Leiden Elasticity Lectures III

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Lattice Elasticity: Preliminaries

Vertices labelled by ℓ are at position $\mathbf{R}_\ell$; b labels a bond of length R_b

$$U_T = \sum_b V(R_b) = \sum_{\langle \ell,\ell' \rangle} V(|\mathbf{R}_{\ell'} - \mathbf{R}_\ell|)$$

$$\mathbf{R}_\ell = \mathbf{R}_{\ell 0} + \mathbf{u}_\ell; \quad \mathbf{R}_b = \mathbf{R}_{b0} + \Delta\mathbf{u}_b; \quad \Delta\mathbf{u}_b = \mathbf{u}_{\ell'} - \mathbf{u}_\ell$$

$$R_{b0} = |\mathbf{R}_{\ell' 0} - \mathbf{R}_{\ell 0}|; \quad v_b = \tfrac{1}{2}(R_b^2 - R_{b0}^2) = \mathbf{R}_{b0} \cdot \Delta\mathbf{u}_b + \tfrac{1}{2}\Delta\mathbf{u}_b \cdot \Delta\mathbf{u}_b$$

Invariant under: $R_{bi} \to O_{ij} R_{bj}; O_{ij}$ is a rotation matrix

v_b: Lattice analog of non-linear strain

Expand to 2nd order in $v_b : V_b(R_b) = V_b\left(\sqrt{R_{b0}^2 + v_b}\right)$

$$\approx R_{b0}^{-1} V_b'(R_{b0}) v_b + \tfrac{1}{2} R_{b0}^{-2}\left[V_b''(R_{b0}) - R_{b0}^{-1} V_b'(R_{b0})\right] v_b^2$$

Linearized Limit

$$\Delta U_T = \sum_b R_{b0}^{-1} \tilde{F}(b) v_b + \tfrac{1}{2} \sum_b k(b) R_{b0}^{-2} v_b^2$$

First term could come from internal or external stresses

$$\tilde{F}(b) = V_b'(R_{b0}) = \text{ Tension in bond}$$

$$k(b) = \left[V_b''(R_{b0}) - R_{b0}^{-1} V_b'(R_{b0}) \right]$$

$$R_{b0}^{-1} V_b'(R_{b0}) v_b \to V_b'(\mathbf{R}_{b0}) \mathbf{e}_{b0} \cdot \Delta \mathbf{u}_b = \tilde{F}_b(\mathbf{R}_{b0}) \cdot \Delta \mathbf{u}_b$$

In Equilibrium, the force at every site must be zero.
Eliminates linear term in v_b in first term in U_T.

$$F_i(\ell) = \frac{\partial U_T}{\partial u_{\ell i}} = \sum\nolimits_{\ell'} \tilde{F}_i(\langle \ell, \ell' \rangle) = 0$$

$$\Delta U_T = \tfrac{1}{2} \sum\nolimits_b [V_b'' e_{b0i} e_{b0j} + R_{b0}^{-1} V_b' (\delta_{ij} - e_{b0i} e_{b0j})] \Delta u_{bi} \Delta u_{bj}$$

$$= \tfrac{1}{2} \sum\nolimits_b [V_b'' (\Delta u_b^{\parallel})^2 + R_{b0}^{-1} V_b' (\Delta u_b^{\perp})^2]$$

Continuum Limit

Reference space vectors : $\mathbf{R}_{b0}$

Target space vectors: $R_{bi} = \Lambda_{i\alpha} R_{b0\alpha}$

$$v_b = R_{b0\alpha} R_{b0\beta} \left(\Lambda^T_{\alpha i} \Lambda_{i\beta} - \delta_{\alpha\beta} \right) = 2 R_{b0\alpha} R_{b0\beta} u_{\alpha\beta}$$

$$u_{\alpha\beta} = \tfrac{1}{2} \left(\partial_\alpha u_\beta + \partial_\beta u_\alpha + \partial_\alpha \mathbf{u} \cdot \partial_\beta \mathbf{u} \right)$$

$$\mathcal{H} \square = \int d^D x \left[\tfrac{1}{2} K_{\alpha\beta\gamma\delta} u_{\alpha\beta} u_{\gamma\delta} + \tilde{\sigma}_{\alpha\beta} u_{\alpha\beta} \right]$$

$$K_{\alpha\beta\gamma\delta} = \tfrac{1}{2v(x)} \sum_{\ell'} k(b) R_{b0}^{-2} R_{b0\alpha} R_{b0\beta} R_{b0\gamma} R_{b0\delta} \, |_{b=\langle \ell,\ell' \rangle}$$

$$\tilde{\sigma}_{\alpha\beta} = \tfrac{1}{2v(x)} \sum_{\ell'} \tilde{F}_\alpha(b) R_{b0\beta} \, |_{b=\langle \ell,\ell' \rangle}$$

$$= \tfrac{1}{2v(x)} \sum_{\ell'} V_b'(R_{b0}) R_{b0}^{-1} R_{b0\alpha} R_{b0\beta} \, |_{b=\langle \ell,\ell' \rangle}$$

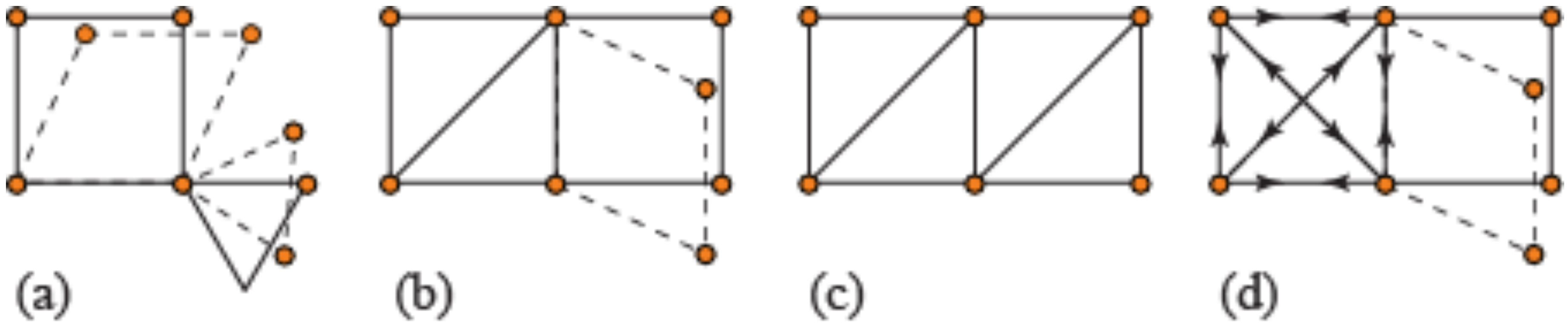
This expression is for the free energy before any relaxation in response to external stress. $K_{\alpha\beta\chi\delta}$ is symmetric under interchange of any pair of indices – Cauchy symmetry.

Maxwell –Calladine Count: No Tension

C. R. Calladine, Int. J. Solids and Struct. **14** (2), 161-172 (1978).

Degrees of freedom: dN; # of constraints: $N_c = N_B = zN/2$

Maxwell: $N_0 = dN - N_c$ -> $z_c = 2d$



(a) N=6, $N_c = 7$: $N_0 = 2x6\text{-}7 = 5 = 3+2$
(b) N=6, $N_c = 8$; $N_0 = 2x6\text{-}8 = 3 +1$
(c) N=6, $N_c = 9$; $N_0 = 3$
(d) N=6, $N_c = 9$; N_0 π 3

(d) Has a state of self stress: bonds can be under stress with net zero force at nodes.

$$N_0 - S = dN - N_B$$

Equilibrium and Compatibility Matrices

$$\Delta U_T = \tfrac{1}{2}\sum\nolimits_b [V_b''(\Delta u_b^{\parallel})^2] \rightarrow \tfrac{1}{2}\sum_b k_b \mathsf{e}_b^2$$

$$\mathsf{e}_b = \Delta u_b^{\parallel} = \hat{\mathbf{b}}_b \cdot \Delta \mathbf{u}_b = \text{ bond extension or stretch}$$

$$\vec{\mathsf{e}}_b = N_b \text{ dimensional vector of bond stretches}$$

$$\Delta U_T = \tfrac{1}{2}\vec{\mathsf{e}}_b^T \overleftrightarrow{k} \vec{\mathsf{e}}_b$$

$$t_b = \frac{\partial U_T}{\partial e_b} = k_b e_b \rightarrow \vec{t}\ (N_b \text{ dim}); \quad f_{\ell i} = \frac{\partial U_T}{\partial u_{\ell i}} \rightarrow \vec{f}\ (dN \text{ dim})$$

$$\overleftrightarrow{\mathsf{C}} \cdot \vec{\mathsf{u}} = \vec{\mathsf{e}}; \quad \overleftrightarrow{\mathsf{Q}} \cdot \vec{\mathsf{t}} = \vec{\mathsf{f}};$$

$\overleftrightarrow{\mathsf{C}}$: Compatibility matrix

$\overleftrightarrow{\mathsf{Q}}$: Equlibrium Matrix

$$\Delta W_{\mathsf{f}} = \vec{\mathsf{f}}^T \cdot \Delta \vec{\mathsf{u}} = \vec{\mathsf{t}}^T \cdot \overleftrightarrow{\mathsf{Q}}^T \cdot \Delta \vec{\mathsf{u}}$$

$$\Delta W_{\mathsf{t}} = \vec{\mathsf{t}}^T \cdot \Delta \vec{\mathsf{e}} = \vec{\mathsf{t}}^T \cdot \overleftrightarrow{\mathsf{C}} \cdot \Delta \vec{\mathsf{u}}$$

$$\Delta W_{\mathsf{t}} = \Delta W_{\mathsf{f}} \Rightarrow \overleftrightarrow{\mathsf{C}} = \overleftrightarrow{\mathsf{Q}}^T$$

$$\Delta U_T = \tfrac{1}{2}\vec{\mathsf{u}}^T \cdot \overleftrightarrow{\mathsf{C}}^T \cdot \overleftrightarrow{\mathsf{k}} \cdot \overleftrightarrow{\mathsf{C}} \cdot \vec{\mathsf{u}}$$

$$= \tfrac{1}{2}\vec{\mathsf{t}}^T \cdot \overleftrightarrow{\mathsf{k}}^{-1} \cdot \vec{\mathsf{t}}$$

$\overleftrightarrow{\mathsf{C}}$: u (dim. dN) to $\vec{\mathsf{e}}$ (dim N_B)

$\Rightarrow dN \times N_B$ Matrix

$\overleftrightarrow{\mathsf{Q}}$: t (dim. N_B) to $\vec{\mathsf{f}}$ (dim dN)

$\Rightarrow N_B \times dN$ Matrix

Calladine Theorem

$\overleftrightarrow{C} \cdot \vec{u} = 0$; Displacements with no stretch:

zero modes = Nullspace (kernel) of $\overleftrightarrow{C}$

$\overleftrightarrow{Q} \cdot \vec{t} = 0$; Tensions with no force:

States of Self Stress = Nullspace (kernel)of $\overleftrightarrow{Q}$.

