

Variational and numerical analysis of a Q-tensor model for smectic-A liquid crystals

Jingmin Xia
University of Oxford

Patrick E. Farrell, University of Oxford

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A recent smectic-A model (Xia et al., 2021)

Smectic order parameter $u : \Omega \rightarrow \mathbb{R}$.

Nematic order parameter $Q : \Omega \rightarrow \mathbb{R}^{d \times d}$, symmetric and traceless.

A unified smectic-A free energy

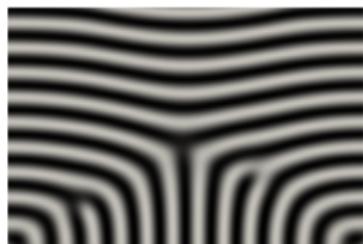
$$\begin{aligned}\mathcal{J}(u, Q) = & \int_{\Omega} \left(\frac{a_1}{2} u^2 + \frac{a_2}{3} u^3 + \frac{a_3}{4} u^4 \right. \\ & \left. + B \left| \mathcal{D}^2 u + q^2 \left(Q + \frac{I_d}{d} \right) u \right|^2 + \frac{K}{2} |\nabla Q|^2 + f_n^b(Q) \right),\end{aligned}\tag{1}$$

where the nematic bulk term is defined as

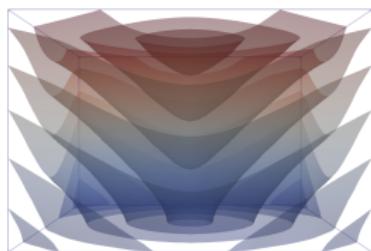
$$f_n^b(Q) := \begin{cases} \left(-I (\text{tr}(Q^2)) + I (\text{tr}(Q^2))^2 \right), & \text{if } d = 2, \\ \left(-\frac{I}{2} (\text{tr}(Q^2)) - \frac{I}{3} (\text{tr}(Q^3)) + \frac{I}{2} (\text{tr}(Q^2))^2 \right), & \text{if } d = 3. \end{cases}$$

I_d is the $d \times d$ identity matrix, \mathcal{D}^2 denote the Hessian operator, $a_1, a_2, a_3, B, K, I, q$ are some known parameters.

Successful implementation examples



Oily Streaks

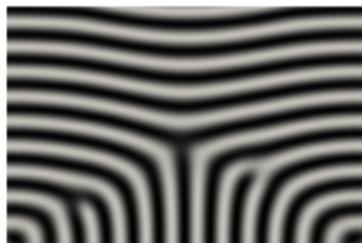


TFCD

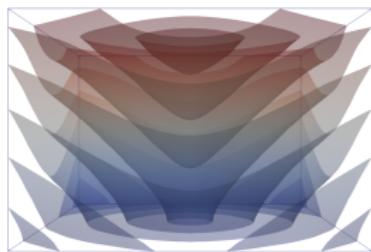
See more details in

J. Xia, S. MacLachlan, T. J. Atherton and P. E. Farrell, *Structural Landscapes in Geometrically Frustrated Smectics*, PRL, 2021.

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Our goal

To answer the following two questions:

- do minimisers exist?
- how do finite element approximations behave?

Section 1. Existence of minimisers

Existence of minimisers

Define the admissible set

$$\begin{aligned}\mathcal{A} = \left\{ u \in H^2(\Omega, \mathbb{R}), Q \in H^1(\Omega, S_0) : \right. \\ Q = s \left(n \otimes n - \frac{I_d}{d} \right) \text{ for some } s \in [0, 1] \text{ and } n \in H^1(\Omega, \mathcal{S}^{d-1}), \\ \left. Q = Q_b \text{ on } \partial\Omega \right\},\end{aligned}$$

with Dirichlet boundary data $Q_b \in H^{1/2}(\partial\Omega, S_0)$.

Theorem

Let \mathcal{J} be of the form (1) with positive parameters a_3, B, q, K, l . Then there exists a solution pair (u^*, Q^*) that minimises \mathcal{J} over the admissible set \mathcal{A} .

