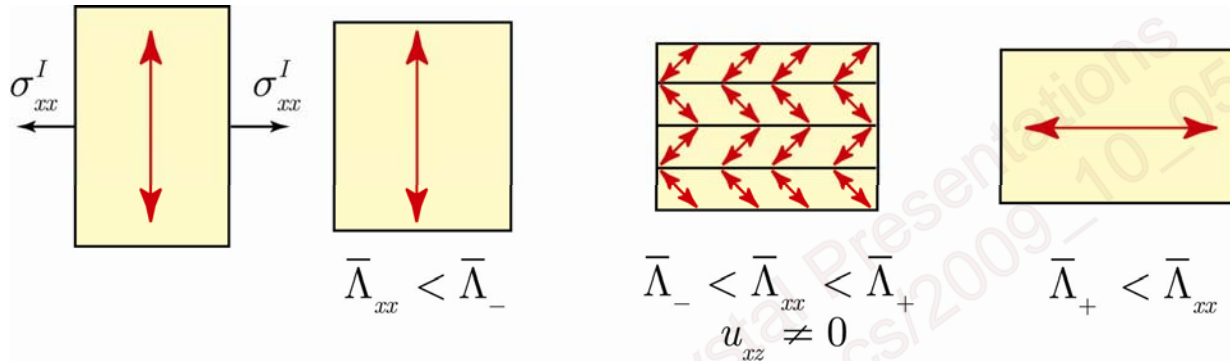


# Ward Identities and Semisoft Elasticity

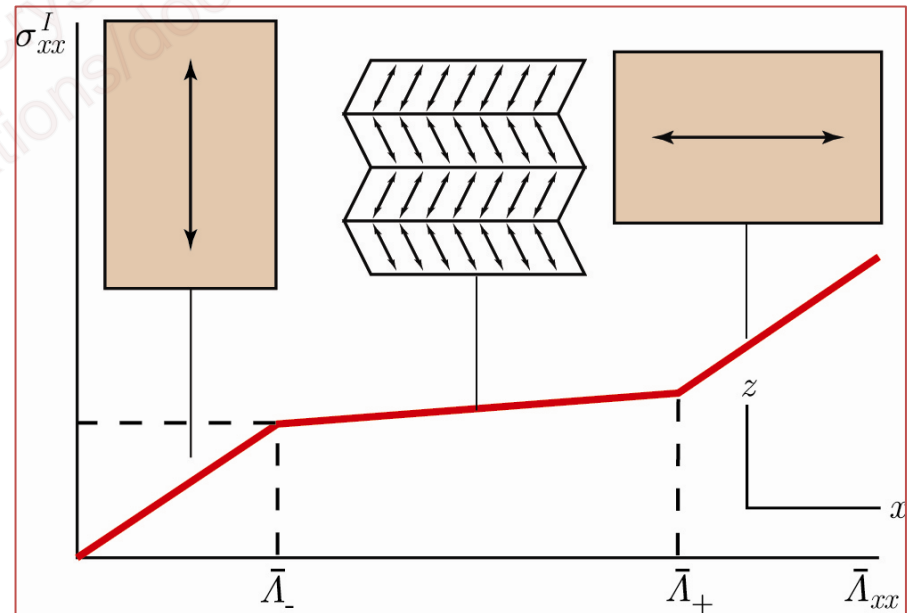
T.C. Lubensky

Fangfu Ye

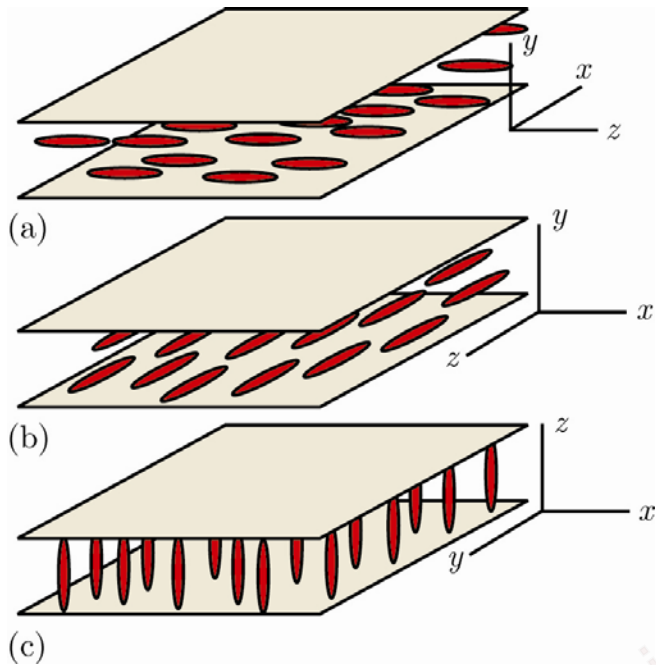
# Semisoft Elastic Response



$\Lambda_-$  and  $\Lambda_+$  signal  
 phase transitions at  
 which  $u_{xz}$ ,  
 respectively,  
 becomes nonzero  
 and vanishes



# Differential Elastic Response



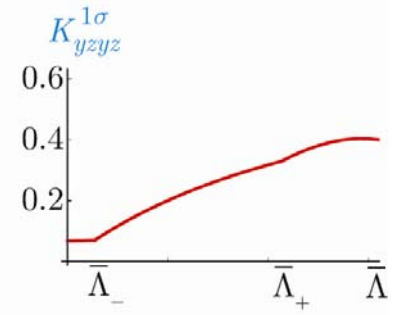
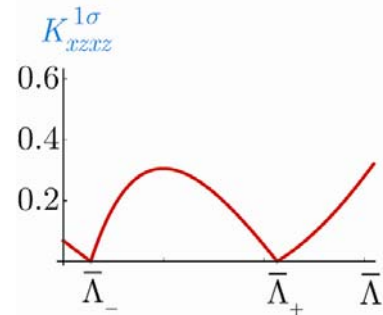
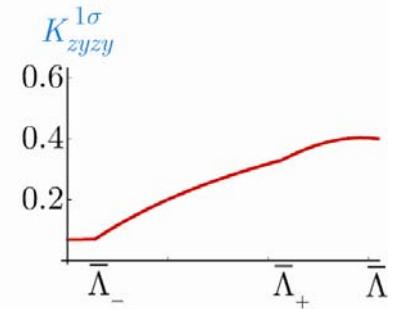
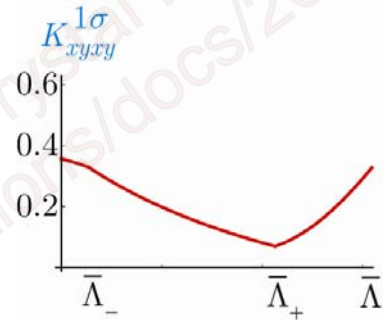
