# Chevron Structures in Liquid Crystal Cells

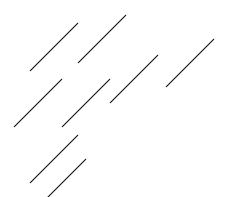
Lei Cheng, Lidia Mrad, Dan Phillips

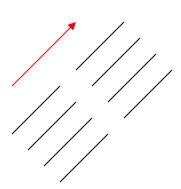
## Liquid Crystal Phases

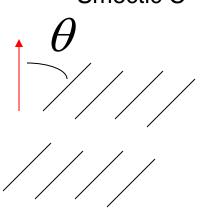
Nematic

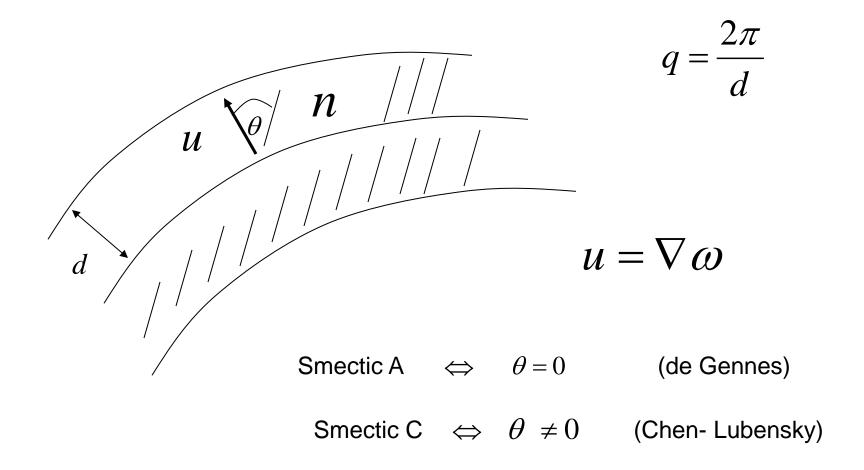
Smectic A

Smectic C









The level curves of  $\omega$  represent layers.

$$\mathcal{F}_q = \int_{\Omega} \left(\frac{1}{q} f_s + f_n + f_e\right)$$

$$f_s = f_s(\psi, \mathbf{n}) , f_n = f_n(\mathbf{n}),$$

$$f_e = f_e(\psi, \mathbf{n})$$

$$\Omega$$
 – material body

$$\psi \colon \Omega \to \mathbb{C}, \qquad \mathbf{n} \colon \Omega \to \mathbb{S}^2$$

 $\psi$  is a complex order parameter,

**n** is the director field

$$\psi(x) = \rho(x)e^{iq\omega(x)}$$

$$\rho = 0$$
 nematic,  $\rho \neq 0$  smectic

 $f_n(\mathbf{n})$  - Frank-Oseen energy

$$f_{\mathbf{n}} = \frac{1}{2}K|\nabla\mathbf{n}|^2$$

The material is "chiral" however the domain  $\Omega$  will be thin and due to this the specific elastic features are not significant.

 $f_e(\mathbf{n}, \psi)$  - Electrostatic energy

Chirality induces a spontaneous polarization field,  $\mathbf{P} = P_0(\nabla \omega \times \mathbf{n})$ .

If **E** is an applied electric field then

$$f_e = -\mathbf{E} \cdot \mathbf{P}$$

 $f_s(\mathbf{n}, \psi)$  - Smectic C energy density

$$f_{s} = \frac{a_{\perp}}{q^{2}} |D \cdot D_{\perp} \psi|^{2} - c_{\perp} |D_{\perp} \psi|^{2}$$

$$+ \frac{a_{\parallel}}{q^{2}} |D \cdot D_{\parallel} \psi|^{2} + c_{\parallel} |D_{\parallel} \psi|^{2}$$

$$+ qg(|\psi|^{2} - 1)^{2}$$

$$a_{\perp}, c_{\parallel}, c_{\perp}, a_{\parallel} > 0, \text{ where } \frac{a_{\perp}}{2c_{\perp}} = \sin^{2} \theta.$$

 $D = \nabla - iq\cos\theta\mathbf{n}, \quad D_{\parallel} = (\mathbf{n}\cdot\nabla - iq\cos\theta)\mathbf{n}$ 

$$D_{\perp} = D - D_{\parallel}.$$

Let  $\psi = e^{iq\omega(\mathbf{x})}$ ,  $\mathbf{n} = \mathbf{n}(\mathbf{x})$ .