Rank-Nullity theorem:

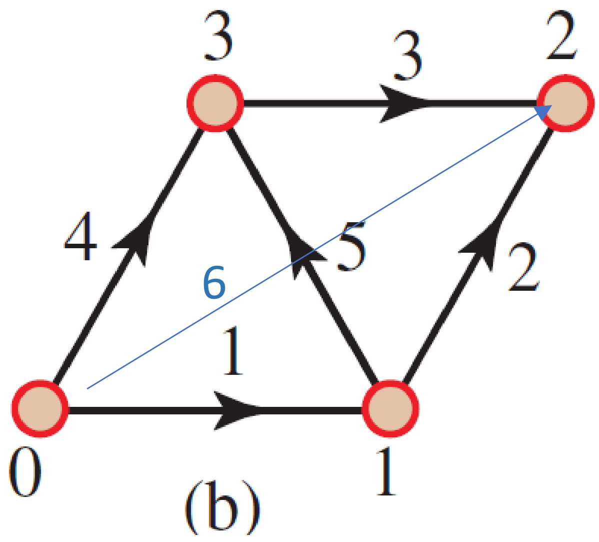
Rank($\overleftrightarrow{M}$)+Dim(ker($\overleftrightarrow{M}$))=No. of columns of $\overleftrightarrow{M}$

Rank($\overleftrightarrow{M}$) $=$ Rank($\overleftrightarrow{M}^T$)

Rank($\overleftrightarrow{C}$)+N_0=dN;   Rank($\overleftrightarrow{Q}$) $+ S = N_B$

$$N_0 - S = dN - N_B$$

An Example



$\hat{\mathbf{b}}_1 = (1,0)$

$\hat{\mathbf{b}}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$

$\hat{\mathbf{b}}_3 = (1,0)$

$\hat{\mathbf{b}}_4 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$

$\hat{\mathbf{b}}_5 = (-\frac{1}{2}, \frac{\sqrt{3}}{2})$

$\hat{\mathbf{b}}_6 = (\frac{\sqrt{3}}{2}, \frac{1}{2})$

Set $\mathbf{u}_0 = 0$, $\mathbf{u}_1 = (u_{1x}, 0)$

$\Rightarrow 3$ constraints,

5 degrees of freedom

Set 1: 5 bonds (no $\mathbf{b}_6$);

Set 2: 6 bonds;

Set 3: 5 bonds (no $\mathbf{b}_5$ or $\mathbf{b}_6$)

$\tilde{\mathrm{u}} = (u_{1x}, u_{2x}, u_{2y,} u_{3x}, u_{3y})$

$e_{\langle \ell, \ell' \rangle} = \hat{\mathbf{b}}_{\langle \ell, \ell' \rangle} \cdot (\tilde{\mathrm{u}}_{\ell'} - \tilde{\mathrm{u}}_{\ell})$

$$\overleftrightarrow{\mathrm{C}}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}$$

No zero modes or SSS;

N_0-S=0=5-5=0

$$\overleftrightarrow{\mathrm{C}}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{1}{2} & 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \end{pmatrix}$$

State of Self stress, no Zero mode: N_0=0, S=1:

N_0-S=-1=5-6=-1

$$\overleftrightarrow{\mathrm{C}}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{pmatrix}$$

One Zero mode, no SSS:

N0=1,S=0: N0-S=1=5-4=1

Periodic Maxwell-Calladine

Periodic Systems:
$\overleftrightarrow{C}(\mathbf{q})\vec{u}(\mathbf{q}) = \vec{e}(\mathbf{q});$
$\vec{Q}(\mathbf{q})\vec{t}(\mathbf{q}) = \vec{f}(\mathbf{q})$
for every $\mathbf{q}$:

Maxwell-Calladine applies for every $\mathbf{q}$

$$n_0(\mathbf{q}) - s(\mathbf{q}) = dn - n_B$$

$n_0(\mathbf{q})$: # zero modes at $\mathbf{q}$
$s(\mathbf{q})$: # SSSs at $\mathbf{q}$
n : sites/unit cell
n_B : bonds/unit cell

Maxwell Periodic lattice:

$$dn = n_B \Rightarrow n_0(\mathbf{q}) = s(\mathbf{q}) \, \forall \, \mathbf{q}$$

In the bulk phonon spectrum, there is exactly one zero mode for each state of self stress!

SSS's and Elasticity I

States of self stress determine elastic response. To see how this comes about, we consider applying an affine strain to a system under periodic boundary conditions. The affine response is not the lowest energy one, so there will be local relaxation. Here we calculate that relaxation and relate it to SSSs.

$$(u_{\ell' i} - u_{\ell i})_{\text{affine}} = \Lambda_{ij}(R_{\ell' 0,j} - R_{\ell 0,j}) = \Lambda_{ij} b_{\langle \ell,\ell' \rangle,j}$$

$$e_{b,\text{affine}} = \hat{b}_{bi} \Lambda_{ij} b_{bj} \text{ (linearized)}$$

$$\vec{\mathsf{e}} = \vec{\mathsf{e}}_{\text{aff}} + \overleftrightarrow{\mathsf{C}} \cdot \vec{\mathsf{u}}$$

$$\Delta U_T = \tfrac{1}{2}(\vec{\mathsf{e}}_{\text{aff}}^T + \vec{\mathsf{u}}^T \cdot \overleftrightarrow{\mathsf{C}}^T) \cdot \overleftrightarrow{\mathsf{k}} \cdot (\vec{\mathsf{e}}_{\text{aff}} + \overleftrightarrow{\mathsf{C}} \cdot \vec{\mathsf{u}})$$

$\vec{\mathsf{u}}$ meaures the deviation from affine strain.

SSS's and Elasticity II

Break $\overleftrightarrow{C}$ into components of its range and null spaces

$$\overleftrightarrow{I}^{dN} = \overleftrightarrow{P}_R + \overleftrightarrow{P}_Z; \quad \overleftrightarrow{I}^{N_B} = \overleftrightarrow{P}_R + \overleftrightarrow{P}_S$$

$$\overleftrightarrow{C} = (\overleftrightarrow{P}_R + \overleftrightarrow{P}_S)\cdot\overleftrightarrow{C}\cdot(\overleftrightarrow{P}_R + \overleftrightarrow{P}_Z) = \overleftrightarrow{C}_{RR} + \overleftrightarrow{C}_{SR} + \overleftrightarrow{C}_{RZ} + \overleftrightarrow{C}_{SZ}$$

$$\overleftrightarrow{C}\cdot\vec{u} = (\overleftrightarrow{C}_{RR} + \overleftrightarrow{C}_{SR})\cdot\vec{u}_R$$

$$\vec{a}\cdot\overleftrightarrow{C}\cdot\vec{u} = \vec{a}\cdot\overleftrightarrow{C}_{RR}\cdot\vec{u} = \vec{a}_R\cdot\overleftrightarrow{C}_{RR}\cdot\vec{u}_R$$

Singular Value Decomposition

$$\Delta U_T = \tfrac{1}{2}(\vec{e}^T_{\text{aff}} + u^T_R\cdot Q_{RR})\cdot\overleftrightarrow{k}\cdot(\vec{e}_{\text{aff}} + \overleftrightarrow{C}_{RR}\cdot\vec{u}_R)$$

$$\frac{\partial\Delta U_T}{\partial u^T_R} = \overleftrightarrow{Q}_{RR}\cdot\overleftrightarrow{k}\cdot(\vec{e}_{\text{aff}} + \overleftrightarrow{C}_{RR}\cdot\vec{u}_R) = 0$$

$$\overleftrightarrow{k}_{RR}\cdot(\vec{e}_{\text{aff},R} + \overleftrightarrow{C}_{RR}\cdot\vec{u}_R) = -\overleftrightarrow{k}_{RS}\cdot\vec{e}_{\text{aff},S}$$

$$(\vec{e}_{\text{aff},R} + \overleftrightarrow{C}_{RR}\cdot\vec{u}_R) = -\overleftrightarrow{k}^{-1}_{RR}\cdot\overleftrightarrow{k}_{RS}\cdot\vec{e}_{\text{aff},S}$$

$$\Delta U_T = \tfrac{1}{2}\vec{e}^T_{\text{aff},S}\cdot(\overleftrightarrow{k}_{SS} - \overleftrightarrow{k}_{SR}\cdot\overleftrightarrow{k}^{-1}_{RR}\cdot\overleftrightarrow{k}_{RS})\cdot\vec{e}_{\text{aff},S} = \tfrac{1}{2}\vec{e}^T_{\text{aff},S}\cdot(\overleftrightarrow{k}^{-1}_{SS})^{-1}\cdot\vec{e}_{\text{aff},S}$$

$$= \tfrac{1}{2}\vec{e}^T_{\text{aff},S}\cdot\hat{t}_n\hat{t}^T_n\cdot(\overleftrightarrow{k}^{-1}_{SS})^{-1}\cdot\hat{t}_m\hat{t}^T_m\cdot\vec{e}_{\text{aff},S} \rightarrow \tfrac{1}{2}k\sum_n(\vec{e}^T_{\text{aff},S}\cdot\hat{t}_n)^2$$

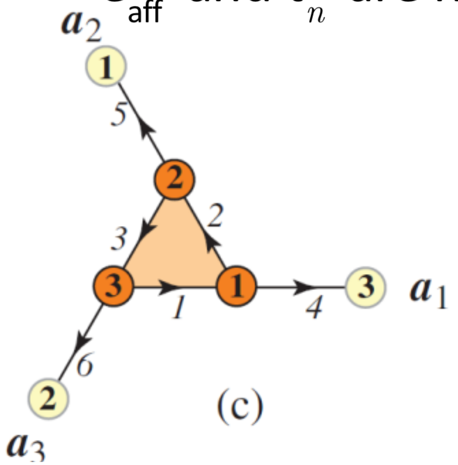
$\hat{t}_n$: Normalized basis vectors for SSS

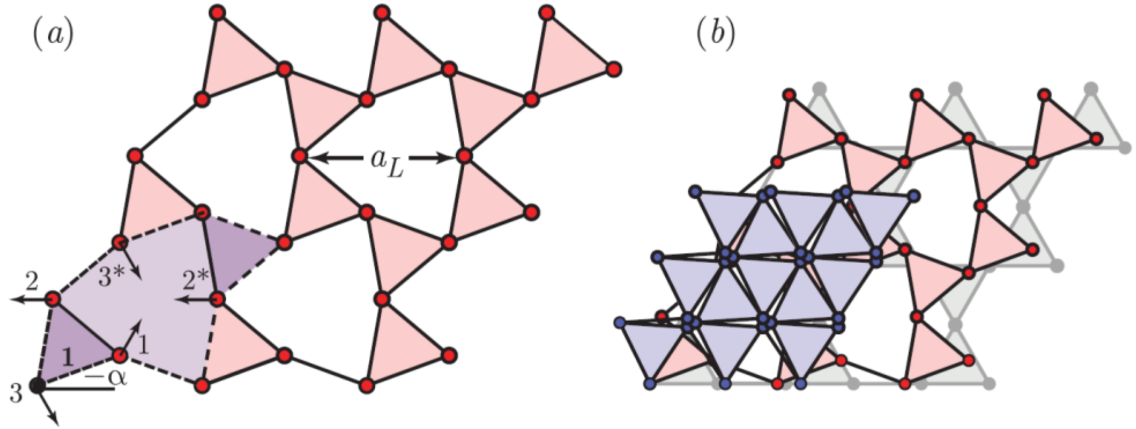
Periodic Lattices

$\Delta\vec{\mathrm{e}}_{\mathrm{aff}}$ is spacially uniform $\Rightarrow$ only $\mathbf{q}=0$ part of $\hat{\mathrm{t}}_n$ contributes.

$$f_{el} = \frac{N_c}{2V}\sum_{n,m} \vec{\mathrm{e}}^T_{\mathrm{aff}} \cdot \hat{\mathrm{t}}_n \hat{\mathrm{t}}^T_n \cdot (\mathrm{k}_{\mathrm{SS}}^{-1})^{-1} \cdot \hat{\mathrm{t}}_n \hat{\mathrm{t}}^T_n \cdot \vec{\mathrm{e}}_{\mathrm{aff}} \rightarrow \frac{N_c}{2V}\sum_n k\,(\vec{\mathrm{e}}^T_{\mathrm{aff}} \cdot \hat{\mathrm{t}}_n)^2$$

$\vec{\mathrm{e}}_{\mathrm{aff}}$ and $\hat{\mathrm{t}}_n$ are now vectors of dimension n_B.





