Multistability for a Reduced Landau–de Gennes Model in the Exterior of 2D Polygons

Yuchen Han and Apala Majumdar

Department of Mathematics and Statistics, University of Strathclyde, G1 1XQ, United Kingdom.

We present a systematic study of nematic equilibria in an unbounded domain, with a two-dimensional regular polygonal hole with $K$ edges in a reduced Landau–de Gennes framework. This complements our previous work on the “interior problem” for nematic equilibria inside regular polygons (SIAM Journal on Applied Mathematics, 80(4):1678–1703, 2020). The two essential model parameters are $\lambda$-the edge length of polygon hole and an additional freedom parameter $\gamma$-the nematic director at infinity. In the $\lambda \to 0$ limit, the limiting profile has a unique interior point defect outside a triangular hole, two interior point defects outside a generic polygon hole, except for a triangle and a square. For a square hole, the equilibria has either no interior defects or two line defects depending on $\gamma$. In the $\lambda \to \infty$ limit, we have at least $[K/2]$ stable states differentiated by the location of two bend vertices and the multistability is enhanced by $\gamma$, compared to the interior problem. Our work offers new methods to tune the existence, location and dimensionality of defects.

I. INTRODUCTION

Nematic liquid crystals (NLCs) are classical examples of partially ordered materials or viscoelastic anisotropic materials, with long-range orientational ordering [11]. The NLC molecules are typically asymmetric in shape e.g. rod-like, and they tend to align along locally preferred directions, referred to as nematic directors in the literature [11]. The optical, mechanical and rheological NLC responses are direction-dependent, with distinguished responses along the nematic directors. Indeed, the anisotropic NLC responses to external stimuli, interfaces and boundaries make them soft, self-organising and the cornerstone of several NLC applications in science and engineering [25]. Nematics in confinement have attracted substantial scientific interest in the academic and industrial sectors [20]. In fact, nematics inside a planar cell are the building block of the celebrated twisted nematic display, and contemporary work has focused on the tremendous potential of NLCs for multistable systems i.e. NLC systems with multiple observable states without applied fields, such that each observable state offers a distinct mode of functionality [23]. Nematic defects play a key role in multistability, where a nematic defect is a point/line/surface where the nematic director cannot be uniquely defined [11]. Nematic defects often organise the space of stable states in multistable systems in the sense that we can classify the stable states in terms of the nature, multiplicity and locations of defects. Additionally, defects have distinct optical signatures and can act as binding sites or “special” sites in materials design or applications. The delicate interplay between geometric frustration, boundary effects, material properties and defects in multistability leads to a suite of challenging mathematical questions at the interface of applied topology, nonlinear partial differential equations and scientific computation (to name a few). Equally, it gives new inroads into engineered soft materials, topological materials or meta-materials which could find new applications in photonics, robotics and artificial intelligence [10].

In this paper, we focus on the mathematical modelling and numerical computation of NLC equilibria outside regular two-dimensional (2D) polygons with homeotropic boundary conditions i.e. the nematic director is constrained to be normal to the polygon boundary. We work in a reduced 2D Landau–de Gennes framework, details of which are given in the next section, and this can capture the nematic directors and the nematic defects in a 2D setting, along with informative insights into how multistability can be tailored by the shape and size of the polygon. This toy mathematical problem models a single colloidal particle, in the shape of a 2D polygon, suspended in an extended NLC medium, which is of both experimental and theoretical interest [23, 8, 29, 13, 25]. In [8, 23, 29], the authors fabricate almost 2D platelets of different polygonal shapes suspended in a NLC medium. Using advanced microfabrication techniques and optical methods, they can track the director profiles and the associated defects. The authors observe multiple types of defects: dipoles, Saturn rings, and various linked or entangled defect loop lines intertwining arrays of embedded inclusions. In fact, in [23], the authors use optical tweezers to manipulate the defect lines, to link them or disentangle them, and in doing so, create various exotic knotted defect patterns. In all cases, the observed states and their defect patterns strongly depend on the geometry and orientation of colloidal particle(s) and their boundary effects, offering excellent examples of organic self-assembled structures in NLC media.

In [10], we study the “interior” problem of multistability for NLCs confined to a regular 2D polygon with tangent boundary conditions i.e. the nematic director is tangent to the polygon edges, in a reduced Landau–de Gennes framework. We use conformal mapping techniques and methods from elliptic partial differential equations, to show that there is a unique Ring solution for small regular polygons, with a single isolated point defect at the centre of the polygon. The only exceptions are the triangle and the square, which are dealt with separately. In fact, the triangle supports a fractional point defect at the centre, if the edge length is sufficiently small, whereas the square supports...
the Well Order Reconstruction Solution (WORS) with two orthogonal defect lines along the square diagonals (also see [19]). As the edge length increases, the Ring solution loses stability and there are at least \( \frac{K}{2} \) classes of distinct NLC equilibria on a \( K \)-polygon with \( K \) edges. In related papers, we comprehensively study NLC solution landscapes on 2D polygons with tangent boundary conditions [17, 18].

We study the complementary “exterior” problem in this paper: asymptotic and numerical studies of NLC equilibria outside a regular polygonal hole, immersed in \( \mathbb{R}^2 \). This problem, and related problems, have received some analytical interest although systematic studies are missing. In [25], the authors study stable NLC profiles outside a square hole with homeotropic boundary conditions. They numerically observe string defects (line defects) pinned to square edges, defects at square vertices and interior point defects, depending on the temperature and square size. In [19], the authors model NLCs with multiple spherical inclusions and numerically investigate how the defect set depends on the spatial organisation and properties of the spherical particles, along with those of the ambient NLC media. In [1], the authors rigorously analyse NLC equilibria outside a spherical particle with homeotropic boundary conditions, in a three-dimensional (3D) Landau–de Gennes framework. They obtain elegant limiting profiles in the small particle and large particle limit, and in fact, produce an analytic expression for the celebrated Saturn ring solution with a distinct defect loop around the spherical particle. We adopt a systematic approach in this paper in 2D, focusing on the effects of shape and size of the polygonal hole on the NLC equilibria. The methodology follows that of [16], the key difference being the extra degree of freedom rendered by the far-field boundary conditions, away from the polygon boundary. As with the interior problem, we have a unique NLC equilibrium for small holes, and multistability for large holes. However, the unique limiting profiles for small holes, are more varied compared to the interior problem, depending on the far-field condition. For a square hole, we can observe either line defects or point defects at the square vertices, depending on the far-field condition. There is qualitative agreement with the numerical results in [25]. In general, the locations of the defects for the unique limiting profile depend on the far-field condition. Using a result from Ginzburg–Landau theory in [2], we show that there are exactly two interior point defects for a generic polygonal hole, \( E_K \) with \( K \) edges and \( K > 4 \), and the location of these defects can be tuned with the far-field condition. For large polygonal holes, we provide a simple estimate for the number of stable NLC equilibria using combinatorial arguments, and multistability is enhanced compared to the interior problem. This is because the exterior problem has lesser symmetry than the interior problem, due to the far-field conditions. For example, there are two rotationally equivalent diagonal NLC equilibria in the interior of a square domain, but we lose the equivalence for the exterior problem since the far-field condition breaks the symmetry.

Applied mathematics focuses on the development of new mathematical methods, and equally elegant applications of known methods to new settings. Our work falls into the second category, where we largely build on previous work, and use techniques from complex analysis, Ginzburg–Landau theory for superconductivity, symmetry results and combinatorial arguments to analyse limiting profiles, complemented by numerical studies to support the theory. In doing so, we adopt a systematic and holistic approach, unravelling beautiful examples of how geometric frustration and nematic defects go hand in hand for tailored multistability. All of this sets the scene for global mathematical studies of NLC solution landscapes in complex geometries with voids, mixed boundary conditions and in some cases, multiple order parameters [14].

The paper is organised as follows. In Section II we review the reduced 2D Landau–de Gennes theoretical framework, which is equivalent to the Ginzburg–Landau theory for superconductivity. In Section III we focus on the small polygon limit i.e. the \( \lambda \to 0 \) limit of minimizers of the reduced Landau–de Gennes free energy, where \( \lambda \) is the polygon edge length. We use the Schwarz–Christoffel mapping to define an associated boundary-value problem on the unit disc, for each regular polygonal hole, and this boundary-value problem is explicitly solved. We can track the defect set of the limiting solution analytically, and study its dependence on \( K \) and the far-field condition. In Section IV, we focus on the \( \lambda \to \infty \) limit and the limiting problem is captured by the Laplace problem for an angle in the plane, with Dirichlet boundary conditions. This angle models the 2D nematic director. The Dirichlet boundary conditions for the angle are not uniquely defined, and this leads to multistability in this limit. We present illustrative examples for a square and a hexagon, accompanied by bifurcation diagrams for solution branches in this model, for a square hole. There are interesting differences between the bifurcation diagrams for the interior problem and those for the exterior problem respectively. We conclude in Section V with a summary and some perspectives.

II. THEORETICAL FRAMEWORK

The Landau–de Gennes (LdG) theory is one of the most powerful continuum theories for nematic liquid crystals. In the LdG framework, the nematic state is described by a macroscopic LdG order parameter - the \( Q \)-tensor order parameter. In three dimensions (3D), the LdG order parameter is a symmetric, traceless \( 3 \times 3 \) matrix with five degrees of freedom. The nematic director is often interpreted as the eigenvector of the LdG \( Q \)-tensor with the largest positive eigenvalue [10]. For thin 3D systems, for which the height is negligible compared to the two-dimensional
(2D) cross-section dimensions, it suffices to work with the reduced Landau–de Gennes (rLdG) model, based on the assumption that the nematic director is in the cross-section plane, and structural details are invariant across the height of the system \[12\]. The rLdG model has been successfully applied for capturing the qualitative properties of physically relevant solutions and for probing into defect cores \[3, 13, 23, 24\]. In the rLdG model, the nematic state in the 2D cross-section/2D domain is described by a reduced order parameter: a symmetric, traceless $2 \times 2$ matrix, $\mathbf{P}$, as given below

$$
\mathbf{P} = \begin{pmatrix} P_{11} & P_{12} \\ P_{12} & -P_{11} \end{pmatrix}.
$$

As is standard in the calculus of variations, the physically observable configurations correspond to local or global minimizers of a suitably defined rLdG free energy. We work at a special temperature, $A = -B^2/3C$, where $A$ is a re-scaled temperature and $B, C$ are positive material-dependent constants \[11\]. At this fixed temperature, we work with the following reduced rLdG free energy:

$$
F[\mathbf{P}] := \int_{\Omega} \frac{L}{2} |\nabla \mathbf{P}|^2 + f_b(\mathbf{P}) \, d\mathbf{A}.
$$

(II.1)

where $\Omega$ is the 2D domain and $L$ is a positive elastic constant. In the remainder of this manuscript, $\Omega$ is the complement of a regular 2D polygon in two-dimensional Euclidean space. Here, we have employed the simplest one-constant approximation for the elastic energy density, which is typically a quadratic and convex function of $|\nabla \mathbf{P}|$, and in the one-constant case, the elastic energy density is $\frac{B}{2} |\nabla \mathbf{P}|^2$, which assumes that all deformations are equally energetically expensive \[11\]. The bulk energy density dictates the planar nematic order as a function of the $\nabla \mathbf{P}$, one-constant approximation for the elastic energy density, which is typically a quadratic and convex function of $|\nabla \mathbf{P}|$, and in the one-constant case, the elastic energy density is $\frac{B}{2} |\nabla \mathbf{P}|^2$, which assumes that all deformations are equally energetically expensive \[11\]. The bulk energy density dictates the planar nematic order as a function of the temperature \[16\]. At this fixed temperature, we work with:

$$
f_b = -\frac{B^2}{4C} \text{tr} \mathbf{P}^2 + \frac{C}{4} (\text{tr} \mathbf{P})^2.
$$