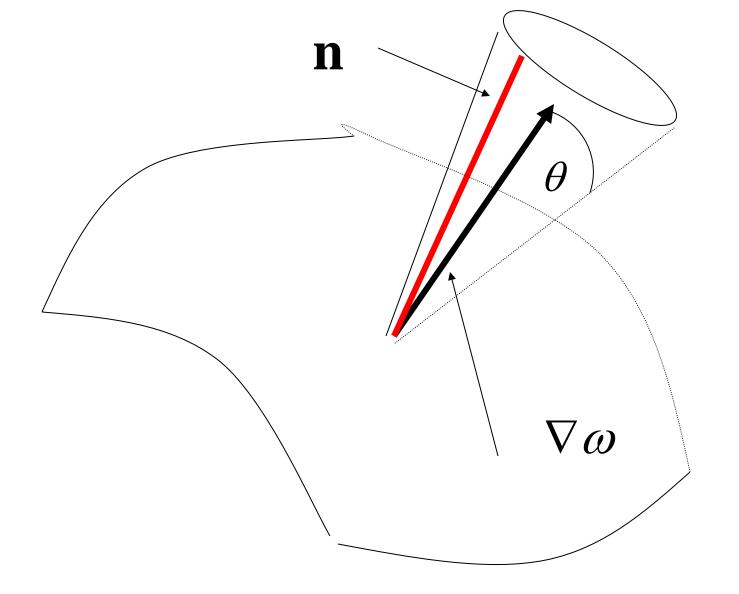
$$\frac{1}{q}f_{s} = \frac{1}{q} \left\{ a_{\perp} \left( \operatorname{div} \left( \nabla \omega - (\mathbf{n} \cdot \nabla \omega) \mathbf{n} \right) \right)^{2} + a_{\parallel} \left( \operatorname{div} \left( \left( (\mathbf{n} \cdot \nabla \omega) - \cos \theta \right) \mathbf{n} \right) \right)^{2} \right\} \right.$$

$$+ q \left\{ a_{\perp} (|\nabla_{\perp} \omega|^{2} - \sin^{2} \theta)^{2} \right.$$

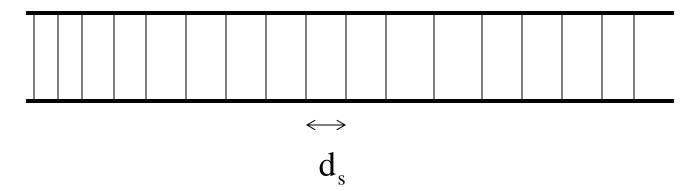
$$+ a_{\parallel} ((\nabla \omega \cdot \mathbf{n}) - \cos \theta)^{4} + c_{\parallel} (\nabla \omega \cdot \mathbf{n} - \cos \theta)^{2} \right\} + \operatorname{const}$$

For q large we see:

- vanishing costs of specific curvatures for the smectic layers ( $\omega = \text{const}$ )
- $\nabla \omega \cdot \mathbf{n} \to \cos \theta$  (fixed tilt)
- $|\nabla \omega| \to 1$  (uniform spacing)



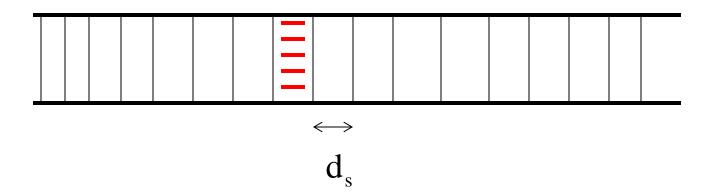
In surface-stabilized cells where the liquid crystals are confined between close glass plates with fixed boundary conditions.



The layer thickness on the boundary is given by  $d_s$ .

In surface-stabilized cells where the liquid crystals are confined between close glass plates with fixed boundary conditions.

## Bookshelf Geometry

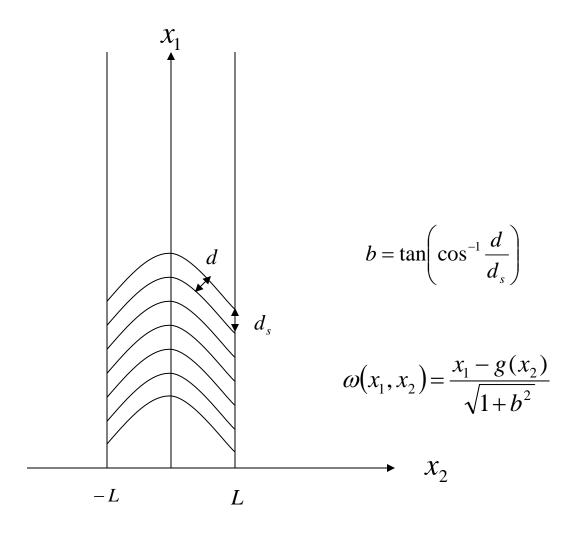


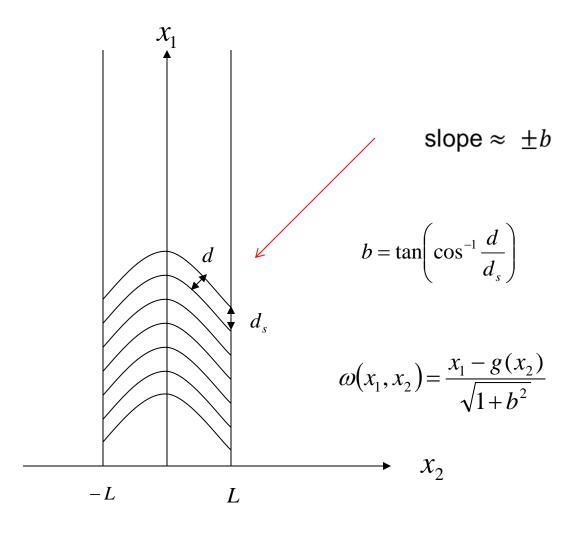
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We assume initially that the l.c. is in the smectic A phase.

- When the temperature is reduced the material enters the smectic C phase and the bookshelf structure deforms into V-shaped (chevron) layers.
- It is caused by two effects. The layers thin as the l.c. molecules tilt. The boundary layer spacing  $d_s$  does not change.
- It causes distortions in director pattern.







