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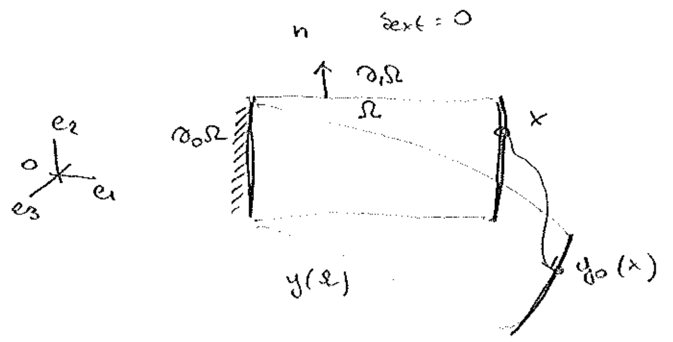
Topics in the Mechanics of Soft and Biological Matter

Contents

1. Nonlinear Elastostatics

Typical BVP for hyperelastic materials

$$\mathrm{Div}\, S + b_0 = 0 \quad \text{in } \Omega$$
$$S n = s_{ext} \quad \text{on } \partial_1 \Omega$$
$$y = y_0 \quad \text{on } \partial_0 \Omega$$



$u(x) = y(x) - x$ displacement at x

where

$y : \Omega \to \mathbb{R}^d$, def. map (globally inv.)

$F = \nabla y$ def. grad, $\det F > 0$

$S(x) = \partial_F W(F(x)) = \partial_F W(\nabla y(x))$

$S_{ij} = \dfrac{\partial}{\partial F_{ij}} W$

W energy density (a free-energy)

S 1st Piola-Kirchhoff stress.

Unknown: $y : \Omega \to \mathbb{R}^d$, def. map.

Data: b_0, s_{ext} given functions of x alone
forces per ref. volume/area at each x
Dead loads: must be indep. of y. How??

y_0 prescribed function on $\partial_0\Omega$

The data involve "traction" and "displacement" BCs. Once y is known, can determine def. field $F(x) = \nabla y(x)$ and stress distribution $S(x) = \partial_F W(\nabla y(x))$.

Solutions of BVP above are stationary points for the energy functional

$$I(y) = \underbrace{\int_\Omega W(\nabla y(x))\,dx}_{\text{stored elastic energy}} \underbrace{- \int_\Omega b(x)\cdot y(x)\,dx - \int_{\partial_1\Omega} s_{ext}\cdot y(x)\,dx}_{-\text{work done by ext. forces}}$$

$: \; -\int_\Omega b_0(x)\cdot(y(x) - x) = -\int_\Omega b_0 \cdot y + \text{const.}$

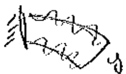
subject to $y = y_0$ on $\partial_0\Omega$.

Take $\delta y = \varepsilon u$, $u = 0$ on $\partial_0\Omega$ and consider

$$I(y+\varepsilon u) = \int_\Omega W(\nabla y + \varepsilon \nabla u) - \int_\Omega b_0 \cdot (y+\varepsilon u) - \int_{\partial_1\Omega} s_{ext} \cdot (y + \varepsilon u)$$

I stationary at y implies

$$\frac{d}{d\varepsilon} I(y+\varepsilon u)\Big|_{\varepsilon=0} = \int_\Omega \underbrace{\partial_F W(\nabla y)}_{S(\nabla y)} \cdot \nabla u - \int_\Omega b_0 \cdot u - \int_{\partial_1\Omega} s_{ext} \cdot u = 0 \qquad \forall u$$


$y(\Omega)$

[virtual work done by int. stresses = virtual work done by ext. forces $\forall$ virt. displ u perturbing $y(\Omega)$]

Since

$$\mathrm{Div}(S^T u) = \mathrm{Div}\, S \cdot u + S \cdot \nabla u \qquad \left[(S_{ji} u_j)_{,i} = S_{ji,i} u_j + S_{ji} u_{j,i} \right]$$

we have

$$0 = \int_\Omega \mathrm{Div}(S^T u) - \int_\Omega (\mathrm{Div}\, S + b_0) \cdot u - \int_{\partial_1\Omega} s_{ext} \cdot u \qquad \forall u .$$

$$= \int_{\partial_1\Omega} (Sn - s_{ext}) \cdot u - \int_\Omega (\mathrm{Div}\, S + b_0) \cdot u$$

Take $u \in C_0^\infty(\Omega)$ to get $\mathrm{Div}\, S + b_0 = 0$, then take u vanishing on $\partial_0\Omega$ but arbitrary on $\partial_1\Omega$ to get $Sn = s_{ext}$ on $\partial_1\Omega$. Thus, crit. pts of I are solutions of the equilibrium pb. For W, I strictly convex, the only crit. pt is the minimizer of I. Conversely is unrealistic, but we'll keep minimizing energy because minimizing free energy is the correct physical principle for equilibrium in isothermal conditions.

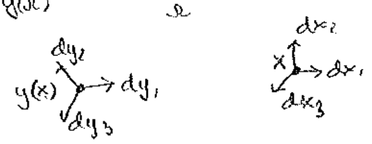
Incompressible case

Under normal loading conditions, rubbers deform experiencing negligible volume changes (shear modulus << bulk modulus)

Volume preserving def's. $\det \nabla y(x) \equiv 1$.

[Rem: formula for change of var's in volume int. involve Jacobian determinant of the map giving transf. of coordinates

$$\int_{y(\Omega)} f(y)\,dy = \int_\Omega f(y(x)) \det \nabla y(x)\, dx$$



$$y(x + dx_i) \simeq y(x) + F dx_i$$

$$\frac{dy}{dx} = \frac{dV_y}{dV_x} = \frac{F dx_1 \times F dx_2 \cdot F dx_3}{dx_1 \times dx_2 \cdot dx_3} = \det F$$]

This places a constraint on admissible def's.

Deal with it using Lagrange multiplier technique

$$\tilde{I}(y,\pi) = I(y) - \int_\Omega \pi(x)(\det \nabla y(x) - 1)\,dx$$

$$\tilde{I}(y+\varepsilon u, \pi+\varepsilon\delta\pi) = \text{---}\,''\,\text{---} - \int_\Omega (\pi+\varepsilon\delta\pi)(\det(\nabla y + \varepsilon\nabla u) - 1)$$

$$\frac{d}{d\varepsilon}\tilde{I}\Big|_{\varepsilon=0} = \text{---}\,''\,\text{---} - \int_\Omega \pi \underbrace{\partial_F \det(\nabla y)}_{\operatorname{cof}\nabla y}\cdot\nabla u - \int_\Omega \delta\pi(\det\nabla y - 1) = 0 \qquad \forall u, \delta\pi$$

[Re: $\operatorname{cof} F$: matrix of $d-1$ minors/cofactors.

For F invertible $\operatorname{cof} F = (\det F)\, F^{-T}$ from $F^{-1} = \frac{1}{\det F}(\operatorname{cof} F)^T$

$$f(F+U) = f(F) + Df(F)[U] + o(U)$$

$$\det(F+U) = \det F + U\cdot\operatorname{cof} F + \operatorname{cof} U\cdot F + \det U$$

$$= \det F + \underbrace{(\operatorname{cof} F)}_{\partial_F \det(F)}\cdot U + o(U)$$]

we obtain

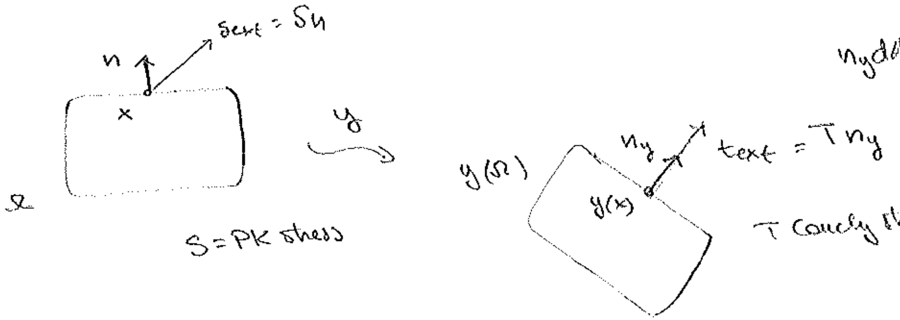
$$\int_\Omega \underbrace{(\partial_F W(\nabla y) - \pi \operatorname{cof}\nabla y)}_{S(\nabla y,\pi)}\cdot\nabla u - \int_\Omega b\cdot u - \int_{\partial_1\Omega} s_{ext}\cdot u - \int_\Omega \delta\pi(\det\nabla y - 1) = 0 \qquad \forall u, \delta\pi$$

Everything as before, except that now the stress is not entirely determined by the deformation. The scalar π, that carries a "reactive part" (reaction to incompressibility constraint), called pressure, is a further unknown of the BVP.

Remark π is the same pressure we are used to think as $-\pi I$ in the real world of Cauchy stresses.

Formula for change of variable in surface integrals.

$$n_y\, dA_y = (\operatorname{cof}\nabla y)\, n_x\, dA_x$$



S = PK stress

T Cauchy stress

$$\int_{\partial y(\Omega)} T(y)\, n_y\, dA_y = \int_{\partial\Omega} \underbrace{T(y(x))\operatorname{cof}\nabla y(x)}\, n_x\, dA_x = \int_{\partial\Omega} \underset{\sim}{S}\, n_x\, dA_x$$

$$S = T\operatorname{cof} F = (\det F)\, T F^{-T}$$

If $T = -\pi I$, then $t_{ext} = -\pi n_y$

$s_{ext} = S n_x = -\pi \operatorname{cof}\nabla y(x)\, n_x$

[same direction of t_{ext} and s_{ext} (!)]

