II Continuum Theories of GFA

Last lecture we introduce GFA from a discrete perspective of particle packing (e.g. triangular/tetrahedral order).

In this lecture, we introduce continuum theories of stressed equilibria of GFA.

Here, we will see how ground states develop gradient order that varies with domain size.

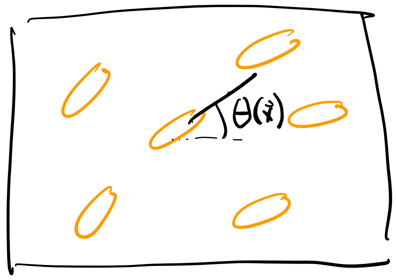
DOF = spatially varying order parameters

Broken symmetries		continuous DOF
orientational (LCs)	$\rightarrow$	rotations
positional (crystalline)	$\rightarrow$	displacements

Ex. 1 2D nematics on curved surface

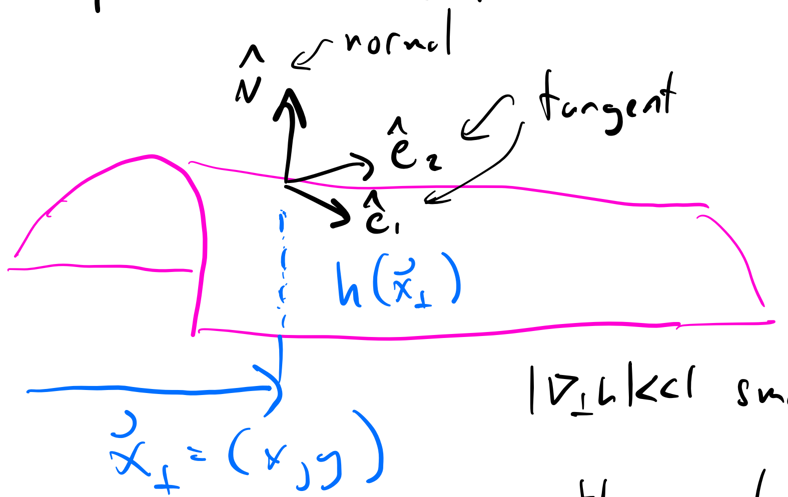
refs. Nelson & Peliti, J. Phys. (1987)
Giomi & Bowick, Adv. Phys. (2009)

Planar case $\hat{n} = \cos\theta(\vec{x})\,\hat{x} + \sin\theta(\vec{x})\,\hat{y}$



Curved surf. (Monge representation)

$\vec{R}(x, y, h(x,y))$



$|\nabla_\perp h| \ll 1$ small slopes

$\hat{n}$ in tangent plane $\{\hat{e}_1, \hat{e}_2, \hat{N}\}$ ← orthonormal frame

$$\hat{n} = \cos\theta(\vec{x})\,\hat{e}_1 + \sin\theta(\vec{x})\,\hat{e}_2$$

When computing strains, we will focus on intrinsic gradients, i.e. changes of $\hat{n}$ in tangent plane

intrinsic derivatives

$$D_i\hat{n} = \partial_i\hat{n} - \hat{N}(\hat{N}\cdot\partial_i\hat{n})$$

← out-of-plane (extrinsic)

* note extrinsic terms can also be important (Helfrich & Prost, PRA 1988; MacKintosh & Lubensky, PRL 1991)

Let's analyze components of $D_i \hat{n}$ in $\{\hat{e}_1, \hat{e}_2\}$ basis

$$\hat{e}_1 \cdot (D_i \hat{n}) = \hat{e}_1 \cdot \left[\partial_i \theta \left(-\sin\theta\, \hat{e}_1 + \cos\theta\, \hat{e}_2 \right) + \cos\theta\, \partial_i \hat{e}_1 + \sin\theta\, \partial_i \hat{e}_2 \right]$$

$$= \sin\theta \left(-\partial_i \theta + \hat{e}_1 \cdot (\partial_i \hat{e}_2) \right) + \cos\theta\, \cancel{\hat{e}_1 \cdot (\partial_i \hat{e}_1)}$$

Likewise, $\partial_i |\hat{e}_1|^2 = 2\, \hat{e}_1 \cdot (\partial_i \hat{e}_1) = 0$

$$\hat{e}_2 \cdot (D_i \hat{n}) = \cos\theta \left(\partial_i \theta + \hat{e}_2 \cdot (\partial_i \hat{e}_1) \right)$$