We consider a reduced setting such that:

• The domain is

$$\Omega = \{(x_1, x_2) | -L < x_2 < L\}.$$

- $\mathbf{n} = (n_1(x_2), n_2(x_2), n_3(x_2)),$
- Let  $\omega(x_1, x_2) = \frac{x_1 g(x_2)}{\sqrt{1 + b^2}}$ , where  $g(x_2)$  is the layer displacement, and  $b = tan(cos^{-1}\frac{d}{ds})$ .
- $\mathbf{E} = (0, E, 0)$

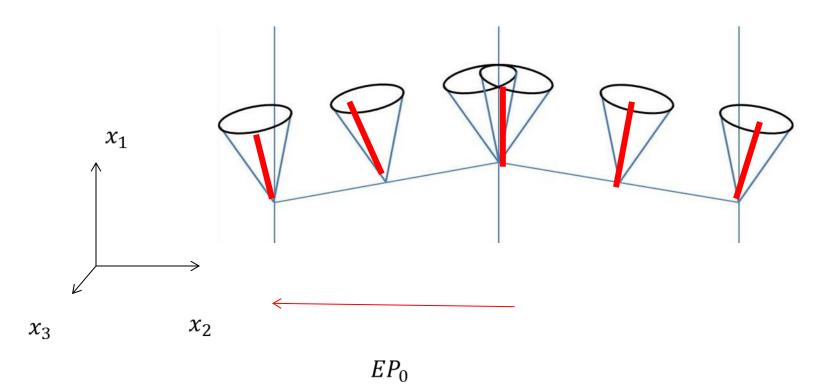
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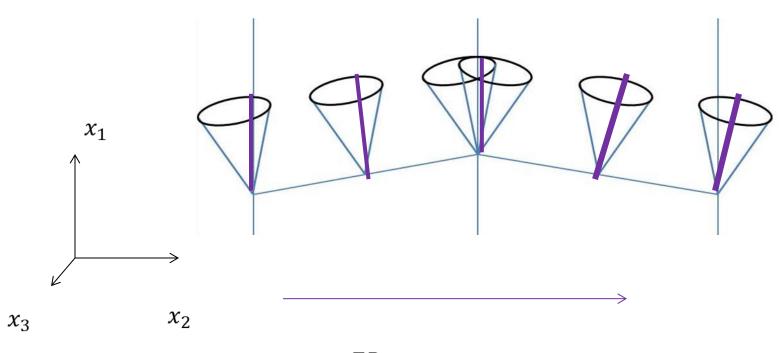
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- $\mathbf{E} = (0, E, 0)$

$$\Rightarrow$$
 that  $-\mathbf{E} \cdot \mathbf{P} = \frac{P_0 E}{\sqrt{1+b^2}} n_3$ .





 $EP_0$ 

Now the total energy can be simplified into

$$\mathcal{F}_{q}(\mathbf{n}, g') = \int_{-L}^{L} \left\{ \frac{1}{q} \left[ \frac{a_{\perp}}{1 + b^{2}} \left( \left( -g' - n_{1}n_{2} + n_{2}^{2}g' \right)' \right)^{2} \right. \right. \\ \left. + \frac{a_{\parallel}}{1 + b^{2}} \left( \left( n_{1}n_{2} - n_{2}^{2}g' - n_{2}\cos\theta\sqrt{1 + b^{2}} \right)' \right)^{2} \right] \\ \left. + q \left[ \frac{a_{\perp}}{(1 + b^{2})^{2}} \left( 1 + (g')^{2} - (n_{1} - n_{2}g')^{2} - \sin^{2}\theta(1 + b^{2}) \right)^{2} \right. \\ \left. + \frac{a_{\parallel}}{(1 + b^{2})^{2}} \left( n_{1} - n_{2}g' - \cos\theta\sqrt{1 + b^{2}} \right)^{4} \right. \\ \left. + \frac{c_{\parallel}}{1 + b^{2}} \left( n_{1} - n_{2}g' - \cos\theta\sqrt{1 + b^{2}} \right)^{2} \right] \\ \left. + \frac{1}{2} K \left( n_{1}'^{2} + n_{2}'^{2} + n_{3}'^{2} \right) \\ \left. + \frac{EP_{0}}{\sqrt{1 + b^{2}}} n_{3} \right\} dx_{2}$$

Our goal is to analyze the minimizers for  $\mathcal{F}_q$  and their limiting behavior.

The admissible set:

$$X = \{ (g', \mathbf{n}) | g' \in \mathbf{L}^2(-L, L), g(-L) = g(L),$$
  
 $\mathbf{n} \in \mathbf{L}^2(-L, L), |\mathbf{n}| = 1 \}$ 

- Can we find the function pairs  $(g'_q, \mathbf{n_q})$  in the admissible set  $\mathbb{X}$  that minimize the energy for q > 0?
- If yes, what do the minimizers look like?
- Is there a limiting problem as  $q \to \infty$ ?