Thm of power expended (conservation of energy).

Given a one-parameter of equilibrium states $\tau \mapsto y(x,\tau)$ [e.g., solutions of BVP under a one-par. family of displacement/traction BCs], then

$$\frac{d}{dt}\int_\Omega W(\nabla y(x,\tau))\,dx = \int_\Omega b_0 \cdot \underbrace{\frac{\partial}{\partial \tau} y}_{\dot y} + \int_{\partial\Omega} Sn \cdot \underbrace{\frac{\partial}{\partial \tau} y}_{\dot y}$$

$\tau \simeq$ time

Proof: Exercise (test equ's against $\dot y$ + integrate by parts) ///

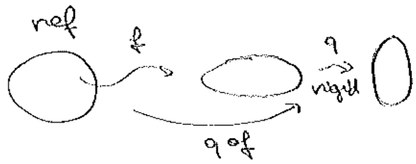
Remarks. Physical meaning: in the absence of dissipations, the rate at which we store energy is exactly the rate at which external work is performed on the system.

- It holds for both compressible and incompressible cases
- Extremely useful in the analysis of BVPs reproducing standard mech tests aiming at characterizing stress-strain response of engineering materials.

Constitutive Theory

a) Frame-indifference (FI): $\forall F$

$$W(QF) = W(F) \qquad \forall Q \in Rot$$



$$\nabla(q \circ f) = QF$$

A basic requirement for physical plausibility (and with a grain of salt: linear elasticity is not FI).

A consequence. Using right polar decomposition of F

$$Q = R^T$$

Re: $F = RU, \quad U = (F^TF)^{1/2} \in PSym$ (polar decomp.)

$$W(F) = W(QF) = W(R^TRU) = W(U)$$

Define

$$\tilde{W}(C) = \hat{W}(F^TF) = W(C^{1/2})$$

get

$$W(F) = \tilde{W}(F^TF)$$

[Frame indifference of W also leads automatically to symmetry of Cauchy stress, which guarantees that also balance of torques is satisfied]

Re: Polar decomposition

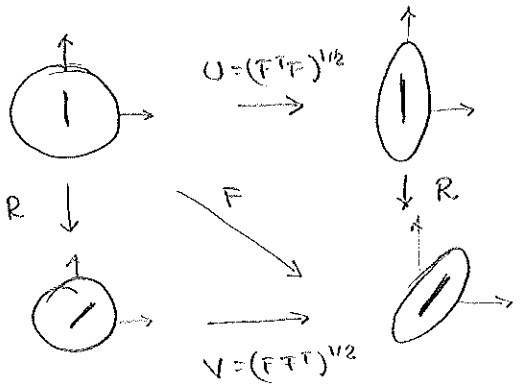
F with $\det F > 0$, then $\exists!\ R \in Rot$, $U, V \in PSym$ s.t.

$$F = RU = VR$$

Since $V = RUR^T$, V has same evalues of U and evectors rotated by R

$$(\omega_i(V), e_i(V)) = (\omega_i(U), R\, e_i(U))$$

Schematic diagram



$$e \mapsto Fe$$

$$|Fe|^2 = Fe \cdot Fe = F^TFe \cdot e$$

$$\max_{|e|=1} \left[\frac{|Fe|^2}{|e|^2}\right]^{1/2} = \max \left[(F^TF)e \cdot e\right]^{1/2} = \omega_{max}^{1/2}(F^TF) = \omega_{max}(U)$$

$\omega_{max}(U)$, $e_{max}(U)$ give direction of material fibre which is maximally stretched by F (reference orientation)

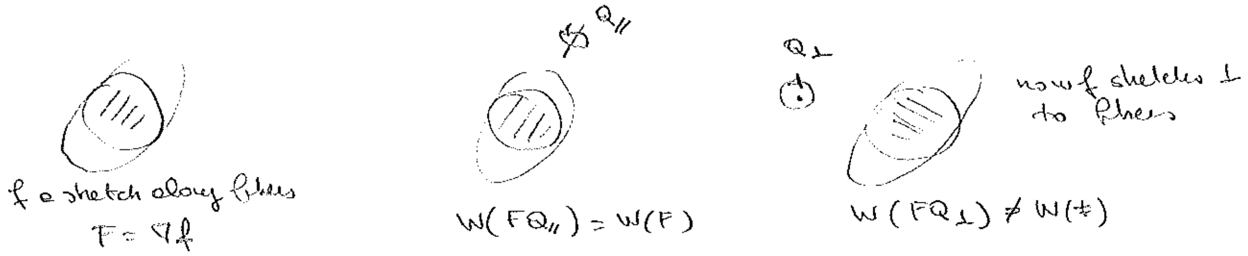
$\omega_{max}(V)$, $e_{max}(V) = R\, e_{max}(U)$ give the current orientation of the direction which is maximally stretched by F. (current orientation = after deformation).

b) Material Symmetry. $Q \in$ symmetry group of the material iff, $\forall F$,

$$W(FQ) = W(F)$$

[rotations of the ref. configurations that are not detectable by energy density, hence by mech. testing].

E.g. for a material with aligned fibres.



Isotropic materials are those with NO special directions at all, i.e. their symmetry group is = Rot

$$\forall F, \quad W(FQ) = W(F) \quad \forall Q \in Rot \quad (150).$$

For isotropic, FI materials, the energy density can only depend on the principal stretches (sq. roots of evalues of $B = FF^T$ or $C = F^TF$) or, equivalently, on the invariants of B or C.

$$\left.\begin{array}{l} W(QF) = W(F) \\ W(FQ) = W(F) \end{array}\right\} \forall Q \in Rot \Rightarrow W(F) = \left\{\begin{array}{l} \tilde{W}(F^TF) \\ \tilde{W}(Q^TF^TFQ) \end{array}\right. \forall Q \in Rot \Bigg\} = \tilde{W}\left(\begin{bmatrix} \lambda_1^2(F) & 0 & 0 \\ 0 & \lambda_2^2(F) & 0 \\ 0 & 0 & \lambda_3^2(F) \end{bmatrix}\right)$$

use Q that diagonalizes F^TF

or

$$W(F) = f(\lambda_1(F), \lambda_2(F), \lambda_3(F)), \quad \text{where } \underbrace{\lambda_i(F)}_{\substack{\text{principal stretches} \\ \text{or singular values of } F}} = \underbrace{\omega_i^{1/2}(C) = \omega_i^{1/2}(B)}_{\text{evalues of } C \text{ and } B}.$$

Rubber Elasticity

Neo-Hookean model

$$W(F) = \frac{1}{2}\mu\left[\mathrm{tr}(FF^T) - 3\right], \quad \det F = 1$$

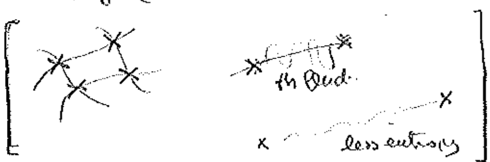
$\mu > 0$ shear modulus

Equivalent expressions: $\frac{1}{2}\mu(F\cdot F - 3)$, $\frac{1}{2}\mu(|F|^2 - 3)$, $\frac{1}{2}\mu[\mathrm{tr}B - 3]$, $\frac{1}{2}\mu(\mathrm{tr}C - 3]$, $\frac{1}{2}\mu[\lambda_1^2(F) + \lambda_2^2(F) + \lambda_3^2(F) - 3]$

$$W(F) = \begin{cases} \frac{1}{2}\mu[\mathrm{tr}(FF^T) - 3] & \text{if } \det F = 1 \\ +\infty & \text{else} \end{cases}$$

Remarks

- W depends only on principal stretches: it's iso and FI
- This is a basic conceptual model, like perfect gas law $p = nRT\frac{1}{V}$, not a tool for designing tires. It can be derived from stat mech: it's entropic elasticity of phantom gaussian chains. Useful, because it leads to $\mu = n k_B T$ (the material stiffens with temperature). Restoring force opposing stretching is due to decrease in entropy (lower number of microscopic realizations for a stretched chain).



- $W(F) \geq 0 \ \forall F$, $W(F) = 0 \Rightarrow F \in Rot$

Nothing to prove if $\det F \neq 1$. If $\det F = 1$, then (≠ between arithmetic and geometric mean) ⟺ strict concavity of the logarithm

$$\underbrace{\lambda_1^2 + \lambda_2^2 + \lambda_3^2}_{\mathrm{tr}B} \geq 3\big(\underbrace{\lambda_1^2\lambda_2^2\lambda_3^2}_{\det F^2 = \det B = 1}\big)^{1/3} = 3$$

$=$ only if $\lambda_1^2 = \lambda_2^2 = \lambda_3^2$ which, together with $\lambda_1\lambda_2\lambda_3 = 1 \Rightarrow \lambda_i = 1,\ i = 1, 2, 3$

This implies $B = I$ and $F = B^{1/2}R \in Rot$.

Mechanical tests. Assume specimen behaves as neohookean. Simulate outcome of mech exp's.

