{Q} \in H^1(B_1^2, \mathbb{S}_0)$ satisfies $\|\mathbf{Q}\|_{L^\infty(B_1^2)} \leq M$ and

$$\phi_0(\mathbf{Q}, A) := \operatorname{ess\,inf}_A (\min\{r_*^{-1}(\lambda_1 - \lambda_2), r_*^{-1}(\lambda_2 - \lambda_3)\}) > 0.$$

Then

$$E_\varepsilon(\mathbf{Q}, B_1^2) \geq \mathcal{E}^*([\varrho \circ \mathbf{Q}|_{\partial B_1^2}]_{\mathcal{N}}) \phi_0^2(\mathbf{Q}, A) \log \frac{1}{\varepsilon} - C(f_b, M),$$

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- **Luckhaus-type lemma for logarithmic energy:** interpolation estimates for manifold-valued maps.

Sketch of the Proof: Logarithmic Energy

Let $0 < \varepsilon < 1$ and let $\mathbf{Q}_\varepsilon \in H^1(\Omega, \mathbb{S}_0)$ be a local minimizer of (sLDG). Define a non-negative Radon measure μ_ε on $\overline{\Omega}$ by

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Then there exist $\mu_0 \geq 0$ and $\varepsilon_n \rightarrow 0^+$ such that

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- **Rectifiability:** Follows from the results in [Arroyo-Rabasa–De Philippis–Hirsch–Rindler, *GAFA*, 2019] and [Ambrosio–Soner, *Ann. Norm. Pisa*, 1997].

Sketch of the Proof: Logarithmic Energy

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 - [Explicit computation](#) of $\mathcal{E}^*(H_i)$, $i \in \{1, 2, 3, 4\}$.
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Sketch of the Proof: Logarithmic Energy

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Sketch of the Proof: Logarithmic Energy

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- **supp μ_0 is a finite union of line segments:**
 - Densities have finite values.
 - Classification of 1-dimensional stationary varifolds [Allard-Almgren, *Invent. Math.*, 1976].
- **Endpoint analysis:** Let $x_0 \in \mathcal{S}_{\text{line}}$ be an endpoint. Choose $r > 0$ such that

$$B_{2r}(x_0) \Subset K, \quad \mathcal{S}_{\text{pts}} \cap \partial B_{2r}(x_0) = \emptyset, \quad \mathcal{S}_{\text{line}} \cap B_{2r}(x_0) = \bigcup_{j=1}^q \ell_{ij}.$$

Let \mathbf{v}_j be the unit **direction vector** of the segment ℓ_{ij} emanating from x_0 , and define $x_j := \ell_{ij} \cap B_r(x_0)$. Choose $0 < \rho < r/10$ such that the balls $B_\rho(x_j)$ are disjoint, and define $\gamma_j := B_\rho(x_j) \cap \partial B_r(x_0)$. Then

$$\sum_{j=1}^q \theta_j \mathbf{v}_j = 0, \quad H_0 \in \prod_{j=1}^q [\mathbf{Q}_0|_{\gamma_j}]_{\mathcal{N}}. \quad (\star)$$

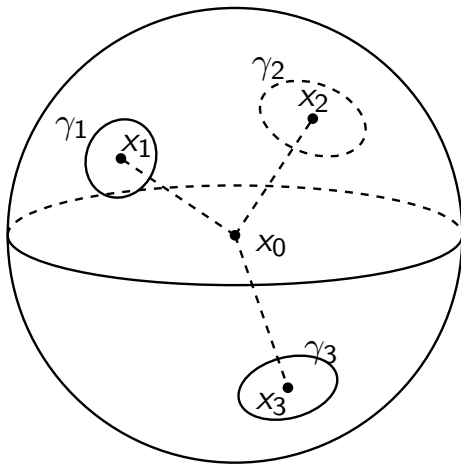


Figure: Geometric configuration near x_0 for $q = 3$.

Proof of (6b)

Let

$$n_0 := \#\{j \in \{1, 2, \dots, q\} : \theta_j = \kappa_*\}.$$

Assume that n_0 is odd. Up to a permutation of the indices,

$$\theta_j = \kappa_*, \quad j \in \{1, 2, \dots, 2q_0 + 1\},$$

where $q_0 \in \mathbb{Z}_{\geq 0}$ and $2q_0 + 1 \leq q$. We deduce that $[\mathbf{Q}_0|_{\gamma_j}]_{\mathcal{N}} \in \{H_1, H_2\}$ for any $j \in \{1, 2, \dots, 2q_0 + 1\}$ and $[\mathbf{Q}_0|_{\gamma_j}]_{\mathcal{N}} \in \{H_3, H_4\}$ for any $j \in \{2q_0 + 2, \dots, q\}$. By the product table, we have

$$\prod_{j=1}^{2q_0+1} [\mathbf{Q}_0|_{\gamma_j}]_{\mathcal{N}} \in \{H_1, H_2\},$$
$$\prod_{j=2q_0+2}^q [\mathbf{Q}_0|_{\gamma_j}]_{\mathcal{N}} \in \{H_0, H_3, H_4\}.$$

This contradicts (\star) , since $H_0 \notin H_i \cdot H_j$ for any $i \in \{1, 2\}$ and $j \in \{0, 3, 4\}$.

Thank you for listening!