Displacement of the top plate relative to the bottom one produces  $xy$  and  $zy$  stress in (a) and (b) and  $xz$  and  $yz$  stresses in (c).

Forms of elastic tensors independent of detailed model: follow from Ward identities.

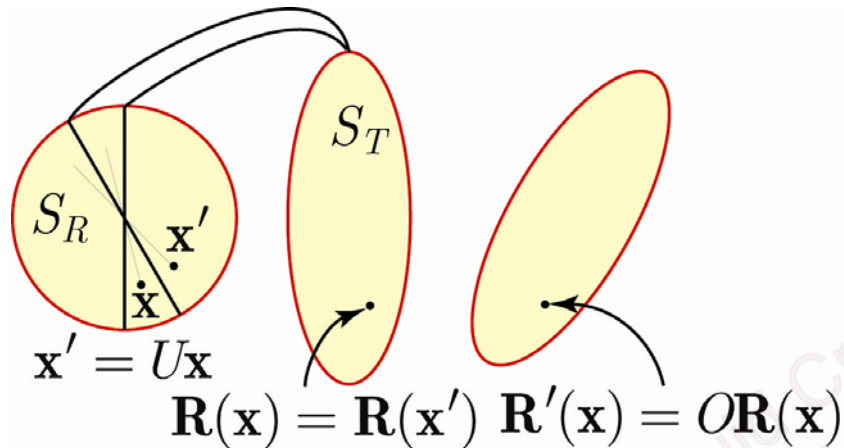
$$\delta\Lambda'_{ij} = K_{ijkl}^{\sigma} \delta\sigma_{kl}^I$$

$$(c) \delta\Lambda'_{zx} = \delta\Lambda'_{zy} = \delta\Lambda'_{xy} \\ = \delta\Lambda'_{yx} = 0$$

$$(a) \delta\Lambda'_{yx} = \delta\Lambda'_{yz} = \delta\Lambda'_{xz} \\ = \delta\Lambda'_{zx} = 0$$