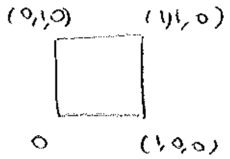
Small specimens, neglect gravity ($b_0 = 0$).

Enforce affine deformations (easier interpretation: def. can be estimated from boundary measurements)

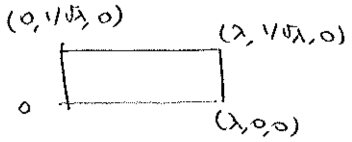
$$F = \text{const.} \Rightarrow S = \partial_F W(F) = \text{const.} \Rightarrow \mathrm{Div}\, S + b_0 = 0 \text{ trivially satisfied.}$$

Equil pb. reduces to checking consistency of F with displacement / traction BCs.

a) Uniaxial extension



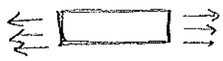
extend along e_1 by λ
leaving $\perp$ directions unconstrained



by symmetry $F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}$

$$[y(x) - 0] = F \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Q: How to realize this? If pull on vertical edges



On lateral surfaces, $Sn = s_{ext} = 0$

[Re: $S_{ij} = Se_j \cdot e_i$]

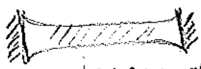
On $x_1 = 0$: $y_1 = \lambda x_1 = 0 \Rightarrow Se_1 \cdot e_1 \neq 0$

y_2, y_3 free $\Rightarrow Se_1 \cdot \{e_2, e_3\} = 0$

On $x_1 = 1$: $y_1 = \lambda x_1 = \lambda \Rightarrow Se_1 \cdot e_1 \neq 0$

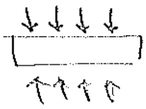
y_2, y_3 free $\Rightarrow Se_1 \cdot \{e_2, e_3\} = 0$

[If const. guarantee the



region of affine def.
but do local measurements
of F, cannot only
rely on boundary
measurements]

Alternatively, could be pushing on lateral faces,
leaving vertical ones free



Analysis of the experiment, assuming ⇇▭⇉

$$F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}, \quad \mathrm{cof}\, F = \underbrace{\det F}_{=1} \underbrace{F^{-T}}_{F^{-1}} = \begin{bmatrix} 1/\lambda & 0 & 0 \\ 0 & \sqrt{\lambda} & 0 \\ 0 & 0 & \sqrt{\lambda} \end{bmatrix}$$

$$W(F) = \frac{1}{2}\mu\,(F \cdot F - 3)$$

[$W(F+U) = (F+U)\cdot(F+U) =$
$= F\cdot F + F\cdot U + U \cdot F + U \cdot U$
$= W(F) + 2F\cdot U + o(U)$]

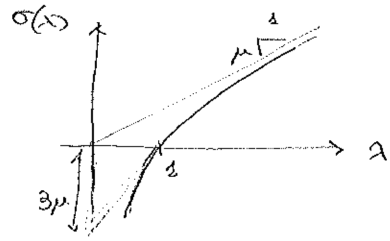
$$S = \partial_F W(F) - \pi\, \mathrm{cof}\, F = \mu F - \pi\, \mathrm{cof}\, F$$

$$= \mu \begin{bmatrix} \lambda & & \\ & 1/\sqrt{\lambda} & \\ & & 1/\sqrt{\lambda} \end{bmatrix} - \pi \begin{bmatrix} 1/\lambda & & \\ & \sqrt{\lambda} & \\ & & \sqrt{\lambda} \end{bmatrix}$$

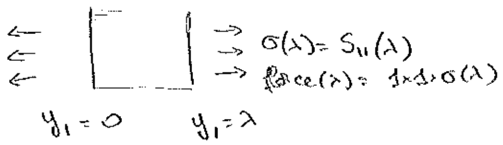
$$S_{22} = S_{33} = 0 \Rightarrow \mu \frac{1}{\sqrt{\lambda}} - \pi \sqrt{\lambda} = 0 \Rightarrow \pi = \frac{\mu}{\lambda}$$

$$S_{11} = \mu\lambda - \pi \frac{1}{\lambda} = \mu\lambda - \mu\frac{1}{\lambda^2} = \mu\left(\lambda - \frac{1}{\lambda^2}\right) = \sigma(\lambda)$$

$$\left.\frac{d}{d\lambda}\sigma(\lambda)\right|_{\lambda=1} = \left.\mu\left(1 + \frac{2}{\lambda^3}\right)\right|_{\lambda=1} = 3\mu$$



Can get $\sigma(\lambda)$ from thm of power expended



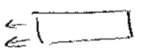
$$\frac{d}{d\lambda}\int_{\Omega} W(F(\lambda)) = 1\times 1\times 1\ \frac{d}{d\lambda}\left(\frac{1}{2}\mu\left(\lambda^2 + \frac{2}{\lambda}\right)\right) = \mu\left(\lambda - \frac{1}{\lambda^2}\right)$$

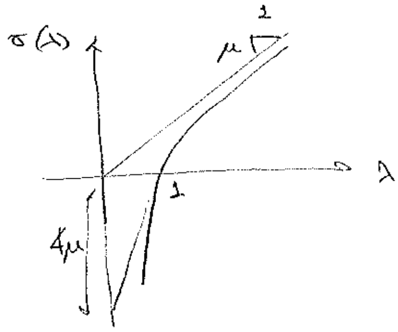
$$\int_{\partial\Omega} S(F(\lambda))\, n \cdot \frac{d}{d\lambda} y = 1\times 1 \cdot S_{11}(\lambda) \cdot 1$$

Remark: Not realistic, Ogden-type energies for stiffening at high stretches.

b) Plane strain extension (or pure shear)

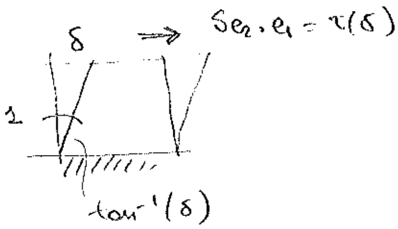
$$F = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\lambda & 0 \\ 0 & 0 & 1 \end{bmatrix},$$ no deformation in e_3 direction.

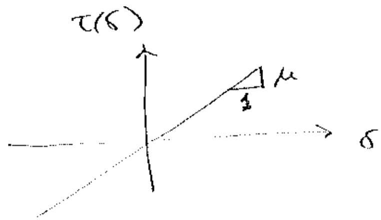
Anyway  $\sigma(\lambda)$ get



c) Simple shear

$$F = \begin{bmatrix} 1 & \delta & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$



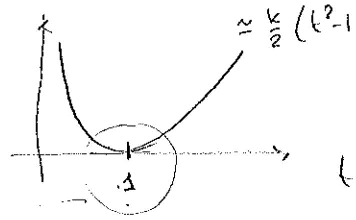


Compressible case

$W = W_{dev}(F)$, $\det F = 1$

$W_{comp}(F) = W_{dev}\left((\det F)^{-1/3} F\right) + W_{vol}(\det F)$

$W_{vol}(t)$



$\simeq \frac{k}{2}(t^2 - 1 - 2\log t)$

E.g., for Neohookean near $B = I$

near 1

$\simeq \frac{k}{2}(\det F - 1)^2$

$k > 0$.

$$W_{comp}(B) = \frac{1}{2}\mu\left((\det B)^{-1/3} \operatorname{tr} B - 3\right) + \frac{k}{2}\left(\det(B^{1/2}) - 1\right)^2$$

Small strain theory (geometrically linear theory)

Assume $B = I + 2E$, E small

$$W_{comp}(B) = \frac{1}{2}\mu\left((\det B)^{-1/3} \operatorname{tr} B - 3\right) + \frac{k}{2}\left(\det(B^{1/2}) - 1\right)^2$$

$$= \frac{1}{2}\mu\left(\left(\det(I+2E)\right)^{-1/3} \operatorname{tr}(I+2E) - 3\right) + \frac{k}{2}\left(\det\left((I+2E)^{1/2}\right) - 1\right)^2$$

$\vdots$ (Ex)

$$\simeq \mu \, |E_d|^2 + \frac{k}{2} (\operatorname{tr} E)^2$$

where $E_d = E - \frac{1}{3}(\operatorname{tr} E) I$ deviatoric part of E. and we have used

$\det(I+H) = 1 + \operatorname{tr} H + \operatorname{tr} \operatorname{cof} H + \det H$

$(I + 2E)^{1/2} = I + E + \dots$

Taylor expansions of various functions.

Since $F = I + \nabla u$

$B = FF^T = (I + \nabla u)(I + \nabla u^T) = I + 2 \operatorname{sym} \nabla u + \nabla u \nabla u^T$

we identify E in $B = I + 2E$ with $\operatorname{sym} \nabla u$ and obtain the variational formulation of isotropic linear elasticity

$$I(u) = \int_\Omega \mu \left|(\operatorname{sym} \nabla u)_d\right|^2 + \frac{k}{2}(\operatorname{div} u)^2 - \int_\Omega b \cdot u - \int_{\partial_s \Omega} s_{ext} \cdot u \quad + \text{BCs}$$

where $u(x) = y(x) - x$ is the displacement

$\mu > 0$ shear modulus

$k > 0$ bulk modulus.