$$\boldsymbol{C}_{\mathrm{sym}}(\boldsymbol{q}) = \begin{pmatrix} \hat{b}_{1x} & \hat{b}_{1y} & 0 & 0 & -\hat{b}_{1x} & -\hat{b}_{1y} \\ -\hat{b}_{2x} & -\hat{b}_{2y} & \hat{b}_{2x} & \hat{b}_{2y} & 0 & 0 \\ 0 & 0 & -\hat{b}_{3x} & -\hat{b}_{3y} & \hat{b}_{3x} & \hat{b}_{3y} \\ -\hat{b}_{4x} & -\hat{b}_{4y} & 0 & 0 & e^{i\boldsymbol{q}\cdot\boldsymbol{a}_1}\hat{b}_{4x} & e^{i\boldsymbol{q}\cdot\boldsymbol{a}_1}\hat{b}_{4y} \\ e^{i\boldsymbol{q}\cdot\boldsymbol{a}_2}\hat{b}_{5x} & e^{i\boldsymbol{q}\cdot\boldsymbol{a}_2}\hat{b}_{5y} & -\hat{b}_{5x} & -\hat{b}_{5y} & 0 & 0 \\ 0 & 0 & e^{i\boldsymbol{q}\cdot\boldsymbol{a}_3}\hat{b}_{6x} & e^{i\boldsymbol{q}\cdot\boldsymbol{a}_3}\hat{b}_{6y} & -\hat{b}_{6x} & -\hat{b}_{6y} \end{pmatrix}. \qquad \text{(C.2)}$$

kagome (3 SSS's): $\lambda = \mu = \dfrac{\sqrt{3}}{8}k$

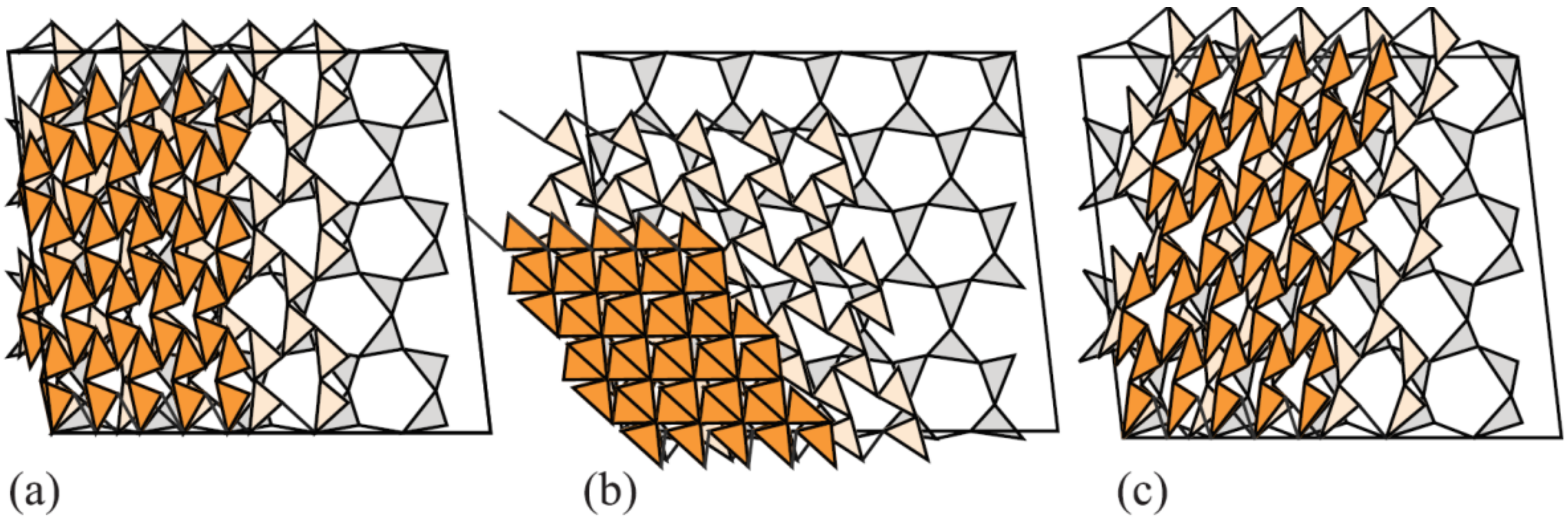
Twisted Kag (2 SSS's): $\lambda = -\mu = \dfrac{\sqrt{3}}{8}k$

$B = \lambda + \mu = 0;$ Bulk Modulus

$$f_{el} = \tfrac{1}{2}\mu\tilde{u}_{\alpha\beta}\tilde{u}_{\alpha\beta}; \quad \tilde{u}_{\alpha\beta} = u_{\alpha\beta} - \tfrac{1}{2}\delta_{\alpha\beta}u_{\gamma\gamma}$$

Guest-Hutchinson Modes

A fully gapped Maxwell lattice (FGML)has exactly d zero modes at $\mathbf{q}=0$ under periodic boundary conditions in d dimensions and thus d $\mathbf{q}=0$ SSS's. $d(d+1)/2$ SSS's are needed for elastic stability. Thus FGMLs have $d(d\text{-}1)/2$ elastic distortions of zero energy – the Guest-Hutchinson modes.



GH modes and phonon dispersion

Let $\underset{\sim}{u}^G = (u^G_{xx}, u^G_{yy}, u^G_{xy})$ be the strain of a 2D Guest mode:

$$\begin{pmatrix} K_{xxxx} & K_{xxyy} & 2K_{xxxy} \\ K_{xxyy} & K_{yyyy} & 2K_{yyxy} \\ 2K_{xxxy} & 2K_{yyxy} & 4K_{xyxy} \end{pmatrix} \begin{pmatrix} u^G_{xx} \\ u^G_{yy} \\ u^G_{xy} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$\underset{\sim}{u}^G(\mathbf{q}) = (iq_x u^G_x, iq_y u^G_y, \frac{1}{2}(q_x u^G_y + q_y u^G_x))$ also zero mode if

$$\frac{q_x u^G_x}{q_y u^G_y} = \frac{u^G_{xx}}{\underset{\sim}{u}^G_{yy}}; \frac{q_x u^G_y + q_y u^G_x}{2q_y u^G_y} = \frac{u^G_{xy}}{u^G_{yy}}$$

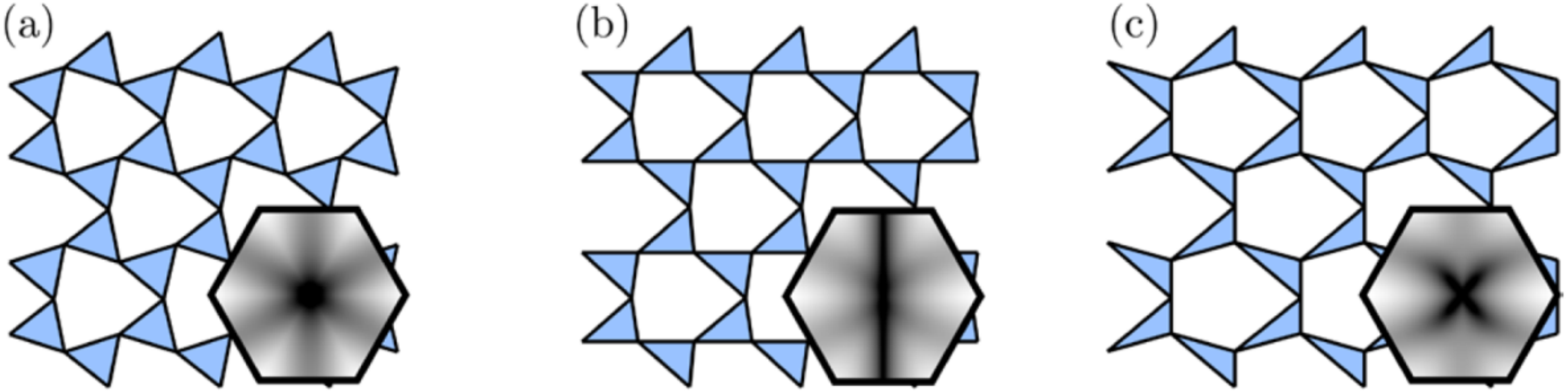
$$\frac{q_y}{q_x} = \frac{1}{u^G_{xx}}\left[u^G_{xy} \pm \sqrt{-\det \underset{\sim}{u}^G}\right]$$

$$\frac{q_y}{q_x} = \frac{1}{u^G_{xx}}\left[u^G_{xy} \pm \sqrt{-\det \underset{\sim}{u}^G}\right]$$

$\det \underset{\sim}{u}^G < (>) 0 : \ \underset{\sim}{u}^G_{yy} \underset{\sim}{u}^G_{yy} < (>) 0,$ i.e., positive (negative)

Poisson ratio if $\underset{\sim}{u}^G_{xy} = 0 : \ \ q_y / q_y$ Real (imaginary - surface mode)

Mode Examples



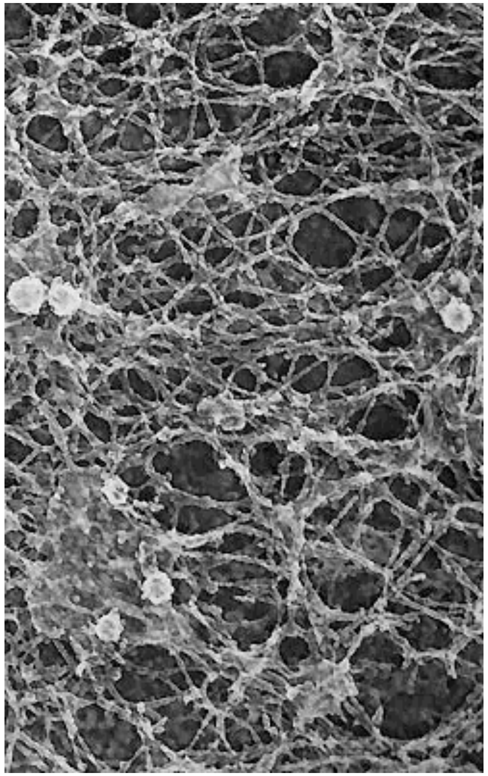
$\det \underset{\sim}{u}^G > 0$ $\det \underset{\sim}{u}^G < 0$

$$u^G_{xy} = 0 \Rightarrow \det \underset{\sim}{u}^G = u^G_{xx} u^G_{yy} \rightarrow \begin{cases} - \Rightarrow \text{Pos. Poisson ratio} \\ + \Rightarrow \text{Neg. Poisson ratio} \end{cases}$$

$\det \underset{\sim}{u}^G < 0:\ q_y / q_x$ real $\Rightarrow$ zero-bulk mode to order q.

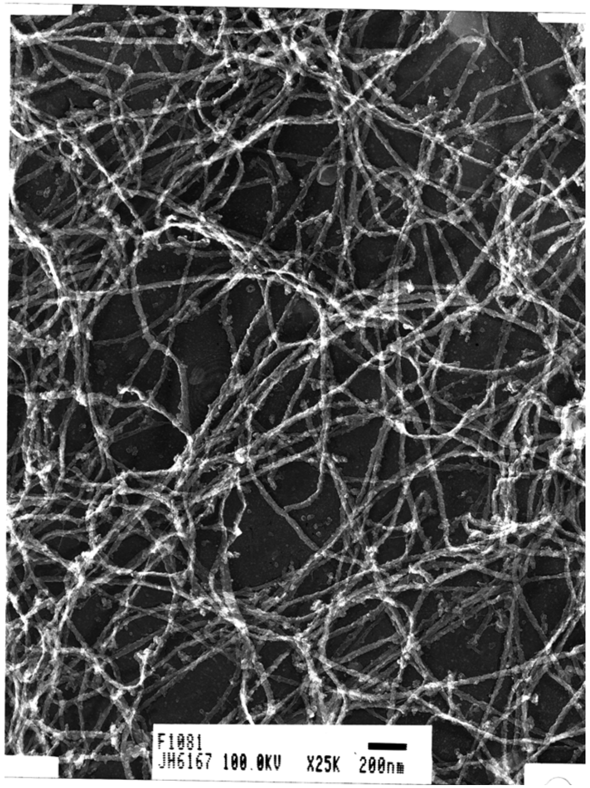
$\det \underset{\sim}{u}^G > 0:\ q_y / q_x$ Imaginary $\Rightarrow$ zero-surface mode at order q.