We choose this temperature, partly for comparison with previous work in \[16\] and \[9\], and partly because for this special temperature, solutions in the rLdG model also exist as solutions for the full LdG model in 3D i.e. the minimizers of the rLdG model at $A = -B^2/3C$ will exist as critical points of the full LdG free energy in 3D settings, for suitably defined boundary conditions. This is generally not true for arbitrary $A < 0$; see \[2\] for more details. More precisely, at $A = -B^2/3C$, we can relate minimizers (or indeed critical points) of (II.1) to critical points of an appropriately defined 3D LdG energy:

$$
I[\mathbf{Q}] := \int_{\Omega \times [0,h]} \frac{L}{2} |\nabla \mathbf{Q}|^2 + F_b(\mathbf{Q}) \, d\mathbf{V}
$$

(II.2)

where $h$ is the height of a 3D domain with $\Omega$ as the 2D cross-section, and $F_b(\mathbf{Q}) := \frac{1}{2} \text{tr} \mathbf{Q}^2 - \frac{B}{6C} (2 \hat{\mathbf{x}} \otimes \hat{\mathbf{x}} - \hat{\mathbf{x}} \otimes \hat{\mathbf{y}} - \hat{\mathbf{y}} \otimes \hat{\mathbf{y}})$. The order parameter $\mathbf{Q}$ is defined as shown below:

$$
\mathbf{Q} = \mathbf{P}_3 - \frac{B}{6C} (2 \hat{\mathbf{x}} \otimes \hat{\mathbf{x}} - \hat{\mathbf{x}} \otimes \hat{\mathbf{y}} - \hat{\mathbf{y}} \otimes \hat{\mathbf{y}}).
$$

The matrix, $\mathbf{P}_3$ is a $3 \times 3$ symmetric traceless matrix, such that $(\mathbf{P}_3)_{ij} = \mathbf{P}_{ij}$ for $i, j = 1, 2$ and all remaining matrix entries are set to zero.

The energy, (II.1) is non-dimensionalised with $\tau = x/\lambda$, where $\lambda$ is the edge-length of the polygonal hole.

$$
F[\mathbf{P}] := \int_{E_K^C} \frac{1}{2} |\nabla \mathbf{P}|^2 + \frac{\lambda^2}{L} f_b(\mathbf{P}) \, d\mathbf{A}.
$$

(II.3)

The working domain is $E_K^C$, the complement of a 2D re-scaled polygon $E_K$ with $K$ edges of unit length, centered at the origin, with vertices

$$
w_k = (\cos (2 \pi (k - 1)/K), \sin (2 \pi (k - 1)/K)), \; k = 1, \ldots, K.
$$

We label the edges counterclockwise as $C_1, \ldots, C_K$, starting from $(1, 0)$. See figure \[1\].

We can also write $\mathbf{P}$ in terms of an order parameter, $s$, and an angle $\gamma$ as shown below -

$$
\mathbf{P} = 2s \left( \mathbf{n} \otimes \mathbf{n} - \frac{1}{2} \mathbf{I}_2 \right),
$$

(II.4)
where \( \mathbf{n} = (\cos \gamma, \sin \gamma)^T \) is the nematic director in the plane, and \( \mathbf{I}_2 \) is the \( 2 \times 2 \) identity matrix. so that

\[
\begin{align*}
P_{11} &= s \cos (2\gamma), \quad P_{12} = s \sin (2\gamma).
\end{align*}
\]

The defect set in simply identified with the nodal set of \( n \), where \( n = 1 \) for all values of \( n \), and \( n = 0 \) otherwise, see [16], interpreted as the set of no planar order in \( E_K \).

We impose homeotropic boundary conditions on \( \partial E_K \), which requires \( n \) in (II.4) to be homeotropic/normal to the edges of \( E_K \). However, there is a necessary mismatch at the corners/vertices. We impose a continuous Dirichlet boundary condition, \( \mathbf{P} = \mathbf{P}_b \), on \( \partial E_K \) as defined below:

\[
\begin{align*}
P_{11b}(w) &= \alpha_k = \left\{ \begin{array}{ll}
\frac{B}{2C} \left[ \left(1 - k\frac{1}{2}\right) \cos \left(\frac{2k-1}{2}\pi\frac{w}{K} \right) + \frac{a}{2} \cos \left(\frac{2k+1}{2}\pi\frac{w}{K} \right) \right], & ||w - w_k|| \geq ||w - w_{k+1}||, \\
\frac{B}{2C} \left[ \left(1 - k\frac{1}{2}\right) \cos \left(\frac{2k-1}{2}\pi\frac{w}{K} \right) + \frac{a}{2} \cos \left(\frac{2k+1}{2}\pi\frac{w}{K} \right) \right], & ||w - w_k|| \leq ||w - w_{k+1}||,
\end{array} \right. \\
P_{12b}(w) &= \beta_k = \left\{ \begin{array}{ll}
\frac{B}{2C} \left[ \left(1 - k\frac{1}{2}\right) \sin \left(\frac{2k-1}{2}\pi\frac{w}{K} \right) + \frac{a}{2} \sin \left(\frac{2k+1}{2}\pi\frac{w}{K} \right) \right], & ||w - w_k|| \geq ||w - w_{k+1}||, \\
\frac{B}{2C} \left[ \left(1 - k\frac{1}{2}\right) \sin \left(\frac{2k-1}{2}\pi\frac{w}{K} \right) + \frac{a}{2} \sin \left(\frac{2k+1}{2}\pi\frac{w}{K} \right) \right], & ||w - w_k|| \leq ||w - w_{k+1}||,
\end{array} \right.
\end{align*}
\]

where \( a(w, \sigma) \in [0, 1], w \in C_k, k = 1, \ldots, K \) is an interpolation function, which is continuous and strictly monotonic about \( ||w - (w_k + w_{k+1})/2|| \), increasing from 0 at the centre of \( C_k \), to 1 at the two vertices of \( C_k \). Further, we take \( 0 < \sigma \leq 1/2 \) and \( a(w, \sigma) \to 0 \) as \( \sigma \to 0 \). At the vertices \( w = w_k \), we set \( \mathbf{P}_b \) to be equal to the average of the two constant values on the two intersecting edges, and at the edge mid-point i.e., \( w = (w_k + w_{k+1})/2 \). As \( \sigma \to 0 \), we work with strictly homeotropic Dirichlet boundary conditions, and the Dirichlet boundary conditions are piece-wise constant, see below

\[
\begin{align*}
P_{11b}(w) &= \hat{\alpha}_k = \frac{B}{2C} \cos \left(\frac{2k-1}{2}\pi\frac{w}{K} \right), \quad P_{12b}(w) = \hat{\beta}_k = \frac{B}{2C} \sin \left(\frac{2k-1}{2}\pi\frac{w}{K} \right), \quad w \in C_k.
\end{align*}
\]

Further, the domain \( E_K \) is unbounded and we impose uniform/constant boundary conditions at infinity as given below:

\[
\lim_{||w|| \to \infty} \mathbf{P} = \mathbf{P}^\ast := s_+ (\mathbf{n}^\ast \otimes \mathbf{n}^\ast - \frac{1}{2} \mathbf{I}_2), \quad \text{II.7}
\]

where \( \mathbf{n}^\ast = (\cos(\gamma^\ast), \sin(\gamma^\ast)) \) is the constant nematic director at infinity. To avoid confusion, we reiterate that \( \gamma \) is the director angle and \( \gamma^\ast \) is associated with the boundary condition at infinity.

FIG. 1: The normalized domain \( E_K^C \), with \( K = 6 \), as an illustrative example.
The corresponding Euler-Lagrange equations are
\[
\Delta P_{11} = \frac{2C\lambda^2}{L} \left( P_{11}^2 + P_{12}^2 - \frac{B^2}{4C^2} \right) P_{11},
\]
\[
\Delta P_{12} = \frac{2C\lambda^2}{L} \left( P_{11}^2 + P_{12}^2 - \frac{B^2}{4C^2} \right) P_{12}.
\]  
(II.8)

The admissible space is
\[
\mathcal{H}_\infty := \mathbf{P}^* + \mathcal{H},
\]
\[
\mathcal{H} := \left\{ \mathbf{H} \in H^1_{\text{loc}}(E_K^C ; S_0) : \int_{E_K^C} |\nabla \mathbf{H}|^2 + \int_{E_K^C} |\mathbf{H}|^2 < \infty \right\}
\]  
(II.9)

The free energy (II.3) is not everywhere finite on the space \(\mathcal{H}_\infty\), since the potential term \(f_b \geq 0\) may very well not be integrable in \(E_K^C\). However, since \(f_b(P^*) = 0\), we may find a compactly supported \(\mathbf{H}\), for which \(\mathbf{P} = \mathbf{P}^* + \mathbf{H}\), \(\mathbf{H} \in \mathcal{H}\) satisfies the boundary condition (II.5). The existence of solution of (II.8) in \(\mathcal{H}\), has been proved in Proposition 3 of [1].

We study two distinguished limits analytically in what follows—the \(\lambda \to 0\) limit which is relevant for nano-scale interior polygonal domains \(E_K\), and the \(\lambda \to \infty\) limit, which is the macroscopic limit relevant for micron-scale or larger interior domain \(E_K\). In the following sections, we study the limiting problems systematically and describe the limiting minimizer profiles, their defect sets and study multistability in the \(\lambda \to \infty\) limit.

### III. The \(\lambda \to 0\) Limit

In Theorem 1 of [1], as \(\lambda \to 0\), the solution of (II.8) converges to the unique solution of (III.1) below, with Dirichlet boundary conditions.
\[
\Delta P_{11}^0 = 0, \quad \Delta P_{12}^0 = 0, \text{ on } E_K^C,
\]
\[
P_{11}^0 = P_{11b}, \quad P_{12}^0 = P_{12b}, \text{ on } \partial E_K,
\]
\[
\mathbf{P} = \mathbf{P}^*, \quad |x| \to \infty.
\]
(III.1)

In other words, we need only solve boundary-value problems for the Laplace equation for \(\mathbf{P}\) on \(E_K^C\), in this limit. This problem is explicitly solvable and in the following sections, we exploit the symmetries of the Laplace equation, the symmetries of the polygon and boundary conditions to beautifully illustrate how the limiting profile depends on \(K\) - the number of polygon edges, and \(\gamma^*\) - the director angle at infinity. In fact, these two parameters tune the existence, location and dimensionality of defects in this limit, amenable to experimental verification in due course.