Establishing the  $\Gamma$ -Convergence result for  $(\mathcal{F}_q)$ 

Theorem 1 (L.Cheng-D.P.) (2015) For every q > 0, set

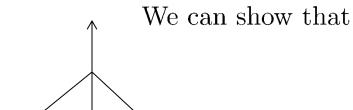
$$\mathcal{F}_q(g', \mathbf{n}) = \begin{cases} \int_{-L}^{L} F_q(g', \mathbf{n}) \, \mathrm{d}x_2 & \text{if } (g', \mathbf{n}) \in \mathbb{X}, g', \mathbf{n} \in W^{1,2}(-L, L) \\ \infty & \text{elsewhere in } \mathbb{X} \end{cases}$$

Then as  $q \to \infty$ , the functionals  $(\mathcal{F}_q)$   $\Gamma$ -converge in  $\mathbb{X}$  to

$$\mathcal{F}_{\infty}(g', \mathbf{n}) = \begin{cases} C_0 \|g'\|_{\mathsf{BV}} + \int_{-L}^{L} (\frac{1}{2}K|\mathbf{n}'|^2 + EP_0n_3) \, \mathrm{d}x_2 & \text{if } (g', \mathbf{n}) \in \mathbb{X} \cap \mathbb{A} \\ \infty & \text{elsewhere in } \mathbb{X} \end{cases}$$

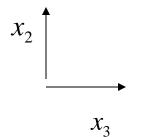
where  $\mathbb{A} = \{(g', \mathbf{n}) | g' \in BV, n_2 = 0 \text{ at jumps of } g', |g'| = b,$ 

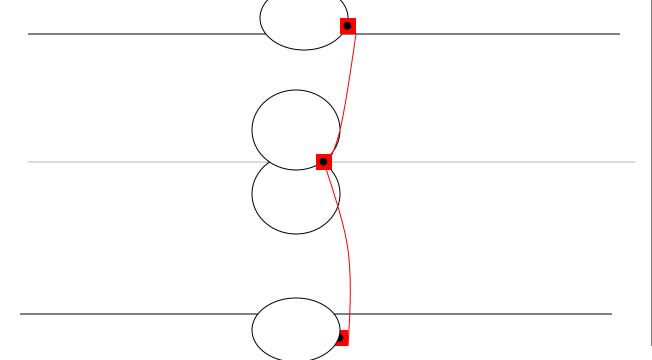
$$n_1 - n_2 g' = \cos \theta \sqrt{1 + b^2}$$
 on  $(-L, L)$ } and  $C_0 = \frac{4a_{\perp} b^2}{3(1 + b^2)^{\frac{3}{2}}}$ 



$$g'(x) = \begin{cases} b & \text{if } x \in (-L, 0) \\ -b & \text{if } x \in (0, L) \end{cases}$$

front





L

 $\mathcal{X}_{2}$ 

-1

• The reduced energy  $\mathcal{F}_{\infty}$  does not have a path allowing switching from  $E \to -E$  with finite energy. This means for large q it takes a very large E to induce switching for the gradient flow for  $\mathcal{F}_q$ .

- The reduced energy  $\mathcal{F}_{\infty}$  however does not have a path allowing switching from  $E \to -E$  with finite energy. This means for large q it takes a very large E to induce switching for the gradient flow for  $\mathcal{F}_q$ .
- To get a theory with a reduced energy that allows switching with a finite energy barrier one needs to work with  $f_s$  replacing the ansatz  $\psi(x_1, x_2) = e^{\frac{q(ix_1 g(x_2))}{\sqrt{1 + b^2}}}$  with  $\psi(x_1, x_2) = e^{\frac{iqx_1}{\sqrt{1 + b^2}}} \tilde{\psi}(x_2)$  such that  $\tilde{\psi}(x_2) \in \mathbb{C}$  and can vanish.

#### Lidia Mrad, Dan Phillips

#### Mathematical Model

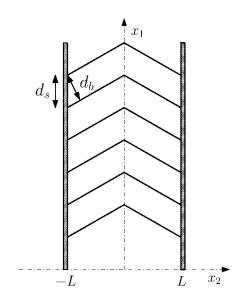
$$\frac{1}{q} f_s(\mathbf{n}, \psi) = G(\mathbf{n}, \psi) + H(|\psi|)$$

$$G(\mathbf{n}, \psi) = \frac{a_{\perp}}{q^3} \left| D \cdot D_{\perp} \psi + \frac{c_{\perp} q^2}{2a_{\perp}} \psi \right|^2 + \frac{a_{\parallel}}{q^3} \left| D \cdot D_{\parallel} \psi \right|^2 + \frac{c_{\parallel}}{q} \left| D_{\parallel} \psi \right|^2$$

$$H(|\psi|) = g(|\psi|^2 - 1)^2 + |\nabla|\psi|^2|^2 + \frac{1}{q^2}|\nabla^2|\psi|^2|^2 + \frac{1}{q^6}|\nabla^3|\psi|^2|^2$$

 $G(\mathbf{n}, \psi)$ : describes how **n** relates to the layers

 $H(|\psi|)$ : describes the energetic cost leaving the smectic phase



We consider a 2-D cross-section of the cell.

