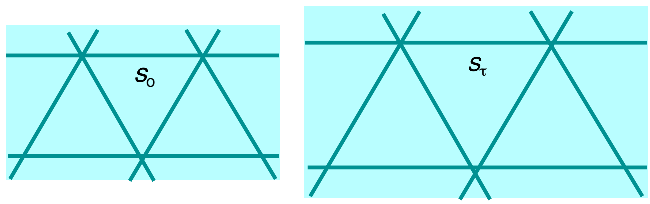
PHYS 4xx Net 3 - Properties of two-dimensional networks

Six-fold spring networks under stress

When the network is placed under a two-dimensional tension τ, s changes from its unstressed value s_o to a new value s_τ. We evaluate this behavior for a spring network.



- calculate s_τ by minimizing the enthalpy H

$$H = E - \tau A \quad (1)$$

- at 3 springs per vertex, the energy per vertex is $(3/2)k_{sp}(s - s_o)^2$

- the area per vertex is

$$A_V = \sqrt{3}\, s^2/2 \quad (2)$$

- hence, the enthalpy per vertex H_V is

$$H_V = (3/2)k_{sp}(s - s_o)^2 - \sqrt{3}\, \tau s^2/2 \quad (3)$$

- take the derivative of H_V to find s_τ:

$$0 = \partial H_V / \partial s = \partial/\partial s\, [(3/2)k_{sp}(s - s_o)^2 - \sqrt{3}\, \tau s^2/2]$$
$$= (3/2) \cdot 2 \cdot k_{sp}(s - s_o) - \sqrt{3} \cdot 2\tau s/2$$
$$= \sqrt{3} \cdot [\sqrt{3}\, k_{sp}(s - s_o) - \tau s]$$

then

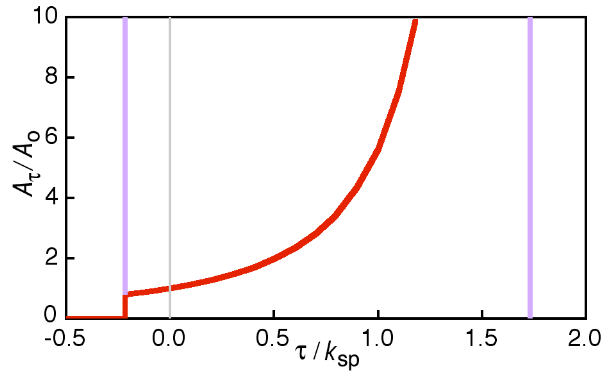
$$[\sqrt{3}\, k_{sp} - \tau]s = \sqrt{3}\, k_{sp} s_o$$
$$s = \sqrt{3}\, k_{sp} s_o / [\sqrt{3}\, k_{sp} - \tau]$$

or

$$s_\tau = s_o / (1 - \tau / [\sqrt{3}\, k_{sp}]) \qquad \text{(six-fold symmetry)} \quad (4)$$

- (4) shows that the network expands without bound as the tension approaches a critical value τ_{exp},

$$\tau_{exp} = \sqrt{3}\, k_{sp} \qquad \text{(six-fold symmetry),} \quad (5)$$



- expansion at large tension because both the energy of the springs and the pressure term τA_v scale like s^2 at large extensions; of course, physical networks could reach a maximum bond length

- the minimum value of the enthalpy per vertex is

$$H_{v,min} = (3/2)k_{sp}(s_\tau - s_o)^2 - \sqrt{3}\ \tau s_\tau^2/2$$
$$= (3/2)k_{sp}s_o^2\ [1/(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ ) - 1]^2 - \sqrt{3}\ \tau s_o^2\ /\ 2(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ )^2$$
$$= \{\ (3/2)k_{sp}s_o^2\ [\tau\ /\ [\sqrt{3}\ k_{sp}]^2 - \sqrt{3}\ \tau s_o^2\ /2\}\ /(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ )^2$$
$$= s_o^2\{k_{sp}\ [\tau\ /\ k_{sp}]^2 - \sqrt{3}\ \tau\}\ /\ 2(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ )^2$$
$$= \tau s_o^2\{\tau\ /\ k_{sp} - \sqrt{3}\ \}\ /\ 2(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ )^2$$
$$= \sqrt{3}\ \tau s_o^2\{\ (\tau/\sqrt{3}\ k_{sp}) - 1\}\ /\ 2(1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ )^2$$

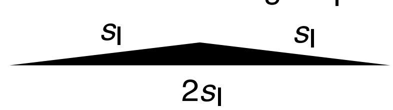
or

$$H_{v,min} = -\ (\sqrt{3}\ /\ 2)\tau s_o^2\ /\ (1 - \tau\ /\ [\sqrt{3}\ k_{sp}]\ ) \quad \text{(equilateral plaquettes)} \quad (6)$$

- Eq. (6) is not the global minimum of H under compression ($\tau < 0$) if shapes other than equilateral plaquettes are considered

- the smallest τA contribution at $\tau < 0$ is given by plaquettes with zero area