#### A. Defect patterns outside a 2D disc

As \(K \to \infty\), the domain, \(E_K^C\), converges to the exterior of a disc, \(D^C\). The Laplace equation in (III.1) can be easily solved on \(D^C\). The conformal mapping from unit disc \(D\) to exterior of disc \(D^C\) is given by
\[
w = f(z) = \frac{1}{z},
\]
Under the mapping \(f^{-1} : D^C \to D\), we define the limiting problem for \(\lambda = 0\) to be
\[
\Delta p_{11} = 0, \quad \Delta p_{12} = 0, \quad z \in D
\]
\[
p_{11} = \frac{B}{2C} \cos(-2\theta), \quad p_{12} = \frac{B}{2C} \sin(-2\theta), \quad z \in \partial D
\]
\[
p_{11} = \frac{B}{2C} \cos(2\gamma^*), \quad p_{12} = \frac{B}{2C} \sin(2\gamma^*), \quad z = 0
\]
(III.2)

where \(z = re^{i\theta}\), \(\theta\) is the azimuthal angle and \(r\) is the radius. The solution of the above equations is given by
\[
p_{11}(re^{i\theta}, \gamma^*) = \frac{B}{2C} \left( r^2 \cos(-2\theta) + \lim_{\epsilon \to 0} \frac{\cos(2\gamma^*)\ln r}{\ln \epsilon} \right),
\]
\[
p_{12}(re^{i\theta}, \gamma^*) = \frac{B}{2C} \left( r^2 \sin(-2\theta) + \lim_{\epsilon \to 0} \frac{\sin(2\gamma^*)\ln r}{\ln \epsilon} \right).
\]
(III.3)
This solution has the rotational symmetry property
\[(p_{11}, p_{12})(re^{i\theta}, \gamma^*) = (p_{11}(re^{i\theta + i\gamma^*}, 0) \cos 2\gamma^* - p_{12}(re^{i\theta + i\gamma^*}, 0) \sin 2\gamma^*, p_{12}(re^{i\theta + i\gamma^*}, 0) \cos 2\gamma^* + p_{11}(re^{i\theta + i\gamma^*}, 0) \sin 2\gamma^*),\] (III.4)
so that it suffices to assume \(\gamma^* = 0\), in order to study the defect or zero set of \(p\). With \(\gamma^* = 0\), the solution in (III.3) reduces to
\[p_{11} = \frac{B}{2C} \left( r^2 \cos(-2\theta) + \lim_{\epsilon \to 0} \frac{\ln r}{\ln \epsilon} \right), \quad p_{12} = \frac{B}{2C} r^2 \sin(-2\theta),\] (III.5)

The zero set of \(p_{12}\) is \(\{re^{i\theta} : \theta \in \{0, \pi/2, \pi, 3\pi/2\}, r \in [0, 1]\}\). For \(\theta = 0\) or \(\theta = \pi\), both terms in \(p_{11}\) are positive in (III.5) and subsequently, \(p_{11}\) is always positive. For \(\theta = \pi/2\) or \(\theta = 3\pi/2\), the first and second term of \(p_{11}\) in (III.5) monotonically decrease from 0 to -1, and from 1 to 0 respectively, i.e., \(p_{11}\) decreases monotonically from 1 to -1, as \(r\) increases from 0 to 1. Hence there exists a \(r^*\), s.t. \(p_{11}(r^*e^{i\pi/2}, 0) = p_{11}(r^*e^{3\pi/2}, 0) = 0\), i.e., there are two point defects along the given disc diameter. The corresponding limiting solution for the exterior of a 2D disc is
\[P(w) = p(f^{-1}(w)) = p(\rho^{-1}e^{-i\psi}) = s_+ \left( \frac{1}{\rho^2} (e_\rho \otimes e_\rho - I_2/2) + \lim_{\epsilon \to 0} \frac{\ln \rho}{\ln 1/\epsilon} (n^* \otimes n^* - I_2/2) \right)\] (III.6)
where \(w = \rho e^{i\psi}, e_\rho = (\cos \psi, \sin \psi)\) is unit radial vector and the constraint at infinity is \(n^* = (\cos \gamma^*, \sin \gamma^*)\).

Next, we compare this limiting 2D solution, in the \(\lambda \to 0\) limit, with the limiting solution on the complement of a unit 3D ball. With regards to the exterior of a 3D spherical colloidal particle, as the proof in [1], the minimizer of 3D Landau–de Gennes free energy, \(Q_{L,W}\), converges to
\[Q_0 = s_+ \left( \frac{1}{\rho^3} (e_\rho \otimes e_\rho - I_3/3) + (1 - \frac{1}{\rho})(n^* \otimes n^* - I_3/3) \right)\] (III.7)
where \(e_\rho = (\sin \phi \cos \psi, \sin \phi \sin \psi, \cos \phi)\) is the unit normal and the constraint at infinity is \(n^* = (\sin \phi^* \cos \gamma^*, \sin \phi^* \sin \gamma^*, \cos \phi^*)\), in the limit of strong anchoring strength and small particle radius. The solutions in (III.6) and (III.7) are a linear combination of the boundary condition on \(\partial D\), and the constraint at infinity. The coefficients are proportional to \(\frac{1}{\rho^3}\) and \(\lim \ln \rho\) for the 2D solution in (III.6), and proportional to \(\frac{1}{\rho^3}\) and \(\frac{\ln \rho}{\ln 1/\epsilon}\) for the 3D solution in (III.7), due to the different dimension of Laplace operator. The 3D solution, in (III.7), for the exterior of a 3D sphere, is called the Saturn ring quadrupole, which is known to be stable for small particles, as also reported in [3].

This method can be easily generalised to piecewise constant boundary conditions on segments of \(\partial D\), relevant for solving the limiting problem in (III.1) on \(E_K^\Lambda\) as we shall see in the next section. Consider the following boundary-value problem on the unit disc \(D\),
\[\Delta u = 0, \quad z \in D,\]
\[u = u_k, \quad on \ z \in D_k, \quad k = 1, \cdots, K,\]
\[u = u_0, \quad on \ z = 0.\] (III.8)
where
\[D_k = \{e^{i\theta}, \theta \in (-2\pi k/K, -2\pi (k+1)/K + 2\pi/K)\}, \quad k = 1, \cdots, K,\] (III.9)
are the segments of \(\partial D\). We write \(u\) as \(u = u_a + u_b\), where \(u_a\) and \(u_b\) are defined by the following boundary-value problems:
\[\Delta u_a = 0, \quad z \in D,\]
\[u_a = u_k, \quad on \ z \in D_k, \quad k = 1, \cdots, K,\]
\[u_a = \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi (k-1)/K}^{2\pi (k+1)/K} u_k d\phi \quad on \ z = 0,\] (III.10)
\[\Delta u_b = 0, \quad z \in D,\]
\[u_b = u_0, \quad on \ z \in D_k, \quad k = 1, \cdots, K,\]
\[u_b = u_0 - \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi (k-1)/K}^{2\pi (k+1)/K} u_k d\phi \quad on \ z = 0.\] (III.11)
Using the Poisson integral, and standard separation of variables method for the Laplace equation on an annulus, with the radius of inner ring (denoted by $\epsilon$) approaching zero, the solution of (III.8) is given by

$$u(re^{i\theta}) = \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi(K-k)/K}^{2\pi(K-k+1)/K} u_k \left( \frac{1 - r^2}{1 - 2r \cos(\phi - \theta)} + r^2 d\phi + \lim_{\epsilon \to 0} \frac{1}{2\pi} \sum_{k=1}^{K} \left( \frac{2\pi(K-k+1)/K}{2\pi(K-k)/K} u_k d\phi \right) \right).$$

(III.12)

### B. Schwarz–Christoffel mapping

The exterior of a disc is a good example that gives useful insights into the limiting profile for the exterior of a regular polygon, $E_K^C$. The conformal mapping from $D$ to $D^C$ is straightforward to construct. The analogous conformal mapping from $D$ to $D^C$ is the following Schwarz–Christoffel mapping: $f(D) = E_K^C$ from the unit disc to the exterior of a regular polygon with $K$ sides of unit length, defined by $[7]$

$$w = f(z) = A - C \int_{z}^{z_K} x^{-2} \prod_{k=1}^{K} \left( 1 - \frac{x}{w_k} \right)^{1-\alpha_k} dx, \ \forall z \in D.$$  

(III.13)

Here $\alpha_k \pi$ is the exterior angle of $E_K^C$ (interior angle of polygon $E_K^C$) and $\omega_k$ are the polygon vertices. In particular, for the mapping from the unit disc to $E_K^C$, $\alpha_k = 1 - 2/K$ $k = 1, \cdots, K$, with the first vertex located at $w_1 = (1,0)$, the Schwarz–Christoffel mapping is uniquely given by

$$w = f(z) = C(K) \int_{z}^{z_K} x^{-2} (1 - x^K)^{2/K} dx,$$

(III.14)

see Fig. 2. The leading term of $f$ in (III.14) is $-C(K)z^{-1}$ and hence, as $z \to 0$, $f(z) \to \infty$ and $f$ is single-valued near the origin $[7]$. The pre-factor, $C(K)$ is real and $|C(K)|$ is the capacity or transfinite diameter of the region $E_K^C$ $[7]$. One can check that $f$ maps the circle, $\partial D$, onto the polygon boundary, $\partial E_K^C = f(\partial D)$.

The mapping $f$ maps the segments of $\partial D$ to the corresponding segments of $\partial E_K^C$, i.e.,

$$f(D_k) = C_k,$$

(III.15)

where $D_k$, $k = 1, \cdots, K$ is defined in (III.9) and maps the origin of $D$, to the infinity of $E_K^C$

$$f(0) = \infty.$$  

(III.16)

The mapping, $f$, has the following properties

$$f(z) = C(K) \int_{z}^{z_K} x^{-2} (1 - x^K)^{2/K} dx = C(K) \int_{x}\pi^{2} (1 - x^K)^{2/K} dx = f(z),$$

(III.17)

$$f(ze^{2\pi i/K}) = C(K) \int_{ze^{2\pi i/K}}^{z_K} x^{-2} (1 - x^K)^{2/K} dx = C(K) \int_{e^{-2\pi i/K}x^{-2}(1 - x^K)^{2/K}}^{e^{2\pi i/K}x^{-2}(1 - x^K)^{2/K}} dx = e^{-2\pi i/K} f(z),$$

(III.18)

which will be useful in studying the properties of solutions of (III.1) on $E_K^C$. 

FIG. 2: Schwarz-Christoffel mapping from unit disc to exterior of hexagon.
C. The limiting problem for $E_K^C$ in terms of a boundary-value problem on $D$

Under the Schwarz-Christoffel mapping $f^{-1}: E_K^C \rightarrow D$, the limiting problem (III.1) can be equivalently written in terms of a rLdG tensor, $p$ on $D$, as

$$\Delta p_{11}^0 = 0, \Delta p_{12}^0 = 0, \text{on } D,$$

$$p_{11}^0 = p_{11b}, \ p_{12}^0 = p_{12b}, \text{ on } D_k,$$

$$p_{11}(0,0) = \frac{B}{2C} \cos(2\gamma^*), \ p_{12}(0,0) = \frac{B}{2C} \sin(2\gamma^*).$$

(III.19)

The Dirichlet boundary conditions (II.5) translate to boundary conditions, on $D_k$, $k = 1, \cdots, K$ defined in (III.9), which are segments of $\partial D$ as shown below:

$$p_{11b} = \alpha_k = \begin{cases} \frac{B}{2C} \left(1 - \frac{\pi}{2}\right) \cos(\frac{2(k-1)\pi}{K}) + \frac{\pi}{2} \cos\left(\frac{2(k+1)\pi}{K}\right), & \theta \in [2\pi(K - k)/K, 2\pi(K - k + 1)/K - \pi/K], \\ \frac{B}{2C} \left(1 - \frac{\pi}{2}\right) \cos(\frac{2(k-1)\pi}{K}) + \frac{\pi}{2} \cos\left(\frac{2(k+1)\pi}{K}\right), & \theta \in [2\pi(K - k + 1)/K - \pi/K, 2\pi(K - k + 1)/K], \end{cases}$$

$$p_{12b} = \beta_k = \begin{cases} \frac{B}{2C} \left(1 - \frac{\pi}{2}\right) \sin(\frac{2(k-1)\pi}{K}) + \frac{\pi}{2} \sin\left(\frac{2(k+1)\pi}{K}\right), & \theta \in [2\pi(K - k)/K, 2\pi(K - k + 1)/K - \pi/K], \\ \frac{B}{2C} \left(1 - \frac{\pi}{2}\right) \sin(\frac{2(k-1)\pi}{K}) + \frac{\pi}{2} \sin\left(\frac{2(k+1)\pi}{K}\right), & \theta \in [2\pi(K - k + 1)/K - \pi/K, 2\pi(K - k + 1)/K], \end{cases}$$

(III.20)

where the interpolation function, $\alpha(z, \sigma), \forall z \in \partial D$ satisfies $\alpha(e^{i(2K-2k+1)\pi/K}, \sigma) = a((w_k + w_{k+1})/2, \sigma) = 0$ and $\alpha(e^{i(2K-K-k)\pi/K}, \sigma) = a(w_{k+1}, \sigma) = 1$. We assume $\alpha \in C^2$ and $\frac{\partial \alpha}{\partial \sigma}$ $\leq 0$. As $\sigma \rightarrow 0$, $\alpha \rightarrow 0$ and the Dirichlet boundary condition approaches $p_{11b} = \alpha_k$, $p_{12b} = \beta_k$ on $D_k$ uniformly, where $\alpha_k$ and $\beta_k$ are given in (II.6).