Periodicity: Reduce to 1-D model as first suggested by Sluckin et al.,  $\widetilde{\psi}(x_1, x_2) = \rho e^{i\frac{q[x_1 - g(x_2)]}{\sqrt{1 + b^2}}}.$ 

Main difference: We reduce the model but keep the 1-D complex-valued parameter in general form:  $e^{\frac{iqx_1}{\sqrt{1+b^2}}}\psi(x_2)$ , allowing for  $|\psi|=0$ .

$$\partial_t(\psi, \mathbf{n}) = -\delta \mathcal{F}_q(\psi, \mathbf{n})$$

where  $(\psi(x_2,0),\mathbf{n}(x_2,0))$  is close to  $(e^{\frac{-iqg(x_2)}{\sqrt{1+b^2}}},\mathbf{n}_0(x_2))$  such that

$$(g', \mathbf{n}_0) \in \mathbb{A} = \{(g', \mathbf{n}) | g' \in BV, n_2 = 0 \text{ at jumps of } g', |g'| = b,$$

$$n_1 - n_2 g' = \cos \theta \sqrt{1 + b^2}$$
 on  $(-L, L)$ 

Existence and uniqueness results for continuous  $L^2$  – gradient flows

$$(\psi(x_2,t), \mathbf{n}(x_2,t))$$
 for:

$$\begin{split} \mathcal{F}_{q}(\psi,\mathbf{n}) &= \int_{-L}^{L} \left\{ \frac{a_{\perp}}{q} | [\frac{\psi'}{q} - (\frac{i}{\sqrt{1+b^{2}}} n_{1}\psi + n_{2}\frac{\psi'}{q}) n_{2}]' - \frac{q}{1+b^{2}} \psi \right. \\ &+ \frac{q}{1+b^{2}} n_{1}^{2} \psi - \frac{i}{\sqrt{1+b^{2}}} n_{1} n_{2} \psi' + q s i n \theta \psi |^{2} \\ &+ \frac{a_{\parallel}}{q} | (\frac{n_{1}}{\sqrt{1+b^{2}}} - c o s \theta) (-\frac{q}{\sqrt{1+b^{2}}} n_{1} \psi + i n_{2} \psi' + q c o s \theta \psi) \\ &+ [(\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \frac{\psi'}{q} - i c o s \theta \psi) n_{2}]' |^{2} + c_{\parallel} |\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \psi' + q c o s \theta \psi |^{2} \\ &+ k (|\psi|^{2} - 1)^{2} + h (|\psi|^{2}')^{2} + \frac{\alpha}{q^{2}} (|\psi|^{2''})^{2} + \frac{\beta}{q^{6}} (|\psi|^{2'''})^{2} \\ &+ \frac{K}{2} |\mathbf{n}'|^{2} + \frac{PE}{\sqrt{1+b^{2}}} |\psi|^{2} n_{3} \right\} dx_{2} \end{split}$$

#### Statics

• We prove coercivity and lower semi-continuity of the energy  $\mathcal{F}_q(\mathbf{n}, \psi)$ .

• We construct well-prepared initial data, ind. of q. (A specific  $(\mathbf{n}, \psi) = (\mathbf{n}_q, \psi_q)$  for which  $\mathcal{F}_q(\mathbf{n}, \psi) \leq C$  where C is ind. of q.)

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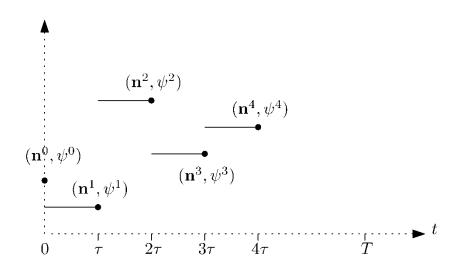
- We construct well-prepared initial data, ind. of q. (A specific  $(\mathbf{n}, \psi) = (\mathbf{n}_q, \psi_q)$  for which  $\mathcal{F}_q(\mathbf{n}, \psi) \leq C$  where C is ind. of q.)
- This is a large class of initial conditions  $\{(\mathbf{n}_q, \psi_q)\}$  that can approximate states with finite numbers of chevrons.

Dynamics: Gradient Flow

To study the dynamic behavior, we construct a discrete-in-time gradient flow following *Rothe's method*.

$$J^{0}(\mathbf{n}, \psi) = \int_{-L}^{L} \left\{ \frac{|\mathbf{n} - \mathbf{n}^{0}|^{2}}{2\tau} + \frac{|\psi - \psi^{0}|^{2}}{2\tau} \right\} dx + \mathcal{F}_{q}(\mathbf{n}, \psi)$$

- Minimize  $J^0$  over  $[0,\tau]$  with initial conditions  $(\mathbf{n}^0,\psi^0)$ .
- Get minimizer  $(\mathbf{n}^1, \psi^1)$ .
- Use  $(\mathbf{n}^1, \psi^1)$  as an initial condition for  $[\tau, 2\tau]$ , minimize  $J^1$  and iterate.
- Get a sequence of minimizers  $\{(\mathbf{n}^m, \psi^m)\}$ .
- Connect these minimizers in a piecewise costant fashion to get the discretized minimizers  $\{(\mathbf{n}^{\tau}, \psi^{\tau})\}$  over [0, T].



We consider a 2-D cross-section of the cell with a piecewise constant in time solution.

#### Energy Dissipation:

$$\frac{1}{2} \sum_{k=1}^{m} \tau(||\delta_{\tau} \mathbf{n}^{k}||_{2}^{2} + ||\delta_{\tau} \psi^{k}||_{2}^{2}) + \mathcal{F}_{q}(\mathbf{n}^{m}, \psi^{m}) \leq \mathcal{F}_{q}(\mathbf{n}^{0}, \psi^{0}) \text{ for } 1 \leq m \leq M \text{ where } M\tau < T.$$

With well-prepared initial data, energy at any later time is controlled (independent of q).