[Rigorous proof by Gamma-convergence, Agostiniani et al, 2011]

2. Nematic Elastomers

NEs want current max stretch $e_{max}(V) \parallel n$, current nematic director

$$\omega_{max}(V) = (a^{1/3})^{e}$$

$F = I \qquad F = L^{1/2}(n)$

$\nearrow n, \ |n| = 1$

$\swarrow\!\!\nearrow \ N = n \otimes n$ ($\pm n$ symmetry)

[de Gennes order tensor, Fundamental symmetry case

$$Q = s\left(n \otimes n - \tfrac{1}{3} I\right)$$

↳ if constant, get Frank's theory]

Spont. stretch $\quad \alpha \, n \otimes n + \frac{1}{\sqrt{\alpha}} (I - n \otimes n)$

$$\alpha = a^{1/3} > 1, \quad \frac{1}{\sqrt{\alpha}} = a^{-1/6} < 1$$

Incompressible $\quad \det B = 1$

Energy minimized if $\quad B = FF^T = \alpha^2 N + \frac{1}{\alpha}(I - N) =: L(n)$

Possible expression $\quad \overline{W}(F, n) = \frac{1}{2}\mu \left[\operatorname{tr}(B L^{-1}(n)) - 3 \right]$

[$\det(BL^{-1}) = 1$

$\operatorname{tr}(BL^{-1})$ minimized at value 3 ↳

$BL^{-1} = I$

$\Longleftrightarrow \ B = L(n)$]

Remarks

- Ref. config. ($F = I$) is the one the system would have if heated to isotropic case

  Spontaneous stretch is $F = L^{1/2}(n)$
- All this is really due to Warner–Terentjev (mid 90's)
- $$\inf_{y, n} \int_\Omega \overline{W}(\nabla y, n) - \cdots$$ + BC of def & traction (not involving n)

$$\inf_{y} \int_\Omega \underbrace{\min_{|n|=1} \overline{W}(\nabla y, n)}_{=: W(\nabla y)} - \cdots + \text{BC's}$$ ~~not involving~~

work mostly with this in the sequel

Some explicit formulas

$$L(n) = a^{2/3} N + a^{-1/3}(I - N)$$

$$\Rightarrow \quad L^{-1}(n) = a^{-2/3} N + a^{1/3}(I - N) = a^{1/3}\Big(I - \underbrace{\big(1 - \tfrac{1}{a}\big)}_{>0} N\Big)$$

$$\bar W(F,n) = \tfrac12 \mu\,\big[\overbrace{B\cdot L^{-1}(n)}^{BL^{-1}\cdot I = B\cdot L^{-1}} - 3\big] = \tfrac12 \mu a^{1/3}\Big[\mathrm{tr}B - \big(1-\tfrac1a\big)\underbrace{B\cdot n\otimes n}_{B_{ij}n_in_j} - 3a^{-1/3}\Big] \geq 0, \quad = 0 \text{ for } B = L(n)$$

$$W(F) = \min_{|n|=1} \bar W(F,n) = \tfrac12 \mu a^{1/3}\Big(\mathrm{tr}B - \big(1-\tfrac1a\big)\underbrace{\max_{|n|=1} \overbrace{Bn\cdot n}}_{} - 3a^{-1/3}\Big]$$

$= \lambda^2_{max}(B)$, max evalue of $B = FF^T$ achieved by

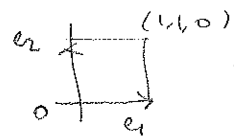
$n^* = e_{max}(B)$

$$= \tfrac12 \mu a^{1/3}\Big[\lambda^2_{min}(F) + \lambda^2_{mid}(F) + \tfrac1a \lambda^2_{max}(F) - 3a^{-1/3}\Big]$$

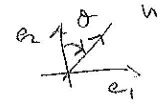
- It's an ISO and FI expression
- Recover NeoH. for $a = 1$, but have changed convex $|F|^2$ into nonconvex expression.

Energy landscape.

2d (plane-strain) perturbations of spont. strain associated with $n = e_2$



$y(x) = 0 + Fx$, $\quad F = \begin{bmatrix} \cdot & \cdot & 0 \\ \cdot & \cdot & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$,



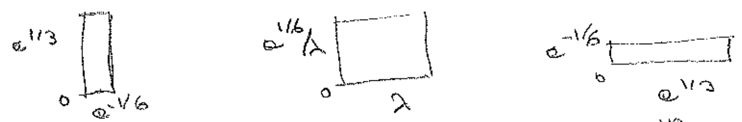
$n = (\sin\theta, \cos\theta, 0)$

$n \in \mathrm{span}\{e_1, e_2\}$

Ω = unit ref. cube

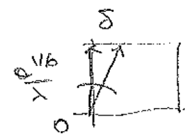
Consider $\lambda \in [a^{-1/6}, a^{1/3}]$

$$F(\lambda,0) = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & a^{1/6}/\lambda & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$$



$F(a^{-1/6},0) = L^{1/2}(e_2)$ $\quad F(\lambda,0)$ $\quad F(a^{1/3},0) = L^{1/2}(e_1)$

$$F(\lambda,\delta) = \begin{bmatrix} \lambda & \delta & 0 \\ 0 & a^{1/6}/\lambda & 0 \\ 0 & 0 & a^{-1/6} \end{bmatrix}$$



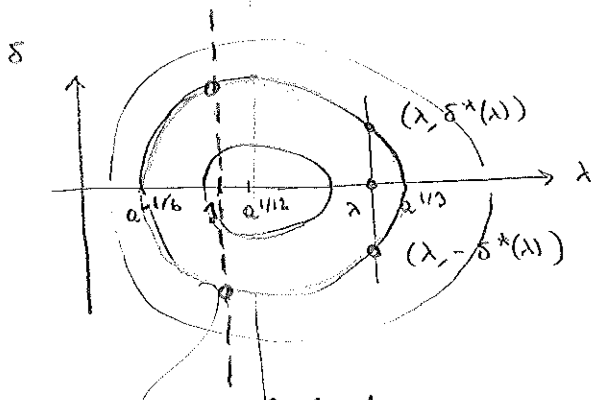
$F(\lambda,\delta)e_2 = \begin{bmatrix} \delta \\ a^{1/6}/\lambda \\ 0 \end{bmatrix}$

$\tan\psi = \dfrac{\lambda}{a^{1/6}}\,\delta$ (shear amplitude)

$$B = FF^T = \begin{bmatrix} \lambda^2+\delta^2 & \delta a^{1/6}/\lambda & 0 \\ \cdot & a^{1/3}/\lambda^2 & 0 \\ \cdot & \cdot & a^{-1/3} \end{bmatrix}$$

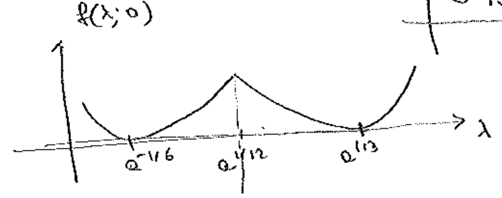
$$\bar W(F(\lambda,\delta), n(\theta)) = \bar f(\lambda,\delta,\theta) = \dots$$

$$\min_\theta \bar W(F(\lambda,\delta), n(\theta)) = W(F(\lambda,\delta)) = f(\lambda,\delta) = \dots \quad \leftarrow \text{plot.}$$

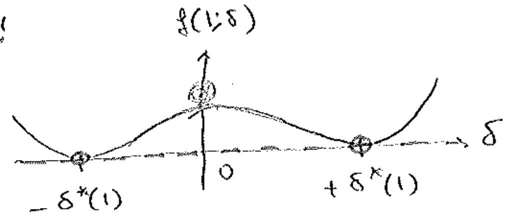


zero-level set
This must come from $B = L(n)$

Section at $\delta = 0$



Section at $\lambda = 1$



$$\mathrm{tr}\, B(\lambda, \delta) = \lambda^2 + \delta^2 + \frac{e^{1/3}}{\lambda^2} + e^{-1/3}$$

$$\mathrm{tr}\, L(n) = e^{2/3} + e^{-1/3} + e^{-1/3}$$

} imposing equality, we obtain

$$\lambda^2 + \delta^2 + \frac{e^{1/3}}{\lambda^2} = e^{2/3} + e^{-1/3} \Rightarrow \delta^2 = \dots = (e^{2/3} - \lambda^2)\left(1 - \frac{e^{-1/3}}{\lambda^2}\right)$$

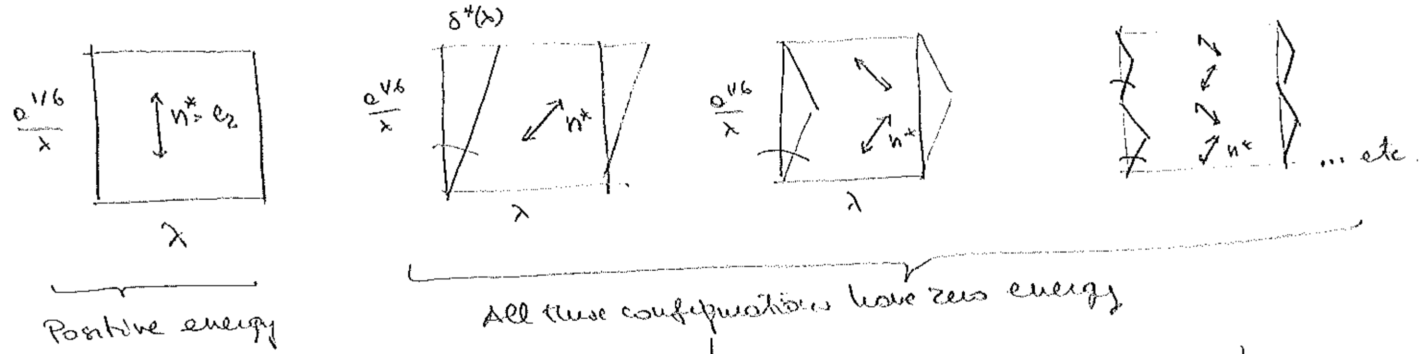
$$\boxed{\delta^*(\lambda) = \left(1 - \frac{e^{-1/3}}{\lambda^2}\right)^{1/2} \left(e^{2/3} - \lambda^2\right)^{1/2}}$$

