

# Extending a complex tensor model for smectics

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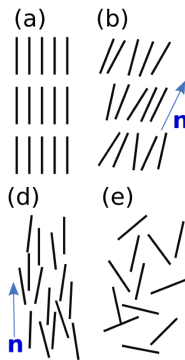
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Two main goals: adapt it for 3D & introduce projection operators to free energy terms

# Smectic liquid crystals

- ▶ Layering of long molecules (simplest case)
- ▶ Smectic A – molecules perpendicular to layers
- ▶ 3 quantities (fields)
  - ▶ How ordered the phase is
  - ▶ Direction of layering – director  $\underline{N}$
  - ▶ Spacing of layers



**Figure:** Crystalline, smectic C, nematic and isotropic phases

# Describing smectics

- ▶ The layering is a density fluctuation

$$\rho(\underline{r}, t) = \sum_{m=-\infty}^{+\infty} \psi_m e^{im\underline{q} \cdot \underline{r}} \simeq \rho_0 + 2 \operatorname{Re}(\psi e^{i\underline{q}_0 \cdot \underline{r}})$$

- ▶ Having  $\psi = |\psi|e^{i\phi}$  gives
  - ▶  $|\psi|$  as the order parameter
  - ▶ Changes in  $\phi$  lead to spacing differences
- ▶  $\underline{N} \propto \underline{q}_0$  , can be an additional parameter or taken as  $\underline{\nabla}\phi$

# E theory – Motivations

## Problems

- ▶  $\underline{N} \leftrightarrow -\underline{N}$  symmetry –  $\underline{N}$  is not a vector
- ▶ Defects lead to undefined  $\underline{N}$  and related problems

## Requirements

- ▶ Incorporate the symmetry
- ▶ Combine the parameters to allow "numerical melting"
- ▶ Keep enough degrees of freedom to have them separate

# E theory

- ▶ Inspiration from Q-tensor and complex  $\psi$
- ▶ Replace the real order parameters  $S$  with complex  $\psi$

$$\underline{\underline{Q}} = S_1(\underline{\underline{N}}\underline{\underline{N}} - \frac{\delta}{d}) \quad \text{uniaxial case}$$

$$\underline{\underline{E}} \sim \psi_1(\underline{\underline{N}}\underline{\underline{N}} - \frac{\delta}{d})$$

$d$  is the number of dimensions, 2 or 3

# E theory

$$\underline{\underline{E}} \sim \psi_1(\underline{N}\underline{N} - \frac{\delta}{d})$$

- ▶ Want to evolve  $\underline{\underline{E}}$  directly
- ▶ In general, it is a  $d$  by  $d$  complex tensor
- ▶ How to keep in the form above?

# Constraints on $\underline{\underline{E}}$

- ▶ Q-tensor is symmetric and traceless – so orthogonally diagonalizable
- ▶ Require  $\underline{\underline{E}}$  be diagonalizable by a unitary matrix
  - ▶ so "normal"  $\leftrightarrow \underline{\underline{E}}\underline{\underline{E}}^\dagger = \underline{\underline{E}}^\dagger \underline{\underline{E}}$
- ▶ and symmetric and traceless

# Constraints on E

Leads to the following form in 3D (equivalent in 2D, but only 1 term)

$$\underline{\underline{E}} = \underline{\underline{U}}^\dagger \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & -\lambda_1 - \lambda_2 \end{pmatrix} \underline{\underline{U}} = \dots = \psi_1(\underline{\underline{N}}\underline{\underline{N}} - \frac{\delta}{3}) + \psi_2(\underline{\underline{M}}\underline{\underline{M}} - \frac{\delta}{3})$$

also using symmetry

- ▶ With  $\underline{\underline{N}}$ ,  $\underline{\underline{M}}$  being real, orthogonal, unit vectors, and

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} \lambda_1 - \lambda_3 \\ \lambda_2 - \lambda_3 \end{pmatrix}$$

- ▶ so the  $\psi$ s are the differences from the third eigenvalue
- ▶ Clearly biaxial form of the E we want!