Networks of Semi-Flexible Polymers (z_m=4)

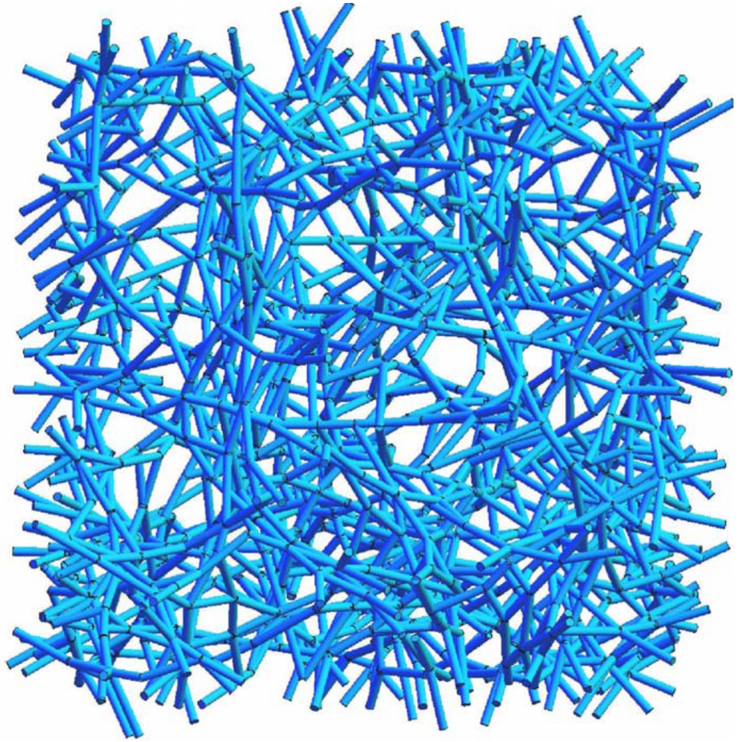


cortical actin gel

Janmey

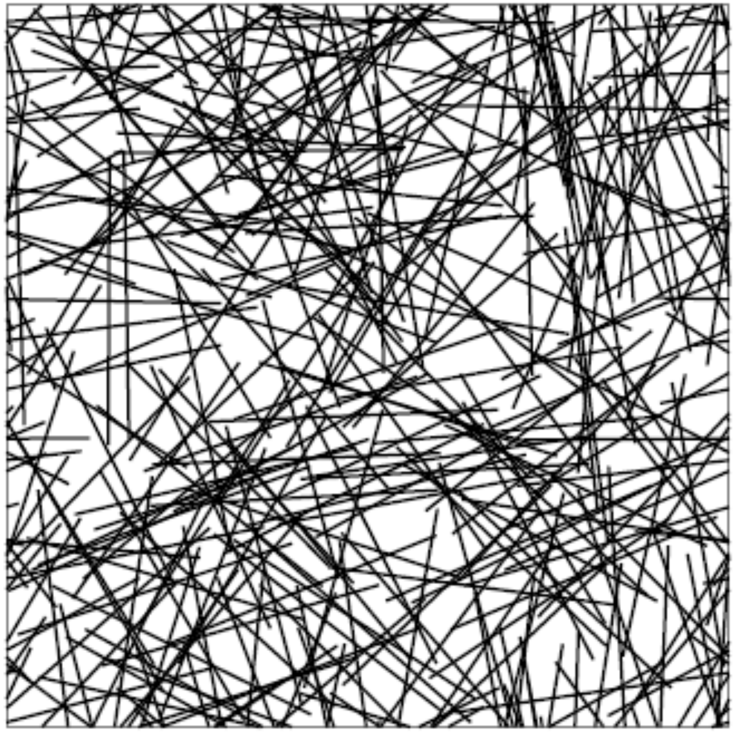


neurofilament network



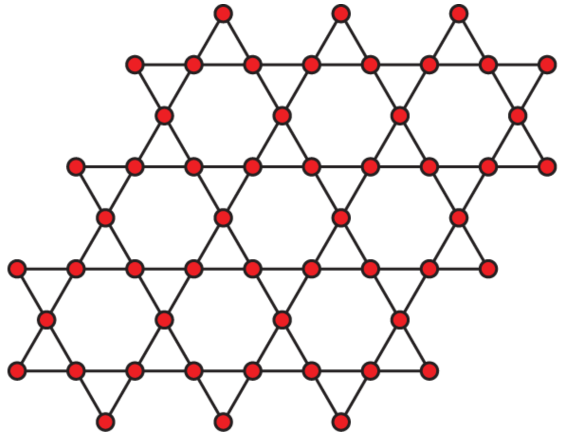
Computer generated Model (Huisman)

Two-dimensional "Straight Models"

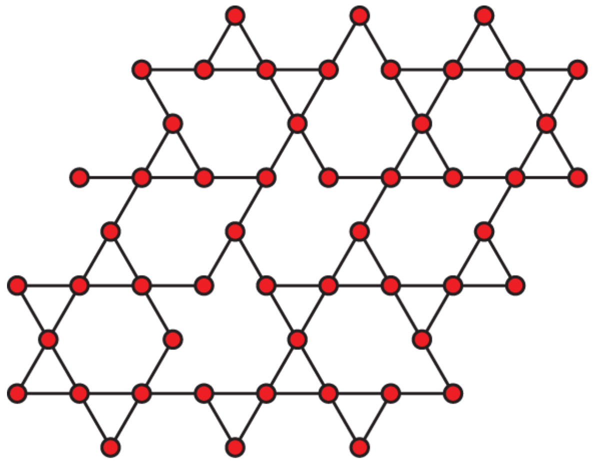


Mikado model (MacKintosh, Frey, Head, Levine, Huessinger)

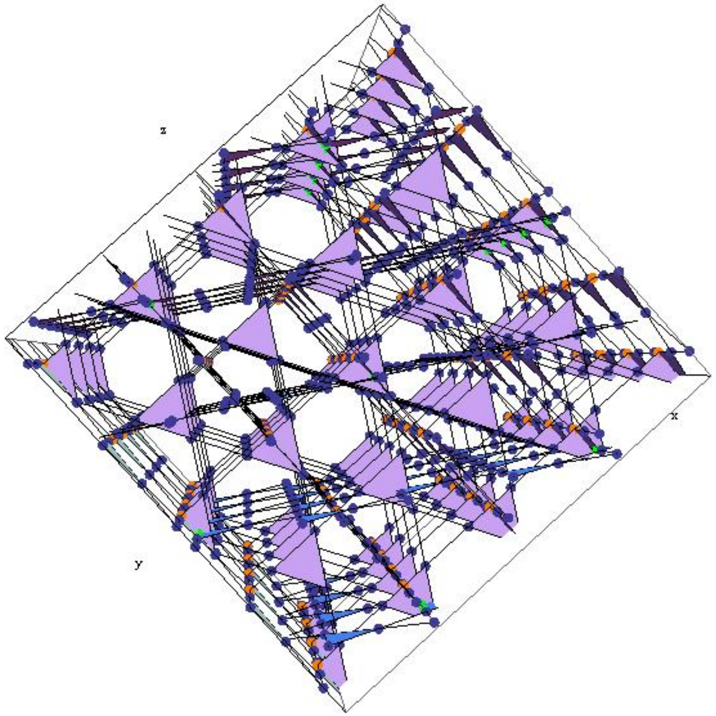
Kagome



Diluted kagome

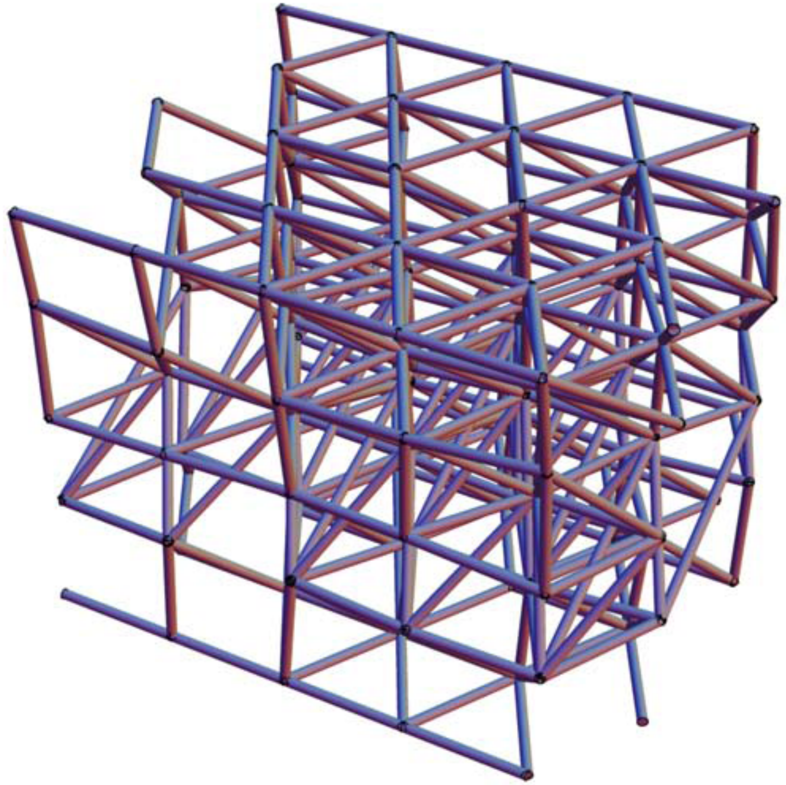


Three-dimensional "Straight Models"



3d kagome (+ diluted)

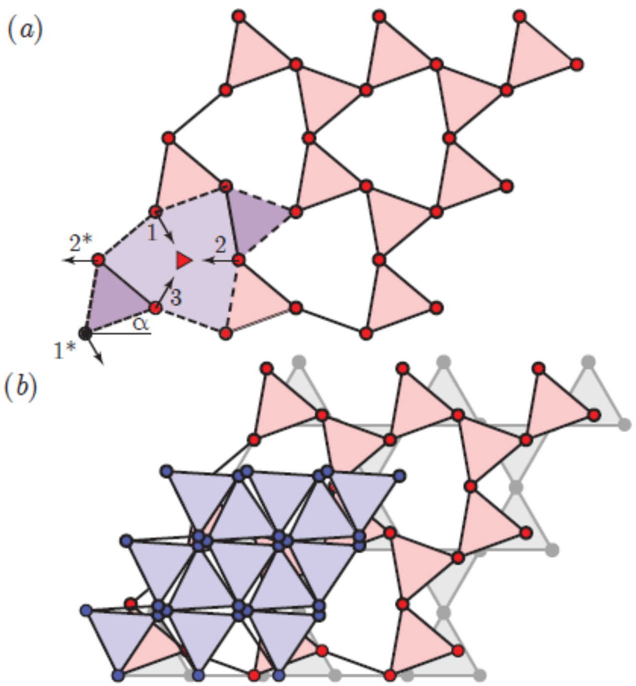
Stenull, TCL



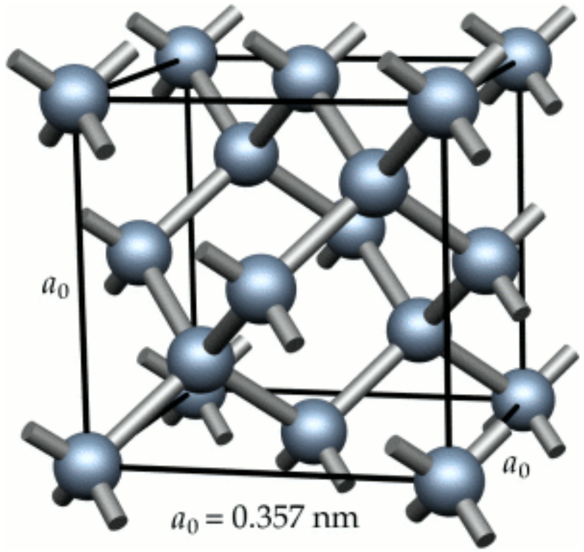
Diluted fcc lattice with cutting rules (Broedersz,Sheinman, and MacKintosh)

"Bent" Lattices

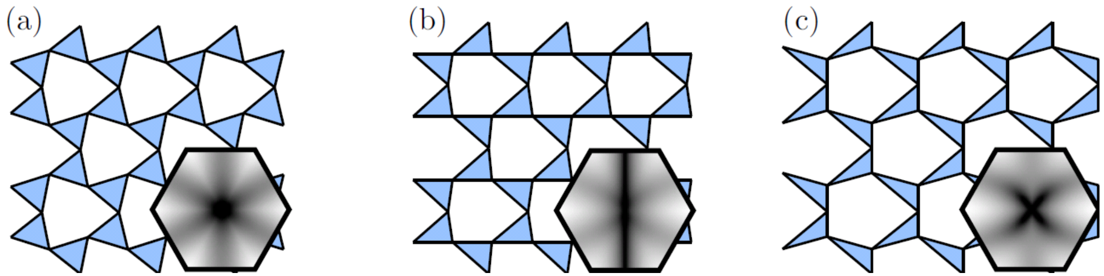
p=1 limit of these lattices are not stable without bending.