For convenience, we extend the definition of $\alpha_k$, $\beta_k$, $k = 1, \cdots, K$, to $k \in \mathbb{Z}$ and use the periodicity of tan, cos and sin to define

$$\alpha_{k+nK} = \alpha_k, \beta_{k+nK} = \beta_k, \text{ } n \in \mathbb{Z}.$$  

(III.21)

One can check the following relations between $\alpha_k$ and $\beta_k$, $\beta_k$ and $\beta_k$ as given below:

$$\alpha_{n+k} = \cos(4\pi n/K)\alpha_k - \sin(4\pi n/K)\beta_k,$$

(III.22)

$$\beta_{n+k} = \sin(4\pi n/K)\alpha_k + \cos(4\pi n/K)\beta_k,$$

(III.23)

$$\alpha_{K-k-1} = \alpha_k,$$

(III.24)

$$\beta_{K-k-1} = -\beta_k.$$  

(III.25)

The constants $\alpha_k$ and $\beta_k$ have similar properties. From (III.25), we have

$$\int_0^{2\pi} p_{12b} d\theta = \sum_{k=1}^{K} \beta_k = -\frac{1}{2} \sum_{k=1}^{K} \beta_k + \frac{1}{2} \sum_{k=1}^{K} \beta_{K-k+1} = 0.$$  

(III.26)

From (III.23) and (III.26), we have

$$\int_0^{2\pi} p_{11b} d\theta = \sum_{k=1}^{K} \alpha_k = \sum_{k=1}^{K} \beta_{k+1} - \cos(4\pi K)\beta_k = \frac{1}{\sin(4\pi K)} \sum_{k=1}^{K} \beta_{k+1} - \frac{1}{\tan(4\pi K)} \sum_{k=1}^{K} \beta_k = 0, \text{ for } K \neq 4.$$  

(III.27)

Additionally, for $K = 4$, $\alpha_k = 0$, i.e., $\int_0^{2\pi} p_{11b} d\theta = 0$.

Hence, following the solution of (III.8) with Dirichlet boundary conditions on $\partial D$, and constraint at origin in
Proposition III.1

The solution to the problem is given by

\[ p_{11}(r, \theta, \gamma^*) = \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi(k-1)/K}^{2\pi k/K} \pi_k \frac{1 - r^2}{1 - 2r \cos(\phi - \theta) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \cos(2\gamma^*) \ln r}{2C} \]

\[ p_{12}(r, \theta, \gamma^*) = \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi(k-1)/K}^{2\pi k/K} \beta_{K-k+1} \frac{1 - r^2}{1 - 2r \cos(\phi - \theta) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \sin(2\gamma^*) \ln r}{2C} \]

In the above, we use (III.24) and (III.25), along with standard changes of variables i.e. \( s - 1 = K - k \), and swap the summation variable from \( k \) to \( s \) etc. The following proposition is crucial for restricting \( \gamma^* \) to a specified range, for a given \( K \), using rotation and reflection symmetries.

Proposition III.1 We can restrict \( \gamma^* \in [0, \frac{\pi}{K}] \), since there are rotation and reflection relations between \((p_{11}, p_{12})|_{(r \in [s-2\pi k/K, \pi^* - \frac{2\pi n}{K}]})\), with \( k = 1, \cdots, K \), \((p_{11}, p_{12})|_{(r \in [s, -\gamma^*])}\) and \((p_{11}, p_{12})|_{(r \in [\gamma^*, \pi^*])}\), respectively.

Proof: From the relationship between \( \pi_k \) and \( \pi_{n+k} \) in (III.22), and the solution \((p_{11}, p_{12})\) in (III.28) and (III.29), one can check

\[ p_{11}(re^{i\theta+2\pi ni/K}, \gamma^* - \frac{2\pi n}{K}) = \frac{1}{2\pi} \sum_{k=1}^{K} \int_{2\pi(k-1)/K}^{2\pi k/K} \pi_k \frac{1 - r^2}{1 - 2r \cos(\phi - \theta - 2\pi n/K) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \cos(2\gamma^* - \frac{4\pi n}{K}) \ln r}{2C} \]

\[ p_{12}(re^{i\theta+2\pi ni/K}, \gamma^* - \frac{2\pi n}{K}) = \cos \left( \frac{4\pi n}{K} \right) p_{11}(re^{i\theta}, \gamma^*) + \sin \left( \frac{4\pi n}{K} \right) p_{12}(re^{i\theta}, \gamma^*) \]
Using the relation between \( \pi_k \) and \( \pi_{K-k+1} \) in [III.24], we have

\[
p_{11}(e^{-i\theta}, -\gamma^*) = \frac{1}{2\pi} \sum_{k=1}^{K} \frac{1}{\pi_{K-k+1}/K} \int_{2\pi(k-1)/K}^{2\pi/k/K} \frac{1 - r^2}{1 - 2r \cos(\phi + \theta) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \cos(-\gamma^*)}{2C} \ln \epsilon
\]

\[
= -\frac{1}{2\pi} \sum_{k=1}^{K} \frac{1}{\pi_{K-k+1}/K} \int_{2\pi(k-1)/K}^{2\pi(k-k+1)/K} \frac{1 - r^2}{1 - 2r \cos(\phi - \theta) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \cos(\gamma^*)}{2C} \ln \epsilon
\]

\[
= \frac{1}{2\pi} \sum_{k=1}^{K} \frac{1}{\pi_{K-k+1}/K} \int_{2\pi(k-1)/K}^{2\pi(k-k+1)/K} \frac{1 - r^2}{1 - 2r \cos(\phi - \theta) + r^2} d\phi + \lim_{\epsilon \to 0} \frac{B \cos(\gamma^*)}{2C} \ln \epsilon
\]

\[
= p_{11}(e^{i\theta}, \gamma^*)
\]

(III.32)

and using analogous arguments, we obtain

\[
p_{12}(e^{-i\theta}, -\gamma^*) = -p_{12}(e^{i\theta}, \gamma^*)
\]

(III.33)

\[\square\]

**Corollary III.1** If \( K \) is even, using [III.30] and [III.31] with \( n = K/2 \), we have the symmetry property \( p(e^{i\theta+i\pi}, \gamma^*) = p(e^{i\theta}, \gamma^*) \). Due to the property of the SC mapping \( f \) in [III.18], \( f(e^{i\theta+i\pi}) = e^{-i\pi}f(e^{i\theta}) \), \( P(e^{i\theta+i\pi}, \gamma^*) = P(e^{i\theta}, \gamma^*) \).

**Corollary III.2** From [III.32] and [III.33] with \( \gamma^* = 0 \), we have

\[
p_{11}(e^{-i\theta}, 0) = p_{11}(e^{i\theta}, 0), \quad p_{12}(e^{-i\theta}, 0) = -p_{12}(e^{i\theta}, 0).
\]

(III.34)

The SC mapping in [III.14] preserves reflection symmetry, \( f(e^{-i\theta}) = f(\bar{e}^{i\theta}) \). We have \( (P_{11}, P_{12})(e^{i\psi}, 0) = (p_{11}, p_{12})(f^{-1}(e^{i\psi}), 0) \), for \( w = e^{i\psi} \in E^*_K \), \( (P_{11}, P_{12}) \) has reflection symmetry about \( \psi = 0 \), i.e.,

\[
P_{11}(e^{-i\psi}, 0) = P_{11}(e^{i\psi}, 0), \quad P_{12}(e^{-i\psi}, 0) = -P_{12}(e^{i\psi}, 0).
\]

(III.35)

**Corollary III.3** With \( \gamma^* = \pi/K \), \( (P_{11}, P_{12}) \) has reflection symmetry about \( \psi = \pi/K \), i.e.,

\[
P_{11}(e^{i\pi/K-i\psi}, \pi/K) = P_{11}(e^{i\pi/K+i\psi}, \pi/K) \cos(4\pi/K) + P_{12}(e^{i\pi/K+i\psi}, \pi/K) \sin(4\pi/K),
\]

\[
P_{12}(e^{i\pi/K-i\psi}, \pi/K) = -P_{12}(e^{i\pi/K+i\psi}, \pi/K) \cos(4\pi/K) + P_{11}(e^{i\pi/K+i\psi}, \pi/K) \sin(4\pi/K)
\]

(III.36)

(III.37)

**Proof:** Use [III.30] and [III.31] with \( \gamma^* = -\pi/K, n = -1 \), and substitute \( \theta + \pi/K \) for \( \theta \) to get

\[
p_{11} \left( e^{-i\pi/K+i\psi}, \pi/K \right) = \cos \left( -\frac{4\pi}{K} \right) p_{11} \left( e^{i\pi/K+i\psi}, -\pi/K \right) + \sin \left( -\frac{4\pi}{K} \right) p_{12} \left( e^{i\pi/K+i\psi}, -\pi/K \right),
\]

(III.38)

\[
p_{12} \left( e^{-i\pi/K+i\psi}, \pi/K \right) = \cos \left( -\frac{4\pi}{K} \right) p_{12} \left( e^{i\pi/K+i\psi}, -\pi/K \right) - \sin \left( -\frac{4\pi}{K} \right) p_{11} \left( e^{i\pi/K+i\psi}, -\pi/K \right).
\]

(III.39)

Combining [III.32] with [III.33], it follows that

\[
p_{11} \left( e^{i\pi/K+i\psi}, -\pi/K \right) = p_{11} \left( e^{-i\pi/K-i\psi}, \pi/K \right), \quad p_{12} \left( e^{i\pi/K+i\psi}, -\pi/K \right) = -p_{12} \left( e^{-i\pi/K-i\psi}, \pi/K \right).
\]

(III.40)
Substituting \[ \text{III.40} \] into \[ \text{III.38} \] and \[ \text{III.39} \], we obtain

\begin{align*}
p_{11}\left(re^{-i\pi/K+i\theta}, \pi/K\right) &= \cos\left(\frac{4\pi}{K}\right) p_{11}(re^{-i\pi/K-i\theta}, \pi/K) + \sin\left(\frac{4\pi}{K}\right) p_{12}(re^{-i\pi/K-i\theta}, \pi/K), \\
p_{12}\left(re^{-i\pi/K+i\theta}, \pi/K\right) &= -\cos\left(\frac{4\pi}{K}\right) p_{12}(re^{-i\pi/K-i\theta}, \pi/K) + \sin\left(\frac{4\pi}{K}\right) p_{11}(re^{-i\pi/K-i\theta}, \pi/K).
\end{align*}

\[ \text{III.41} \]

\[ \text{III.42} \]

Using \[ \text{III.17} \] and \[ \text{III.18} \], the SC mapping in \[ \text{III.14} \] preserves reflection symmetry, \( f(re^{-i\pi/K-i\theta}) = f(re^{-i\pi/K+i\theta}) = e^{2i\pi/K} f(re^{-i\pi/K+i\theta}) \). We have for any \( \rho e^{i\theta} \in E_K^r \) satisfying \( f(re^{-i\pi/K-i\theta}) = \rho e^{i\theta} \) and \( f(re^{-i\pi/K+i\theta}) = \rho e^{i\pi-K+i\theta} \), \( (P_{11}, P_{12})(\rho e^{i\pi-K+i\theta}, \pi/K) = (p_{11}, p_{12})(re^{-i\pi/K-i\theta}, \pi/K) \) and \( (P_{11}, P_{12})(\rho e^{i\pi-K+i\theta}, \pi/K) = (p_{11}, p_{12})(re^{-i\pi/K+i\theta}, \pi/K) \). Hence \( (P_{11}, P_{12}) \) has reflection symmetry about \( \psi = \pi/K \).