#### smectic elastic term

$$\begin{split} \mathcal{F}_{q}(\psi,\mathbf{n}) &= \int_{-L}^{L} \left\{ \frac{a_{\perp}}{q} | [\frac{\psi'}{q} - (\frac{i}{\sqrt{1+b^{2}}} n_{1}\psi + n_{2}\frac{\psi'}{q}) n_{2}]' - \frac{q}{1+b^{2}} \psi \right. \\ &+ \frac{q}{1+b^{2}} n_{1}^{2} \psi - \frac{i}{\sqrt{1+b^{2}}} n_{1} n_{2} \psi' + q s i n \theta \psi |^{2} \\ &+ \frac{a_{\parallel}}{q} | (\frac{n_{1}}{\sqrt{1+b^{2}}} - c o s \theta) (-\frac{q}{\sqrt{1+b^{2}}} n_{1} \psi + i n_{2} \psi' + q c o s \theta \psi) \\ &+ [(\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \frac{\psi'}{q} - i c o s \theta \psi) n_{2}]' |^{2} + c_{\parallel} | \frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \psi' + q c o s \theta \psi |^{2} \\ &+ k (|\psi|^{2} - 1) + h (|\psi|^{2'})^{2} + \frac{\alpha}{q^{2}} (|\psi|^{2''})^{2} + \frac{\beta}{q^{6}} (|\psi|^{2'''})^{2} \\ &+ \frac{K}{2} |\mathbf{n}'|^{2} + \frac{PE}{\sqrt{1+b^{2}}} |\psi|^{2} n_{3} \right\} dx_{2} \end{split}$$

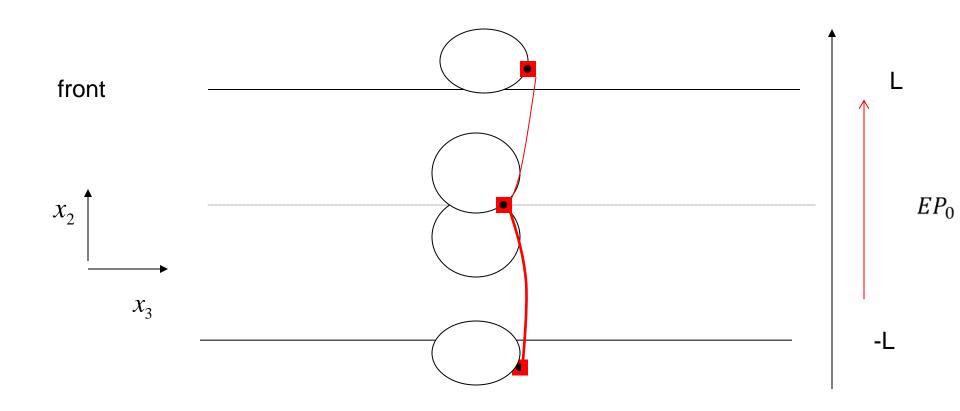
term determining the bulk phase

$$\begin{split} \mathcal{F}_{q}(\psi,\mathbf{n}) &= \int_{-L}^{L} \left\{ \frac{a_{\perp}}{q} | [\frac{\psi'}{q} - (\frac{i}{\sqrt{1+b^{2}}} n_{1}\psi + n_{2}\frac{\psi'}{q}) n_{2}]' - \frac{q}{1+b^{2}} \psi \right. \\ &+ \frac{q}{1+b^{2}} n_{1}^{2} \psi - \frac{i}{\sqrt{1+b^{2}}} n_{1} n_{2} \psi' + q s i n \theta \psi |^{2} \\ &+ \frac{a_{\parallel}}{q} | (\frac{n_{1}}{\sqrt{1+b^{2}}} - c o s \theta) (-\frac{q}{\sqrt{1+b^{2}}} n_{1} \psi + i n_{2} \psi' + q c o s \theta \psi) \\ &+ [(\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \frac{\psi'}{q} - i c o s \theta \psi) n_{2}]' |^{2} + c_{\parallel} |\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \psi' + q c o s \theta \psi |^{2} \\ &+ k (|\psi|^{2} - 1)^{2} + h (|\psi|^{2}')^{2} + \frac{\alpha}{q^{2}} (|\psi|^{2}'')^{2} + \frac{\beta}{q^{6}} (|\psi|^{2}''')^{2} \\ &+ \frac{K}{2} |\mathbf{n}'|^{2} + \frac{PE}{\sqrt{1+b^{2}}} |\psi|^{2} n_{3} \right\} dx_{2} \end{split}$$