Proof: by the direct method of calculus of variations.

(Davis and Gartland, 1998, Theorem 4.3) & (Bedford, 2014, Theorem 5.19)

Section 2. A priori error estimates

Finite element approximations in (Xia et al., 2021)

Essentially...

we are solving a *second order* PDE (for Q) and *fourth order* PDE (for u), coupled together.

- For the second order PDE \Leftarrow common continuous Lagrange elements ✓
- For the fourth order PDE \Leftarrow a *practical* choice of finite elements?

Solution: use continuous Lagrange elements for u !

By adding the following penalty term (Engel et al., 2002; Brenner and Sung, 2005) in the total energy:

$$\sum_{e \in \mathcal{E}_I} \int_e \frac{B\epsilon}{h_e^3} (\llbracket \nabla u \rrbracket)^2 .$$

Two independent problems when $q = 0$

For tensor-valued Q : a second order PDE

$$(P1) \quad \begin{cases} -K\Delta Q + 2I(2|Q|^2 - 1)Q = 0 & \text{in } \Omega \subset \mathbb{R}^2, \\ Q = Q_b & \text{on } \partial\Omega. \end{cases}$$

For real-valued u : a fourth order PDE

$$(P2) \quad \begin{cases} 2B\nabla \cdot (\nabla \cdot \mathcal{D}^2 u) + a_1 u + a_3 u^3 = 0 & \text{in } \Omega, \\ u = u_b & \text{on } \partial\Omega, \\ \mathcal{D}^2 u = \mathcal{D}^2 u_b & \text{on } \partial\Omega. \end{cases}$$

Here, we take $a_2 = 0$ to only analyse the cubic nonlinearity for simplicity.

A priori estimates for tensor Q

(Davis and Gartland, 1998, Theorem 6.3) (Regularity)

Let Ω be an open, bounded, Lipschitz and convex domain. If the Dirichlet data $Q_b \in H^{1/2}(\partial\Omega, S_0)$, then any solution of $(\mathcal{P}1)$ belongs to $H^2(\Omega, S_0)$.

(Davis and Gartland, 1998, Theorem 7.3)(H^1 error estimate)

If $Q \in H^2 \cap H_b^1(\Omega, S_0)$ and $Q_h \in V_h$ (consisting of piecewise linear polynomials) represents an approximated solution to Q , it holds that

$$\|Q - Q_h\|_1 \lesssim h \|Q\|_2.$$

Theorem (L^2 error estimate)

Let Q be a regular solution of the nonlinear weak form for $(\mathcal{P}1)$ and $Q_h \in V_h$ is an approximated solution to Q , there holds that

$$\|Q - Q_h\|_0 \lesssim h^2 (2 + (3 + 2h + 2h^2) \|Q\|_2^2) \|Q\|_2.$$

To derive L^2 error estimates for Q

Given $G \in L^2$, consider the linear dual problem to the primary problem ($\mathcal{P}1$): find $N \in H_0^1$ such that

$$\begin{cases} -K\Delta N + 4I|Q|^2N + 8I(Q : N)Q - 2/N = G & \text{in } \Omega, \\ N = 0 & \text{on } \partial\Omega. \end{cases} \quad (2)$$

Weak formulation of (2): find $N \in H_0^1$ such that

$$\langle \mathcal{D}\mathcal{N}^n(Q)N, \Phi \rangle := A^n(N, \Phi) + 3B^n(Q, Q, N, \Phi) + C^n(N, \Phi) = (G, \Phi)_0 \quad (3)$$

for all $\Phi \in H_0^1$.

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Weak formulation of (2): find $N \in H_0^1$ such that

$$\langle \mathcal{DN}^n(Q)N, \Phi \rangle := A^n(N, \Phi) + 3B^n(Q, Q, N, \Phi) + C^n(N, \Phi) = (G, \Phi)_0 \quad (3)$$

for all $\Phi \in H_0^1$.