In the next sub-sections, we apply these results to \( K = 3, 4 \) and generic \( E_K^r \) with \( K > 4 \). These specific examples demonstrate the interplay between \( K \) and \( \gamma^* \), and how this can be exploited to tailor defect sets in reduced 2D problems.

1. The limiting profile for \( E_3^\gamma \) - exterior of an equilateral triangle

We first consider the solution of \[ \text{III.1} \] on \( E_3^\gamma \), the complement of a regular, re-scaled equilateral triangle with homeotropic boundary conditions. Recall the SC mapping from the unit disc \( D \) to \( E_3^\gamma \) given by \( f(z) = f(re^{i\theta}) = \rho e^{i\psi} = w \).

From Corollary \[ \text{III.2} \] for any \( K \), with \( \gamma^* = 0 \), we have \( p_{12}(r, 0) = 0 \) on \( \theta = 0 \) or \( \pi \). The boundary condition in \[ \text{III.20} \], \( p_{12} = \beta_k \leq 0 \) with \( K = 3 \) on \( \partial D \cap \{ \theta \in [0, \pi] \} \). From the maximum principle for the Laplace equation on \( D \cap \{ \theta \in [0, \pi] \} \), \( p_{12} = 0 \) if and only if \( \theta = 0 \) or \( \pi \). Analogously, on \( D \cap \{ \theta \in [\pi, 2\pi] \} \), \( p_{12} = 0 \) if and only if \( \theta = \pi \) or \( 2\pi \). In conclusion, defects can only appear on the diameter \( z = r, \ r \in (-1, 1) \). Using \[ \text{III.27} \], we obtain \( p_{11}(0, \gamma^*) - \frac{B}{2C} \cos(2\gamma^*)c(r) = \frac{1}{2} \int_0^r p_{11}(t, \theta) \, dt = 0 \), where \( c(r) = \lim_{\theta \to 0} \frac{\int_{\theta r}^{\pi - \theta r} \cos(2\gamma^*) \, d\theta}{\pi} \). For \( K = 3 \), with \( \gamma^* = 0 \), as in Lemma 4.5 in \[ 13 \], we show that as \( r \) increases from 0 to 1, \( p_{11}(r, 0) - \frac{B}{2C} c(r) \) monotonically decreases from 0 to \( \pi_1 = \frac{B}{2C} (1 - \pi/2) \cos(2\pi/3) + \pi/2 \cos(-2\pi/3) = \frac{B}{2C} \cos(2\pi/3) = -\frac{B}{2C} \). The term, \( \frac{B}{2C} c(r) \), monotonically decreases from \( \frac{B}{2C} \) to 0. Hence, \( p_{11}(r, 0) \) monotonically decreases from \( B/2C \) to \(-B/4C \). There exists a \( r^* \) such that \( p_{11}(r^*, 0) = 0 \), i.e. there is a defect on \( \theta = 0 \). As \( r \) increases from 0 to 1, \( p_{11}(-r, 0) - \frac{B}{2C} c(r) \) monotonically increases from 0 to \( \pi_2 = \frac{B}{2C} (1 - \pi/2) \cos(\pi) = \frac{B}{2C}, \) since \( \pi = 0 \) at the middle of \( D_2 \). So with \( \gamma^* = 0 \), under the SC mapping \( f^{-1} \), the defect set of the limiting profile consists of a single isolated point, on \( E_3^\gamma \).

Using the rotation-based relations in \[ \text{III.30} \], with \( \gamma^* = 0, \theta = 0, n = 1 \), and \( (p_{11}, p_{12})(r^*, 0) = 0 \), we obtain \( (p_{11}, p_{12})(r^* e^{i2\pi/3}, \pi/3) = (p_{11}, p_{12})(r^* e^{i2\pi+3}, -2\pi/3) = 0 \), i.e., for \( \gamma^* = \pi/3 \), there is a unique defect on \( \theta = 2\pi/3 \), and consequently for \( \psi = -2\pi/3 \) in the limiting profile \( (P_{11}, P_{12})(\rho e^{i\psi}, \gamma^*) \). For \( \gamma^* = (0, \pi/3) \), the defect smoothly rotates between \( \psi = 0 \) and \( \psi = -2\pi/3 \) in the limiting profile (see Fig. 3) and this is a good example of how \( \gamma^* \) can tune the location of the defect for the limiting profile.

2. The limiting profile for \( E_4^\gamma \) - exterior of a unit square

In \[ 16 \], the authors study the limiting profiles for rLDG minimizers on \( E_K \) i.e. the interior of \( K \)-regular polygons with tangent boundary conditions on the polygon edges, as \( \lambda \to 0 \). They find the universal \( \text{Ring} \) solution for all \( K > 4 \) and in the special case of \( K = 4 \), the authors report that the limiting profile is the WORS (Well Order Reconstruction Solution) with two defect lines along the square diagonals. Hence, we consider the case \( K = 4 \) separately and study whether the line defects survive on \( E_4^\gamma \), with homeotropic boundary conditions and different choices of \( \gamma^* \). We note that the boundary conditions \[ \text{III.5} \] necessarily imply that there are 4 defects at the square vertices, on \( E_4^\gamma \).

**Proposition III.2** The solution of \[ \text{III.1} \] on \( E_4^\gamma \) has two line defects for \( \gamma^* = \pi/4 + n\pi/2, n \in \mathbb{Z} \), and no interior defects otherwise.

**Proof:** Substituting \( K = 4 \) into the Dirichlet boundary condition \[ \text{III.20} \], \( \sigma_k = 0, k = 1, \cdots, 4 \). According to \[ \text{III.28} \], the solution of \[ \text{III.19} \] on \( E_4^\gamma \) is given by

\[ p_{11}(re^{i\theta}, \gamma^*) = \frac{B}{2C} \cos(2\gamma^*)c(r). \]

\[ \text{III.43} \]
As in Proposition III.1, we can assume that
we have
Since
Using (III.33), we obtain
Combining (III.45) and (III.46), we get the desired conclusion,
Similarly, we prove that on \( \theta = 3\pi/2 \), i.e., \( x = 0 \) and \( y \leq 0 \), \( p_{12}(re^{i3\pi/2}, \gamma^*) - \frac{B}{2C} \sin(2\gamma^*)c(r) \equiv 0 \). Using (III.31) with \( n = 1 \), \( K = 4 \), \( \theta = \pi \), and \( \gamma = \pi/4 \), we have

\[
p_{12}(re^{i3\pi/2}, -\pi/4) = \cos(\pi)p_{12}(re^{i\pi}, \pi/4) = -p_{12}(re^{i\pi}, \pi/4).
\]
From (III.47), \( p_{12}(re^{i\pi}, \pi/4) = \frac{B}{2C} \sin(\pi/2) c(r) \) and hence,

\[
p_{12}(re^{i\pi/2}, \gamma^*) - \frac{B}{2C} \sin(2\gamma^*)c(r) = p_{12}(re^{i\pi/2}, -\pi/4) - \frac{B}{2C} \sin(-\pi/2)c(r) = -p_{12}(re^{i\pi}, \pi/4) + \frac{B}{2C} \sin(\pi/2)c(r) = 0. \tag{III.48}
\]

On the quadrant \( \theta \in [\pi, 3\pi/2] \) or the quarter disc, \( D_q = D \cap \{ x \leq 0 \} \cap \{ y \leq 0 \} \) (see Fig. 5), the function, \( p_{12}(re^{i\theta}, \pi/4) - \frac{B}{2C} \sin(\pi/2)c(r) \), is the solution of

\[
\Delta u_a = 0, \quad \text{on } D_q,
\]

\[
u_a = \beta_2, \quad \text{on } D_2,
\]

\[
u_a = 0, \quad \text{on } x = 0 \text{ and } y = 0. \tag{III.49}
\]

where \( D_2 \) is the segment of \( \partial D \) with \( x \leq 0 \) and \( y \leq 0 \), \( \beta_2 \leq 0 \) is the corresponding Dirichlet boundary condition of \( p_{12} \) on \( D_2 \). Following the arguments from Lemma 4.5 in \cite{5}, the first step is to show that \( u_a \) is non-increasing in the \( r \) direction, i.e.

\[
u_a(r, \theta) \geq u_a(\tau r, \theta), \quad \forall \tau > 1, \quad (r, \theta) \in D_q. \tag{III.50}
\]

We consider Problem (III.51), the analogue of Problem (III.49) on the extended domain, \( D_q^\tau = (\tau r, \theta) \) where \((r, \theta) \in D_q^\tau\),

\[
\Delta u_a^\tau = 0, \quad \text{on } D_q^\tau,
\]

\[
u_a^\tau = \beta_2, \quad \text{on } D_2^\tau,
\]

\[
u_a^\tau = 0, \quad \text{on } x = 0 \text{ and } y = 0. \tag{III.51}
\]

where \( D_2^\tau = (\tau r, \theta) \), with \((r, \theta) \in D_2 \). By scaling invariance, the unique non-negative solution to Problem (III.51) is given by

\[
u_a^\tau(r, \theta) := u_a(r, \theta) \text{ for any } (r, \theta) \in D_q. \tag{III.52}
\]

Moreover, the function

\[
u_a^\tau(r, \theta) = \left\{ \begin{array}{ll}
u_a \text{ on } D_q, \\
\beta_2(\theta), & \text{on } \{ r > 1 \} \cup \{ x \leq 0 \} \cup \{ y \leq 0 \}
\end{array} \right. \tag{III.53}
\]

is a subsolution of (III.49), with \( \frac{\partial^2 u_a^\tau}{\partial r^2} \leq 0 \), so that

\[
u_a^\tau(r, \theta) \geq u_a^\tau(r, \theta) \text{ for any } (r, \theta) \in D_q \text{ s.t. } (\tau r, \theta) \in D_q \tag{III.54}
\]
Recalling (III.52) and using $u_i^* = u_a$ on $D_q$, we conclude the proof of (III.50). Let $v_a = \partial u_a / \partial r$. By (III.50), $v_a \leq 0$ on $D_q$; we want to prove that the strict inequality holds. We differentiate Equation (III.49) with respect to $r$, so that $\nabla v_a = 0$ on $D_q$. By the strong maximum principle, we deduce that either $v_a \equiv 0$ or $v_a < 0$ in $D_q$. The first possibility is clearly inconsistent with the boundary conditions for $u_a$ in (III.49), and hence, $v_a$ must be strictly negative inside $D_q$.