$\hat{e}_2 \cdot (\partial_i \hat{e}_1) = -\hat{e}_1 \cdot (\partial_i \hat{e}_2)$ since $\partial_i (\hat{e}_1 \cdot \hat{e}_2) = \hat{e}_1 \cdot (\partial_i \hat{e}_2) + \hat{e}_2 \cdot (\partial_i \hat{e}_1) = 0$

$$\boxed{\begin{gathered}\text{Spin connection (frame rotations)} \\ A_i \equiv \hat{e}_1 \cdot (\partial_i \hat{e}_2) = -\hat{e}_2 \cdot (\partial_i \hat{e}_1)\end{gathered}}$$

$$D_i \hat{n} = (\hat{N} \times \hat{n}) (\partial_i \theta - A_i)$$

rotation of frame

angle changes

$\hat{N} \times \hat{n} = -\sin\theta\, \hat{e}_1 + \cos\theta\, \hat{e}_2$

Mermin-Ho relation: gradients (curl) of A_i are constrained by K_G

Let's see this by direct calculation: Tangent vectors of surface (not $\hat{e}_1$ & $\hat{e}_2$)

$$\partial_x \vec{R} = \hat{x} + \partial_x h\, \hat{z} \;; \quad \partial_y \vec{R} = \hat{y} + \partial_y h\, \hat{z}$$

Construct frame vectors: $\hat{e}_1 \overset{?}{\neq} \dfrac{\hat{x} + \partial_x h \hat{z}}{\sqrt{1+(\partial_x h)^2}}$
(to order $|\nabla_\perp h|^2 << 1$)

$$\begin{cases} \hat{e}_1 \simeq \hat{x}\left(1 - \frac{1}{2}(\partial_x h)^2\right) + \partial_x h \hat{z} - \frac{1}{2} \partial_x h\, \partial_y h \hat{y} \\ \hat{e}_2 \simeq \hat{y}\left(1 - \frac{1}{2}(\partial_y h)^2\right) + \partial_y h \hat{z} - \frac{1}{2} \partial_x h\, \partial_y h \hat{x} \end{cases}$$

$$\hat{N} = \hat{e}_1 \times \hat{e}_2 \simeq \hat{z}\left(1 - \frac{1}{2}(\nabla_\perp h)^2\right) - \underbrace{\nabla_\perp h}_{= \partial_x h \hat{x} + \partial_y h \hat{y}}$$

not $\perp$ to order $(\nabla_\perp h)^2$

need to subtract off

$$\partial_i \hat{e}_2 \simeq -\partial_y h\, \partial_i \partial_y h \hat{y} + \partial_i \partial_y h \hat{z} - \frac{1}{2} \partial_i (\partial_x h\, \partial_y h) \hat{x}$$

$$A_i = \hat{e}_1 \cdot (\partial_i \hat{e}_2) \simeq \partial_x h\, \partial_i \partial_y h - \frac{1}{2} \partial_i (\partial_x h\, \partial_y h)$$

$$\boxed{A_i \simeq \frac{1}{2}\left(\partial_x h\, \partial_i \partial_y h - \partial_y h\, \partial_i \partial_x h\right)}$$

Consider 2D curl

$$\begin{aligned}
\nabla_\perp \times \vec{A} &= \partial_x A_y - \partial_y A_x \\
&\simeq \frac{1}{2}\left[\partial_x\left(\partial_x h\, \partial_y^2 h - \partial_y h\, \partial_y \partial_x h\right) - \partial_y\left(\partial_x h\, \partial_x \partial_y h - \partial_y h\, \partial_x^2 h\right)\right] \\
&= \frac{1}{2}\Big[\partial_x^2 h\, \partial_y^2 h + \cancel{\partial_x h\, \partial_x \partial_y^2 h} - (\partial_x \partial_y h)^2 - \cancel{\partial_y h\, \partial_y \partial_x^2 h} \\
&\quad - (\partial_x \partial_y h)^2 - \cancel{\partial_x h\, \partial_x \partial_y^2 h} + \partial_y^2 h\, \partial_x^2 h + \cancel{\partial_y h\, \partial_y \partial_x^2 h}\Big) \\
&= \partial_x^2 h\, \partial_y^2 h - (\partial_x \partial_y h)^2 = \det(K_{ij})
\end{aligned}$$

$$\boxed{\begin{array}{l}\text{Mermin-Ho relation:}\\ \nabla_\perp \times \vec{A} = K_G\end{array}}$$

Curvature tensor
$K_{ij} = \partial_i \partial_j h$

coordinate independent

$\vec{A}$ must have gradients if $K_G \neq 0$, no matter choice of $\hat{e}_1$ & $\hat{e}_2$. This a way of encoding incompatibility between straight & parallel curves on non-Euclidean surfaces.

