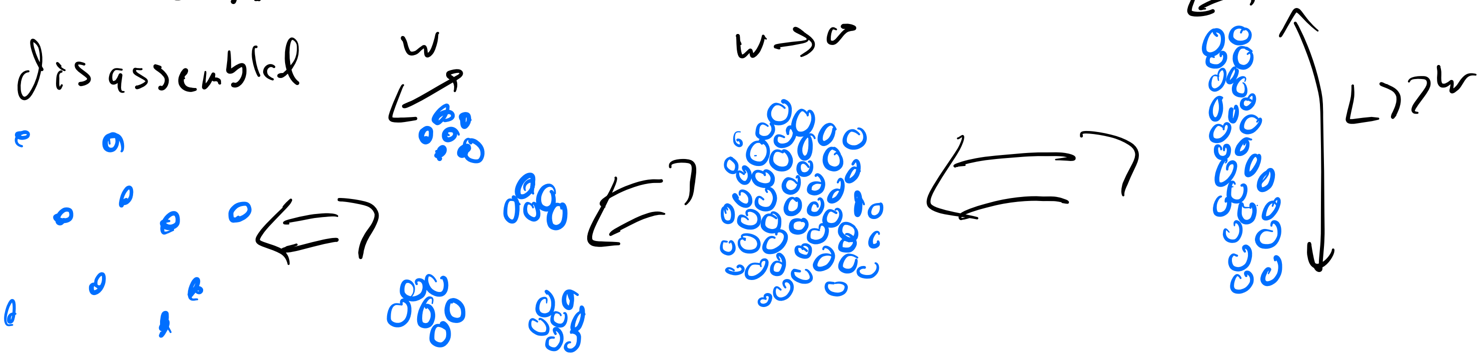
III GFA Consequences: Shape & Size Selection

In "canonical view" of GF (see Sadoc & Mosseri) the ordered domain itself is considered fixed, and usually assumed to take bulk dimensions (i.e. $L \to \infty$). In assemblies, size and shape of domain become important degrees of freedom (in addition to internal order).



Let's start with a simple assembly model, short-range, cohesive interactions $= -u_0$

Interaction energy of clusters:

bulk surface # @ surface $\propto W^{d-1}$

$$E_{int} = -u_0 \frac{\langle z \rangle}{2} N_p + \frac{u_0}{2} \Delta z \, N_s$$

avg. # neighbors # particles decrease in neighbor @ surf.

$N_p \propto W^d$

Canonical ensemble $\Rightarrow$ Fixed N_{tot}

For simplicity, assume n_c clusters of size W

$N_{tot} = n_c N_p$

$$F_{tot} = n_c E_{int}(W) = N_{tot}\left(\frac{E_{int}}{N_p}\right) = N_{tot}\,\epsilon_{int}(w)$$

consider $T \to 0$

energy/particle (intensive)

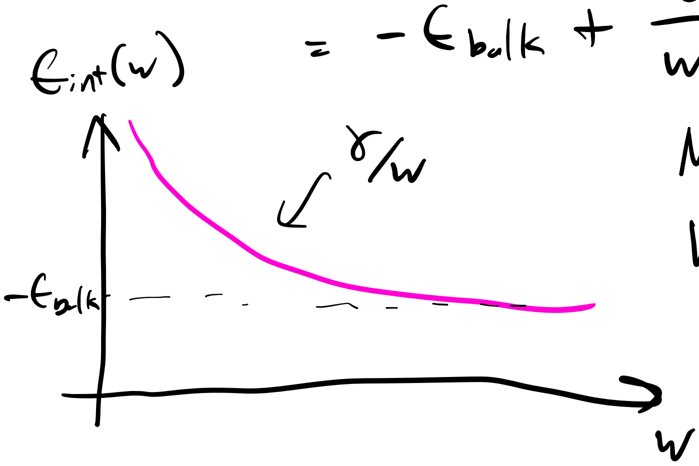
In simple model (short-range cohesion):

$$\epsilon_{int}(w) = -u_0\frac{\langle z\rangle}{2} + \frac{u_0}{2}\Delta z\left(\frac{N_s}{N_p}\right) \sim \propto \frac{w^{d-1}}{w^d} = \frac{1}{w}$$

const.