Weak formulation of $(\mathcal{P}1)$ \implies find $Q \in H_b^1$ such that

$$\mathcal{N}^n(Q)P := A^n(Q, P) + B^n(Q, Q, Q, P) + C^n(Q, P) = 0$$

for all $P \in H_0^1$, where the bilinear forms are

$$A^n(Q, P) := K \int_{\Omega} \nabla Q : \nabla P, \quad C^n(Q, P) := -2I \int_{\Omega} Q : P,$$

and the nonlinear operator is given by

$$B^n(\Psi, \Phi, \Theta, \Xi) := \frac{4I}{3} \int_{\Omega} ((\Psi : \Phi)(\Theta : \Xi) + 2(\Psi : \Theta)(\Phi : \Xi)).$$

Sketch proof of the L^2 -error rates for Q

Lemma

For $Q \in H^2 \cap H_b^1$, $N \in H^2 \cap H_0^1$ and $I_h Q \in V_h \subset H_b^1$, it holds that

$$A^n(I_h Q - Q, N) \lesssim h^2 \|Q\|_2 \|N\|_2.$$

Lemma

The solution N to the weak form (3) of the dual linear problem belongs to $H^2 \cap H_0^1$ and it holds that $\|N\|_2 \lesssim \|G\|_0$.

A standard technique in the Aubin–Nitsche argument:

taking $G = I_h Q - Q_h$ and the test function $\Phi = I_h Q - Q_h$ in the weak dual form (3).

- Optimal rates in the H^1 norm. ✓
- Optimal rates in the L^2 norm. ✓

Remark: it also holds for higher order (> 1) approximations by following similar steps in (Maity, Majumdar, and Nataraj, 2020).

Now, consider problem $(\mathcal{P}2)$ for u

Continuous weak form of $(\mathcal{P}2)$ \implies find $u \in H^2(\Omega) \cap H_b^1(\Omega)$ s.t.

$$\mathcal{N}^s(u)v := A^s(u, v) + B^s(u, u, v) + C^s(u, v) = L^s(v) \quad \forall v \in H^2 \cap H_0^1, \quad (4)$$

where for $v, w \in H^2(\Omega)$,

$$A^s(v, w) = 2B \int_{\Omega} \mathcal{D}^2 v : \mathcal{D}^2 w, \quad C^s(v, w) = a_1 \int_{\Omega} vw,$$
$$L^s(v) := 2B \int_{\partial\Omega} (\mathcal{D}^2 u_b \cdot \nabla v) \cdot \nu,$$

and for $\mu, \zeta, \eta, \xi \in H^2(\Omega)$,

$$B^s(\mu, \zeta, \eta, \xi) = a_3 \int_{\Omega} \mu \zeta \eta \xi.$$

Newton linearisation \implies find $v \in H^2 \cap H_0^1$ such that

$$\langle \mathcal{D}\mathcal{N}^s(u)v, w \rangle_{H^2} := A^s(v, w) + 3B^s(u, v, w) + C^s(v, w) = L^s(w)$$

for all $w \in H^2 \cap H_0^1$.

Finite element discretisation for u

- C^0 interior penalty methods (Brenner, 2011).
- We take the H^2 -nonconforming but still continuous approximation $u_h \in W_{h,b} \subset H^2(\mathcal{T}_h) \cap H_b^1(\Omega)$ for the solution u of the continuous weak form (4).

Here,

$$W_{h,b} := \{v \in H^2(\mathcal{T}_h) \cap H^1(\Omega) : v = u_b \text{ on } \partial\Omega, v \in \mathbb{Q}_{\deg}(T) \forall T \in \mathcal{T}_h\}.$$

- Denote the mesh-dependent H^2 -like semi-norm for $v \in W_h$

$$\|v\|_h^2 := \sum_{T \in \mathcal{T}_h} |v|_{H^2(T)}^2 + \sum_{e \in \mathcal{E}_I} \int_e \frac{1}{h_e^3} |\llbracket \nabla v \rrbracket|^2.$$

Here, $\llbracket \nabla w \rrbracket = (\nabla w)_- \cdot \nu_- + (\nabla w)_+ \cdot \nu_+$.