- isosceles triangles with two short sides of length s_l and a long side of length $2s_l$



have the lowest spring energy at zero area

$$H_{iso} = (k_{sp}/2)\bullet\ [(2s_l - s_o)^2 + 2(s_l - s_o)^2\ ]$$

- minimum value of H_{iso} as a function of s_l is at $\partial H / \partial s = 0$, or

$$0 = \partial/\partial s\ [(2s_l - s_o)^2 + 2(s_l - s_o)^2\ ]$$
$$= 2\bullet 2\bullet(2s_l - s_o) + 2\bullet 2\bullet(s_l - s_o)$$
$$= 8s_l - 4s_o + 4s_l - 4s_o \qquad = 12s_l - 8s_o$$

or

$$s_l = 2s_o/3$$

- Thus

$$H_{iso} = (k_{sp}/2)\bullet [(4s_o/3- s_o)^2 + 2(2s_o/3 - s_o)^2] = k_{sp}s_o^2/2 [(1/3)^2 + 2(1/3)^2]$$
$$= k_{sp}s_o^2/6 \quad (7)$$

Thus, the enthalpy per vertex of the equilateral network rises with pressure ($\tau < 0$) according to Eq. (6) until it exceeds Eq. (7) at a collapse tension τ_{coll}

$$H_{V,min} = k_{sp}s_o^2/6$$

that is

$$- (\sqrt{3} / 2)\tau s_o^2 / (1 - \tau / [\sqrt{3}\ k_{sp}]) = k_{sp}s_o^2/6$$
$$- (\sqrt{3} / 2)\tau = (k_{sp}/6)\bullet(1 - \tau / [\sqrt{3}\ k_{sp}])$$
$$- \tau = (k_{sp}/3\sqrt{3})\bullet(1 - \tau / [\sqrt{3}\ k_{sp}])$$
$$- \tau = k_{sp}/3\sqrt{3} - \tau /9$$
$$- (8/9)\tau = k_{sp}/3\sqrt{3}$$

or

$$\tau_{coll} = - (\sqrt{3} /8)\ k_{sp} \qquad \text{(six-fold symmetry)}, \quad (8)$$

or, equivalently, at an equilateral spring length $s_\tau/s_o = 8/9$.

Elastic moduli for networks under stress

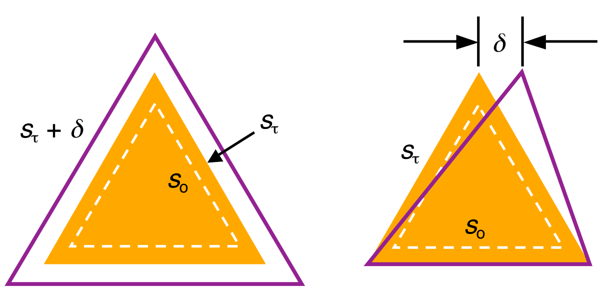
Elastic moduli can be obtained by the same method as in Net 2 for springs at zero temperature and no stress. For variety, we take a different approach for the compression modulus, going back to its definition

$$K_A^{-1} = A^{-1}\ \partial A /\partial\tau = (1/s_\tau^2)\ \partial s_\tau^2 /\partial\tau = (2/s_\tau)\ \partial s_\tau /\partial\tau$$
$$= (2/s_\tau)\ \partial/\partial\tau\{ / (1 - \tau / [\sqrt{3}\ k_{sp}])\}$$
$$= (2s_o/s_\tau)\ (-1)(-1/\sqrt{3}\ k_{sp})(1 - \tau / [\sqrt{3}\ k_{sp}])^{-2}$$
$$= (2/\sqrt{3}\ k_{sp})(1 - \tau / [\sqrt{3}\ k_{sp}])^{-1}$$

thus

$$K_A = (\sqrt{3}\ k_{sp}/2)\bullet(1 - \tau / [\sqrt{3}\ k_{sp}]) \quad (9)$$

(this returns our previous expression when $\tau = 0$)



The shear modulus can be obtained following the same route as before

$\mu = (\sqrt{3}\ k_{sp}/4) \bullet (1 + \sqrt{3}\ \tau / k_{sp})$, (10)

- the Poisson ratio is a measure of how a material contracts in a transverse direction when stretched longitudinally; in two dimensions (stress along the *x*-axis)
  $\sigma_p = - u_{yy} / u_{xx}$, (11)

- (the negative sign gives $\sigma_p > 0$ for conventional materials)

- we can show, from the 3D result in Appendix D, that in 2D:
  $\sigma_p = (K_A - \mu) / (K_A + \mu)$. (12)

- a triangular network at zero temperature and stress has $K_A / \mu = 2$ ---> $\sigma_p = 1/3$

- (9) and (10) give
  $\sigma_p = [1 - 5\tau / (\sqrt{3}\ k_{sp})] / [3 + \tau / (\sqrt{3}\ k_{sp})]$ (six-fold symmetry). (13)

- thus, σ_p becomes negative over the range $\sqrt{3} / 5 < \tau / k_{sp} < \sqrt{3}$