$$= -\epsilon_{bulk} + \frac{\gamma}{w}$$

surface energy

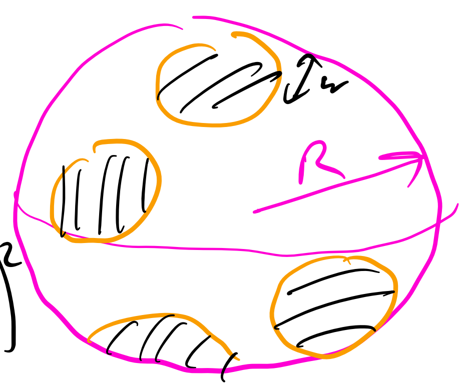


Minimal E_{TOT}

$W_* \to \infty$; single, macroscopic cluster

For GFA $E_{int}(w)$ has additional terms due to accumulation of internal stress

Ex. 2D Nematic domains (defect-free) on sphere



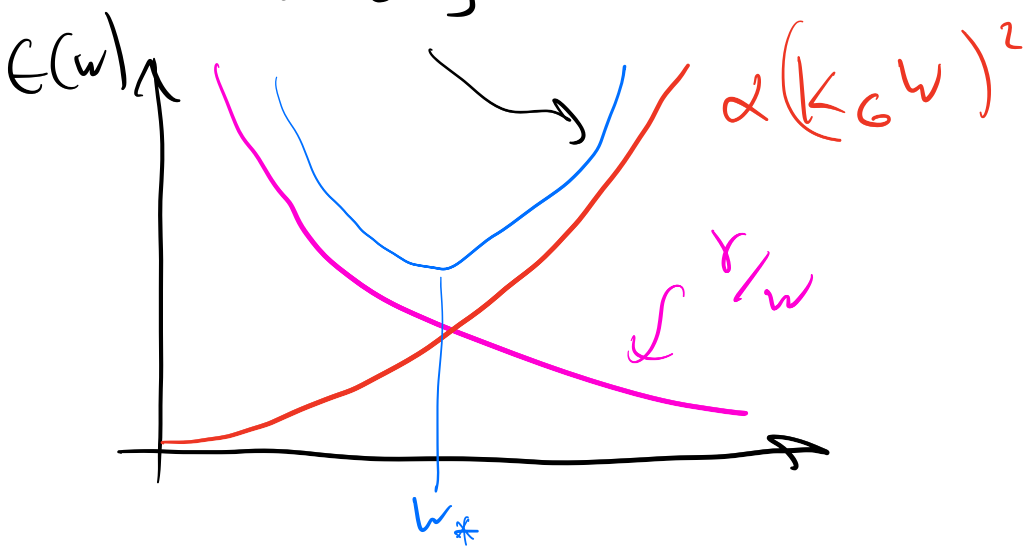
last lecture: $F_{elas} = \frac{Kf}{16}(\text{Area})\left(\frac{W}{R^2}\right)^2$

$$\epsilon(w) = -\epsilon_{bulk} + \frac{\gamma}{w} + \frac{F_{elas}}{\rho_0 (\text{Area})}$$

$\rho_0 \rightarrow$ density of particles

"excess" energy density $\rightarrow$

$$\epsilon_{ex}(w) = \frac{K_f}{16 \rho_0} \left(\frac{W}{R^2} \right)^2$$



$$\frac{\partial \epsilon}{\partial w} = -\frac{\gamma}{W_*^2} + \frac{K_f}{8 \rho_0} \frac{W}{R^4} \Rightarrow W_* = \left(\frac{8\gamma}{K_f} \rho_0 \right)^{1/3} R^{4/3}$$

Self-limited assembly:

finite domain size W_*

subunit size $\ll W_* \ll$ bulk

Note $\lim_{K_G \to 0} W_* \to \infty$, unlimited for frustration-free limit

2nd Ex. Crystalline domains on spheres (Schneider & Gompper, EPL 2005)

$$\epsilon_{ex}(w) = \frac{Y}{384\, \rho_0} \left(\frac{w}{R}\right)^4$$

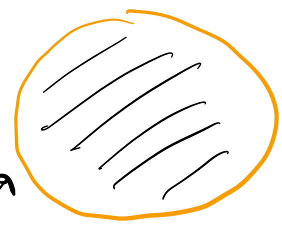
$$\Rightarrow w_* \propto \underbrace{\left(\frac{\gamma \rho_0}{Y}\right)^{1/5}}_{\text{cohesion/stiffness}} \underbrace{K_G^{-2/5}}_{\text{frustration}}$$

Shapes of domains

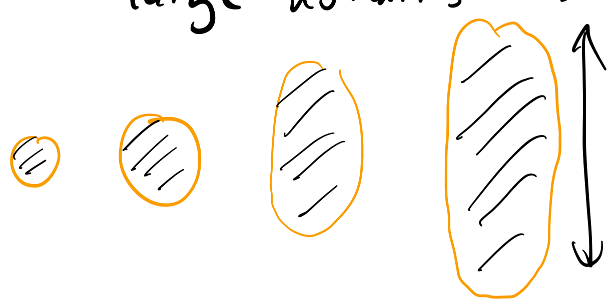
So far we have tacitly assumed compact (circular) domains. Why?