To see consequences, consider 1-constant approximation $K_1 = K_3 = K_f$

$$F = \frac{K_f}{2} \int dx\, dy \sqrt{g} \left((D_i \hat{n}) \cdot (D^i \hat{n}) \right)$$

$$\hat{=} \frac{K_f}{2} \int dx\, dy \left(\nabla_\perp \theta - \vec{A} \right)^2$$

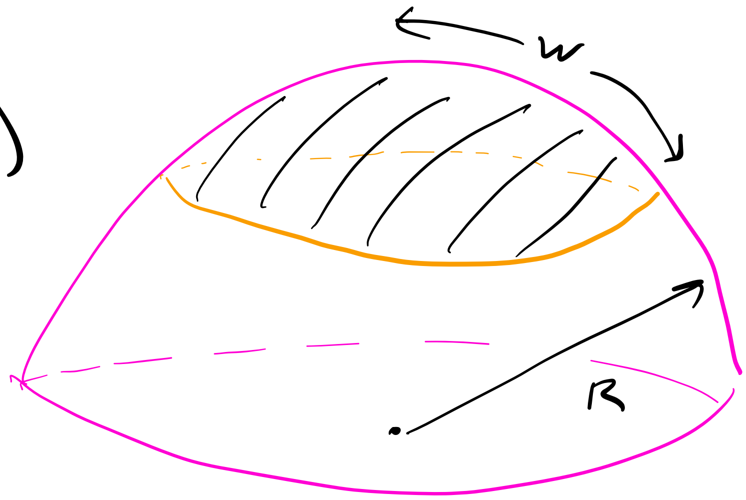
$g_{ij} \hat{=} \delta_{ij}$
(small slopes)

This encodes frustration. Why?
Ground state favors $\nabla_\perp \theta - \vec{A} = 0$

However $\nabla_\perp \times (\nabla_\perp \theta - \vec{A}) = \cancel{\nabla_\perp \times (\nabla_\perp \theta)}^{\,0} - \nabla_\perp \times \vec{A} = -K_G \neq 0!$

$\nabla(\text{strain}) \approx -K_G$

Ex. Nematic domain on sphere (paraboloid)



$$h(x,y) = h_0 - \frac{x^2+y^2}{2R}$$

$$\partial_x h = \frac{-x}{R} \; ; \; \partial_y h = \frac{-y}{R}$$

$$A_x = \frac{1}{2}\Big[\partial_x h\, \partial_x \partial_y h - \underset{\underset{-\frac{y}{R}}{\parallel}}{\partial_y h}\, \underset{\underset{-\frac{1}{R}}{\parallel}}{\partial_x^2 h}\Big] = -\frac{1}{2}\frac{y}{R^2}$$

$$A_y = \frac{1}{2}\frac{x}{R^2}$$

$$\vec{A} = \frac{1}{2R^2}\left(-y\hat{x} + x\hat{y}\right) = \frac{r}{2R^2}\hat{\phi}$$

$$\nabla_\perp \times \vec{A} = \frac{1}{2R^2}\left[+1 - (-1)\right] = \frac{1}{R^2} \checkmark$$

$$\nabla_\perp \cdot \vec{A} = 0$$

Minimize F: $$\frac{\delta F}{\delta \theta} = -\nabla_\perp \cdot \left(\nabla_\perp \theta - \vec{A}\right) = -\nabla_\perp^2 \theta = 0$$

B.C. (free): $$\left(\nabla_\perp \theta - \vec{A}\right)\cdot \hat{r}\Big|_{r=w} = 0$$

$$\theta = ax + by + cxy + d$$

$$a = b = c = 0 \longrightarrow \left(\nabla_\perp \theta\right)\cdot\hat{r}\Big|_{r=w} = 0$$