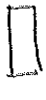
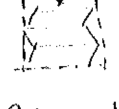
[this gives energy minima at prescribed λ. will do this many times again in the future]

Use of the plot

Fix $\lambda \in [e^{-1/6}, e^{1/12})$ and verify that, in this range $\boxed{e_{max}(B(\lambda, 0)) = n^* = e_2}$ (EX)

The energy $\delta \mapsto f(\lambda; \delta)$ is even, hence stationary at $\delta = 0$.
This means that, at frozen λ, the state $\delta = 0, \theta = 0$ is an equilibrium. But $\left.\frac{\partial^2}{\partial \delta^2} f(\lambda; \delta)\right|_{\delta = 0} < 0$ shows that this unsheared state is unstable towards shears and shear banding.



[Idea: compress  inside a box  ≃ accordion/concertina pattern!

This explains the "stripe-domain" instability observed in experiments.
(optical contrast with transparent/opaque horizontal bands due to spatial oscillations of the nematic director).

A calculation in the same spirit by de Gennes (mid 80's) gave the inspiration to synthesize NEs (early 90's).

P.G de Gennes' version · expand around $\delta = \theta = 0$, an equilibrium state $\forall \lambda$ fixed.

[SKIP?]

$$\bar{f}(\lambda;\delta,\theta) = \bar{f}(\lambda;0,0) + \underbrace{\frac{\partial \bar{f}}{\partial \delta}(\lambda;0,0)}_{=0}\delta + \underbrace{\frac{\partial \bar{f}}{\partial \theta}(\lambda;0,0)}_{=0}\theta$$

$$+\frac{1}{2}\Big\{ \underbrace{\frac{\partial^2 \bar{f}}{\partial \delta^2}(\lambda,0,0)}_{G_{\delta\delta}}\delta^2 + 2\underbrace{\frac{\partial^2 \bar{f}}{\partial \delta \partial \theta}(\lambda;0,0)}_{G_{\delta\theta}}\delta\theta + \underbrace{\frac{\partial^2 \bar{f}}{\partial \theta^2}(\lambda;0,0)}_{G_{\theta\theta}}\theta^2 \Big\} + \text{h.o.t.}$$

$$G_{\theta\theta} = \mu a^{1/3}\left(\frac{a-1}{a}\right)\left(\frac{a^{1/3}}{\lambda^2} - \lambda^2\right) > 0 \text{ if } \lambda < a^{1/12}$$

Find $\theta^*(\delta)$ (equil. value of θ, as a function of δ, λ. It depends on λ as well, but omit from notation.) frozen stretching parameter

$$\frac{\partial}{\partial \theta}\frac{1}{2}\left\{G_{\delta\delta}\delta^2 + 2G_{\delta\theta}\delta\theta + G_{\theta\theta}\theta^2\right\} = G_{\delta\theta}\delta + G_{\theta\theta}\theta = 0 \Rightarrow \theta^* = -\frac{G_{\delta\theta}}{G_{\theta\theta}}\delta$$

Plug back into $\bar{f}$

$$\bar{f}(\lambda;\delta,\theta^*(\delta)) = \text{const.} + \frac{1}{2}\left\{G_{\delta\delta}\delta^2 - 2\frac{G^2_{\delta\theta}}{G_{\theta\theta}}\delta^2 + G_{\theta\theta}\frac{G^2_{\delta\theta}}{G^2_{\theta\theta}}\delta^2\right\} + \text{h.o.t}$$

$$\simeq \frac{1}{2}\underbrace{\left\{G_{\delta\delta} - \frac{G^2_{\delta\theta}}{G_{\theta\theta}}\right\}}_{G_{eff}}\delta^2$$

$G_{eff} = \mu a^{1/3}(1 - g(\lambda)) < 0$ for $\lambda > a^{-1/6}$

a strictly increasing function starting from $g(\lambda)\big|_{\lambda = a^{-1/6}} = 1$

Compare with

$$\bar{f}(\lambda,\delta,\theta=0) \simeq \frac{1}{2}G_{\delta\delta}\delta^2$$

$G_{\delta\delta} = \mu a^{1/3} > 0.$

$G_{eff} < G_{\delta\delta}$ always, because of elasto-nematic coupling.

Conclude:

- Director mobility always decreases shear modulus: $G_{eff} < G_{\delta\delta}$ (LCEs first synthesized in early 90s)
  On this basis, de Gennes proposed in the mid 80's that a rubbery solid with embedded nematic mesogens could have interesting mech. properties because of soft modes arising from elasto-nematic coupling.
- The cause for the instability $G_{eff} < 0$ is the mobility of the director, which reduces the effective shear modulus to zero or to negative values, as soon as λ enters the range $(a^{-1/6}, a^{1/12})$

In reality, one sees instabilities and vanishing of shear moduli only past a stretch threshold $\lambda_c > a^{-1/6}$.

Not surprising. There exist a preferred direction $n_0 = e_z$, the director orientation at crosslinking.

$$\bar W_\beta(F,n) = \frac{1}{2}\mu\left\{\left(\mathrm{tr}\, B L^{-1}(n) - 3\right) + \beta\left(\mathrm{tr}\, C L^{-1}(n_0) - 3\right)\right\}, \qquad \det B = \det C = 1$$

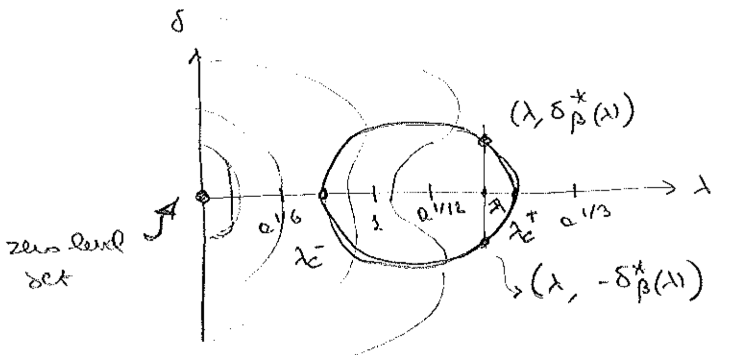
$\bar W_\beta \geq 0$, $= 0$ only if both $B = L(n)$ and $C = L(n_0)$

$B = L(n) \Rightarrow F = VR = L^{1/2}(n)R = \left[\alpha\, n\otimes n + \frac{1}{\sqrt{\alpha}}(I - n\otimes n)\right]R$ (Ex)

$C = L(n_0) \Rightarrow F = QU = Q L^{1/2}(n_0) = Q\left[\alpha\, n_0\otimes n_0 + \frac{1}{\sqrt{\alpha}}(I - n_0\otimes n_0)\right]$

equality of RHSs $\Rightarrow$ $Q = R$ and $\boxed{n = \pm R n_0, \quad F = R L^{1/2}(n_0)}$

Energy landscape in (λ,δ) plane similar as before, except that region of nonconvexity and instabilities are shifted past λ_c.



$$\lambda_c = \lambda_c^- = \left(\frac{1+\beta}{a+\beta}\right)^{1/2} a^{1/6}$$

$$\delta^*_\beta(\lambda) = \frac{1}{\lambda}\left(\frac{a^{1/3}}{\lambda_c^2} - \lambda^2\right)\left(\lambda^2 - \lambda_c^2\right)^{1/2} \qquad \text{(skip)}$$

$$\lambda_c^+ = \frac{a^{1/6}}{\lambda_c}$$

Small strain theory

Assume that spontaneous distortions and Cauchy-Green strains are small perturbations of I

$$a^{1/3} = 1 + \gamma, \qquad \gamma \ll 1$$

$$C = B = I + 2E, \qquad |E| = \gamma \ll 1$$

Taylor expand up to γ^2:

$$\frac{1}{2}\mu\left[(\det B)^{-1/3} B\cdot L^{-1}(n) - 3\right] + \frac{1}{2}\mu\beta\left[(\det C)^{-1/3} C\cdot L^{-1}(n_0) - 3\right] + \frac{k}{2}\left(\det(B^{1/2}) - 1\right)^2$$

$$\downarrow \qquad\qquad \downarrow \qquad\qquad \downarrow$$

$$\bar\varphi_\beta(E,n) = \mu\,|E_d - E_0(n)|^2 + \mu\beta\,|E_d - E_0(n_0)|^2 + \frac{k}{2}(\mathrm{tr}\, E)^2$$