Twisted kagome +
3d generalization



Diamond Lattice



Topological Lattices

Show movie

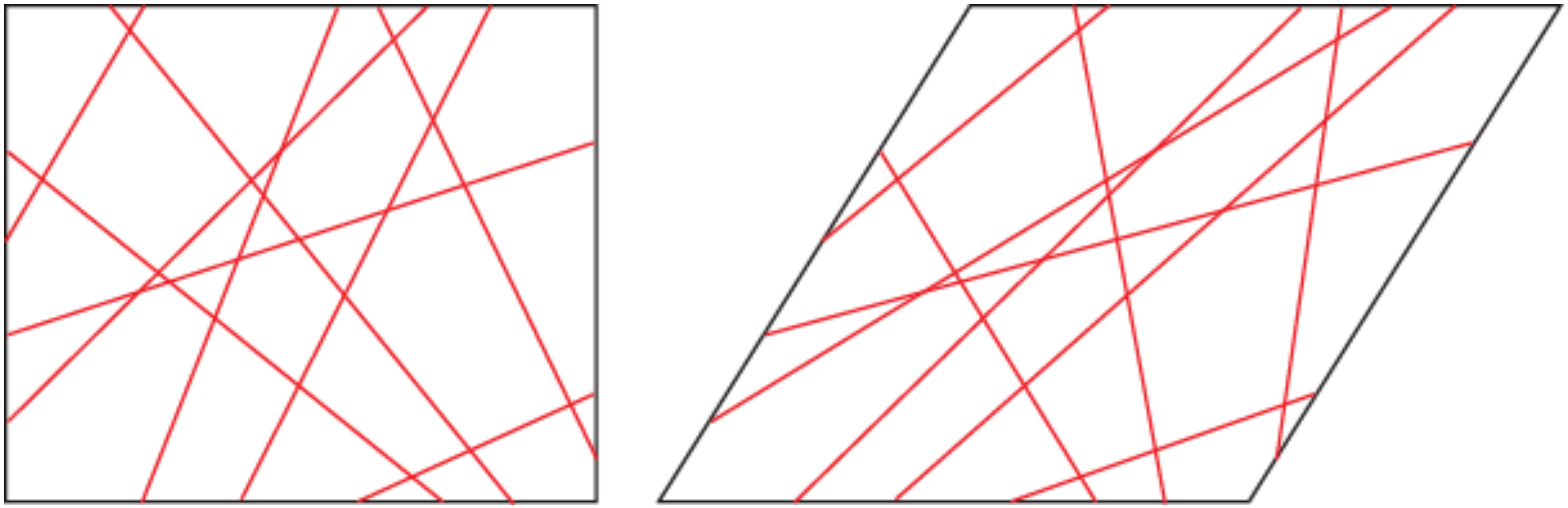
2d and 3d lattices and Isostaticity ($z = 2d$)

2d kagome: z=4 – Just isostatic: support of shear not unreasonable. Bending forces essential for stability when lattice is diluted.

3d Kagome: z=4 – subisostatic. There is an extensive number of zero modes. Nonetheless, the undiluted lattice supports macroscopic compression and shear. How is this possible? Bending forces necessary to keep diluted lattice rigid.

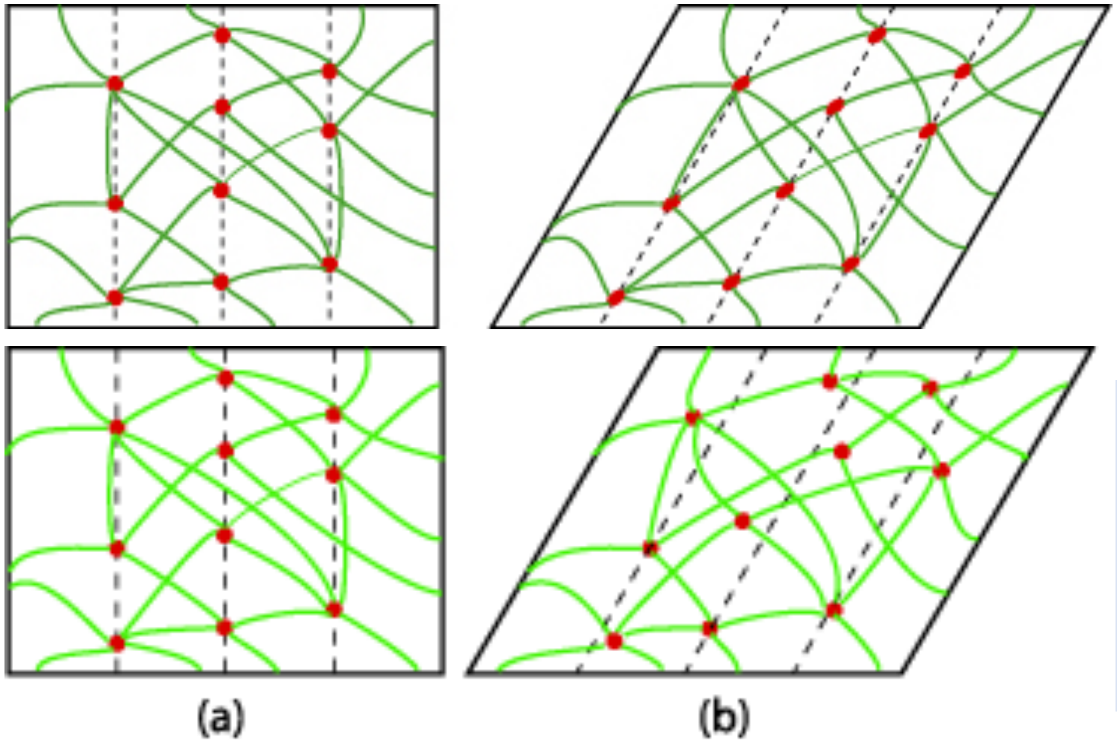
2d triangular (z=6>4) and 3d FCC (z=12>6): overconstrained: have a central-force rigidity threshold.

Affine Response



Straight lines are mapped to straight lines: No bending. Any lattice with sample crossing straight lines along enough independent directions (3 in 2d) and affine response will have nonvanishing elastic central-force elastic moduli.

Non-affine Response



Affine response: microscopic strain is the same as macroscopic strain. Response to uniform stress in Bravais lattices and homogeneous solids.

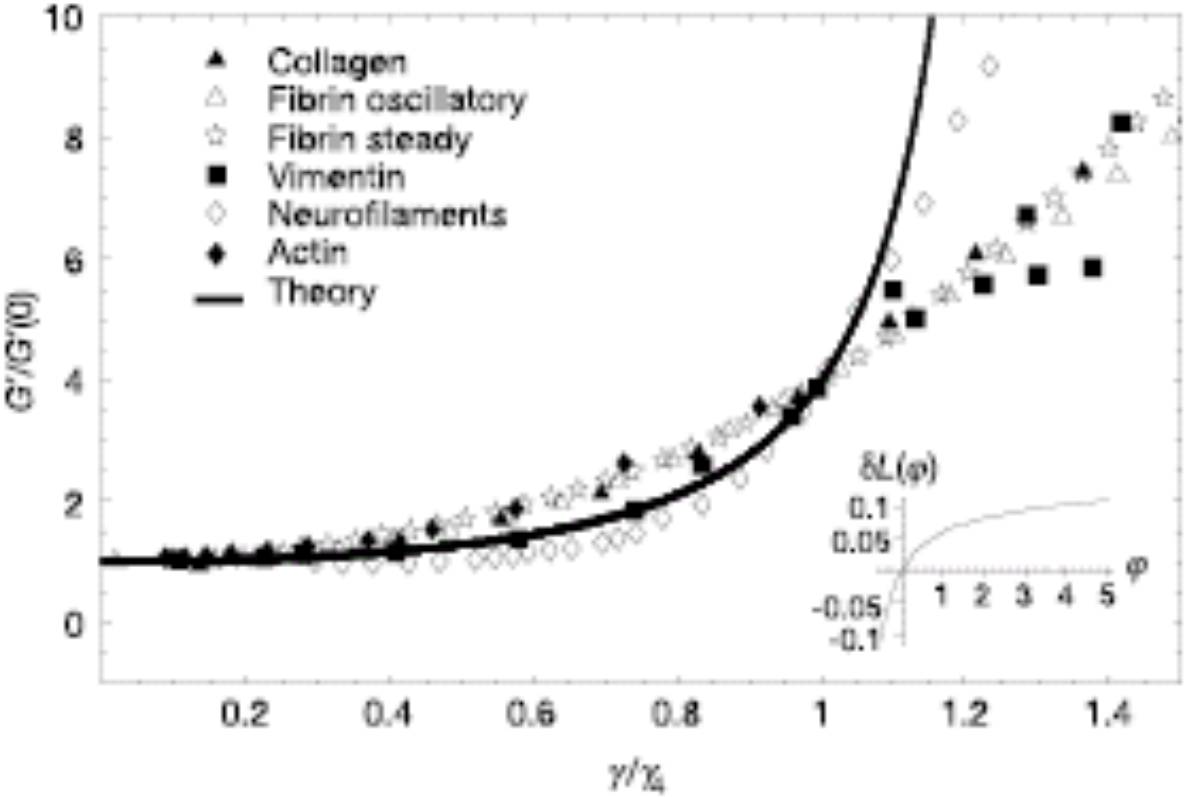
Non affine response: local and macroscopic strains differ. Response in and multi-atom periodic unit cells and in random systems

$$R_{i,\text{affine}} = \gamma_{ij} x_j = x_i + u_{i,\text{affine}}$$

$$\delta u_i(\mathbf{x}) = u_i(\mathbf{x}) - u_{i,\text{affine}}$$

$$\Gamma = \langle (u_i(\mathbf{x}) - u_{i,\text{affine}})^2 \rangle \,/\, \gamma^2$$

Non-linear elastic response



Infinite μ (no stretch) theory Good up to $\gamma/\gamma_4 \sim 1$. Thermal bending fluctuations only

For $\gamma/\gamma_4 > 1$, stretch is needed

γ_4= strain at which $G' = 4G'(0)$

Data from Janmey's lab
Storm et al., Nature **435** (7039), 191-194 (2005).

Filament Energies

Wormlike chain

$$E = \frac{1}{2}\kappa\int_0^L ds\left(\frac{d\theta}{ds}\right)^2$$

$$l_p = \frac{\kappa}{k_B T} = \text{ persistence length;}$$

$$L = \text{ contour length} >> l_p$$

$$k(L) = \frac{\kappa^2}{TL^4} = \text{elastic constant}$$

Elastic beam model

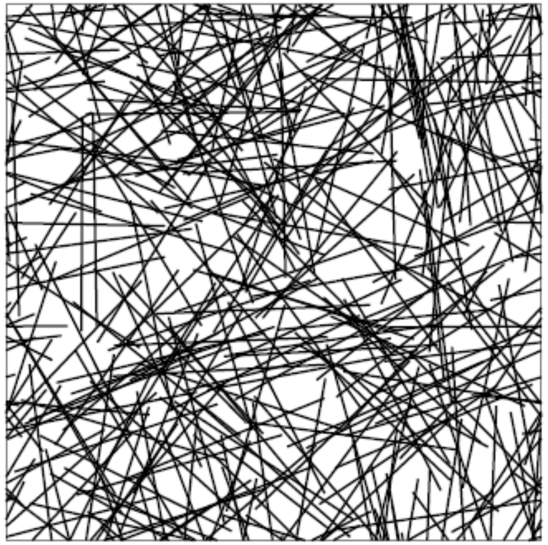
$$E_{\text{beam}} = \frac{1}{2}\int_0^L ds\left[\mu\left(\frac{du}{ds}\right)^2 + \kappa\left(\frac{d^2u}{ds^2}\right)^2\right]$$

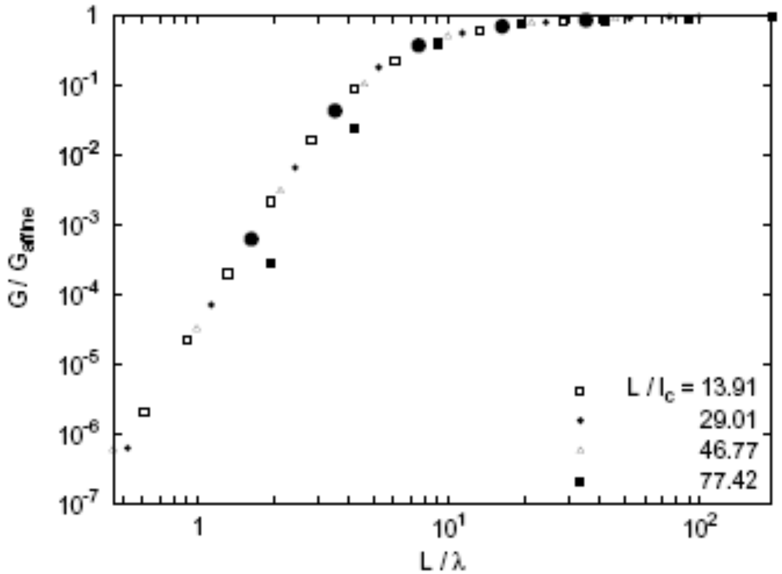
$$u = \gamma s, \quad u(L) - u(0) = \Delta L = \gamma L$$