$$\boxed{\theta = \theta_0 = \text{const.}}$$

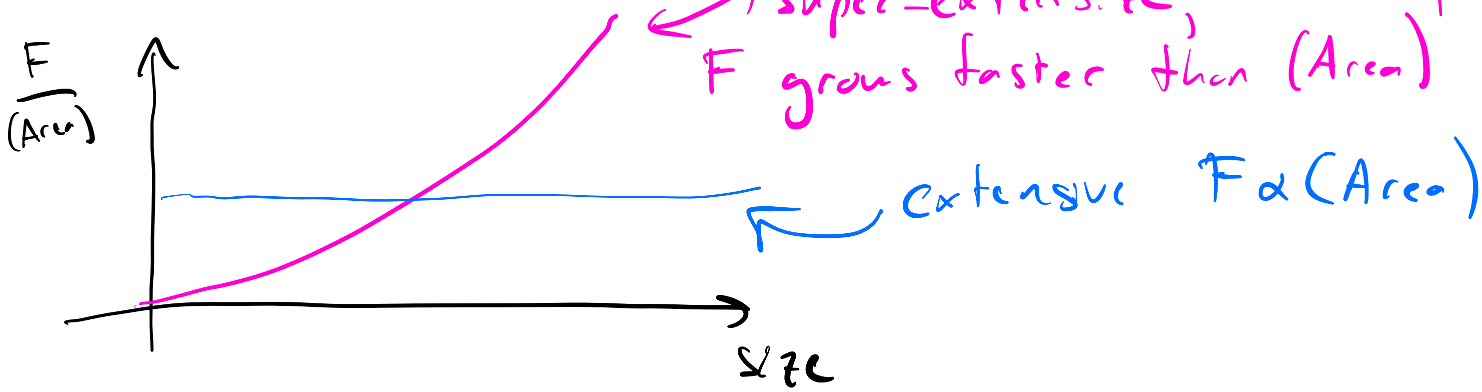
Is solution uniform? $\underline{\text{No}}$. $|\vec{A}| \propto \frac{r}{R^2} = r K_G$

$\Theta = 0 \quad \hat{n} = \hat{e}_1$ * compute and sketch field lines. (where's splay/bend)?

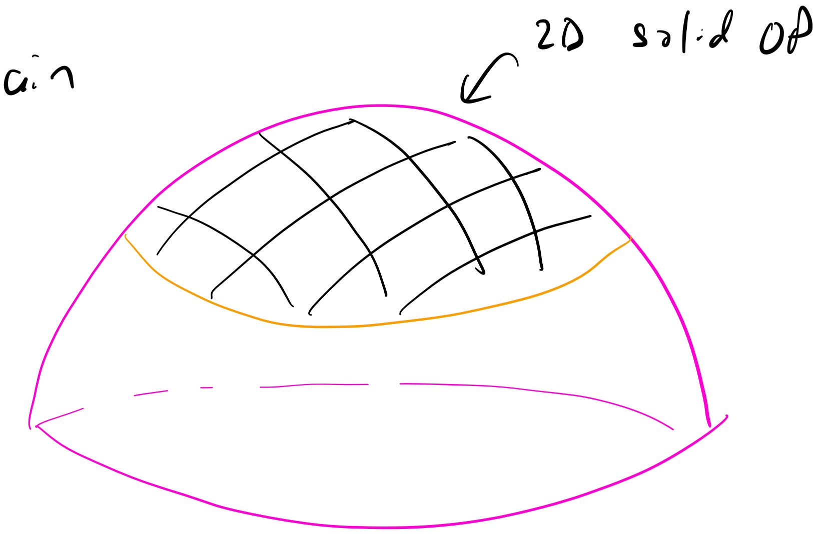
$$|\vec{A}|^2 = \frac{1}{4R^2}(x^2+y^2) = \frac{r^2}{4R^4}$$

$$F = \frac{K_f}{2}\int dA\, |\vec{A}|^2 = \frac{K_f}{2}\int d\phi \int_0^W r\, dr\, \frac{r^2}{4R^4}$$

$$= \frac{K_f}{16}(\pi W^2)\frac{W^2}{R^4} \propto K_G^2 (\text{Area})^2$$



2nd Ex. Crystalline domain on sphere



Here we will briefly summarize key elements of continuum theory, referring back to M. Moshe's lectures on plate elasticity.

