Extending a complex tensor model for smectics

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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

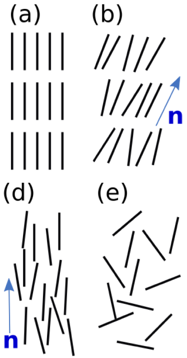

Figure: Crystaline, smectic C, nematic and isotropic phases

Describing smectics

- The layering is a density fluctuation

$$\rho(\underline{r},t) = \sum_{m=-\inf}^{+\inf} \psi_m e^{im\underline{q}\cdot\underline{r}} \simeq \rho_0 + 2\,\mathrm{Re}(\psi e^{i\underline{q_0}\cdot\underline{r}})$$

- Having $\psi = |\psi| e^{i\phi}$ gives
  - $|\psi|$ as the order parameter
  - Changes in ϕ lead to spacing differences
- $\underline{N} \propto \underline{q_0}$, can be an additional parameter or taken as $\underline{\nabla}\phi$

E theory

- Inspiration from Q-tensor and complex ψ

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

- Replace the real order parameters S with complex ψ

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

- Incorporates $\underline{N} \leftrightarrow -\underline{N}$ symmetry
- One object – allows numerical melting
- $\underline{N}$, $|\psi|$ and $\arg(\psi)$ are separate degrees of freedom

d is the number of dimensions, 2 or 3

E theory numerics

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

- Want to evolve $\underline{\underline{E}}$ directly as a dxd complex tensor
- Enforce the form above?
- Inspiration from $\underline{\underline{Q}}$ – symmetric and traceless
  - real so can be diagonalized
- Require $\underline{\underline{E}}$ be unitarily diagonalizable (normal), symmetric and traceless

Constraints on E

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

$$\underline{\underline{E}} = \underline{\underline{U}}^\dagger \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & -\lambda_1 - \lambda_2 \end{pmatrix} \underline{\underline{U}} \underbrace{= \cdots =}_{\text{also using symmetry}} \psi_1(\underline{N}\,\underline{N} - \frac{\underline{\underline{\delta}}}{3}) + \psi_2(\underline{M}\,\underline{M} - \frac{\underline{\underline{\delta}}}{3})$$

- With $\underline{N}$, $\underline{M}$ 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 ψs are the differences from the third eigenvalue
- Clearly biaxial form of the E we want!

Biaxial E

- Theory suggests a biaxial E in 3D
- Perpendicular layering?
  - Happens at interfaces in numerics – we get similar features to other studies using a tetratic order parameter
- No clear constraint to force it uniaxial

E theory – Ginzburg-Landau

- Dynamics using Ginzburg-Landau theory
- Need a free energy in terms of $\underline{\underline{E}}$
- Use $\frac{\partial E_{ij}}{\partial t} = -\mu \frac{\delta F}{\delta E_{ij}^*}$ + Lagrange multipliers for constraints

The free energy – bulk

- F must be real – need to match $\underline{\underline{E}}$ and $\underline{\underline{E}}^*$, simplest is

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

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

The free energy – elastic terms

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

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

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

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

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 $\underline{\nabla} \to a\underline{\underline{\Pi}} \cdot \underline{\nabla} + b\underline{\underline{T}} \cdot \underline{\nabla}$ a, b being some constants

$$
\begin{aligned}
E_{ij,k}E^*_{ij,k} &\to f_{\text{comp}} = b_1^{\parallel}\Pi_{kl}E_{ij,k}E^*_{ij,l} + b_1^{\perp}T_{kl}E_{ij,k}E^*_{ij,l} \\
E_{ij,kk}E^*_{ij,ll} &\to f_{\text{curv}} = b_2^{\parallel}\Pi_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm} + b_2^{\perp}T_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} \\
&\qquad + b_2^{\parallel\perp}(\Pi_{kl}E_{ij,lk}T_{mn}E^*_{ij,nm} + T_{kl}E_{ij,lk}\Pi_{mn}E^*_{ij,nm})
\end{aligned}
$$

Projection operators

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

$$\underline{\underline{\Pi}} = \sqrt{\frac{d-1}{d\underline{\underline{E}} : \underline{\underline{E}}}}\underline{\underline{E}} + \frac{\underline{\underline{\delta}}}{d}$$

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

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

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

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

$$
\begin{aligned}
\frac{\delta F_{\mathsf{bulk}}}{\delta E^*_{ij}} &= \frac{1}{2}(A + C E_{ab} E^*_{ab}) E_{ij} \\
\frac{\delta F_{\mathsf{comp}}}{\delta E^*_{ij}} &= -(b_1^{\|} - b_1^{\perp})(\Pi_{kl,l} E_{ij,k} + \Pi_{kl} E_{ij,kl}) - b_1^{\perp} E_{ij,kk} \\
\frac{\delta F_{\mathsf{curv}}}{\delta E^*_{ij}} &= (b_2^{\|} + b_2^{\perp} - 2 b_2^{\|\perp}) \Big((\Pi_{kl}\Pi_{po,po} + 2\Pi_{kl,o}\Pi_{po,p} + \Pi_{kl,po}\Pi_{po}) E_{ij,lk} \\
&\qquad + 2(\Pi_{kl,o}\Pi_{po} + \Pi_{kl}\Pi_{po,o}) E_{ij,lkp} + \Pi_{kl}\Pi_{po} E_{ij,lkpo} \Big) \\
&\quad + (b_2^{\|\perp} - b_2^{\perp}) \Big(\Pi_{po,po} E_{ij,kk} + 2\Pi_{po,o} E_{ij,kkp} + \Pi_{po} E_{ij,kkpo} \\
&\qquad + \Pi_{kl,oo} E_{ij,lk} + 2\Pi_{kl,o} E_{ij,lko} + \Pi_{kl} E_{ij,lkoo} \Big) \\
&\quad + b_2^{\perp} E_{ij,kkoo}
\end{aligned}
$$

Lagrange multipliers

- Back to enforcing the constraints

Minimize $$\int \left(f(\underline{\underline{E}}, \nabla \underline{\underline{E}}, \ldots) + \lambda_s g_s(\underline{\underline{E}}) + \lambda_t g_t(\underline{\underline{E}}) + \lambda_n g_n(\underline{\underline{E}}) \right) \mathrm{d}V$$

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

$$\begin{aligned} g_s &= |E_{ij} - E_{ji}|^2 \\ g_t &= |E_{ii}|^2 \\ g_n &= |E_{ik} E^*_{kj} - E^*_{ik} E_{kj}|^2 \end{aligned}$$

- Decide what to use for λs – analytic guess, soft constraints etc.

Thank you for your attention

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

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

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