# Biaxial E

- ▶ Our theory clearly suggests a biaxial E in 3D
- ▶ Can a smectic be biaxial? Does that make it a crystal?
- ▶ No clear constraint to force it uniaxial

# E theory – summary

- ▶ So we use a normal, symmetric and traceless complex tensor  $\underline{\underline{E}}$
  - ▶ We know how to interpret it
  - ▶ It might be biaxial
- 
- ▶ Now dynamics – Ginzburg-Landau theory
  - ▶ Need a free energy in terms of  $\underline{\underline{E}}$
  - ▶ Then use  $\frac{\partial E_{ij}}{\partial t} = -\mu \frac{\delta F}{\delta E_{ij}^*}$
  - ▶ Need to enforce constraints – Lagrange multipliers

# The free energy – bulk

- ▶  $F$  must be real – need to match  $\underline{\underline{E}}$  and  $\underline{\underline{E}}^*$
- ▶ Largely taken from previous work – terms inspired by Q

$$f_{\text{bulk}}(E_{ij}E_{ij}^* = \text{Tr}(\underline{\underline{E}}\underline{\underline{E}}^*)) = \frac{A}{2}E_{ij}E_{ij}^* + \frac{C}{4}(E_{ij}E_{ij}^*)^2$$

- ▶ In the uniaxial case  $E_{ij}E_{ij}^* \propto |\psi|^2$

# The free energy – elastic terms

- ▶ Need gradients
- ▶ Take all to be of form  $|\cdot|^2$  (Frobenius norm)
- ▶ Only allow a single  $\underline{\underline{E}}$ , and 1 or 2  $\underline{\nabla}$

$$|\underline{\nabla}\underline{\underline{E}}|^2 = E_{ij,k}E_{ij,k}^* \quad \text{Simplest term}$$

$$|\underline{\nabla} \cdot \underline{\underline{E}}|^2 = E_{ij,j}E_{ik,k}^* \quad \text{Divergence like, new}$$

$$|\underline{\nabla}^2 \underline{\underline{E}}|^2 = E_{ij,kk}E_{ij,ll}^* \quad \text{Simplest double gradient, considered}$$

# Projection operators for $F$

- ▶ Gradients in different directions have different energy costs
- ▶ For **uniaxial**  $\underline{\underline{E}}$ , special direction is  $\underline{N}$
- ▶ Projection operator  $\underline{\underline{\Pi}} = \underline{N}\underline{N}$ , rest is  $\underline{\underline{T}} = \underline{\underline{\delta}} - \underline{\underline{\Pi}}$
- ▶ Consider  $\underline{\nabla} \rightarrow a\underline{\underline{\Pi}} \cdot \underline{\nabla} + b\underline{\underline{T}} \cdot \underline{\nabla}$   $a, b$  being some constants

$$E_{ij,k}E_{ij,k}^* \rightarrow f_{\text{comp}} = b_1^{\parallel} \Pi_{kl} E_{ij,k} E_{ij,l}^* + b_1^{\perp} T_{kl} E_{ij,k} E_{ij,l}^*$$

$$E_{ij,kk}E_{ij,ll}^* \rightarrow f_{\text{curv}} = b_2^{\parallel} \Pi_{kl} E_{ij,lk} \Pi_{mn} E_{ij,nm}^* + b_2^{\perp} T_{kl} E_{ij,lk} T_{mn} E_{ij,nm}^* \\ + b_2^{\parallel\perp} (\Pi_{kl} E_{ij,lk} T_{mn} E_{ij,nm}^* + T_{kl} E_{ij,lk} \Pi_{mn} E_{ij,nm}^*)$$

# Projection operators

- ▶ Need a form for  $\underline{\underline{\Pi}}$  in terms of  $\underline{\underline{E}}$
- ▶ Have 2 forms which work for uniaxial  $\underline{\underline{E}}$

$$\underline{\underline{\Pi}} = \sqrt{\frac{d-1}{d\underline{\underline{E}}:\underline{\underline{E}}}} \underline{\underline{E}} + \frac{\delta}{d}$$
$$\underline{\underline{\Pi}} = \frac{d-1}{d-2} \left( \frac{\underline{\underline{E}} \cdot \underline{\underline{E}}^*}{\underline{\underline{E}}:\underline{\underline{E}}^*} - \frac{\frac{\delta}{d}}{d(d-1)} \right)$$

- ▶ First is significantly easier to work with
- ▶ Lead to seemingly different functional derivatives – why?
- ▶ First form only has  $\underline{\underline{E}}$ , how about  $\underline{\underline{E}} \rightarrow \underline{\underline{E}}^*$ ?
- ▶ How well do they work for biaxial  $\underline{\underline{E}}$ ?