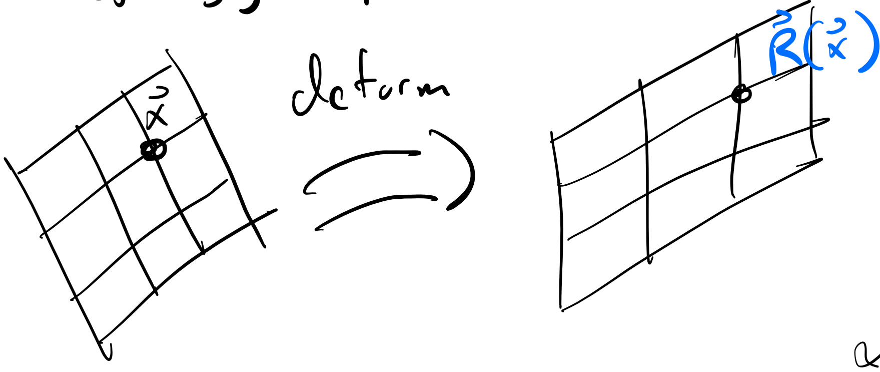
$$E_{el} = E_{strain} + E_{bend}$$

$$= \frac{1}{2}\int dA \left[\varepsilon_{ij}\,\sigma_{ij} + B\,(2H)^2 \right]$$

(2D) strain — stress — mean curvature

$$H \simeq \frac{1}{2}\nabla_\perp^2 h = \frac{1}{2}(K_{xx} + K_{yy}) = \frac{1}{R}$$

$i,j = x,y$ in-plane ref. coords.



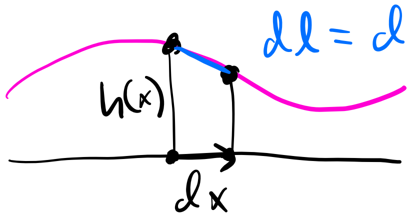
$$\vec{R}(\vec{x}) - \vec{x} = \vec{u}(\vec{x})$$

displacement

out-of-plane contribution.

$$\varepsilon_{ij} = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i + \partial_i h\,\partial_j h\right)$$

$$dl = dx\sqrt{1+(\partial_x h)^2} \simeq dx\left(1 + \frac{1}{2}(\partial_x h)^2\right)$$



Euler-Lagrange eq. ($h(\vec{x})$ fixed to sphere)

$$\frac{\delta E}{\delta u_j} = 0 \Rightarrow \partial_i \sigma_{ij} = 0 \qquad \sigma_{ij} = \lambda\,\delta_{ij}\,\varepsilon_{kk} + 2\mu\,\varepsilon_{ij}$$

dilation — shear

$\sigma_{xy} = \sigma_{yx}$ $\quad$ $\sigma_{ij} \Rightarrow 3$ components

$$\partial_i \sigma_{ix} = \partial_i \sigma_{iy} = 0 \quad 2 \text{ equations.}$$

+1 compatibility

$$\partial_x^2 \varepsilon_{yy} + \partial_y^2 \varepsilon_{xx} - 2\,\partial_x\partial_y\,\varepsilon_{xy} = (\partial_x\partial_y h)^2 - (\partial_x^2 h)(\partial_y^2 h)$$

$$= -\det(K_{ij}) = -K$$

Can use σ_{ij} and $\partial_i \sigma_{ij} = 0$ to show

$$\boxed{\frac{1}{Y}\nabla_\perp^2 \sigma_{kk} = -K_G}$$

$$Y = \frac{4\mu(\lambda+\mu)}{(\lambda+2\mu)}$$

2D Youngs modulus.

(* $\sigma_{ij} = \epsilon_{il}\epsilon_{jm}\partial_l\partial_m \chi$

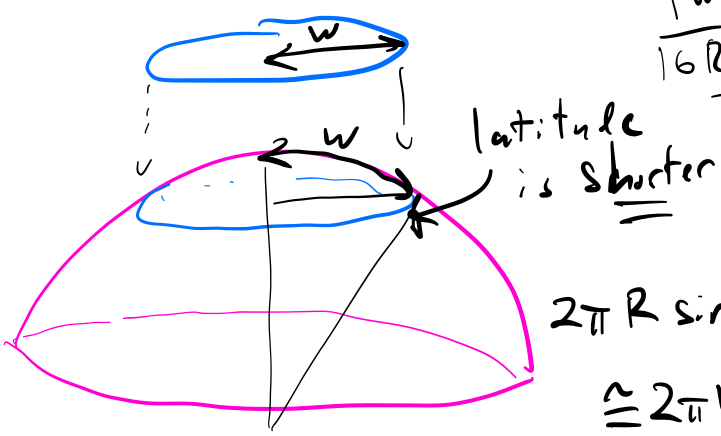
$\Rightarrow \sigma_{kk} = \nabla_\perp^2 \chi \Rightarrow \frac{1}{Y}\nabla_\perp^4 \chi = -K_G$)