Note that $\|\cdot\|_h$ is indeed a norm on $W_{h,0}$.

Discrete weak form of u

Find $u_h \in W_{h,b}$ such that

$$\begin{aligned}\mathcal{N}_h^s(u_h)v_h &:= A_h^s(u_h, v_h) + P_h^s(u_h, v_h) + B^s(u_h, u_h, u_h, v_h) + C^s(u_h, v_h) \\ &= L^s(u_h) \quad \forall v_h \in W_{h,0},\end{aligned}\tag{5}$$

where for all $u, v \in W_h$,

$$A_h^s(u, v) := 2B\left(\sum_{T \in \mathcal{T}_h} \int_T \mathcal{D}^2 u : \mathcal{D}^2 v - \sum_{e \in \mathcal{E}_I} \int_e \left\{\left\{\frac{\partial^2 u}{\partial \nu^2}\right\}\right\} [\![\nabla v]\!] - \sum_{e \in \mathcal{E}_I} \int_e \left\{\left\{\frac{\partial^2 v}{\partial \nu^2}\right\}\right\} [\![\nabla u]\!]\right),$$

and

$$P_h^s(u, v) := \sum_{e \in \mathcal{E}_I} \frac{2B\epsilon}{h_e^3} \int_e [\![\nabla u]\!] [\![\nabla v]\!].$$

Here, ϵ is the penalty parameter, $\left\{\left\{\frac{\partial^2 u}{\partial \nu^2}\right\}\right\} = \frac{1}{2} \left(\frac{\partial^2 u_+}{\partial \nu^2} \Big|_e + \frac{\partial^2 u_-}{\partial \nu^2} \Big|_e \right)$.

Linearisation \implies Seek $v_h \in W_{h,0}$ such that

$$\langle \mathcal{D}\mathcal{N}_h^s(u_h)v_h, w_h \rangle = L^s(w_h) \quad \forall w_h \in W_{h,0},$$

where $\langle \mathcal{D}\mathcal{N}_h^s(u_h)v_h, w_h \rangle := A_h^s(v_h, w_h) + P_h^s(v_h, w_h) + 3B_h^s(u_h, u_h, v_h, w_h) + C_h^s(v_h, w_h)$.

Convergence in the $\|\cdot\|_h$ -norm

Brouwer's fixed point theorem \implies the existence and local uniqueness result of the discrete solution u_h .

Theorem

Let u be a regular isolated solution of the nonlinear problem (4). For a sufficiently large ϵ and a sufficiently small h , there exists a unique solution u_h of the discrete nonlinear problem (5) within the local ball

$\mathcal{B}_{R(h)}(I_h u) := \{v_h \in W_h : \|I_h u - v_h\|_h \leq R(h)\}$. Furthermore, we have

$$\|u - u_h\|_h \lesssim h^{\min\{\deg - 1, \mathbb{k}_u - 2\}}.$$

Here, $R(h) = \mathcal{O}(h^{\min\{\deg - 1, \mathbb{k}_u - 2\}})$, \deg indicates the degree of the approximating polynomials and $\mathbb{k}_u \geq 3$ represents the regularity of u .

\implies optimal rates in the $\|\cdot\|_h$ -norm. ✓

Auxiliary results for $\|\cdot\|_h$ -error estimates

- We define the nonlinear map $\mu_h : W_h \rightarrow W_h$ by

$$\langle \mathcal{DN}_h^s(I_h u) \mu_h(v_h), w_h \rangle = 3B_h^s(I_h u, I_h u, v_h, w_h) + L^s(w_h) - B_h^s(v_h, v_h, v_h, w_h).$$

Lemma (mapping from a ball to itself)

Let u be a regular isolated solution of the continuous nonlinear weak problem (4). For a sufficiently large ϵ and a sufficiently small mesh size h , there exists a positive constant $R(h) = \mathcal{O}(h^{\min\{\deg-1, \mathbb{k}_u-2\}})$ such that:

$$\|v_h - I_h u\|_h \leq R(h) \Rightarrow \|\mu_h(v_h) - I_h u\|_h \leq R(h) \quad \forall v_h \in W_{h,0}.$$