Therefore, on the quadrant $\theta \in [\pi, 3\pi/2]$, $p_{12}(re^{i\theta}, \pi/4) - \frac{B}{2r} \sin(\pi/2)c(r)$ is monotonically decreasing in $r$ directions from $0$ to $\overline{\beta}_2$. Using analogous arguments, $p_{12}(re^{i\theta}, \pi/4) - \frac{B}{2r} \sin(\pi/2)c(r)$ is monotonically decreasing in the $r$-direction, from $0$ to $\overline{\beta}_4$ for $\theta \in [0, \pi/2]$, and monotonically increasing in $r$, from $0$ to $\overline{\beta}_1$ or $\overline{\beta}_3$, on the quadrants $\theta \in [\pi/2, \pi] \cup [3\pi/2, 2\pi]$.

Moreover, $\frac{B}{2r} \sin(\pi/2)c(r)$ is monotonically decreasing from $\frac{B}{2r}$ to $0$, hence there exists $r^*(\theta)$ for each $\theta \in [0, \pi/2] \cup [\pi, 3\pi/2]$ s.t. $p_{12}(r^*(\theta)e^{i\theta}, \pi/4) = 0$, so that there are two line defects in limiting profile for $E^*_K$ with $\gamma^* = \pi/4$. Using (III.30) and (III.31), $(p_{11}, p_{12})(re^{i\theta+2\pi n/K}, \gamma^* - \frac{2\pi n}{\pi})$, $n \in \mathbb{Z}$, can be obtained by rotating $(p_{11}, p_{12})(re^{i\theta}, \gamma^*)$. Hence, for $\gamma^* = \pi/4 + n\pi/2$, $n \in \mathbb{Z}$, there are two line defects in the limiting profile $(p_{11}, p_{12})(re^{i\psi}, \gamma^*)$ for $E^*_K$.

We plot the mapped solution of (III.19) on $D$ with $K = 4$ and corresponding limiting solution of (III.1) on $E^*_K$ with $\gamma^* = 0$ and $\pi/4$ in Fig. 6. On $E^*_4$, with $\gamma^* = \pi/4$, there are two line defects; for $\gamma^* = 0$, there are no interior defects on $E^*_4$, as in Proposition (III.2).

### 3. The limiting profile for $E^*_K$ with $K > 4$

**Lemma III.3** For $\gamma^* \in [0, \pi/K]$, $K \in \mathbb{Z}$ and $K > 4$, the solution of (III.1) has no defect on $D_{q1} = D \cup \{2\pi - \frac{\pi}{K} \leq \theta \leq 2\pi\}$ and $D_{q2} = D \cup \{\pi - \frac{\pi}{K} \leq \theta \leq \pi\}$.

**Proof:** As in Proposition (III.2), we can prove that on $D_{q1}$ and $D_{q2}$, $p_{12}(re^{i\theta}, \gamma^*) - \frac{B}{2r} \sin(2\gamma^*)c(r)$ increases monotonically in the $r$-direction from $0$ to $\beta_1 > 0$, as $r$ increases from $0$ to $1$. Hence, $p_{12}(re^{i\theta}, \gamma^*) - \frac{B}{2r} \sin(2\gamma^*)c(r)$ is positive for $r > 0$ on $D_{q1}$ and $D_{q2}$. For $K > 4$ and $K \in \mathbb{Z}$, $\frac{B}{2r} \sin(2\gamma^*)c(r)$ is non-negative, and is zero if and only if $r = 1$, i.e., on $\partial D$. Hence, $p_{12}$ is nonzero on $D_{q1}$ or $D_{q2}$, i.e., there is no defect on $D_{q1}$ or $D_{q2}$.

As $p_{12}$ and $p_{11}$ are analytic on $D$, the angle $\gamma = \arctan(p_{12}/p_{11})/2$ is continuous. We can separate the disc into four parts by two smooth curves (see Fig. 7): on curve$_1$ (from $z = e^{i(K-1)\pi/K}$ to $z = 0$ to $z = 1$), $\gamma$ decreases from $\pi/K$ to $\gamma^*$ monotonically, and on curve$_2$ (from $z = -1$ to $z = 0$ to $z = e^{-i\pi/K}$), $\gamma$ increases from $0$ to $\gamma^*$, and then to $\pi/K$ monotonically. Since there is no defect on $D_{q1}$ and $D_{q2}$ as proved in Lemma III.3, there is no defect on curve$_1$ and curve$_2$. We define $D_{q}$ to be the part of $D$ above curve$_1$, and $D_{q2}$ to be the part of $D$ below curve$_2$. The boundary $\partial D_{q}$ consists of a segment of $\partial D$ and the interior curve curve$_1$ (curve$_2$). In the following, we prove that the director angle $\gamma$ is strictly monotonic on $\partial D$ and subsequently, that $\gamma$ is strictly monotonic on either $\partial D_{q1}$ or $\partial D_{q2}$, and rotates by $\pi$.

**Lemma III.4** On $\partial D$, the angle $\gamma = \arctan(p_{12}/p_{11})/2$ is strictly monotonic, and there is no defect.
Theorem III.1  If \( p \) is a minimizer of \( J = \int_{D_u} |\nabla p|^2 dA \) in \( A = \{ p \in W^{1,2}(D_u; \mathbb{R}^2) : p = p_{bu} \text{ on } \partial D_u \} \), then there is a unique point defect in \( D_u \). Similarly, there is a unique point defect in \( D_b \). Under the SC mapping \( f \) (III.14), there are two point defects in exterior of regular polygon with \( K > 4 \) edges.

Proof: Let \( Y(l) \) for \( 0 \leq l \leq L \) be a one-to-one parametrization of \( \partial D_u \) with respect to arclength. Considering the Dirichlet data, \( (p_{11bu}, p_{12bu}) \), in \( C^{2,\mu}(\partial D_u; \mathbb{R}^2) \), we have

\[
(p_{11bu}, p_{12bu})(Y(l)) = (s(l)\cos 2\gamma(l), s(l)\sin 2\gamma(l)).
\]
As proved in Lemma III.3 and III.4 we have
\[ s(l) > 0, \quad \gamma^*(l) \neq 0 \quad \text{for all } l \in [0, L], \quad \text{and } |2\gamma(L) - 2\gamma(0)| = 2\pi. \] (III.63)

For \( \alpha \in \mathbb{R} \) and \( p \), a minimizer for \( J \) in \( A \), set
\[ \omega_{\alpha}(X) = -p_{11}(X) \sin(\alpha) + p_{12}(X) \cos(\alpha). \] (III.64)

Define the nodal set of \( \omega_{\alpha} \) by
\[ N_{\alpha} \equiv \{ X \in \bar{D}_u : \omega_{\alpha}(X) = 0 \}. \] (III.65)

Note that for any pair \( \alpha_1, \alpha_2 \) with \( 0 \leq \alpha_1 < \alpha_2 < \pi \), the set of zeros of \( p \) is just \( \Gamma(p) = N_{\alpha_1} \cap N_{\alpha_2} \). Thus as \( \alpha \) varies, \( \Gamma(p) \) is the subset of \( N_{\alpha} \) that remains fixed. Analogous to Lemma 2.2 in [2], we can prove for each \( \alpha \in [0, 2\pi] \), \( N_{\alpha} \) is a \( C^1 \) imbedded curve in \( \bar{D}_u \) which enters and exits \( \partial D_u \) at distinct points of \( \partial D_u \). The following proof is identical to Theorem 2.3 in [2]. Let \( \{P_1, P_2\} = N_0 \cap \partial D_u \) and assume without loss of generality that \( \sin(2\gamma)/p_1 = 0 \) with \( \cos(2\gamma)/p_1 < 0 \) and \( \sin(2\gamma)/p_2 = 0 \) with \( \cos(2\gamma)/p_2 > 0 \). The points \( P_1 \) and \( P_2 \) partition \( \partial D_u \) into two arcs, \( (\partial D_u)^- \equiv \{ X \in \partial D : \sin(2\gamma)|_X \leq 0 \} \) and \( (\partial D_u)^+ \equiv \{ X \in \partial D : \sin(2\gamma)|_X \geq 0 \} \). Starting at \( P_1 \) and moving along \( N_0 \), let \( X_0 \) be the first point reached in \( \Gamma(p) \). Since \( X_0 \in N_{\alpha} \) for all \( \alpha \), each \( N_{\alpha} \) can be parametrized by arclength, \( X = (\tau, \alpha) \), such that
\[ a(\alpha) < \tau < b(\alpha), \quad a(\alpha) < 0, \quad X(a(\alpha), \alpha) \in (\partial D_u)^-, \quad b(\alpha) > 0, \quad X(b(\alpha), \alpha) \in (\partial D_u)^+, \quad \left| \frac{\partial X}{\partial \tau} \right| = 1, \quad \text{and } X(0, \alpha) = X_0. \] (III.66)

Set \( D = \{ (\tau, \alpha) : a(\alpha) \leq \tau \leq b(\alpha), 0 \leq \alpha \leq \pi \} \). In part 1 of Theorem 2.3, the authors proved \( X \in C^1(D) \), and \( a(\alpha) \) and \( b(\alpha) \) are in \( C^1([0, \pi]) \). In part 2, they have that for all \( \alpha \in [0, \pi] \) and \( \tau < 0 \), \( X(\tau, \alpha) \notin \Gamma(p) \). In particular, \( X(\tau, \pi) \notin \Gamma(p) \). In part 3, now \( X(\tau, 0) \) and \( X(\tau, \pi) \) are each parametrizations of \( N_0 \) in opposite directions. Since \( X_0 \) is the first point in each direction along \( N_0 \) that is in \( \Gamma(p) \), we conclude that \( \Gamma(p) = X_0 \), i.e., there is a unique point defect in \( D_u \). Similarly, there is a unique point defect in \( D_b \). Under the SC mapping \( f \) (III.14), there are two point defects in exterior of regular polygon with \( K > 4 \) edges.

Remark: Theorem III.1 does not work for \( E_K^C \) with \( K = 3 \) or 4. For \( K = 3 \), since there exists a \( \tau^* \) s.t. \( (p_{11}, p_{12})(\tau^* e^{2\pi/3}, \pi/3) = (p_{11}, p_{12})(\tau^*, 0) = 0 \), we may have a defect on \( D_{q_1} \) or \( D_{q_2} \) which does not satisfy Lemma III.3. For \( K = 4 \), with the given boundary conditions, we have defects at the four vertices, \( (p_{11}, p_{12}) = \frac{p_{12}}{2} (\cos(\frac{2\pi}{K}), (1 - \pi) \sin(\frac{2\pi}{K})) = (0, 1 - \pi(0)) = (0, 0) \), which does not satisfy Lemma III.3 and III.4.

The mapped solution of (III.19) with \( K = 3, 4, 5, 6, \infty \), and the corresponding solutions of (III.1) in the exterior of a triangle, square, pentagon, hexagon and disc, with \( \gamma^* = 0 \) and \( \gamma^* = \pi/k \), are plotted in Fig. 3, Fig. 6 and Fig. 8 respectively. With even \( K \), the solutions have the symmetry property in Corollary III.1. With \( \gamma^* = 0 \) and \( \pi/k \), the solutions have the symmetry properties in Corollary III.2 and Corollary III.3 respectively. The mapped solution has two \(-1/2\) defects on two sides of \( \theta = \gamma^* + \pi/2 \) as in Theorem III.1 for \( K > 4 \).