# Deformations and Strains



$$\mathbf{R}(\mathbf{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x})$$

$$\Lambda_{i\alpha} = \frac{\partial R_i}{\partial x_\alpha} = \delta_{i\alpha} + \eta_{i\alpha}$$

$$\eta_{i\alpha} = \partial_\alpha u_i$$

$$dR^2 - dx^2 = 2u_{\alpha\beta} dx_\alpha dx_\beta$$

$$\underline{u} = \frac{1}{2} (\underline{\Lambda}^T \underline{\Lambda} - \underline{\delta}) \approx \frac{1}{2} (\underline{\eta} + \underline{\eta}^T)$$

$$u_{\alpha\beta} = \frac{1}{2} (\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha u_k \partial_\beta u_k)$$

$u_{\alpha\beta}$  is invariant under rotations in target space – used to describe systems without aligning stresses

# Elastic Energy

Decompose free energy into an isotropic part invariant under rotations in  $S_R$  (i.e. of  $\underline{x}$ ) and an anisotropic part (Assume Maier Saupe order parameter  $Q_{ij}$  has been integrated out).

$$f(\underline{u}) = f_{\text{iso}}(\underline{u}) + f_{\text{ani}}(\underline{u})$$

$$f_{\text{ani}}(\underline{u}) = -h u_{zz}$$

Add “internal” or second PK stress:  
still invariant w.r.t. to rotations in  $S_T$

$$g(\underline{u}) = f(\underline{u}) - \sigma_{ij} u_{ij}$$

New equilibrium deformation  
and strain

$$u_{ij}^0 = \frac{1}{2} \left( \Lambda_{ki}^0 \Lambda_{kj}^0 - \delta_{ij} \right)$$

$$\Lambda_{ij}^0 = \begin{pmatrix} \Lambda_{xx}^0 & 0 & \Lambda_{xz}^0 \\ 0 & \Lambda_{yy}^0 & 0 \\ 0 & 0 & \Lambda_{zz}^0 \end{pmatrix}$$

# Elastic Tensor

Energy of “harmonic” deviations from equilibrium

$$\delta g = \frac{1}{2} C_{ijkl} \delta u_{ij} \delta u_{kl}$$

New reference position

$$x'_i = \Lambda_{ij}^0 x_j; \quad \Lambda_{ik} = \Lambda'_{ik} \Lambda_{kj}^0$$

Strain w.r.t. to new reference pos.

$$\delta \underline{u} = \underline{\Lambda}^{0T} \cdot \underline{u}' \cdot \underline{\Lambda}$$

$$\delta g' = \frac{1}{2} C'_{ijkl} \delta u'_{ij} \delta u'_{kl}$$

Elastic tensor w.r.t to new reference space – symmetric under interchange of  $i$  and  $j$  and  $k$  and  $l$

$$C'_{ijkl} = \frac{1}{\det \underline{\Lambda}^0} \Lambda_{ip}^0 \Lambda_{kr}^0 C_{pqrs} \Lambda_{qj}^{0T} \Lambda_{sl}^{0T}$$

# Elastic Tensor for Deformations

External 1<sup>st</sup> PK stress induces deformation: Defines a direction in  $S_T$ :  $\sigma_{xx}^I$  is the force along  $x$  in the target space per unit area of the reference space

$$g^I = f(\underline{u}) - \sigma_{ij}^I \Lambda_{ij}$$

First PK stress tensor  
(in equilibrium)

$$\sigma_{ij}^I = \frac{\partial f}{\partial \Lambda_{ij}} = \Lambda_{ik} \frac{\partial f}{\partial u_{kj}}$$