Lemma (contraction result)

For a sufficiently large ϵ , a sufficiently small mesh size h and any $v_1, v_2 \in \mathcal{B}_{R(h)}(I_h u)$, there holds

$$\|\mu_h(v_1) - \mu_h(v_2)\|_h \lesssim h^{\min\{\deg-1, \mathbb{k}_u-2\}} \|v_1 - v_2\|_h.$$

To derive L^2 error estimates

We consider the linear dual problem to the primary nonlinear problem $(\mathcal{P}2)$:

$$\begin{cases} 2B\nabla \cdot (\nabla \cdot (\mathcal{D}^2\chi)) + a_1\chi + 3a_3u^2\chi = f_{dual} & \text{in } \Omega, \\ \chi = 0, \quad \mathcal{D}^2\chi = 0 & \text{on } \partial\Omega, \end{cases}$$

for $f_{dual} \in L^2$.

Weak form: find $\chi \in H^2 \cap H_0^1$ such that

$$\langle \mathcal{DN}^s(u)\chi, v \rangle_{H^2} = \langle \mathcal{DN}_h^s(u)\chi, v \rangle = (f_{dual}, v)_0,$$

for any $v \in H^2 \cap H_0^1$.

Using the standard Aubin–Nitsche technique: take $f_{dual} = I_h u - u_h$ and $v = I_h u - u_h$ in the above weak form.

L^2 error estimate for u

Theorem

Under the same conditions as in the theorem of the $\|\cdot\|_h$ -error rates, the discrete solution u_h approximates u such that

$$\|u - u_h\|_0 \lesssim \begin{cases} h^{\min\{\deg + 1, \mathbb{k}_u\}} & \text{for } \deg \geq 3, \\ h^{2\min\{\deg - 1, \mathbb{k}_u - 2\}} = h^2 & \text{for } \deg = 2. \end{cases}$$

\implies optimal L^2 error rates (only suboptimal for quadratic approximations) for polynomials with degree (≥ 3). ✓

Remark: suboptimal rates with quadratic approximations are also observed for biharmonic equations (Süli and Mozolevski, 2007).

Section 3. Numerical verifications

Convergence tests via MMS

- Exact solutions:

$$Q_{11}^e = \left(\cos \left(\frac{\pi(2y-1)(2x-1)}{8} \right) \right)^2 - \frac{1}{2},$$

$$Q_{12}^e = \cos \left(\frac{\pi(2y-1)(2x-1)}{8} \right) \sin \left(\frac{\pi(2y-1)(2x-1)}{8} \right),$$

$$u^e = 10((x-1)x(y-1)y)^3.$$

Manufactured equations to be solved:

$$\begin{cases} 4Bq^4 u^2 Q_{11} + 2Bq^2 u (\partial_x^2 u - \partial_y^2 u) - 2K\Delta Q_{11} - 4/Q_{11} + 16/Q_{11} (Q_{11}^2 + Q_{12}^2) = f_1, \\ 4Bq^4 u^2 Q_{12} + 4Bq^2 u (\partial_x \partial_y u) - 2K\Delta Q_{12} - 4/Q_{12} + 16/Q_{12} (Q_{11}^2 + Q_{12}^2) = f_2, \\ a_1 u + a_2 u^2 + a_3 u^3 + 2B\nabla \cdot (\nabla \cdot (\mathcal{D}^2 u)) + Bq^4 (4(Q_{11}^2 + Q_{12}^2) + 1) u + 2Bq^2(t_1 + t_2) = f_3, \end{cases}$$

with

$$t_1 := (Q_{11} + 1/2)\partial_x^2 u + (-Q_{11} + 1/2)\partial_y^2 u + Q_{12}\partial_x \partial_y u,$$

$$t_2 := \partial_x^2(u(Q_{11} + 1/2)) + \partial_y^2(u(-Q_{11} + 1/2)) + 2\partial_x \partial_y(uQ_{12}).$$

Here, f_1, f_2, f_3 are source terms derived from substituting the exact solutions to the left hand sides.