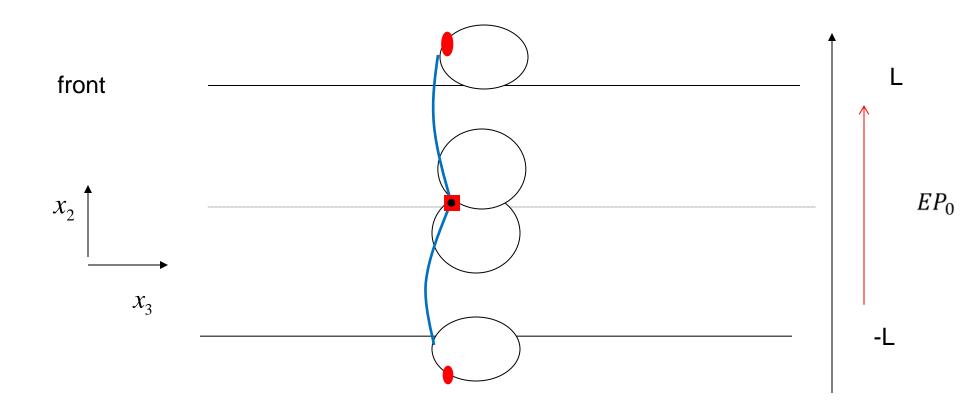
### electrostatic forcing term

$$\begin{split} \mathcal{F}_{q}(\psi,\mathbf{n}) &= \int_{-L}^{L} \left\{ \frac{a_{\perp}}{q} | [\frac{\psi'}{q} - (\frac{i}{\sqrt{1+b^{2}}} n_{1}\psi + n_{2} \frac{\psi'}{q}) n_{2}]' - \frac{q}{1+b^{2}} \psi \right. \\ &+ \frac{q}{1+b^{2}} n_{1}^{2} \psi - \frac{i}{\sqrt{1+b^{2}}} n_{1} n_{2} \psi' + q s i n \theta \psi |^{2} \\ &+ \frac{a_{\parallel}}{q} | (\frac{n_{1}}{\sqrt{1+b^{2}}} - c o s \theta) (-\frac{q}{\sqrt{1+b^{2}}} n_{1} \psi + i n_{2} \psi' + q c o s \theta \psi) \\ &+ [(\frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \frac{\psi'}{q} - i c o s \theta \psi) n_{2}]' |^{2} + c_{\parallel} | \frac{i}{\sqrt{1+b^{2}}} n_{1} \psi + n_{2} \psi' + q c o s \theta \psi |^{2} \\ &+ k (|\psi|^{2} - 1) + h (|\psi|^{2'})^{2} + \frac{\alpha}{q^{2}} (|\psi|^{2''})^{2} + \frac{\beta}{q^{6}} (|\psi|^{2'''})^{2} \\ &+ \frac{K}{2} |\mathbf{n}'|^{2} + \frac{PE}{\sqrt{1+b^{2}}} |\psi|^{2} n_{3} \right\} dx_{2} \end{split}$$

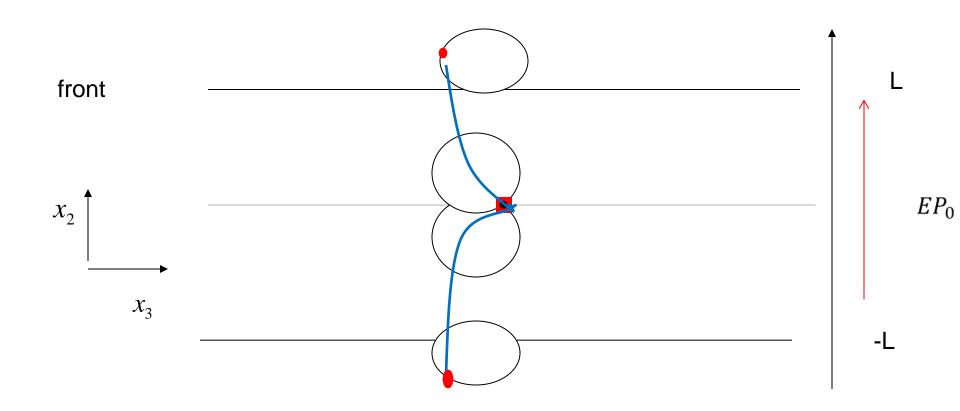
The idea is to have a flow that can go from here at t=0



to here for t >> 0.



As opposed to tending to this...



Idea of Proof:

We need to prove the convergence of the discrete gradient flow.

$$\int_0^T \int_{-L}^L \left[ \delta_{\tau} \mathbf{n} + U_1^{\tau} \right] \mathbf{u} + U_2^{\tau} \mathbf{u}' \, dx dt = 0$$

To get an idea of the nonlinearity of  $U_1^{\tau}$ :

$$U_1^{\tau} = 2\Re\left\{\frac{a_{\perp}}{q} \left(\frac{i}{\sqrt{b^2 + 1}} n_2^{\tau'} \overline{\psi^{\tau}} + \ldots\right) \left(\frac{\psi^{\tau''}}{q} + \ldots\right)\right\} + \ldots$$
$$= C n_2^{\tau'} \Im\left\{\overline{\psi^{\tau}} \psi^{\tau''}\right\} + \ldots$$

It is enough to prove:

$$U_1^{\tau} \to U_1^{\tau} \text{ in } L^1(\Omega_T)$$
 $U_1^{\tau} \text{ is bounded in } L^2(\Omega_T)$ 

$$\Rightarrow U_1^{\tau} \underset{\tau \to 0}{\rightharpoonup} U_1 \text{ in } L^2(\Omega_T).$$

- We get this convergence with two types of estimates.
- Higher order estimates in x:

We can show there are constants  $q_0(C)$  and M(C,q) so that

$$\int_0^T \int_{-L}^L |\mathbf{n}^{\tau''}|^2 + |\psi^{\tau'''}|^2 + ||\psi^{\tau}|^{2(5)}|^2 dx dt \le M(C, q), \text{ uniformly in } \tau > 0$$

provided that  $\mathcal{F}_q(\mathbf{n}^0, \psi^0) < C$  and  $q_0(C) < q$ .

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We can show there are constants  $q_0(C)$  and M(C,q) so that

$$\int_0^T \int_{-L}^L |\mathbf{n}^{\tau''}|^2 + |\psi^{\tau'''}|^2 + ||\psi^{\tau}|^2|^2 dx dt \le M(C, q), \text{ uniformly in } \tau > 0$$

provided that  $\mathcal{F}_q(\mathbf{n}^0, \psi^0) < C$  and  $q_0(C) < q$ .