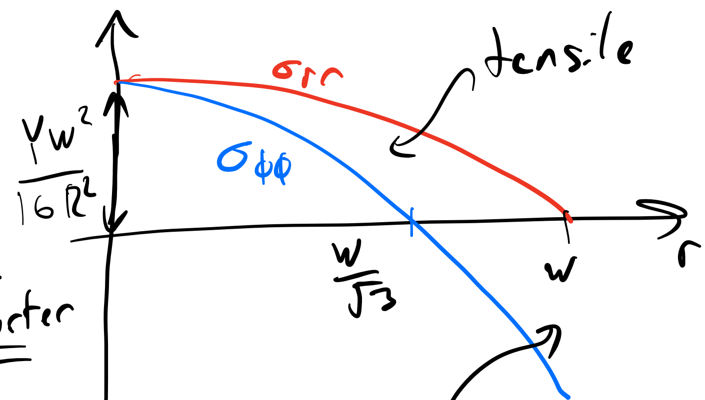
Here, second derivative of strain (i.e. σ_{kk}/Y) is proportional to K_G. (frustration).

Axi-symmetric solution (show as exercise)

$$\sigma_{rr} = \frac{Y}{16R^2}\left(W^2 - r^2\right), \quad \sigma_{\phi\phi} = \frac{Y}{16R^2}\left(W^2 - 3r^2\right), \quad \sigma_{r\phi} = 0$$

satisfies free BC $\quad \sigma_{ri}\Big|_{r=W} = 0$





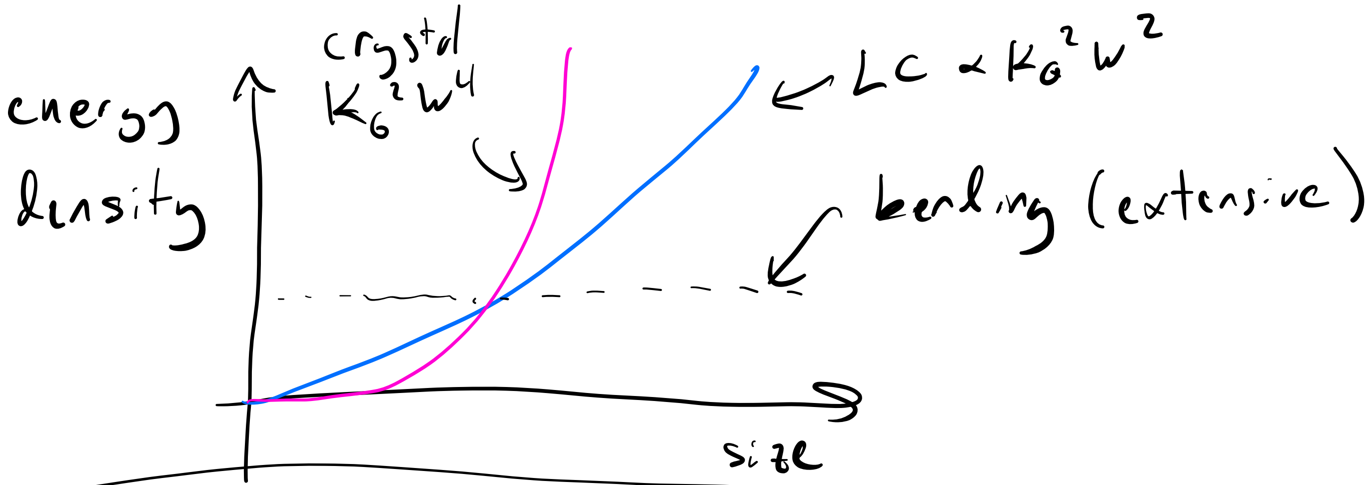
$$2\pi R \sin\left(\frac{W}{R}\right) \simeq 2\pi W\left[1 - \frac{1}{3!}\left(\frac{W}{R}\right)^2\right]$$

$\sigma_{\phi\phi} < 0$ (compressive) Why?

$$E_{strain} = \frac{1}{2}\int dA\, \varepsilon_{ij}\sigma_{ij} \simeq \int dr\, r\, \frac{\sigma^2(r)}{Y} \simeq Y\left(\frac{\pi}{4}W^2\right) \times \frac{W^4}{R^4}$$

$$\varepsilon \simeq \frac{\sigma}{Y}$$

$$\propto Y\,(\text{Area})^3 K_G^2$$



LC (orientation strain) $\propto K_G w$

Crystal (position strain) $\propto K_G w^2$

why is this higher power?