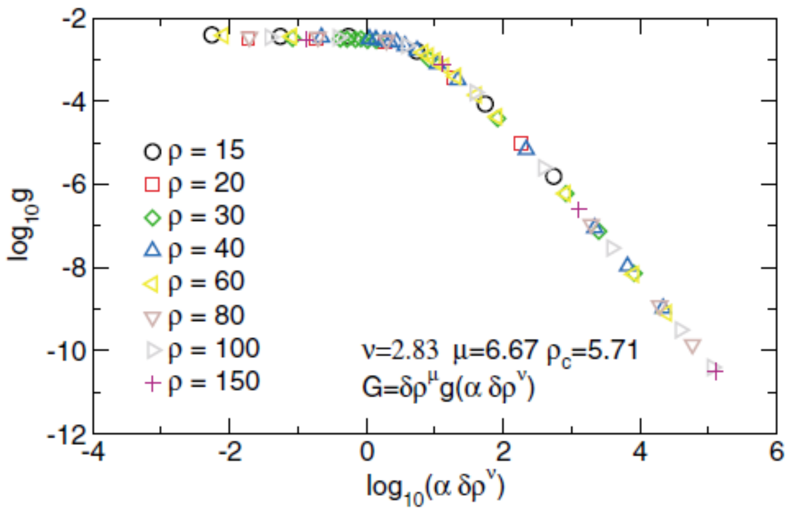
$$\Rightarrow \gamma = \Delta L / L \Rightarrow E_{\text{beam}} = \frac{1}{2}\frac{\mu}{L}(\Delta L)^2 \Rightarrow k(L) = \frac{\mu}{L}$$

$$l_b = \sqrt{\frac{\kappa}{\mu}} = \text{bending length}$$

Networks of Semi-flexible Polymers







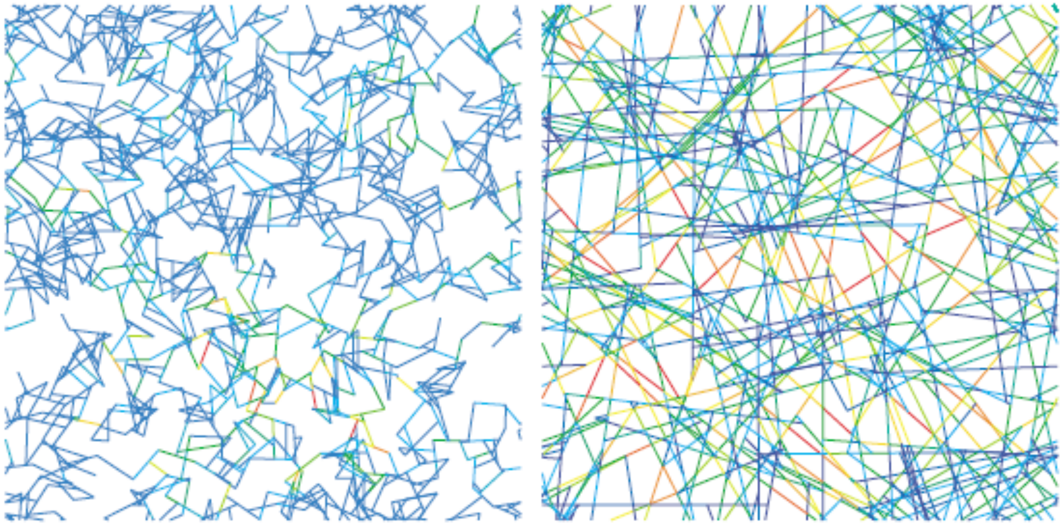
$G \to G_{\text{affine}}$ as $L \to \infty$

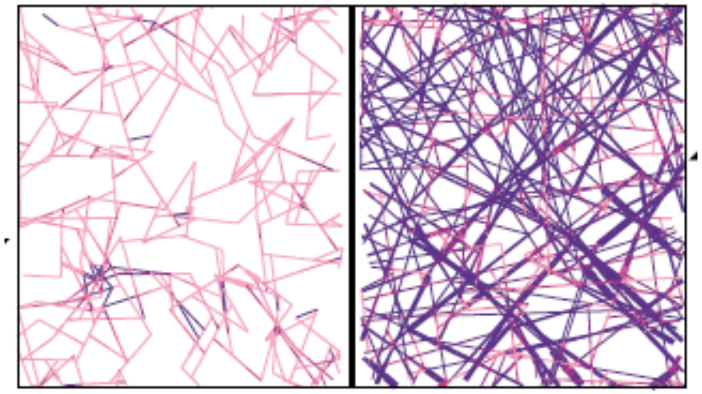
Possible because $G \to G_{\text{affine}}$ when $\kappa=0$ and $L = \infty$. But Why?

Nonaffice response for random systems expected.

Wilhelm and Frey, PRL 91, 108103 (2003);
Head, Levine, MacKintosh, PRL 91, 108102

Non-Affine Response in 2d Networks





Wilhelm and Frey, PRL 91, 108103 (2003);
Head, Levine, MacKintosh, PRL 91, 108102

Mikado vs Diluted Lattice

Mikado

L: Filament length, fixed

l_c: Average distance between crosslinks; Changes with density of filaments

W: System size; $L < W$

$L \to \infty$ limit not directly accessed

Lattice

$L = a/(1-p)$: diverges at $p = 1$

$l_c \approx a$: changes very little with p

W: For any $W < \infty$, there is a a non-zero probability of sample crossing filaments $\Rightarrow$ Affine stretching controlled elasticity

$L \to \infty$ directly accessed at $p = 1$.

Finite-size effects near $p = 1$.

Both: Rigidity percolation critical point at $L/l_c = (L/l_c)_b$; central-force affine behavior at $L > W$. Fixed point at $L \to \infty$. Scaling collapse expected only near fixed points.

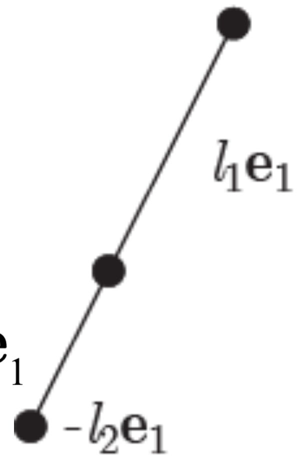
Properties of Beam Model

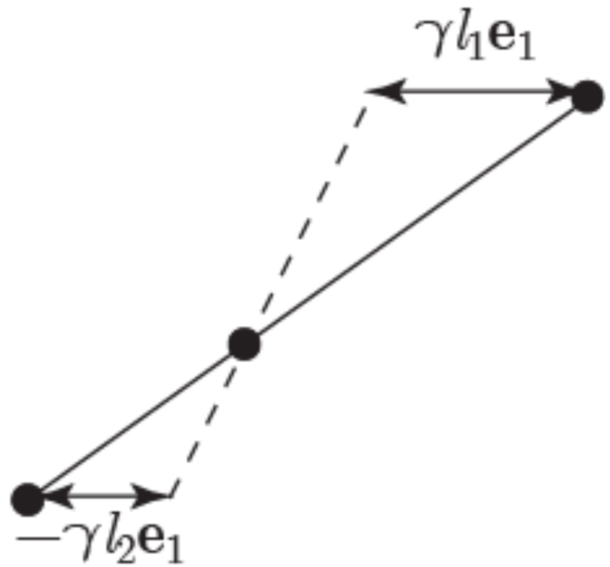
Force on interior nodes with two neighbors along each filament is zero under affine distortion.

$$\delta l_1 = l_1 e_{1i}\gamma_{ij}e_{1j}; \quad \delta l_2 = l_2 e_{1i}\gamma_{ij}e_{ij}$$

$$\mathbf{f}_1 = k(l_1)\delta l_1 \mathbf{e}_1; \quad \mathbf{f}_2 = -k(l_2)\delta l_2 \mathbf{e}_1$$

$$\mathbf{f}_1 + \mathbf{f}_2 = 0 \;\; \text{if}\, k(l) \sim l^{-1}$$

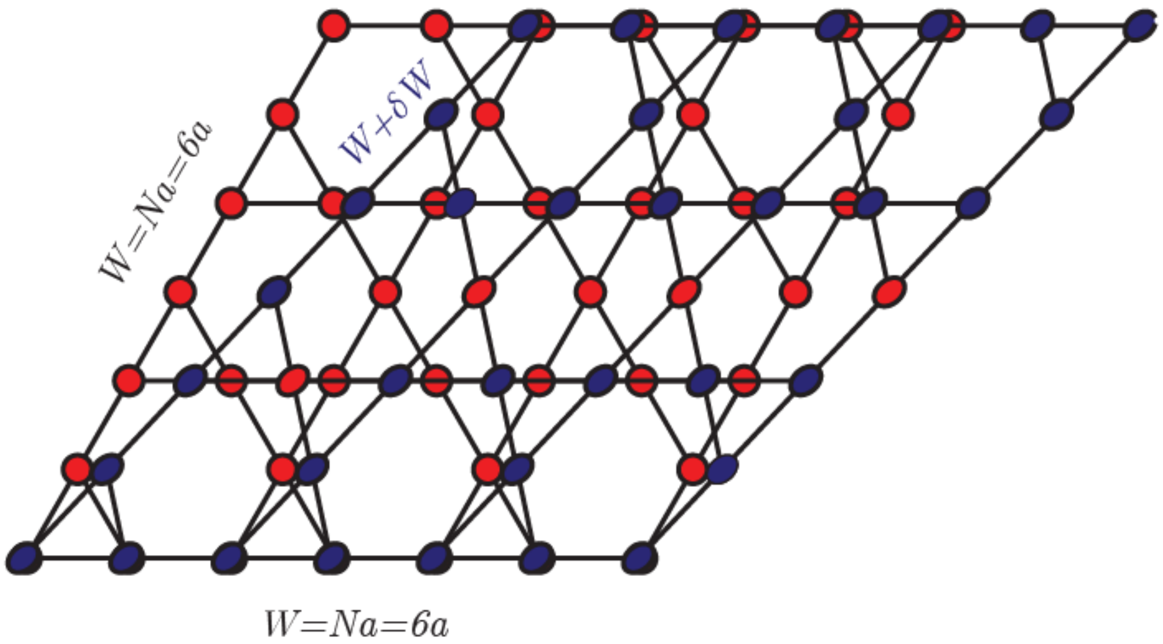




Inverse spring constants of two filament segments add in series: Important for lattice models

$$k^{-1}(l_1) + k^{-1}(l_2) = \mu^{-1}(l_1 + l_2) = k^{-1}(l) = \mu^{-1} l$$

Shearing the kagome lattice



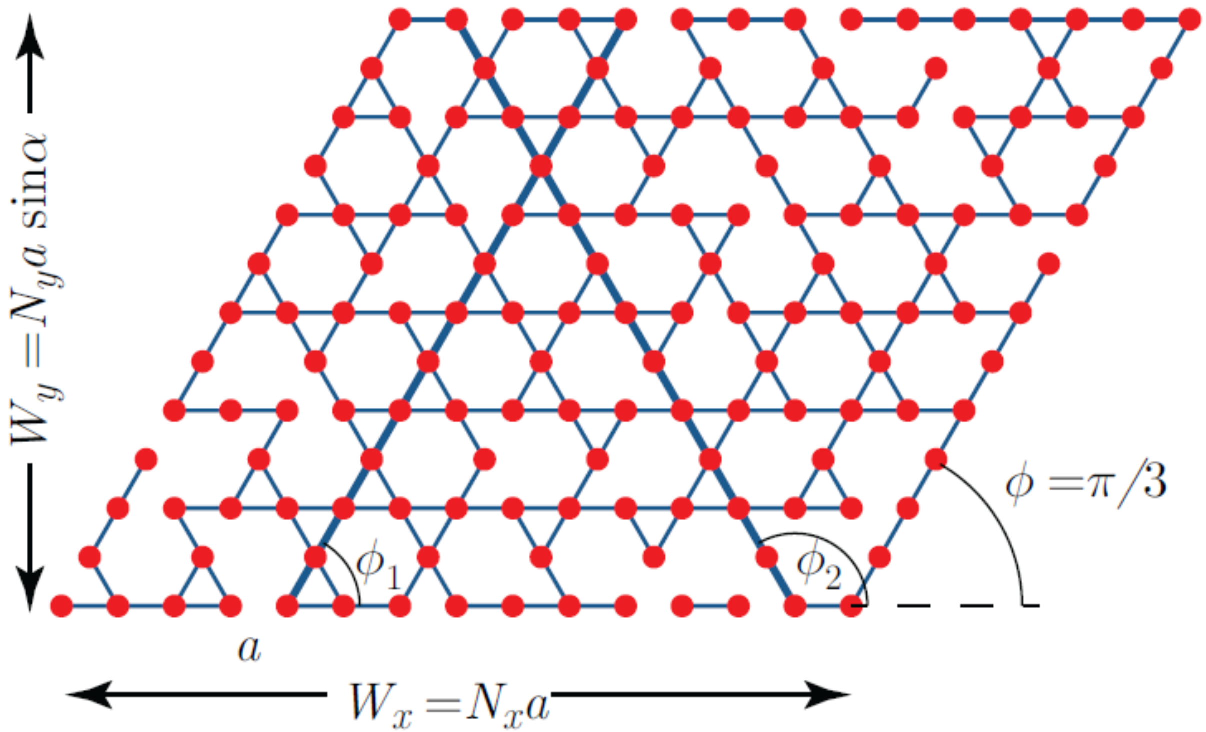
$$N_{\text{fil}} = P(p)N = P(p)W / a$$

$$= \text{Number of filaments crossing sample}$$

$$P(p) = p^N$$

$$= \text{Probability filament crosses sample}$$

Diluted Kagome



$$\delta W = W e_i(\phi) \gamma_{ij} e_j(\phi)$$

Central-force kagome shear modulus

$$E_{\text{fil}} = \frac{1}{2}k(W)(\delta W)^2 = \frac{1}{2}\frac{\mu}{W}(e_i(\phi)\gamma_{ij}e_j(\phi)W)^2 = \frac{1}{2}\mu W\gamma_{xy}^2\sin^2\phi\cos^2\phi$$