FIG. 8: The mapped solution of (III.19) on \( D \) with \( K = 5, 6, \infty \) and the corresponding limiting solution of (III.1) on \( E_K^C \), the complement or exterior domain of a pentagon, hexagon and disc with (a) \( \gamma^* = 0 \) and (b) \( \gamma^* = \pi/K \).
IV. THE $\lambda \to \infty$ LIMIT

In the $\lambda \to \infty$ limit, minimizers of the rLdG energy converge (in an appropriately defined sense) to minimizers of the bulk energy

$$f_b(P) = -\frac{B^2}{4C} \text{tr} P^2 + \frac{C}{4} (\text{tr} P^2)^2.$$

More precisely, it has been proved in Theorem 2 of [1] that the solution $P$ of (II.8) converges strongly in $W^{1,2}$ to

$$P^\infty = \frac{B}{C} \left( n^\infty \otimes n^\infty - \frac{1}{2} I_2 \right),$$

where

$$n^\infty = (\cos \gamma^*, \sin \gamma^*), \quad (IV.1)$$

and $\gamma$ is the solution of the following equations

$$\Delta \gamma = 0, \text{ on } E_K^C$$
$$\gamma = \gamma_b, \text{ on } \partial E_K$$
$$\gamma = \gamma^*, |x| \to \infty,$$

(IV.2)

everywhere away from the vertices of $E_K$. The convergence is actually stronger but that is not the focus of this paper.

There are multiple choices of Dirichlet conditions for $\gamma_b$ consistent with the homeotropic boundary conditions in (II.6) as $\sigma \to 0$, which implies that there are multiple candidates for local/global minima of (II.3), for large $\lambda$. We present a simple estimate of the number of limiting stable states if we restrict $\gamma_b$ so that $\gamma$ rotates by either $2\pi/K$ or $2\pi/K - \pi$ at a vertex (see Fig. 9; referred to as “splay” and “bend” vertices respectively). We impose an additional restriction, namely $\text{deg}(n_b, \partial E_K) = 0$, where $n_b = (\cos \gamma_b, \sin \gamma_b)$, so that if $n_b$ denotes the number of “bend” vertices, then we necessarily have

$$(K - n_b)(2\pi/K) + n_b(2\pi/K - \pi) = 0,$$

equivalent to $n_b = 2$. We can have cases when the the degree of $n_b$ is non-zero, where $n_b$ is as above, but it is reasonable to conjecture that energy minimizers have the simplest admissible topology. We set

$$\gamma_b = \gamma_k, \text{ on } C_k, \quad k = 1, \cdots, K, \quad (IV.3)$$

where

$$\gamma_1 = \frac{\pi}{K}; \quad \gamma_{k+1} = \gamma_k + \text{jump}_k, \quad k = 1, \cdots, K - 1,$$

and the different stable states are distinguished by the different locations of the two bend vertices, where $\gamma$ rotates as in Fig. 9(b). If the chosen corner is between $C_k$ and $C_{k+1}$, then $\text{jump}_k = 2\pi/K - \pi$, otherwise $\text{jump}_k = 2\pi/K$, $k = 1, \cdots, K - 1$. The constraint at infinity is in (II.7).

For $K = 4$, there are 6 different choices for the two “bend” vertices, (i) 2 of which correspond to the two pairs of diagonally opposite vertices, (ii) 4 of which correspond to pairs of adjacent vertices. We refer to (i) as $D$ states, (ii) as $R$ states.

The diagonal states are defined by the following choices of $\gamma_b$ on $E_4$:

$$\gamma_{b1} = \begin{cases} 
\frac{\pi}{4}, \text{ on } C_1, \\
-\frac{\pi}{4}, \text{ on } C_2, \\
\frac{\pi}{4}, \text{ on } C_3, \\
-\frac{\pi}{4} \text{ on } C_4,
\end{cases} \quad \gamma_{b2} = \begin{cases} 
\frac{\pi}{4}, \text{ on } C_1, \\
\frac{3\pi}{4}, \text{ on } C_2, \\
\frac{\pi}{4}, \text{ on } C_3, \\
\frac{3\pi}{4} \text{ on } C_4.
\end{cases}$$

(IV.4)
FIG. 10: The limiting profiles for $E_4$, in the $\lambda \to \infty$ limit, with $\gamma^* = n\pi$ (a) and $\gamma^* = n\pi + \pi/4$ (b). The diagonal states are plotted in the first row of (a) and (b). The rotated states are plotted in the second row of (a) and (b).

The choice $\gamma_{b1}$ corresponds to what we call the $D1$ state for $\gamma^* = 0$ (for which there are no interior defects) and the $St$ state (for which there are two line defects) for $\gamma^* = \pi/4$. The choice, $\gamma_{b2}$ corresponds to what we call $D2$ states, for example, see the first row of Fig. 10(a), where we plot $D2$ for two choices of $\gamma^*$, i.e., $\gamma^* = \pi$ (the second configuration) and $\gamma^* = 0$ (the third configuration).

The rotated states correspond to different choices for $\gamma_b$ and the four different choices of $\gamma_b$ are enumerated below; the rotated states are plotted in the second row of Fig. 10(a) and (b) from left to right.

$$\gamma_b = \begin{cases} 
\pi/4, & \text{on } C_1, \\
-\pi/4, & \text{on } C_2, \\
\pi/4, & \text{on } C_3, \\
3\pi/4, & \text{on } C_4,
\end{cases}$$

$$\gamma_b = \begin{cases} 
\pi/4, & \text{on } C_1, \\
3\pi/4, & \text{on } C_2, \\
\pi/4, & \text{on } C_3, \\
-\pi/4 & \text{on } C_4,
\end{cases}$$

$$\gamma_b = \begin{cases} 
\pi/4, & \text{on } C_1, \\
-\pi/4, & \text{on } C_2, \\
-3\pi/4, & \text{on } C_3, \\
-\pi/4 & \text{on } C_4,
\end{cases}$$

$$\gamma_b = \begin{cases} 
\pi/4, & \text{on } C_1, \\
3\pi/4, & \text{on } C_2, \\
5\pi/4, & \text{on } C_3, \\
3\pi/4 & \text{on } C_4.
\end{cases}$$

Discarding rotation and reflection symmetries, there are three distinct classes of solutions: $D1$, $D2$ and $R$ with $\gamma^* = n\pi$, and four distinct classes of solutions: $St$, $D$, $R1$, and $R2$ with $\gamma^* = \pi/4 + n\pi$. All the diagonal- and rotated states in Fig. 10 are locally stable in the sense that the corresponding second variation of $\mathcal{L}_\lambda$

$$\partial^2 F_\lambda[\eta] = \int_{[-10,10]^2 \setminus E_4} |\nabla \eta|^2 + \frac{\lambda^2}{4} \left( |P|^2 - \frac{B^2}{2C^2} \right) |\eta|^2 + \frac{\lambda^2}{2} (P \cdot \eta)^2$$

(IV.6)
is strictly positive according to our numerical computations.

We can repeat the same combinatorial arguments for $K = 6$, to get simple estimates for the number of stable states on $E^C_6$, in the $\lambda \to \infty$ limit. When $\gamma^* = \pi/6 + n\pi$, we recover at least six different classes of limiting profiles, as plotted in Fig. [11]. In contrast, the authors report three classes of stable solutions for the interior problem on $E_6$ with tangent boundary conditions in [16]. On $E^C_6$, there are two classes of $Para$ solutions - $Para_1$ and $Para_2$ with two diagonally opposite bend vertices. $Para_2$ is distinguished in the sense that the diagonal connecting the bend vertices is orthogonal to the direction $\mathbf{n}^* = (\cos \gamma^*, \sin \gamma^*)$. There are two classes of $Meta$ states: $Meta_1$ and $Meta_2$, for which the two bend vertices are separated by one vertex, and two further classes: $Ortho_1$ and $Ortho_2$ with two "adjacent" bend vertices connected by an edge. The unique $P$-solution for small enough $\lambda$, is $Para_2$ with two diagonally opposite bend vertices on the diagonal orthogonal to the fixed director at infinity; see Fig. [11](b). $Para_2$ is stable for all $\lambda$. The energy of the different solutions depends on both the location of splay and bend vertices, and $\gamma^*$, again giving us new control on multistability and the solution landscapes.

The asymptotic analysis and estimates in Sections [III] and [IV] give us excellent initial conditions for numerical solvers. In [16], the authors compute the bifurcation diagram for the rLG model on $E_4$ with tangent boundary conditions on the square edges, following previous work in [22] and [27]. They find the unique WORS solution for small $\lambda$, which is globally stable for small $\lambda$ and loses stability as $\lambda$ increases. At a critical value of $\lambda$, the WORS bifurcates into the stable diagonal solutions and the unstable $BD$ solutions. The $BD$ states are distinguished by two interior line defects in the square interior, along a pair of opposite square edges. The $BD$ states eventually bifurcate to the rotated solutions, which gain stability as $\lambda$ increases. In the $\lambda \to \infty$ limit, there are two classes of stable equilibria: the diagonal solutions for which the nematic director is aligned along a square diagonal, and rotated solutions for which the director rotates by approximately $\pi$ radians in the square interior.

We plot the bifurcation diagrams on $E^C_4$ with $\gamma^* = n\pi$ and $n\pi + \pi/4$ in Fig. [12] and Fig. [13]. We numerically compute the solutions of the Euler–Lagrange equations (II,8), subject to the Dirichlet boundary conditions (II,5), which are necessarily critical points of (II,3). We use the popular open-source computing software FEniCS [21] which allows us to solve the weak form of the Euler–Lagrange equations, in the first order Lagrange element function space by using Newton’s method. The convergence may be highly sensitive to the choice of initial condition. We take the solution of (II,1) (IV,2) on $[-10, 10]^2 \setminus E_4$ as the initial conditions for finite but small (large) $\lambda^2$. The domain $[-10, 10]^2 \setminus E_4$ is used to approximate the unbounded domain, $E^C_4$. We perform an increasing $\lambda^2$ sweep for the unique branch (in the $\lambda \to 0$ limit) and decreasing $\lambda^2$ sweep for the distinct diagonal- and rotated-branches. The stability of the solutions is also numerically calculated by evaluating the smallest real eigenvalue of the Hessian of the reduced energy in (IV,6).

In Figure 12, we plot the bifurcation diagram on $E^C_4$ with $\gamma^* = n\pi$. The distinct solution branches are distinguished in terms of the measure, $\int P_{12}(1+x+y/2)dx dy$, and we plot this measure versus $\lambda^2$ for the distinct solution branches.
FIG. 12: Bifurcation diagram for (II.3) on $E^C_4$ with $\gamma^* = n\pi$. Left: plot of $\int P_{12}(1 + x + y/2) \, dx \, dy$ versus $\lambda^2 = 2C\lambda^2/L$, with plots for the corresponding solution branches (the configuration of $D$ is zoomed in). Right: the plot of the rLdG energy versus $\lambda^2$, where the solid lines represent stable solution branches.

For small $\lambda^2$, we have a unique solution of the system (II.8) on the domain $[-10, 10]^2 \setminus E_4$, subject to the boundary conditions (II.5) and constraint $\gamma^* = n\pi$. The unique $P$-solution is the $D1$ state, with two bend vertices along the diagonal on $x = 0$. This solution branch is computed using the limiting profile in Section III, i.e. the solution of (III.1) on $E^C_4$ and then using continuation methods for large $\lambda$. This solution branch remains stable for all $\lambda^2 > 0$. When $\lambda^2$ is large enough, we observe two stable $D2$ states with two bend vertices along the diagonal on $y = 0$, and four stable rotated solutions. The energy of $D1$ solution is always lower than the $D2$ solution and the rotated solutions have higher energies than the diagonal solutions. The solution branches are disconnected according to our simulations. The solution branches are recovered by solving the boundary-value problem (IV.2) for the prescribed choices of $\gamma_b$ above, and using these limiting profiles as initial conditions for large $\lambda$, and then using continuation methods for smaller values of $\lambda$.