# Functional derivatives using $\underline{\underline{\Pi}}$

- Results using the square root version of  $\underline{\underline{\Pi}}$

$$\frac{\delta F_{\text{bulk}}}{\delta E_{ij}^*} = \frac{1}{2}(A + CE_{ab}E_{ab}^*)E_{ij}$$

$$\frac{\delta F_{\text{comp}}}{\delta E_{ij}^*} = -(b_1^{\parallel} - b_1^{\perp})(\Pi_{kl,l}E_{ij,k} + \Pi_{kl}E_{ij,kl}) - b_1^{\perp}E_{ij,kk}$$

$$\begin{aligned} \frac{\delta F_{\text{curv}}}{\delta E_{ij}^*} = & (b_2^{\parallel} + b_2^{\perp} - 2b_2^{\parallel\perp}) \left( (\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po})E_{ij,lk} \right. \\ & \left. + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o})E_{ij,lkp} + \Pi_{kl}\Pi_{po}E_{ij,lkpo} \right) \\ & + (b_2^{\parallel\perp} - b_2^{\perp}) \left( \Pi_{po,po}E_{ij,kk} + 2\Pi_{po,o}E_{ij,kkp} + \Pi_{po}E_{ij,kkpo} \right. \\ & \left. + \Pi_{kl,oo}E_{ij,lk} + 2\Pi_{kl,o}E_{ij,lko} + \Pi_{kl}E_{ij,lkoo} \right) \\ & + b_2^{\perp}E_{ij,kkoo} \end{aligned}$$

# Lagrange multipliers

- ▶ Back to enforcing the constraints

$$\text{Minimize} \quad \int \left( f(\underline{\underline{E}}, \underline{\nabla} \underline{\underline{E}}, \dots) + \lambda_s g_s(\underline{\underline{E}}) + \lambda_t g_t(\underline{\underline{E}}) + \lambda_n g_n(\underline{\underline{E}}) \right) dV$$

- ▶ Need real, non-negative  $g_i(\underline{\underline{E}})$  that reflect the constraints:

$$g_s = |E_{ij} - E_{ji}|^2$$

$$g_t = |E_{ii}|^2$$

$$g_n = |E_{ik} E_{kj}^* - E_{ik}^* E_{kj}|^2$$

- ▶ Decide what to use for  $\lambda$ s – analytic guess, soft constraints etc.



Thank you for your attention

# Gradients of $\underline{\underline{\Pi}}$

- Results using the square root version of  $\underline{\underline{\Pi}}$

$$\Pi_{kl} = \frac{sE_{kl}}{\sqrt{E_{ab}E_{ab}}} + \frac{\delta_{kl}}{d}$$

$$\Pi_{kl,m} = \frac{s}{\sqrt{E_{ab}E_{ab}}} \left( E_{kl,m} - \frac{E_{kl}E_{cd}E_{cd,m}}{E_{ab}E_{ab}} \right)$$

$$\begin{aligned} \Pi_{kl,mn} = \frac{s}{\sqrt{E_{ab}E_{ab}}} & \left( E_{kl,mn} \right. \\ & - \frac{E_{kl,n}E_{cd}E_{cd,m} + E_{kl,m}E_{cd}E_{cd,n} + E_{kl}(E_{cd,n}E_{cd,m} + E_{cd}E_{cd,mn})}{E_{ab}E_{ab}} \\ & \left. + 3 \frac{E_{kl}E_{cd}E_{cd,m}E_{ef}E_{ef,n}}{(E_{ab}E_{ab})^2} \right) \end{aligned}$$