$$K_{ijkl} = \left. \frac{\partial^2 f}{\partial \Lambda_{ij} \partial \Lambda_{kl}} \right|_{\underline{\Lambda} = \underline{\Lambda}^0} \\ = \delta_{ik} \sigma_{jl} + \Lambda_{ip}^0 \Lambda_{kr}^0 C_{pjrl}$$

$$\sigma_{ij} = (\Lambda^0)^{-1}_{ik} \sigma_{kj}^I$$

# Deformation Tensor Relative to New State

$$\Lambda_{ik} = \Lambda'_{ik} \Lambda^0_{kj}$$

$$\delta g'^I = \frac{1}{2} K'_{ijkl} \delta \Lambda'_{ij} \delta \Lambda'_{kl}; \quad K'_{ijkl} = \delta_{ik} \sigma'_{jl} + C'_{ijkl}$$

$$\sigma'_{jl} = \frac{1}{\det \underline{\Lambda}^0} \Lambda^0_{jp} \sigma_{qs} \Lambda^{0T}_{sl}$$

Cauchy Stress Tensor

$K'_{ijkl}$  has a symmetric part  $C'_{ijkl}$  and an anti-symmetric part, which defines preferred direction in  $S_T$

Small

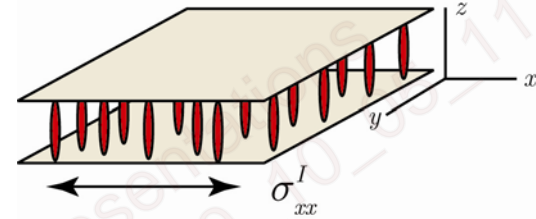
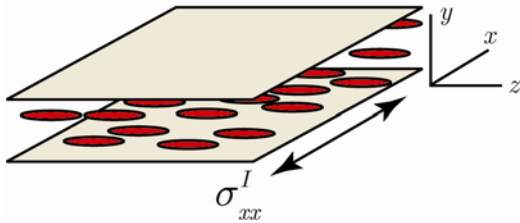
Deformations:

$$\delta g'^I = \frac{1}{2} [\sigma'_{xx} (\delta \theta_y - \varepsilon_{xz})^2 + 4C'_{xzxz} \varepsilon_{xz}^2]$$

$$\delta \theta_y = \frac{1}{2} (\Lambda'_{xz} - \Lambda'_{zx}); \quad \varepsilon_{xz} = \frac{1}{2} (\Lambda'_{xz} + \Lambda'_{zx})$$



# Elastic Moduli at “Constant Stress”



$$\delta\Lambda'_{yx} = \delta\Lambda'_{yz} = \delta\Lambda'_{xz} = \delta\Lambda'_{zx} = 0$$

$$\delta\sigma_{xy} \text{ or } \delta\sigma_{zy} \neq 0; \text{ and}$$

$$\delta\sigma_{xx} = \delta\sigma_{yy} = \delta\sigma_{zz} = 0$$

$$\delta\Lambda'_{zx} = \delta\Lambda'_{zy} = \delta\Lambda'_{xy} = \delta\Lambda'_{yx} = 0$$

$$\delta\sigma_{xz} \text{ or } \delta\sigma_{yz} \neq 0; \text{ and}$$

$$\delta\sigma_{xx} = \delta\sigma_{yy} = \delta\sigma_{zz} = 0$$

$$xx = 1; yy = 2; zz = 3;$$

$$xz = 4; zy = 5; xy = 6.$$

$$K'_{ab} \delta\Lambda'_b = \delta\sigma'^I_a$$

$$\delta\Lambda'_a = S'_{ab} \delta\sigma'^I_b; \quad \underline{S}' = \underline{K}'^{-1}$$

$$K'_{aa} = \frac{\partial \sigma'^I_a}{\partial \Lambda'_b} = \frac{1}{S'_{aa}}$$

# Ward Identities for $C'_{ijkl}$

$$f(\underline{u}) = f_{\text{iso}}(\underline{u}) - hu_{zz}$$

$f_{\text{iso}}(\underline{u})$  is invariant under  $\underline{u} \rightarrow \underline{U}\underline{u}\underline{U}^{-1}$

$$U^a_{ij} = \delta_{ij} - \theta_a \varepsilon_{ajk}$$

$$u_{ij} \rightarrow u_{ij} + \theta_a (\varepsilon_{aki} u_{kj} + \varepsilon_{akj} u_{ik})$$