Convergence tests via MMS: settings

- $\Omega = [0, 1] \times [0, 1]$.
- Mesh size $h = \frac{1}{N}$ with $N = 6, 12, 24, 48$.
- Define numerical errors in L^2 and H^1 norms as

$$\|\mathbf{e}_u\|_0 = \|u^e - u_h\|_0, \quad \|\mathbf{e}_u\|_1 = \|u^e - u_h\|_1, \quad \|\mathbf{e}_u\|_h = \|u^e - u_h\|_h,$$

$$\|\mathbf{e}_Q\|_0 = \|(Q_{11}^e, Q_{12}^e) - (Q_{11,h}, Q_{12,h})\|_0,$$

$$\|\mathbf{e}_Q\|_1 = \|(Q_{11}^e, Q_{12}^e) - (Q_{11,h}, Q_{12,h})\|_1.$$

- Choose parameters: $a_1 = -10$, $a_2 = 0$, $a_3 = 10$, $B = 10^{-5}$, $K = 0.3$ and $l = 30$.

Convergence rates for $q = 0$

Approximating tensor Q:

$N = \frac{1}{h}$	$\ \mathbf{e}_Q\ _0$	rate	$\ \mathbf{e}_Q\ _1$	rate
$[\mathbb{Q}_1]^2$	6	8.12e-04	–	3.78e-02
	12	2.02e-04	2.01	1.88e-02
	24	5.05e-05	2.00	9.39e-03
	48	1.26e-05	2.00	4.69e-03
$[\mathbb{Q}_2]^2$	6	2.92e-05	–	1.11e-03
	12	3.90e-06	2.90	2.71e-04
	24	5.02e-07	2.96	6.72e-05
	48	6.36e-08	2.99	1.68e-05
$[\mathbb{Q}_3]^2$	6	3.02e-07	–	2.25e-05
	12	2.17e-08	3.80	2.72e-06
	24	1.45e-09	3.90	3.34e-07
	48	9.33e-11	3.96	4.13e-08

⇒ optimal rates in the H^1 and L^2 norms. ✓

Convergence rates for $q = 0$

Approximating u with $\epsilon = 1$:

$N = \frac{1}{h}$	$\ \mathbf{e}_u\ _0$	rate	$\ \mathbf{e}_u\ _1$	rate	$\ \mathbf{e}_u\ _h$	rate	
Q_2	6	1.17e-05	–	3.46e-04	–	1.36e-02	–
	12	2.60e-06	2.17	9.81e-05	1.82	7.25e-03	0.91
	24	6.37e-07	2.03	2.54e-05	1.95	3.54e-03	1.03
	48	1.82e-07	1.80	6.88e-06	1.88	1.76e-03	1.01
Q_3	6	4.73e-06	–	1.32e-04	–	4.98e-03	–
	12	3.32e-07	3.83	1.41e-05	3.23	9.96e-04	2.32
	24	2.12e-08	3.97	1.63e-06	3.12	2.46e-04	2.02
	48	1.32e-09	4.00	1.99e-07	3.03	6.14e-05	2.00
Q_4	6	2.01e-07	–	7.76e-06	–	3.94e-04	–
	12	5.40e-09	5.22	4.30e-07	4.17	4.88e-05	3.01
	24	1.68e-10	5.00	2.68e-08	4.00	6.11e-06	2.99
	48	5.27e-12	4.99	1.68e-09	3.99	7.64e-07	3.00

⇒ optimal rates in the $\|\cdot\|_h$, $\|\cdot\|_1$ and $\|\cdot\|_0$ norms (only suboptimal in the $\|\cdot\|_0$ norm with quadratic approximations). ✓

Convergence rates for $q = 30$

Approximating tensor Q (fixing the approximation \mathbb{Q}_3 for u with $\epsilon = 5 \times 10^4$):