• An estimate on  $|\psi'|$ .

• This is due to a Modica-Mortola type estimate:

There is a K(C) so that if  $\mathcal{F}_q(\mathbf{n}, \psi) \leq C$  and  $1 \leq q$  then  $\frac{|\psi'|}{q} \leq K$ .

- We need this to show the energy is coercive.
- In the static problem we assumed the ansatz  $\psi(x) = e^{iqg(x)}$  and showed  $|g'(x)| \leq K$ .

This came from:

$$\int_{-L}^{L} \left\{ \frac{1}{q} (g''(x))^2 + qC_0 \left[ \left( (g'(x))^2 - b^2 \right)^+ \right]^2 \right\} dx \le C_1 \mathcal{F}_q + C_2 \le C_3$$

$$\Rightarrow$$

$$|g'(x)| \le K$$

• For this case note that since  $\mathcal{F}(\mathbf{n},\psi) \leq \mathcal{F}(\mathbf{n}^0,\psi^0)$  we have

$$\int_{-L}^{L} ((|\psi|^4 + (|\psi|^{2\prime})^2 + \frac{1}{q^2} (|\psi|^{2\prime\prime\prime})^2 + \frac{1}{q^6} (|\psi|^{2\prime\prime\prime\prime})^2) \, dx \le C.$$

- It follows that  $\left|\frac{|\psi|^{2''}}{2q^2}\right| + \frac{b^2}{1+b^2}|\psi|^2 \le M$  where C and M are independent of q for  $q \ge 1$ .
- If  $(\alpha, \beta) \subset [-L, L]$  is a maximal interval on which  $|\psi| > 0$  we get

$$\int_{\alpha}^{\beta} \frac{1}{q} \left| \Im \left\{ \frac{\psi'' \overline{\psi}}{q} \right\} \right|^{2} |\psi|^{-2} + q \left| \Re \left\{ \frac{\psi'' \overline{\psi}}{q^{2}} \right\} + \frac{b^{2}}{1 + b^{2}} |\psi|^{2} \right|^{2} |\psi|^{-2} dx \le C$$

Using the fact that the initial energy is bounded, and after carrying out some algebraic manipulations on the energy, we get

• From these inequalities we have a Modica-Mortola type estimate,

$$\int_{\alpha}^{\beta} \left| \left( \Re\{\frac{\psi'\overline{\psi}}{q|\psi|}\} \right)' \left[ \left( \Re\{\frac{\psi'\overline{\psi}}{q|\psi|}\} \right)^2 - 2M \right]^+ \right| \, dx \le C$$

• If  $\Phi$  is such that  $\Phi'(y) = [y^2 - 2M]^+$ , then

$$\underset{(\alpha,\beta)}{osc} \ \Phi\left(\frac{|\psi|'}{q}\right) = \underset{(\alpha,\beta)}{osc} \ \Phi\left(\Re\{\frac{\psi'\overline{\psi}}{q|\psi|}\}\right) \leq C.$$

- If  $|\psi(\alpha)| = |\psi(\beta)| = 0$  it follows that  $|\psi(x)|' = 0$  for some  $x \in (\alpha, \beta)$ .
- If either  $\alpha = -L$  or  $\beta = L$  then it follows from the boundary conditions that  $|\psi|' = 0$  at that point.
- In either case it follows that  $\left|\frac{|\psi|'}{q}\right|$  is uniformly bounded independent of q and the interval  $(\alpha, \beta)$ .

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- A similar reasoning can be applied to the imaginary part  $\frac{1}{q}\Im\{\frac{\psi'\overline{\psi}}{q|\psi|}\}.$
- $[-L, L] \setminus \{\bigcup_j [\alpha_j, \beta_j]\}$  are accumulation points for  $\{\psi = 0\}$  so  $\psi' = 0$  on this set.

- How does this relate to prior work?
- $\bullet$   $\check{C}$ opi $\check{c}$  etal. consider

$$\mathcal{F}_q(\mathbf{n}, \psi) = \int_{-L}^{L} \left\{ f_s(\mathbf{n}, \psi) + f_\mathbf{n}(\mathbf{n}) + f_e(n_3) \right\} dx,$$

with q fixed and choose sufficiently small elasticity constants for  $f_s$  in their simulations so that the three terms are of the same order.

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with q fixed and choose sufficiently small elasticity constants for  $f_s$  in their simulations so that the three terms are of the same order.

• We use q as a parameter

$$\mathcal{F}_q(\mathbf{n}, \psi) = \int_{-L}^{L} \left\{ \frac{1}{q} f_s(\mathbf{n}, \psi) + f_\mathbf{n}(\mathbf{n}) + f_e(n_3) \right\} dx,$$

where

$$q = \frac{1}{\text{layer thickness}} \to \infty.$$

With this weighting the three energies have the same order for large q.

## Results

- existence
- uniqueness (independent of the choice of minimizers as well as the particular discretization used)
- $\bullet$  a simple picture when the wave number q is a sufficiently large constant.

- How can we use it?
- Characterization of and the dynamics for the limiting problem i.e. when  $q \to \infty$ .
- We now have a set-up allowing switching at the chevron tip.
- We expect to identify regions of melting around the chevron tip, where **n** decouples from the cone and switches continuously.