But E_{int} also includes elastic cost of frustration.

circular minimizes boundary



For large domains $\Rightarrow$ symmetry breaking



$L \gg w$ sometimes called "filamentation"

Why would strip be better? Consider 2D nematic example again

$$F = \frac{K_f}{2}\int dA\left(\nabla_\perp \theta - \vec{A}\right)^2 \qquad \text{Recall: } \vec{A} = \frac{1}{2R^2}\left(-y\hat{x} + x\hat{y}\right)$$

E.L. equation $\nabla_\perp^2 \theta = 0$ B.C. $\left(\partial_y \theta - A_y\right)\Big|_{y=\pm\frac{w}{2}} = 0$

$$\theta = Ax + Bx + Cxy + D \qquad = \partial_y \theta\Big|_{y=\pm\frac{w}{2}} - \frac{x}{2R^2}$$

$$A = B = 0 \qquad C = -\frac{1}{2R} \qquad = -Cx - \frac{x}{2R^2}$$

strain gradient: $\left(\nabla_\perp \theta - \vec{A}\right) = -2 \times \frac{1}{2R^2} y\hat{x}$

can check $\nabla_\perp \times \left(\nabla_\perp \theta - \vec{A}\right) = -K_G$

grows $\perp$ to long direction

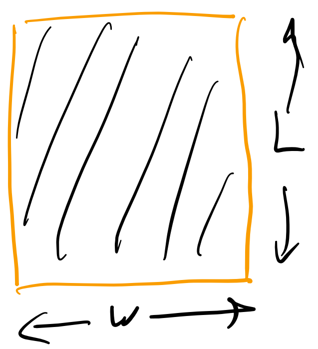
Frustration requires strain gradient. Energetics selects <u>direction</u> of gradient

$$F = \frac{K_f}{2} L \int_{-w/2}^{+w/2} dy \left(\frac{x}{R^2}\right)^2 = \frac{K_f}{8}\underbrace{(Lw)}_{\text{Area}}\left(\frac{w}{R^2}\right)^2 \propto L^1 w^3$$

faster growth in $\perp$ direction

Crude model of shape selection.

$\Rightarrow$ Assume rectangular shape, fixed $N_p \propto LW$



$$E_{tot} \propto \frac{F_{tot}}{\text{Area}} \simeq -\epsilon_{bulk} + \frac{\gamma(\overbrace{\text{perimeter}}^{2w+2L})}{Lw}$$

$$+ \frac{K_f}{8}\left(K_G w\right)^2$$

assume still holds for $w \lesssim L$

$$= \text{const.} + 2\gamma\left(\frac{1}{w} + \frac{w}{\text{Area}}\right) + \frac{K_f}{8}\left(K_G w\right)^2$$

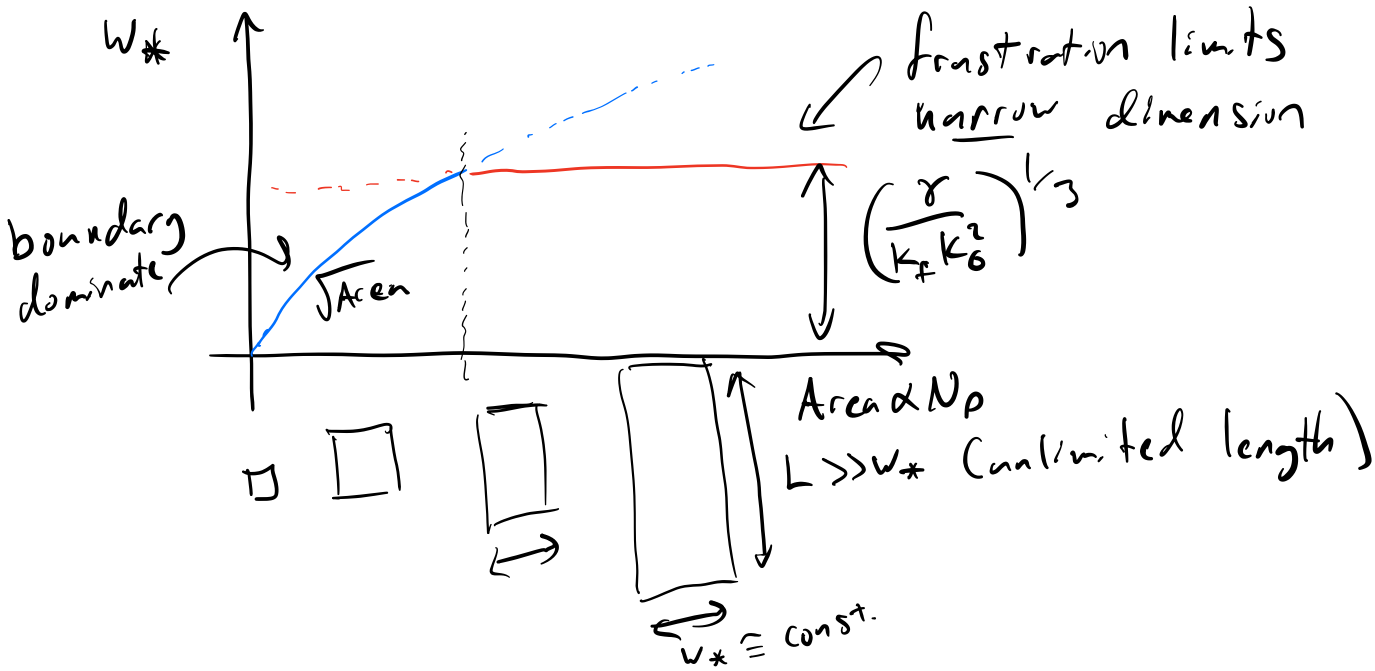
Equilibrium shape $\left.\frac{\partial E}{\partial w}\right|_{Area} = 2\gamma\left(-\frac{1}{w^2} + \frac{1}{Area}\right) + \frac{K_f}{4} K_G^2 W$