	$N = \frac{1}{h}$	$\ \mathbf{e}_Q\ _0$	rate	$\ \mathbf{e}_Q\ _1$	rate
$[\mathbb{Q}_1]^2$	6	8.12e-04	–	3.78e-02	–
	12	2.02e-04	2.01	1.88e-02	1.01
	24	5.05e-05	2.00	9.39e-03	1.00
	48	1.26e-05	2.00	4.69e-03	1.00
$[\mathbb{Q}_2]^2$	6	2.92e-05	–	1.11e-03	–
	12	3.90e-06	2.90	2.71e-04	2.04
	24	5.02e-07	2.96	6.72e-05	2.01
	48	6.37e-08	2.98	1.68e-05	2.00
$[\mathbb{Q}_3]^2$	6	3.02e-07	–	2.25e-05	–
	12	2.17e-08	3.80	2.72e-06	3.05
	24	1.45e-09	3.90	3.34e-07	3.03
	48	9.32e-11	3.96	4.13e-08	3.01

\implies optimal rates in the H^1 and L^2 norms. ✓

Convergence tests for $q = 30$

Approximating u with $\epsilon = 5 \times 10^4$ (fixing the approximation $[\mathbb{Q}_2]^2$ for Q):

$N = \frac{1}{h}$	$\ \mathbf{e}_u\ _0$	rate	$\ \mathbf{e}_u\ _1$	rate	$\ \mathbf{e}_u\ _h$	rate	
\mathbb{Q}_2	6	1.21e-05	–	3.59e-04	–	1.37e-02	–
	12	3.98e-06	1.61	1.42e-04	1.34	8.30e-03	0.72
	24	1.57e-06	1.35	4.99e-05	1.51	3.89e-03	1.09
	48	2.58e-07	2.60	9.07e-06	2.46	1.78e-03	1.13
\mathbb{Q}_3	6	7.36e-06	–	2.25e-04	–	9.10e-03	–
	12	4.13e-07	4.16	1.86e-05	3.60	1.11e-03	3.03
	24	4.23e-08	3.29	2.24e-06	3.05	2.53e-04	2.14
	48	3.01e-09	3.81	2.28e-07	3.29	6.15e-05	2.04

\implies almost optimal (with some fluctuations) in the $\|\cdot\|_h$ and $\|\cdot\|_0$ norms
 (almost suboptimal in the L^2 -norm for quadratic approximations).

Section 4. Conclusions and future work

Conclusions

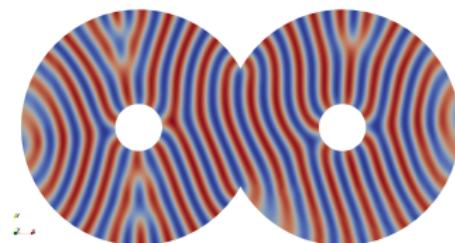
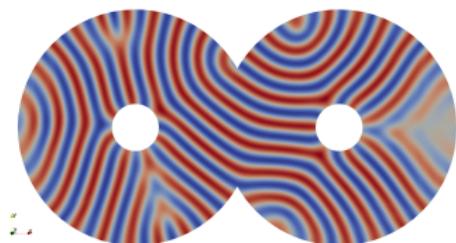
- Existence of minimisers is proven for the proposed smectic-A model in (Xia et al., 2021).
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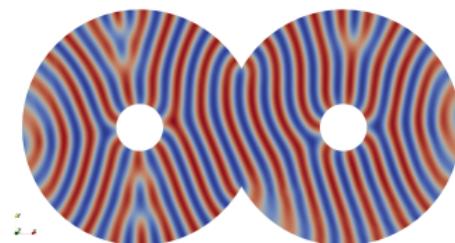
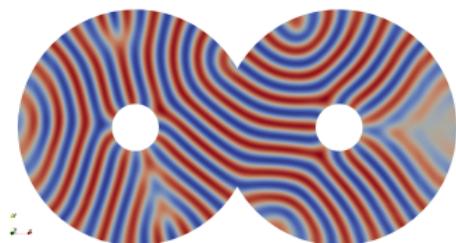


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Thank you for your attention!