Incompressible version

$\mathrm{tr}\, E = 0$

$$\bar\varphi(E,n) = \mu\,|E - E_0(n)|^2$$

$$\bar\varphi_\beta(E,n) = \bar\varphi(E,n) + \mu\beta\,|E - E_0(n_0)|^2$$

where $E_0(n) = \frac{3}{2}\gamma\left(n\otimes n - \frac{1}{3}I\right)$

$= \frac{3}{2}\frac{\gamma}{S}\, S\left(n\otimes n - \frac{1}{3}I\right) = \tilde\gamma\, Q$ ↑ order tensor

$= \gamma\, n\otimes n - \frac{\gamma}{2}(I - n\otimes n)$

$|E_0(n)| = \left(\gamma^2 + 2\frac{\gamma^2}{4}\right)^{1/2} = \sqrt{\frac{3}{2}}\,\gamma$

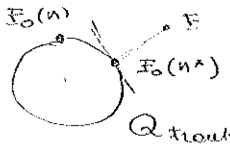
As n spans S^2, $E_0(n)$ spans symm, traceless, uniaxial tensors of magnitude $\sqrt{\frac{3}{2}}\,\gamma$

$\left\{E \in M^{3\times 3}_{sym},\ \mathrm{tr}\, E = 0,\ \text{uniaxial},\ |E| = \sqrt{\tfrac{3}{2}}\,\gamma\right\} =: Q_{\text{Frank}}$

Geometric structure of the energy landscape (case tr E = 0)

$$\bar{\varphi}(E,n) = \mu\,|E - E_0(n)|^2$$

$$\varphi(E) = \min_{|n|=1} \mu\,|E - E_0(n)|^2 = \mu\, \mathrm{dist}^2(E, Q_{trough})$$



Q_{trough} = { symm, traceless, uniaxial tensor of magnitude $\sqrt{\tfrac{3}{2}}\,\gamma$ }

$\bar{\varphi}$ penalizes relative deformations $E^e = E - E_0(n)$

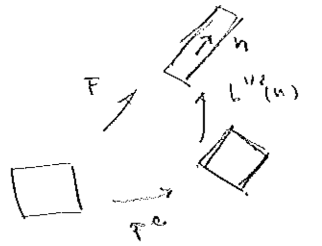
Looking back at nonlinear energy

$$FF^T L^{-1}(n)\cdot I = L^{-1/2} F F^T L^{-1/2}(n)\cdot I = \underbrace{(L^{-1/2}F)}_{F^e}\underbrace{(L^{-1/2}F)^T}_{F^{e\,T}}\cdot I = \mathrm{tr}(F^e F^{e\,T})$$

(sup)

Nonlinear energy penalizes "relative" deformations $F^e = L^{-1/2}(n)\,F$

$\frac{1}{2}\mu\,\{\mathrm{tr}(F^e (F^e)^T) - 3\}$



$F = L^{1/2}(n)\,F^e$

Many of the things we'll discover by analyzing the geometrically linear theory have close analogs in the geometrically nonlinear theory.

Energy landscape in small strain theory

$n \in \mathrm{span}\{e_1, e_2\}$

2d pert. of $E_0(e_2)$: $\quad E = E_0(e_2) + \left[\begin{array}{c|c} F & 0 \\ \hline 0 & 0 \end{array}\right]$, $\quad \mathrm{tr}\, E = 0 \Rightarrow \mathrm{tr}\, F = 0$

$$= \frac{3}{2}\gamma \begin{bmatrix} -1/3 & & \\ & 2/3 & \\ & & -1/3 \end{bmatrix} + \frac{3}{2}\gamma \left[\begin{array}{cc|c} \varepsilon & \delta & 0 \\ \delta & -\varepsilon & 0 \\ \hline & 0 & 0 \end{array}\right]$$

$\varepsilon = 0, \delta = 0 \rightarrow E_0(e_2)$

$\varepsilon = 1, \delta = 0 \rightarrow E_0(e_1)$

$$= \frac{3}{2}\gamma \begin{bmatrix} \varepsilon - 1/3 & \delta & 0 \\ \delta & 2/3 - \varepsilon & 0 \\ 0 & 0 & -1/3 \end{bmatrix} \longleftarrow$$

$\bar{\varphi}(E, n) = \mu \, |E - E_0(n)|^2$

$\bar{\varphi}_\beta(E, n) = \bar{\varphi}(E, n) + \mu\beta \, |E - E_0(e_2)|^2$

$$\varphi(E) = \min_{|n|=1} \mu \, |E - E_0(n)|^2 \overset{(EX)}{=} \mu \left[(\omega_{max}(E) - \gamma)^2 + (\omega_{mid} + \gamma/2)^2 + (\omega_{min} + \gamma/2)^2 \right]$$

2d version: $E = E_0(e_2) + \left[\begin{array}{c|c} F & 0 \\ \hline 0 & 0 \end{array}\right]$

$\bar{f}(F, n) = \mu \, |E_0'(e_2) + F - E_0'(n)|^2$

$f(F) = \min_{|n|=1} \bar{f}(F, n) \overset{(EX)}{=} 2\mu \left[\omega_{max}(E_0'(e_2) + F) - \gamma \right]^2$

$f_\beta(F) = f(F) + \beta\mu \, |F|^2$

Define and plot.

$\tilde{f}(\varepsilon, \delta) = f(F(\varepsilon, \delta)) = 2\mu \, (\omega_{max} - \gamma)^2 = \ldots\ldots$ plot....

$$\left[\quad = \frac{9}{2}\mu\gamma^2 \left(r(\varepsilon, \delta) - \frac{1}{2} \right)^2 \right.$$

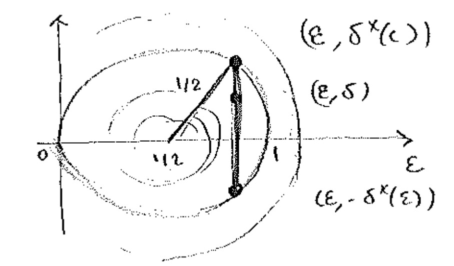
$$|(\varepsilon, \delta) - (1/2, 0)| = \sqrt{(\varepsilon - 1/2)^2 + \delta^2}$$

$$\tilde{f}_\beta(\varepsilon, \delta) = f_\beta(F(\varepsilon, \delta)) = \tilde{f}(\varepsilon, \delta) + \beta\mu \underbrace{|F|^2}_{\frac{9}{2}\gamma^2(\varepsilon^2 + \delta^2)}$$

$= \ldots\ldots$ plot...

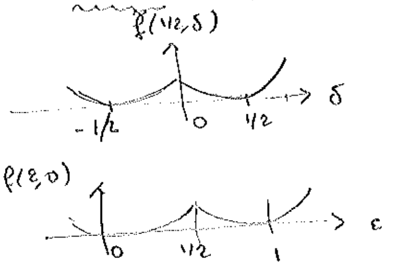
$$= \frac{9}{2}\mu\gamma^2 \left[(1+\beta) \left(r(\varepsilon, \delta) - \frac{1}{2}\frac{1}{1+\beta} \right)^2 + \beta \left(\varepsilon - \frac{1}{4}\frac{\beta}{1+\beta} \right) \right]$$

Isotropic case $f(\varepsilon,\delta)$



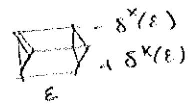
$$\delta^*(\varepsilon) = \sqrt{\left(\tfrac{1}{2}\right)^2 - \left(\varepsilon - \tfrac{1}{2}\right)^2}$$

Sections (two parabolas)

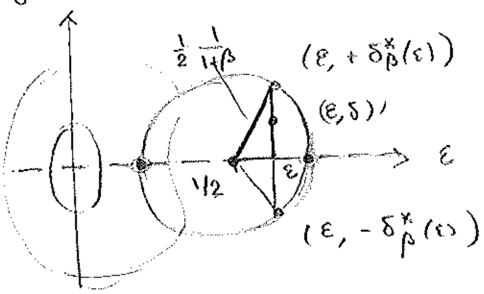


- level sets are circles because $\omega_{max}(\varepsilon,\delta)$ = const are circles centered at $(1/2, 0)$
- zero level set is $\omega_{max} = r$ $\iff$ $r(\varepsilon,\delta) = 1/2$

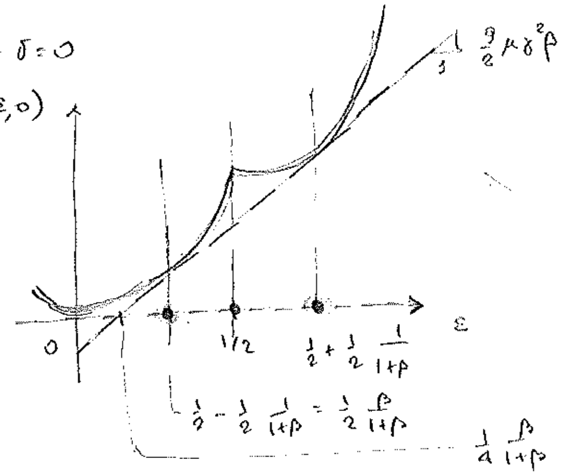
- the energy is proportional to the square of the distance from circle of radius 1/2 centered at $(1/2, 0)$ $\Big\} =: \mathcal{C} = \mathcal{C}_{(1/2,0)}(1/2)$
- Its convex envelope is obtained by replacing with distance from $\operatorname{conv}(\mathcal{C})$
- can achieve it by "layering" $\pm\,\delta^*(\varepsilon)$ at fixed ε