These conditions must hold:

$$\frac{df}{d\theta_a} = \frac{\partial f}{\partial u_{ij}} \frac{du_{ij}}{d\theta_a} = \frac{df_{\text{ani}}}{d\theta_a} = -h_{ij} \frac{du_{ij}}{d\theta_a}$$

$$\begin{aligned} 2u_{yz} h &= 0, & a &= x; \\ 2u_{xz} (h - \sigma_{xx}) &= 0, & a &= y; \\ 2u_{xy} \sigma_{xx} &= 0, & a &= z. \end{aligned}$$

$$(\varepsilon_{ari} u_{rj} + \varepsilon_{arj} u_{ir})(\sigma_{ij} + h_{ij}) = 0$$

Hence

$$u_{xz} = 0 \text{ or } h = \sigma_{xx}$$

# Ward Identities for $C_{ijkl}$

$$\frac{\partial}{\partial u_{kl}} (\varepsilon_{ari} u_{rj} + \varepsilon_{arj} u_{ir}) (\sigma_{ij} + h_{ij}) = 0$$

$$2\varepsilon_{ari} u_{rj} C_{ijkl} + \varepsilon_{aki} (\sigma_{il} + h_{il}) + \varepsilon_{ali} (\sigma_{ik} + h_{ik}) = 0$$

$$u_{xz} = 0$$

$$C_{xyxy} = \frac{1}{2} \frac{\sigma_{xx}}{u_{xx} - u_{yy}};$$

$$C_{yzyz} = \frac{1}{2} \frac{h}{u_{zz} - u_{yy}};$$

$$C_{xzxz} = \frac{1}{2} \frac{h - \sigma_{xx}}{u_{zz} - u_{xx}}.$$

$$u_{xz} \neq 0$$

$$C_{xyxy} = \frac{u_{zz} - u_{yy}}{u_{xx} - u_{yy}} C_{yzyz} = \frac{1}{2} \frac{h}{\Delta};$$

$$C_{xzxz} = (C_{zzzz} - 2C_{xxzz} + C_{xxxx}) \frac{u_{xz}}{(u_{zz} - u_{xx})^2};$$

$$C_{xxxz} = (C_{xxzz} - C_{xxxx}) \frac{u_{xz}}{u_{zz} - u_{xx}};$$

$$\Delta = (u_{xx} - u_{yy})(u_{zz} - u_{yy}) - u_{xz}^2$$

# Ward Identities for $C'_{ijkl}$

$$u_{xz} = 0$$

$$\begin{aligned} C'_{xyxy} &= K'_{xyxy} = \frac{1}{\det \underline{\Lambda}} \frac{\Lambda_{xx}^2 \Lambda_{yy}^2 \sigma_{xx}}{\Lambda_{xx}^2 - \Lambda_{yy}^2}; \\ C'_{yzyz} &= K'_{yzyz} = \frac{1}{\det \underline{\Lambda}} \frac{\Lambda_{yy}^2 \Lambda_{zz}^2 h}{\Lambda_{zz}^2 - \Lambda_{yy}^2}; \\ C'_{xzxz} &= K'_{xzxz} = \frac{1}{\det \underline{\Lambda}} \frac{\Lambda_{zz}^2 \Lambda_{xx}^2 (h - \sigma_{xx})}{\Lambda_{zz}^2 - \Lambda_{xx}^2} \end{aligned}$$

When  $u_{xz}$  is nonzero, expressions are complicated

# Minimal Model

$$f_{\text{iso}} = \frac{1}{2} B u_{\alpha\alpha}^2 + \frac{1}{2} r \text{Tr} \underline{\tilde{u}}^{\sim 2} - w \text{Tr} \underline{\tilde{u}}^{\sim 3} + v \left( \text{Tr} \underline{\tilde{u}}^{\sim 2} \right)^2$$

