E theory

- Building a smectic analogoue to nematic Q tensor
- Replace the real order parameters S with complex ψ
- Mainly thinking about uniaxial case

$$\underline{\underline{Q}} = S_1(\underline{N}\,\underline{N} - \frac{\underline{\underline{\delta}}}{d}) + \underbrace{\boxed{S_2(\underline{M}\,\underline{M} - \frac{\underline{\underline{\delta}}}{d})}}_{S_2 = 0 \text{ makes it uniaxial}}$$

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

- This allows the order to numerically melt at defects
- Preserves the $\underline{N} \to -\underline{N}$ symmetry

Relation to the density fluctuations

- $|\psi|$ represents quality of layers
- q_0 the base layering and ϕ the local offset from it
- $\underline{N}$ is the director, normal to the layering

$$\rho \sim \rho_0 + 2\,\mathrm{Re}(|\psi| e^{i\phi} e^{iq_0 \underline{N}\cdot\underline{r}})$$

- In $\underline{\underline{E}}$ theory these are all degrees of freedom, unlike when $\underline{N} = \frac{\underline{\nabla}\phi}{|\underline{\nabla}\phi|}$ is used
- Using $\underline{\underline{E}}$ makes melting in defect cores easier in numerical simulations

Thinking about constraints, and biaxiality

- Q is real, so symmetry makes it diagonalizable – this leads to the biaxial form
- If a complex matrix is normal ($\underline{\underline{E}}\,\underline{\underline{E}}^\dagger = \underline{\underline{E}}^\dagger \underline{\underline{E}}$) it can be diagonalized by a unitary matrix

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

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

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

- Overall 2*2 + 2 + 1 = 7 dof, 4 if uniaxial

The free energy

- Using the simplest terms
- We need to match $\underline{\underline{E}}$ and $\underline{\underline{E}}^*$ to make it real

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

- Elastic terms need gradients – below are "single elastic constant" terms

$|\underline{\nabla}\underline{\underline{E}}|^2 = E_{ij,k}E^*_{ij,k}$ the main term

$|\underline{\nabla}\cdot\underline{\underline{E}}|^2 = E_{ij,j}E^*_{ik,k}$ not considered in Jacks' work, possibly surface term?

$|\nabla^2\underline{\underline{E}}|^2 = E_{ij,kk}E^*_{ij,ll}$ the only double gradient term considered

Projection operators

- Gradients in different directions have different energy costs
- Working with uniaxial $\underline{\underline{E}}$ (or nearly so) – special direction is $\underline{N}$
- Projection operator $\underline{\underline{\Pi}} = \underline{N}\,\underline{N}$
- Perpendicular projections are then $\underline{\underline{T}} = \underline{\underline{\delta}} - \underline{\underline{\Pi}}$
- Adapt the free energies by $\underline{\nabla} \to \underline{\underline{\Pi}} \cdot \underline{\nabla} + \underline{\underline{T}} \cdot \underline{\nabla}$

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

Projection operators

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

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

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

- 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 $\underline{\underline{E}}$?

Dynamics and functional derivatives

- Starting from $\mu \frac{\partial E_{ij}}{\partial t} = -\frac{\delta F}{\delta E^*_{ij}}$, but need to preserve constraints
- If $\frac{\delta F}{\delta E^*_{ij}}$ is symmetric and traceless, then so will $\underline{\underline{E}}$
- Either treat $\underline{\underline{E}}$ as symmetric, or symmetrize after
- Normality is more complicated, Lagrange multiplier from Djorde's work
- It might be nice to constrain it to be unaxial too

Functional derivatives

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

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

Functional derivatives

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

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