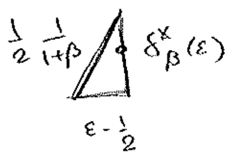


Anisotropic case $f_\beta(\varepsilon,\delta)$



Section at $\delta = 0$





$$\delta^*_\beta(\varepsilon) = \sqrt{\left(\frac{1}{2}\,\frac{1}{1+\beta}\right)^2 - \left(\varepsilon - \frac{1}{2}\right)^2}$$

- this is a function proportional to distance from circle of radius $\frac{1}{2}\frac{1}{1+\beta}$ centered at $(1/2, 0)$ $\Big\} =: \mathcal{C}_\beta$ + linear function

SUMMARY:

$$\tilde{f}^c_\beta(\varepsilon,\delta) = \begin{cases} \tilde{f}_\beta(\varepsilon,\delta) & \text{if } r \geq \frac{1}{2}\frac{1}{1+\beta} \\ \frac{9}{2}\mu\gamma^2\left(\varepsilon - \frac{1}{4}\frac{\beta}{1+\beta}\right) & \text{else} \end{cases} \quad \Leftarrow \Big\{$$

- Its convex envelope is obtained by replacing the first summand with distance from $\operatorname{conv}(\mathcal{C}_\beta)$.
- This can be achieved with $\tilde{f}^c_\beta(\varepsilon,\delta) = \tilde{f}_\beta(\varepsilon, \pm\delta^*_\beta(\varepsilon))$

3. Relaxation results and quasiconvex envelopes

[Put drawing [ ] in a corner
$\tilde f_\beta^c(\varepsilon,\delta) = \tilde f_\beta(\varepsilon, \pm\delta^*)$]

2d perturbations of state of spontaneous strain associated with $e_2 = n_0$.

$$u(x) = \underbrace{u_1(x_1,x_2)\,e_1 + u_2(x_1,x_2)\,e_2}_{u'(x')} - \frac{\gamma}{2}x_3\, e_3$$

$$\nabla u = \left[\begin{array}{c|c} \nabla' u' & 0 \\ \hline 0 & -\gamma/2\end{array}\right] = E_0(e_2) + \left[\begin{array}{c|c} F' & 0\\ \hline 0 & 0\end{array}\right] \qquad E_0(e_2) = \frac32\gamma \begin{bmatrix} -1/3&0&0\\0&2/3&0\\0&0&-1/3\end{bmatrix}$$

$$F' = \nabla' u' - E_0'(e_2) = \nabla'(\underbrace{u' - E_0'(e_2)x'}_{v'(x')}) = \nabla' v'$$

(v' is the real unknown of the problem. Once we know v, we recover u' and hence u)

$$= \frac12 (\mathrm{tr} F')I' + (\mathrm{sym} F')_d + \mathrm{skew}\, F'$$

$$(\mathrm{sym}F')_d = \frac32\gamma \begin{bmatrix}\varepsilon & \delta\\ \delta & -\varepsilon\end{bmatrix} ; \qquad \begin{aligned}\varepsilon &= \varepsilon(F) = \cancel{\tfrac12}(F_{11}-F_{22})\frac{\cancel{2}}{3\gamma}\\ \delta &= \delta(F) = \cancel{\tfrac12}(F_{12}+F_{21})\frac{\cancel{2}}{3\gamma}\end{aligned}$$

Drop primes from notation and work with 2×2 matrices.

$F \in M^{2\times2}$, arbitrary, define

$$\bar h_\beta(F,n) := \bar f_\beta((\mathrm{sym}F)_d, n) + \frac{k}{2}(\mathrm{tr}F)^2$$

$$= \mu\,|E_0'(e_2) + (\mathrm{sym}F)_d - E_0'(n)|^2 + \mu\beta\,|(\mathrm{sym}F)_d|^2 + \frac{k}{2}(\mathrm{tr}F)^2$$

$$h_\beta(F) = \min_{|n|=1} \bar h_\beta(F,n) = f_\beta((\mathrm{sym}F)_d) + \frac k2 (\mathrm{tr}F)^2$$

Observe that, for $F\in \mathrm{Sym}$, $\mathrm{tr}F = 0$, we have $h_\beta(F) = f_\beta(F)$, so that h_β is an extension to non-symmetric, non traceless matrices of our energy.

Since

$$\mathrm{tr}\nabla u = \underbrace{\mathrm{tr}\,E_0(e_2)}_{=0} + \mathrm{tr}F = \mathrm{div}\, v$$

the incompressible case "$k = +\infty$" is obtained by enforcing constraint $\mathrm{div}\, v = 0$. We'll worry about incompressibility after having dealt with compressible case.

$$\inf_{\substack{v\in H^1(\Omega,\mathbb R^2)\\ + BC}} H(v) := \int_\Omega h_\beta(\nabla v(x))\,dx = \int_\Omega f_\beta((\mathrm{sym}\nabla v)_d) + \frac k2(\mathrm{div}\, v)^2$$

ill-posed problem because of non-convexity of f_β (min. seq. may develop increasingly fine spatial oscillations: stripe-domain instability).

f_β controlled by quadratic fns both from above and from below

$\Rightarrow$ Classical relaxation thms apply.

$\bar{H} = \sup \{ G : G \text{ is } H^1\text{-wslsc},\ G \le H \}$ relaxation of H

$\min_{v \in H^1} \bar{H}(v) = \inf_{v \in H^1} H(v)$ minimizers of $\bar{H}$ give inf of H, they represent wk. limits of minimizing sequences of H

$$\bar{H}(v) = \inf \{ \liminf_{k\to\infty} H(v_k) : v_k \rightharpoonup v \text{ in } H^1(\Omega, \mathbb{R}^2) \}$$

$$\bar{H}(v) = \int_\Omega h_p^{qc}(\nabla v(x))\,dx$$

where

$$h_p^{qc}(F) = \inf_{w \in W_0^{1,\infty}} \left\{ \frac{1}{|\omega|} \int_\omega h_p(F + \nabla w(x))\,dx \right\} \qquad (\omega \text{ arbitrary})$$

$$= \sup \{ g(F) : g \le h_p,\ g \text{ quasiconvex} \}$$

Pb: what to do with this, given that there is no algorithmic characterization of quasiconvexity ?

Some facts about convexity

f quasiconvex at F if

$$f(F) \le \frac{1}{|\omega|} \int_\omega f(F + \nabla w(x))\,dx, \quad \forall w \in W_0^{1,\infty}(\Omega, \mathbb{R}^2) \quad (\omega \text{ arbitrary}) \qquad (*)$$

$\frac{1}{|\omega|} \int_\omega (F + \nabla w(x))\,dx$

- Jensen's inequality for convex fn's for gradient perturbations of F with average F (so conv $\Rightarrow$ qconv)
- A notion of material stability. Affine extension to ω of F enforced on $\partial\omega$ gives energy minimum. If violated, f^{qc} gives the smallest energy the system can attain, compatibly with BC $y(x) = Fx$ on $\partial\omega$, by developing Lipschitz modulations in the interior of ω.

f is rank-one convex if

$$f((1-\nu)\xi_1 + \nu\xi_2) \le (1-\nu) f(\xi_1) + \nu f(\xi_2) \quad \forall \nu \in [0,1],\ \forall \xi_1, \xi_2 \in M^{2\times 2} \text{ with rank}(\xi_2 - \xi_1) \le 1$$

rank-one conv hull of f

$$f^{rc}(\xi) = \sup \{ g(\xi) : g \le f,\ g \text{ rc-convex} \}$$

$$f^{c}(\xi) = \sup \{ g(\xi) : g \le f,\ g \text{ conv} \}$$

(so, weaker notion of convexity) out of qconvexity. Use ω → $w(x)$ $\xi_1, \xi_2, \xi_1, \xi_2$ w/ cut-off near $\partial\omega$

$\xi_2 = \xi_1 + a \otimes n$, → n

Since $c \Rightarrow qc \Rightarrow rc$ (but not viceversa), then are more rc, than qc, than c and

$$f^c \le f^{qc} \le f^{rc} \qquad (**)$$

Contrary to f^{qc}, there are "algorithmic" characterizations for f^c and f^{rc}, so can at least bound f^{qc}.
If the bounds match, we have f^{qc}.

$$f^c(\xi) = \inf\left\{ \sum_{i=1}^{k} \lambda_i f(\xi_i) : \sum \lambda_i \xi_i = \xi, \ \sum \lambda_i = 1, \ \lambda_i \in [0,1] \right\}$$

where $k = N+1$ if $\xi \in \mathbb{R}^N$

$$f^{rc}(\xi) := \inf \bigcup_{k=2}^{\infty} \left\{ \sum_{i=1}^{k} \lambda_i f(\xi_i) : \lambda_i, \xi_i \text{ define a laminate of "order } k\text{"} \right\}$$

def. by deduction on k → "condition H_k", see Dacorogna

any finite order, e.g. "order 2"

$$\leq \inf\{ \text{— " —} : \ldots \text{ " — "order 2"} \}$$

$$= \inf\{ (1-\nu) f(\xi_1) + \nu f(\xi_2), \ (1-\nu)\xi_1 + \nu \xi_2 = \xi, \ \nu \in [0,1], \ \mathrm{rank}(\xi_2 - \xi_1) \leq 1 \}$$

Recall, for $F \in M^{2\times 2}$

$$h_\beta(F) := f_\beta((\mathrm{sym}\, F)_d) + \frac{k}{2} (\mathrm{tr}\, F)^2 \qquad \varepsilon = \frac{1}{3\gamma}(F_{11} - F_{22}), \quad \delta = \frac{1}{3\gamma}(F_{12} + F_{21})$$

Define

$$\tilde{h}_\beta(\varepsilon, \delta, \mathrm{tr} F) := \tilde{f}_\beta(\varepsilon, \delta) + \frac{k}{2} (\mathrm{tr} F)^2$$

$$\tilde{j}_\beta(\varepsilon, \delta, \mathrm{tr} F) := \tilde{f}^c_\beta(\varepsilon, \delta) + \frac{k}{2} (\mathrm{tr} F)^2$$

$$j_\beta(F) := \tilde{j}_\beta(\varepsilon(F), \delta(F), \mathrm{tr} F)$$

Theorem (Cesana, DS) $h_\beta^{qc} = h_\beta^c = j_\beta$

Proof To show

$$(h_\beta)^{rc} \leq j_\beta \leq (h_\beta)^c \qquad (*)$$

since by $(**)$

$$(h_\beta)^c \leq (h_\beta)^{qc} \leq (h_\beta)^{rc}$$

and then $(*)$ would imply that all are $=$, and thesis follows.