Ye, et al. PRL **98**,  
147801 (2007)

$$\tilde{u}_{\alpha\beta} = u_{\alpha\beta} - \frac{1}{3} \delta_{\alpha\beta} u_{\gamma\gamma}$$

$$B \rightarrow \infty \Rightarrow u_{\alpha\alpha} = 0$$

$f_{\text{iso}} \rightarrow$  Maier - Saupe - de Gennes

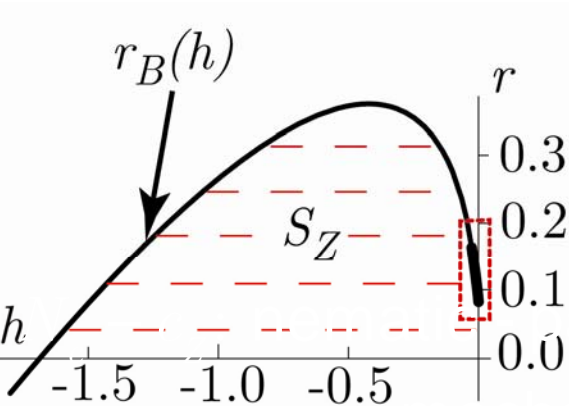
$$g = f_{\text{iso}}(\underline{\tilde{u}}) - h u_{zz} - \sigma_{xx} u_{xx}$$

$$\sigma_{ij} = \frac{\partial f}{\partial u_{ij}} : 2^{\text{nd}} \text{ Piola - Kirchhoff Stress tensor}$$

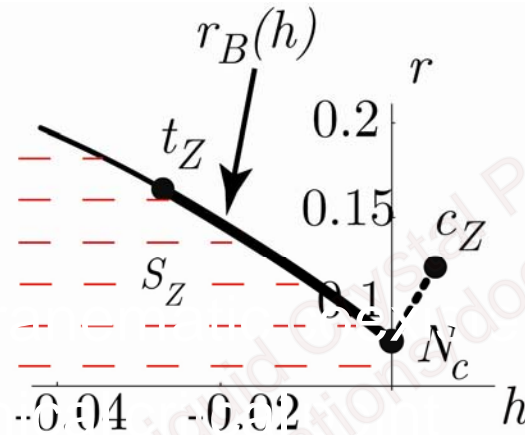
Return to Eng. and Cauchy stress later

- Not full incompressibility
- Nematic in crossed electric and magnetic fields

# Phase diagram at $\sigma_{xx}=0$



(a)



(b)

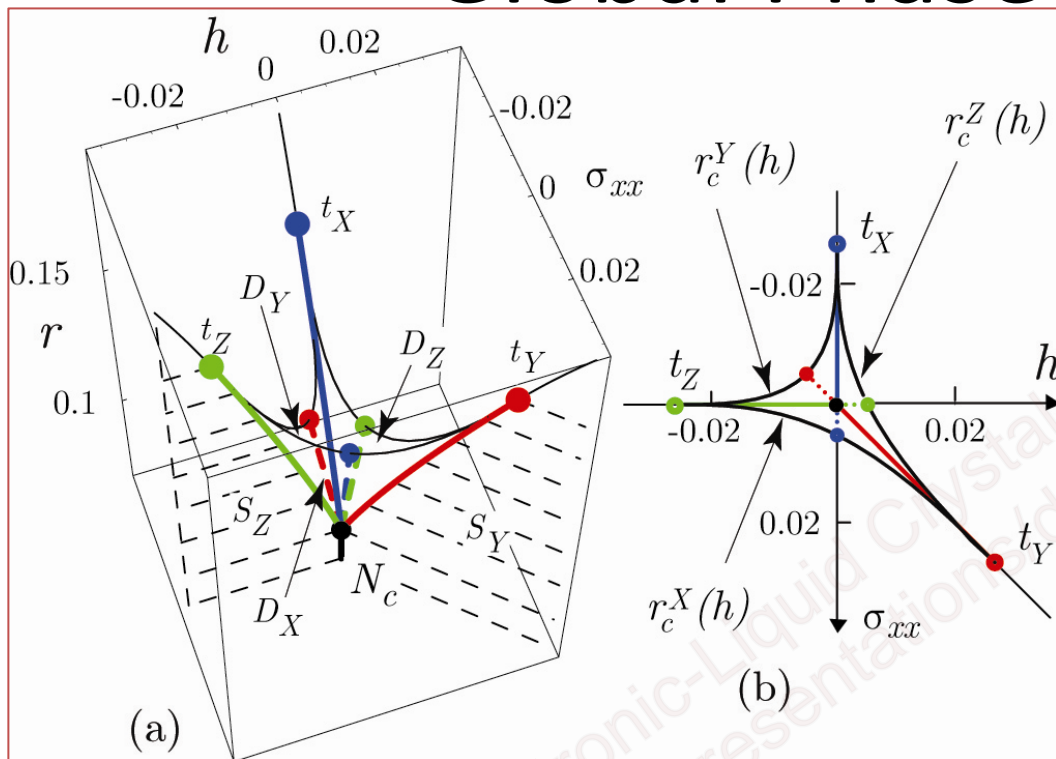
$$\tilde{u} = \begin{pmatrix} -\frac{S}{3} + \eta_1 & \eta_2 & 0 \\ \eta_2 & -\frac{S}{3} - \eta_1 & 0 \\ 0 & 0 & \frac{2S}{3} \end{pmatrix}$$