The case of $\gamma^* = \pi/4 + n\pi$ is different (see Fig. 13). The unique $P$-solution is the $St$-branch with two line defects near opposite square edges, parallel to the direction in infinity. This solution branch exists for all $\lambda^2 > 0$. As $\lambda^2$ increases, $St$ loses stability and bifurcates into two stable diagonal solutions with two diagonally opposite splay vertices. The $St$-branch further bifurcates into two stable $R1$ solutions, with two bend vertices connected by the edge of square, and this edge is perpendicular to $(\cos \gamma^*, \sin \gamma^*)$. There are two stable $R2$ solutions, with two bend vertices along the square edge, which is parallel to $(\cos \gamma^*, \sin \gamma^*)$ and this solution branch only exists for $\lambda^2$ large enough. The energy of the diagonal solution is always lower than $R1$, which in turn is energetically preferable to the $R2$ solution branches. The bifurcation diagram with $\gamma^* = \pi/4$ is similar to the bifurcation diagram on $E_4$ reported in [16], with the $St$-branch being analogous to the WORS, although there is no analogue of the $BD$ state on $E^C_4$, and the $R2$ branch is disconnected from the $St$-branch. For $\gamma^* = n\pi$, we do not observe bifurcation points as such, and simply observe the different stable solution branches and this could well be a limitation of the numerical methods.

In [25], the authors present a computational study of a single square particle embedded in a nematic medium, using the 3D LdG framework. They report the $St$ state for a small square particle and the $R1$ state ($Su$) for large square particles. The authors find a new stable state, $Sb$, with two interior point defects for large square particle. This stable $Sb$ state doesn’t exist for our problem, which could be an artefact of our reduced rLdG model or the fact that we are modelling a large domain with a square hole, such that the outer boundary is sufficiently far from the square boundary. If the two boundaries are close to each other, then new states such as the $Sb$ state may be observable, owing to the geometric frustration and conflicting boundary conditions.
We focus on nematic equilibria in the exterior of a regular 2D polygon, in a reduced LdG framework. The planar director profiles are modelled by minimizers of a rLdG free energy (II.3), in terms of a reduced order parameter, $P$ with two degrees of freedom. We focus on 2D polygonal holes with homeotropic boundary conditions, although our methods will work with generic boundary conditions. The methods heavily rely on our previous work for the interior of 2D polygons in [16], the essential difference being the additional degree of freedom rendered by the fixed boundary condition at infinity, captured by $\gamma^\ast$. This extra degree of freedom plays a crucial role in tuning the limiting profiles, for very small ($\lambda \to 0$) and large ($\lambda \to \infty$) polygonal holes. In fact, the delicate interplay between $K$-the number of edges of the polygon, and $\gamma^\ast$ dictates the existence of interior defects, the multiplicity, location and dimensionality of defects in the limiting cases. For a given $K$ and $\gamma^\ast$, the limiting profile is unique, with a single interior point defect for $K = 3$ and two interior point defects for $K > 4$, in the $\lambda \to 0$ limit. For $K = 4$, the choice of $\gamma^\ast$ determines whether we have line defects or not in the $\lambda \to 0$ limit. It is noteworthy that the physically relevant range of $\gamma^\ast$ depends on $K$, so that we need only restrict ourselves to $\gamma^\ast \in [0, \pi/K]$. In the $\lambda \to \infty$ limit, we have at least $\lfloor K/2 \rfloor$ stable states for each choice of $\gamma^\ast$, differentiated by the location of the two bend vertices. However, we have reduced symmetry equivalences compared to the interior problem on $E_K$ in [16]. For example, we only have two rotationally equivalent classes of stable equilibria on a square domain with tangent boundary conditions: the diagonal and rotated solutions. For $E_C^4$, we have at least 3 different classes of stable equilibria for different choices of $\gamma^\ast$, which are not related by rotations and reflections. Similarly, there are three rotationally equivalent classes of stable equilibria on $E_6^C$: the Para, Meta and Ortho solutions. There are at least six distinct classes of stable equilibria on $E_6^C$ with homeotropic boundary conditions, distinguished not only by the locations of the bend vertices, but also by the orientation of the line connecting the bend vertices relative to the fixed boundary condition at infinity. Hence, there is enhanced multistability in the $\lambda \to \infty$ limit for the exterior problem, compared to the interior problem studied in [16].

This work beautifully complements the work in [10]. The work in Section [11] heavily relies on the symmetry of the Laplacian operator in two dimensions. We expect the limiting profiles in Section [11] to be good approximations for materials with small elastic anisotropy as in [15], although the elastic anisotropy will destroy some of the symmetries of the limiting profiles. A further extension concerns arrays of polygonal exclusions [26] or fully 3D systems, which offer exotic possibilities for defect structures such as linked defect lines etc. Our overarching goal is to propose universal theoretical frameworks for solution landscapes of confined partially ordered systems, with multiple order parameters. These solution landscapes crucially depend on the symmetries of the mathematical model, phenomenological parameters, the domain and the boundary condition, and this work goes some way in illustrating the interesting differences between interior and exterior problems, and how this could be used for tailored solution landscapes in the future.
Acknowledgments AM and YH thank Ingo Dierking and Adam Draude for suggesting this problem to them, complemented by their experimental work. AM gratefully acknowledges support from the University of Strathclyde New Professors Fund and a University of Strathclyde Global Engagement Grant. AM is also supported by a Leverhulme International Academic Fellowship IAF-2019-009, a Daiwa Foundation Small Grant and a Royal Society Newton Advanced Fellowship. Part of this work was facilitated by a London Mathematical Research Reboot grant awarded to AM. YH acknowledges support from a Royal Society Newton International Fellowship.

[1] S. Alama, L. Bronsard, and X. Lamy. Minimizers of the Landau–de Gennes energy around a spherical colloid particle. *Archive for Rational Mechanics and Analysis*, 2016.

[2] P. Bauman, N. N. Carlson, and D. Phillips. On the zeros of solutions to Ginzburg–Landau type systems. *SIAM Journal on Mathematical Analysis*, 24(5):1281–1293, 1993.

[3] A. Brodin, A. Nych, U. Ongysta, B. Lev, Y. Nazarenko, M. Škarabot, and I. Muševeci. Melting of 2D liquid crystal colloidal structure. *Condensed Matter Physics*, 13(3), 2010.

[4] G. Canevari, J. Harris, A. Majumdar, and Y. W. Wang. The well order reconstruction solution for three-dimensional wells, in the Landau–de Gennes theory. *International Journal of Nonlinear Mechanics*, 119:103342, 2020.

[5] G. Canevari, A. Majumdar, and A. Spicer. Order reconstruction for nematics on squares and hexagons: A Landau–de Gennes study. *SIAM Journal on Applied Mathematics*, 77(1):267–293, 2017.

[6] S. B. Chernysheku and B. I. Lev. Theory of elastic interaction of colloidal particles in nematic liquid crystals near one wall and in the nematic cell. *Physical Review E*, 84(1):011707, 2011.

[7] T. A. Driscoll and L. N. Trefethen. *Schwarz-Christoffel mapping*, volume 8. Cambridge University Press, 2002.

[8] J. S. Evans, C. N. Beier, and I. Smalyukh. Alignment of high-aspect ratio colloidal gold nanoplatelets in nematic liquid crystals. *Journal of Applied Physics*, 110(3):033535, 2011.

[9] L. Fang, A. Majumdar, and L. Zhang. Surface, size and topological effects for some nematic equilibria on rectangular domains. *Mathematics and Mechanics of Solids*, 25(5):1101–1123, 2020.

[10] Y. Geng, R. Kizhakidathazhath, and J. P. F. Lagerwall. Encoding Hidden Information onto Surfaces Using Polymerized Cholesteric Spherical Reflectors. *Advances in Functional Materials*, page 2100399, 2021.

[11] P. G. de Gennes and J. Prost. *The physics of liquid crystals*, volume 83. Oxford university press, 1995.

[12] D. Golovaty, J. A. Montero, and P. Sternberg. Dimension reduction for the Landau–de Gennes model on curved nematic thin films. *Journal of Nonlinear Science*, 27(6):1905–1932, 2017.

[13] G. Gupta and A. D. Rey. Texture formation mechanisms in carbon–carbon composites based on mesophase precursor matrices. *Carbon*, 43(7):1400–1406, 2005.

[14] Y. C. Han, J. Harris, J. Walton, and A. Majumdar. Tailored nematic and magnetization profiles on two-dimensional polygons. *Physical Review E*, 103(5):052702, 2021.

[15] Y. C. Han, J. Harris, L. Zhang, and A. Majumdar. Elastic anisotropy of nematic liquid crystals in the two-dimensional Landau–de Gennes model. *arXiv preprint arXiv:2105.10253*, 2021.

[16] Y. C. Han, A. Majumdar, and L. Zhang. A reduced study for nematic equilibria on two-dimensional polygons. *SIAM Journal on Applied Mathematics*, 80(4):1678–1703, 2020.

[17] Y. C. Han, J. Y. Yin, Y. C. Hu, A. Majumdar, and L. Zhang. Solution landscapes of the simplified Ericksen–Leslie model and its comparison with the reduced Landau–de Gennes model. *Proceedings of the Royal Society A*, 477(2253):20210458, 2021.

[18] Y. C. Han, J. Y. Yin, P. W. Zhang, A. Majumdar, and L. Zhang. Solution landscape of a reduced Landau–de Gennes model on a hexagon. *Nonlinearity*, 34(4):2048, 2021.

[19] S. Kralj and A. Majumdar. Order reconstruction patterns in nematic liquid crystal wells. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 470(2169):20140276, 2014.

[20] J. P. F. Lagerwall and G. Scalia. A new era for liquid crystal research: applications of liquid crystals in soft matter nano- and microtechnology. *Current Applied Physics*, 12(6):1387–1412, 2012.

[21] Wells G. E. Logg A., Mardal K. A. *Automated solution of differential equations by the finite element method: the FEniCS book*, volume 84. Springer Science and Business Media, 2012.

[22] C. Luo, A. Majumdar, and R. Erban. Multistability in planar liquid crystal wells. *Physical Review E*, 85(6):061702, 2012.

[23] I. Mušević and M. Škarabot. Self-assembly of nematic colloids. *Soft Matter*, 4(2):195–199, 2008.

[24] I. Mušević, M. Škarabot, U. Tkalec, M. Ravnik, and S. Zumer. Two-dimensional nematic colloidal crystals self-assembled by topological defects. *Science*, 313(5789):954–958, 2006.

[25] P. M. Phillips and A. D. Rey. Texture formation mechanisms in faceted particles embedded in a nematic liquid crystal matrix. *Soft Matter*, 7(5):2052–2063, 2011.

[26] A. Pim. A conservation law for liquid crystal defects on manifolds. *arXiv preprint arXiv:2106.01447*, 2021.

[27] M. Robinson, C. Luo, P. E. Farrell, R. Erban, and A. Majumdar. From molecular to continuum modelling of bistable liquid crystal devices. *Liquid Crystals*, 44(14-15):2267–2284, 2017.

[28] T. J. Spencer, C. M. Care, R. M. Amos, and J. C. Jones. Zenithal bistable device: Comparison of modeling and experiment. *Physical Review E*, 82(021702), 2010.

[29] Y. Yuan, Q. Liu, B. Senyuk, and I. Smalyukh. Elastic colloidal monopoles and reconfigurable self-assembly in liquid
crystals. Nature, 570(7760):214–218, 2019.