Second inequality easy, because

$$\left.\begin{array}{l} \tilde{j}_\beta \leq \tilde{h}_\beta \\ j_\beta \text{ convex} \end{array}\right\} \Rightarrow \quad j_\beta \leq (h_\beta)^c$$

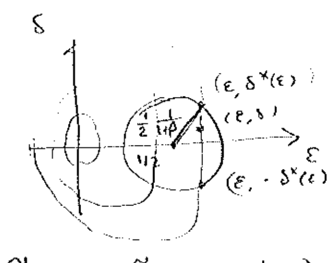
we are left to show that $(h_\beta)^{rc} \leq j_\beta$

Since $(h_\beta)^{rc} \leq h_\beta$, at all F where $h_\beta = j_\beta$ there is nothing to prove

Concentrate on $h_\beta \neq j_\beta$, i.e. where $\tilde{f}^c_\beta \neq \tilde{f}_\beta$, i.e. where

$$r(\varepsilon, \delta) < \frac{1}{2} \frac{1}{1+\beta}$$

where we use a lamination construction.



$$\tilde{f}^c_\beta(\varepsilon, \delta) = \tilde{f}_\beta(\varepsilon, \pm\delta^*(\varepsilon))$$

Take $F \in M^{2\times 2}$ s.t.

$$r(\varepsilon,\delta) < \frac{1}{2}\,\frac{1}{1+\beta} \qquad (*)$$

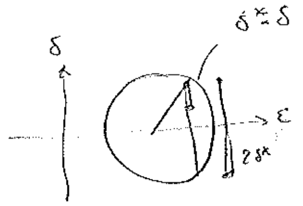
and find F_1, F_2, rank$(F_2 - F_1) \le 1$, $\nu \in [0,1]$ s.t.

(i) $F = (1-\nu)F_1 + \nu F_2$

(ii)
$$\begin{aligned} j_\beta(F) &= (1-\nu)\, h_\beta(F_1) + \nu\, h_\beta(F_2) \\ &\ge \inf\{\textstyle\sum \lambda_i h_\beta(F_i) : \text{laminates of all orders}\} \\ &= (h_\beta)^{rc} \end{aligned}$$

To this end, write

$$F_1 = \Delta E_1 + \frac{\operatorname{tr} F}{2} I + \Delta W - \tilde{W}$$
$$F_2 = \Delta E_2 + \frac{\operatorname{tr} F}{2} I - \Delta W + \tilde{W}$$



where

$$\Delta E_1 = \frac{3}{2}\gamma \begin{bmatrix} \varepsilon & \delta^*(\varepsilon) \\ \delta^*(\varepsilon) & -\varepsilon \end{bmatrix}, \qquad \Delta E_2 = \frac{3}{2}\gamma \begin{bmatrix} \varepsilon & -\delta^*(\varepsilon) \\ -\delta^*(\varepsilon) & -\varepsilon \end{bmatrix}$$

$$\Delta W = \frac{3}{2}\gamma \begin{bmatrix} 0 & \delta^* \\ -\delta^* & 0 \end{bmatrix}, \qquad \tilde{W} = \operatorname{skew} F - (1-2\nu)\Delta W$$

$$\delta^*(\varepsilon) = \sqrt{\left(\frac{1}{2}\,\frac{1}{1+\beta}\right)^2 - \left(\varepsilon - \frac{1}{2}\right)^2}, \qquad \nu = \frac{\delta^* - \delta}{2\delta^*} \in [0,1] \quad \text{by } (*), \text{ or by picture}$$

and verify that rank$(F_2 - F_1) \le 1$ and (i), (ii) are satisfied.

Notice that

$$h_\beta(F_1) = h_\beta(F_2) = \tilde{f}_\beta(\varepsilon, \pm\delta^*(\varepsilon)) + \frac{k}{2}(\operatorname{tr} F)^2 = \tilde{f}_\beta^{\,c}(\varepsilon,\delta) + \frac{k}{2}(\operatorname{tr} F)^2 = j_\beta(F) \qquad ///$$

<u>The incompatible core.</u>

<u>Theorem</u> (Braides) Under suitable assumptions on f, verified by $f(F) = f_\beta(\operatorname{sym} F)$, consider

$$F^k(v) = \int_\Omega f(\nabla v) + \frac{k}{2}(\operatorname{div} v)^2$$

$$F(v) = \begin{cases} \int_\Omega f(\nabla v) & \text{if } \operatorname{div} v = 0 \\ +\infty & \text{else} \end{cases}$$

Then $\bar{F} = \sup_k \overline{F^k}$ and

$$\bar{F}(v) = \begin{cases} \int_\Omega g(\nabla v) & \text{if } \operatorname{div} v = 0 \\ +\infty & \text{else.} \end{cases}$$

where

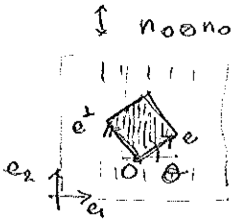
$$g(A) = \sup_{k \in \mathbb{N}} \left\{ \left(f(A) + \frac{k}{2}(\operatorname{tr} A)^2\right)^{qc} \right\} \longleftarrow g(A) = \sup_{k \in \mathbb{N}} \{ j_\beta(A) \} = \begin{cases} \tilde{f}_\beta^{\,c}(\varepsilon(A), \delta(A)) & \text{if } \operatorname{tr} A = 0 \\ +\infty & \text{else} \end{cases}$$

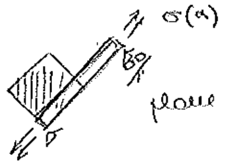
and, if $\operatorname{tr} A = 0$, then

$$g(A) = \inf_{\substack{w \in W_0^{1,\infty} \\ \operatorname{div} w = 0}} \left\{ \frac{1}{|\omega|} \int_\omega f(A + \nabla w(x))\, dx \right\}$$

Applications.

- stress-strain response in conditions of affine deformations.





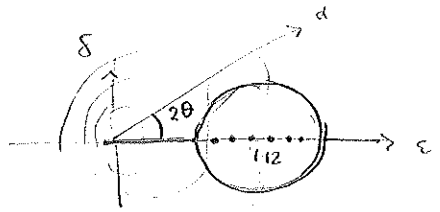
plane strain extension along e: $\frac{3}{2}\gamma\alpha\left(e\otimes e - e^\perp \otimes e^\perp\right) = \Delta E$

$e = (\cos\theta, \sin\theta)$

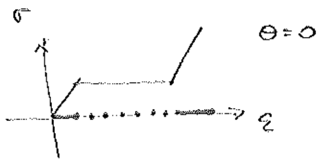
$e^\perp = (-\sin\theta, \cos\theta)$

$\varepsilon(\Delta E) = \alpha \cos 2\theta$

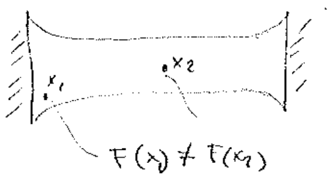
$\delta(\Delta E) = \alpha \sin 2\theta$

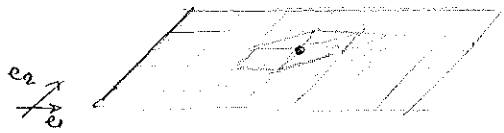


Use thm of power expected to obtain $\sigma(\alpha) = \frac{d}{d\alpha} f_p^c(\varepsilon(\alpha), \delta(\alpha))$



- stress-strain response in conditions of heterogeneous deformations, through "multiscale" finite elements





triangulation

piecewise linear basis function.

constant gradient in

If we use $W^{qc}(F)$ instead of $W(F)$, have accounted correctly for the energetics of energy minimizing states, including microstructures, without having to resolve their kinematics explicitly.

Quality of their features can be accessed from knowledge of the F_i's s.t.

$$W^{qc}\left(\sum \lambda_i F_i\right) = \sum \lambda_i W(F_i)$$

- Other materials: coupling between elastic strains and order tensor/vector variable: magnetostriction, ferroelectrics, magnetic shape-memory, ...