$$\phi = 0, \pi/3, 2\pi/3$$

$$\sin^2\phi\cos^2\phi = \frac{1}{4}\sin^2 2\phi = \frac{1}{4}\sin^2(\pi/3)$$

$$f = \frac{N_{\text{fil}}E_{\text{fil}}}{W^2\sin\pi/3} = \frac{1}{8}\frac{P(p)\mu}{a}\gamma_{xy}^2\frac{\sin^2 2\pi/3}{\sin\pi/3} = \frac{1}{2}G(p)\gamma_{xy}^2$$

$$G(p) = p^{W/a}\frac{\sqrt{3}}{8}\frac{\mu}{a}\xrightarrow{W\to\infty}0; \quad G(p=1) = \frac{\sqrt{3}}{8}\frac{\mu}{a} \equiv G_0$$

p=1: first-order transition for the CF kagome model

Diluted Kagome near p=1: EMT+ 1st-order

$$G_{EMT}(p) = G_0 g(\tau); \qquad \tau = \frac{\kappa}{\mu a^2}\frac{1}{(1-p)^2} = \frac{l_b^2 L^2}{a^4}$$

$$g(\tau) = (1-\sqrt{1+A\tau})^2 / A\tau = \begin{cases} 1 & \text{if } \tau \to \infty \\ A\tau/4 & \text{if } \tau \to 0 \end{cases}$$

Note order of limits:

$$\lim_{\kappa\to 0}\lim_{p\to 1} G_{EMT} = G_0 \propto \frac{\mu}{a}$$

$$\lim_{p\to 1}\lim_{\kappa\to 0} G_{EMT} = 0$$

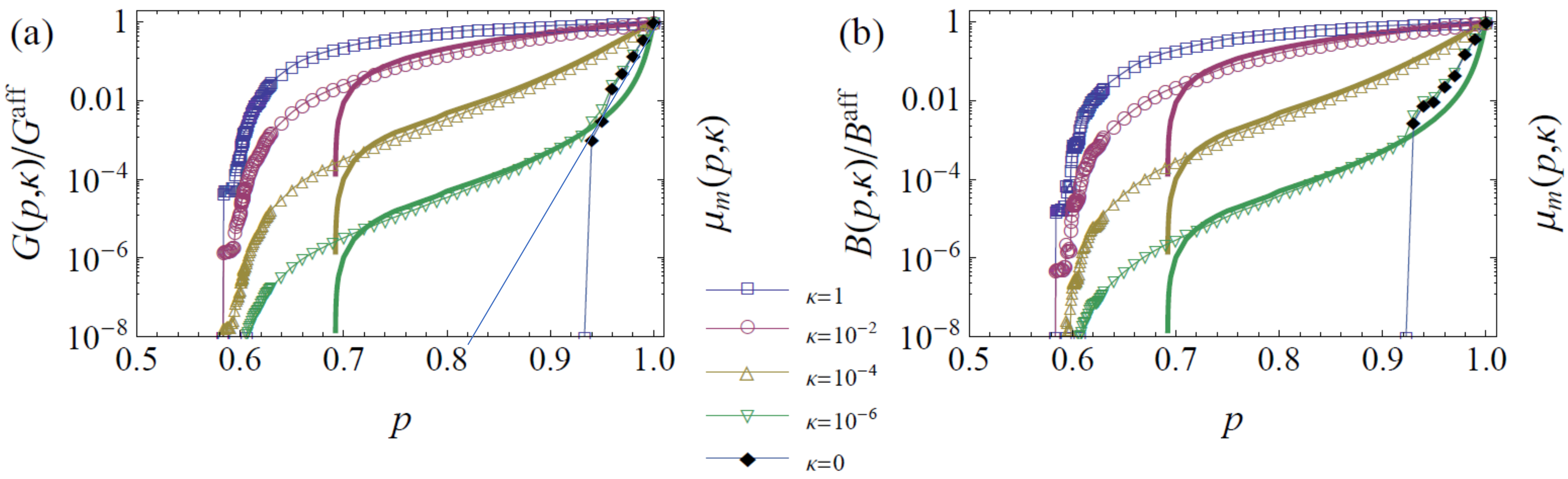
$$G_{EMT} \to \frac{\kappa}{a^3}\frac{L^2}{a^2} \text{ for } \frac{\kappa L^2}{\mu a^4} \ll 1$$

See Broedersz, Sheinman, and MacKintosh

$$G(p,\mu,\kappa,W,a) = \max[G(\mu,\kappa,p,\infty,a), G(\mu,0,p,W,a)]$$
$$\to G_0 \max[g(\tau), p^{W/a}]$$

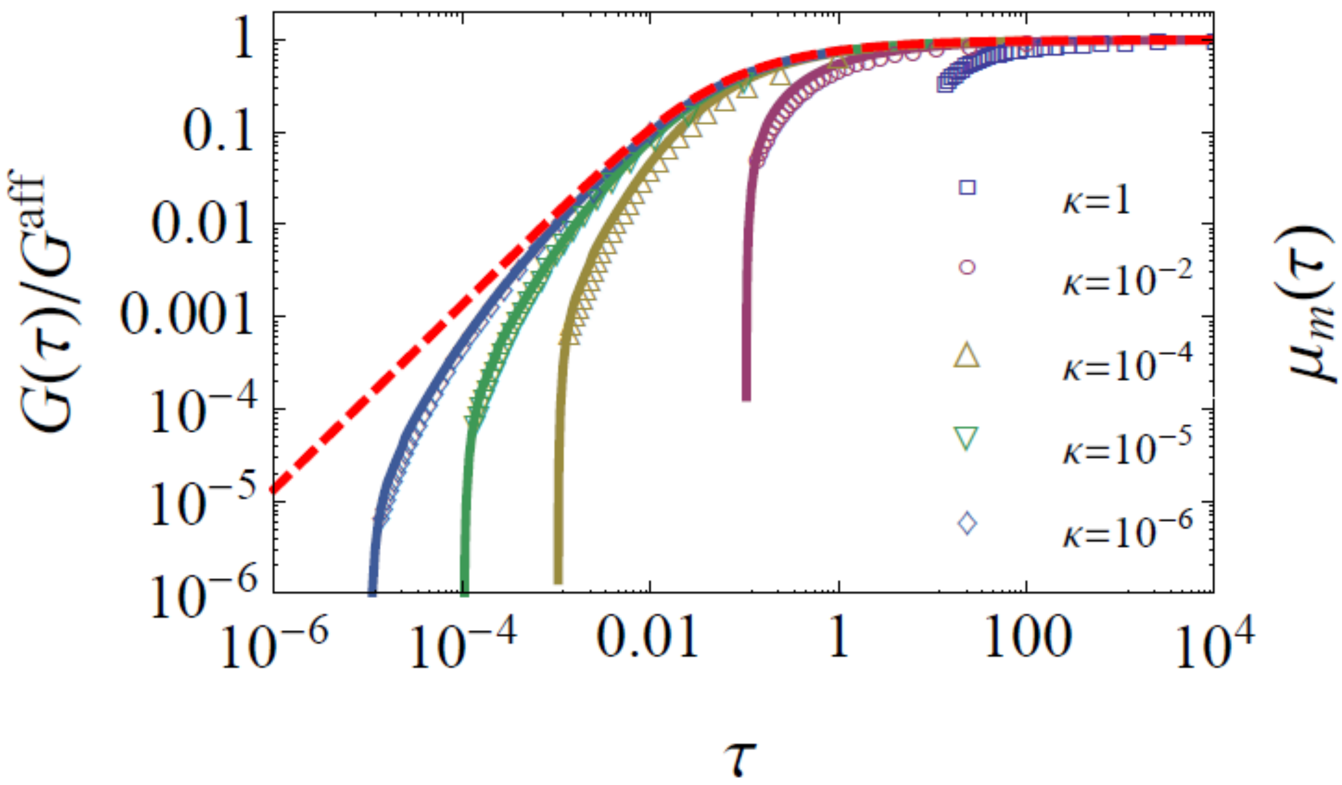
Note: Reasonable expectation that EMT provides a good description of p=1 fixed point. The jamming transition with an isostatic critical point is a MF transition with EMT exponents.

Comparison of EMT and Simulations



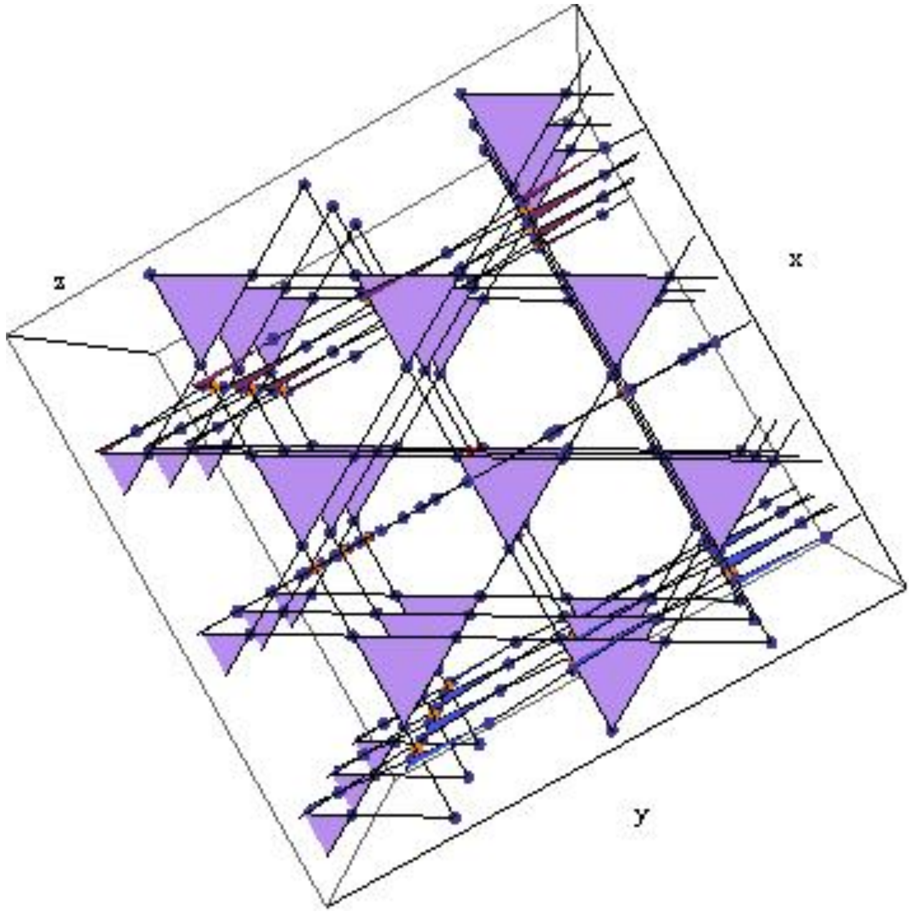
Simulations and EMT, with first-order correction, follow closely down to p~0.73. EMT misses the value of the bending-dominated rigidity threshold.