$$\begin{aligned} h > 0 & : S > 0 \\ h < 0 & : S < 0 \end{aligned}$$

$S_Z$  : Biaxial coexistence -  $\vec{\eta} = (\eta_1, \eta_2) = \eta(\cos 2\theta, \sin 2\theta)$   
 $\eta$  attains equilibrium value

$t_Z$  : Tricritical point;  $N_Z - t_Z$  - First - order line

# Global Phase Diagram



$D_X, D_Y, D_Z$  : Coexistence of discrete biaxial phases

$S_X, S_Y, S_Z$  : Coexistence of continuous biaxial phases

$$\tilde{u} = \begin{pmatrix} -\frac{S}{3} + \eta_1 & 0 & \eta_2 \\ 0 & \frac{2S}{3} & 0 \\ \eta_2 & 0 & -\frac{S}{3} - \eta_1 \end{pmatrix}$$

Order parameter near

$S_Y$  with  $S < 0$

R.G. Priest, Phys. Lett. A 47 475 (1974);  
Friskén, Bergersen, Palfy-Muhoray, Mol. Cryst. Liq. Cryst. 148, 45 (1987).

$$hu_{zz} + \sigma_{xx} u_{xx} = -hu_{yy} + (\sigma_{xx} - h)u_{xx}$$

$$g(r, h, \sigma_{xx}) = g(r, -h, \sigma_{xx} - h)$$

$$\text{Plane } h = \sigma_{xx} \equiv \text{Planes } h = 0, \sigma_{xx} = 0$$

# Modulus at “Constant Stress”

$$xx = 1; yy = 2; zz = 3;$$

$$xz = 4; zy = 5; xy = 6.$$

$$\underline{K}' = \begin{pmatrix} \sigma'_{xx} + C'_{11} & C'_{13} & C'_{14} & 0 \\ C'_{13} & C'_{33} & C'_{34} & 0 \\ C'_{14} & C'_{34} & C'_{44} & 0 \\ 0 & 0 & 0 & C'_{55} \end{pmatrix}$$

$$\begin{aligned} \sigma_{yy} &= 0 \\ \delta\Lambda_{ij} &= 0 \text{ for } ij \neq xz; yy & K'^{1\sigma}_{xzxz} &= C'_{44} \\ \delta\Lambda_{ij} &= 0 \text{ for } ij \neq yz; yy & K'^{1\sigma}_{yzyz} &= C'_{55} \end{aligned}$$

$$\begin{aligned} \sigma_{yy} = \delta\sigma_{zz} = \delta\sigma_{xx} &= 0 \\ \delta\Lambda_{ij} &= 0 \text{ for } ij \neq xx, yy, zz, xz & K'^{2\sigma}_{xzxz} &= \frac{\det \underline{K}'_{\parallel}}{C'_{33}(\sigma'_{xx} + C'_{11}) - (C'_{13})^2} \\ \delta\Lambda_{ij} &= 0 \text{ for } ij \neq xx, yy, zz, yz & K'^{2\sigma}_{yzyz} &= C'_{55} \end{aligned}$$



# Moduli Again

The general behavior of Elastic moduli shown below is independent of model details.