For small area, surface term dominates

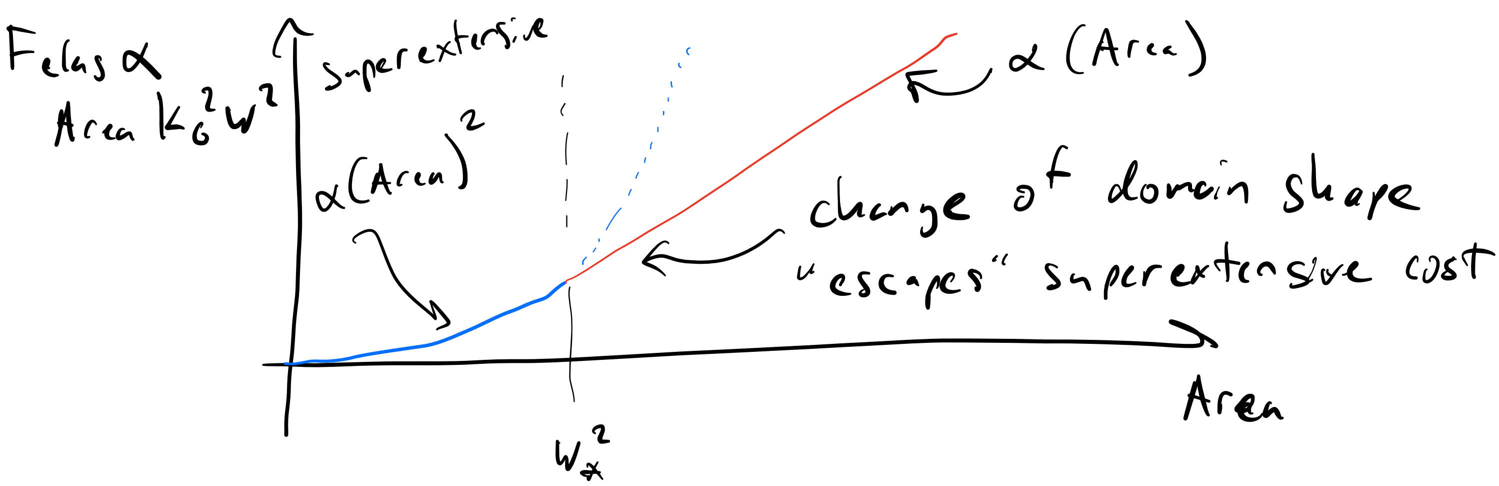
$$\Rightarrow \quad W_* \simeq \sqrt{Area} = L_x \quad (\text{square})$$

For large area, frustration balances edge energy

$$W_* \simeq \left(\frac{4\gamma}{K_f K_G^2}\right)^{1/3} \quad \text{independent of Area}$$



Notice the cross over in elastic energy vs. area



This is the first example of "frustration escape": groundstate avoids superextensive growth of elastic energy via some morphological motif (a.k.a. mode).

Here, transition from compact to extended (a.k.a. "filamented") domain shape.