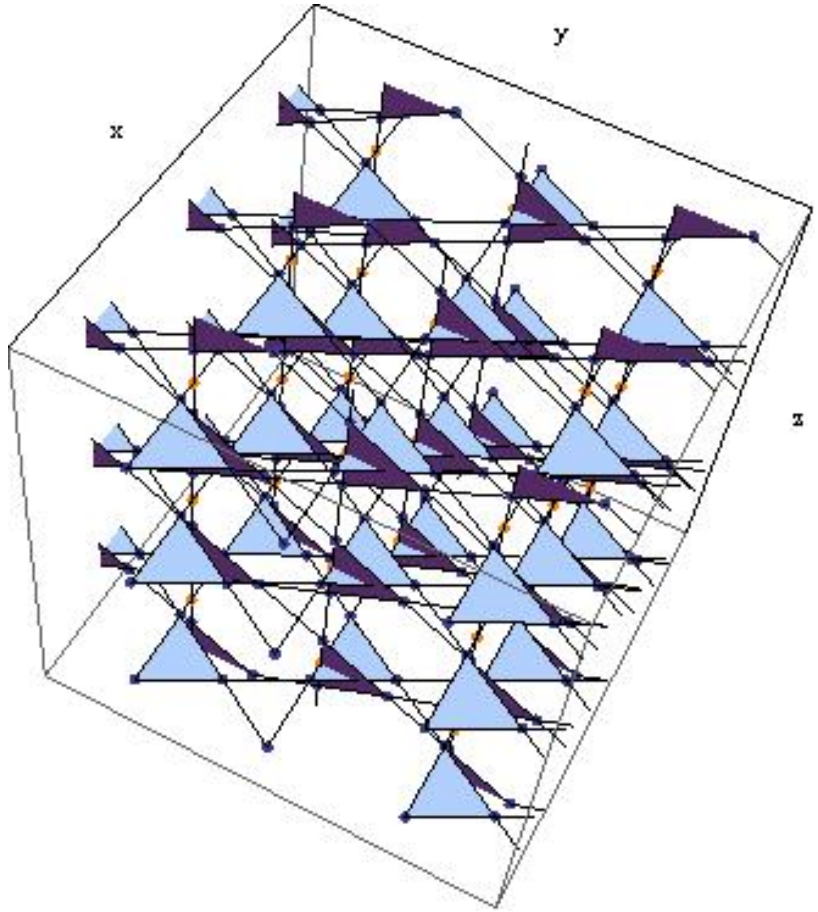
Fits of EMT and Simulations to Scaling



Simulations follow numerical solution to EMT, and both break away from the scaling curve at $\tau \sim 10\,\kappa/\mu a^2$.

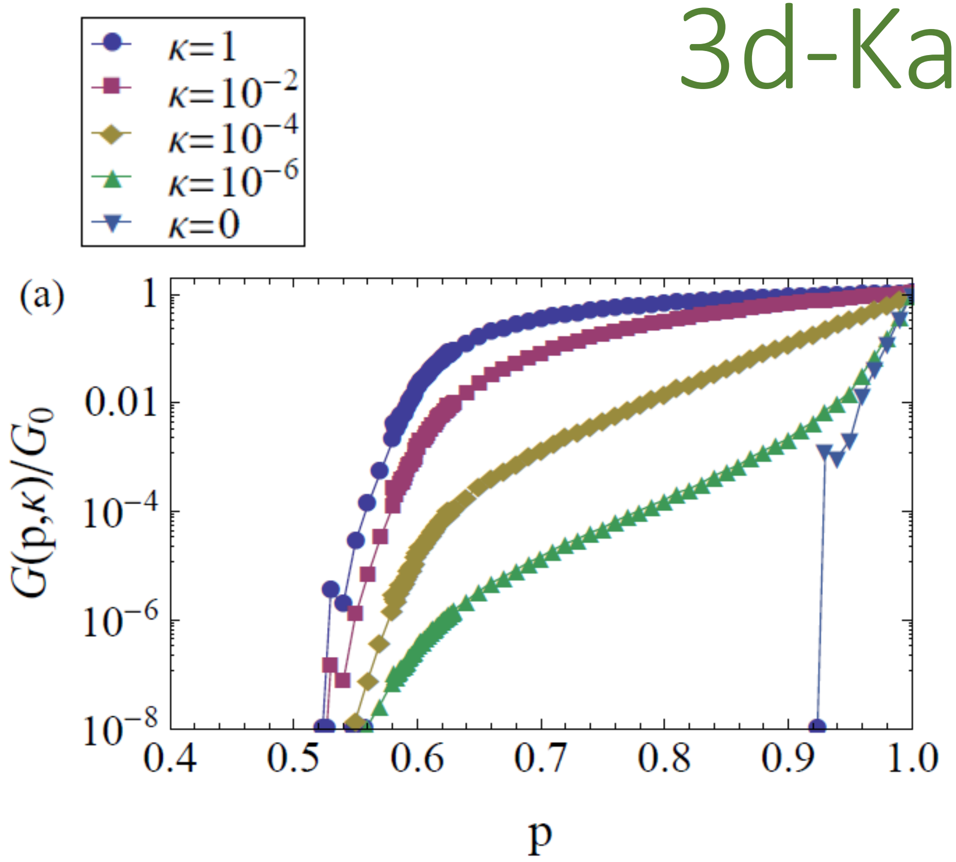
Z=4 Lattice with Straight Filaments

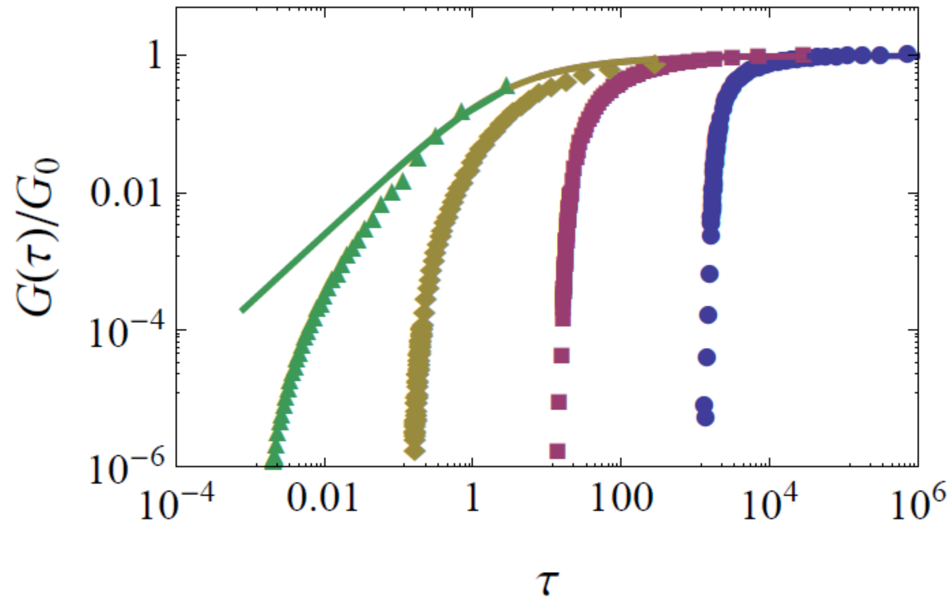




Olaf Stenull, TCL

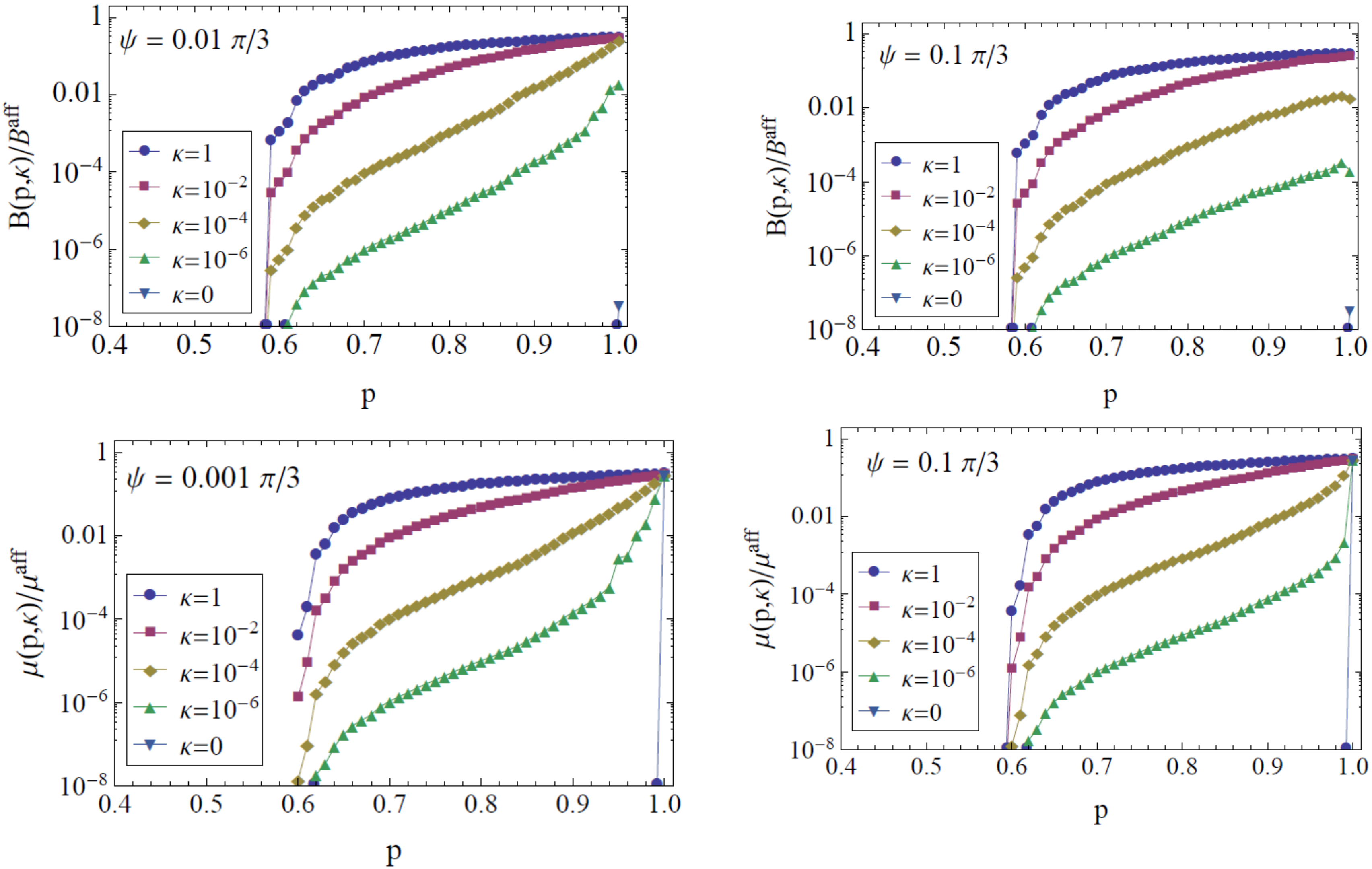
3d-Kagome





- 3d undiluted kagome : straight, sample traversing filaments.
- Affine response; all elastic moduli are nonzero and scale as μ/a^2.
- Data near p=1 collapse onto the kagome EMT curves with a different scale factor.
- There is a regime in which $G \sim \kappa L^2/l_c^4$

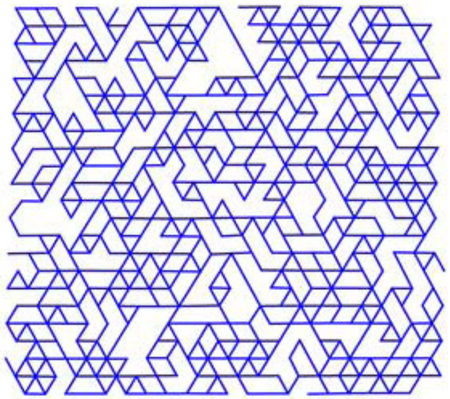
Twisted kagome



Note: The bulk modulus is zero at $\kappa=0$ and m is finite at $p=1$ but zero as p-> 1^-.

Rigidity Percolation with Bending:Triangular lattice

Two critical points: central force at $\kappa = 0$ and bending at $\kappa > 0$. Interesting crossover at $\kappa = 0$ critical point



New bending

CPA (X. Mao)

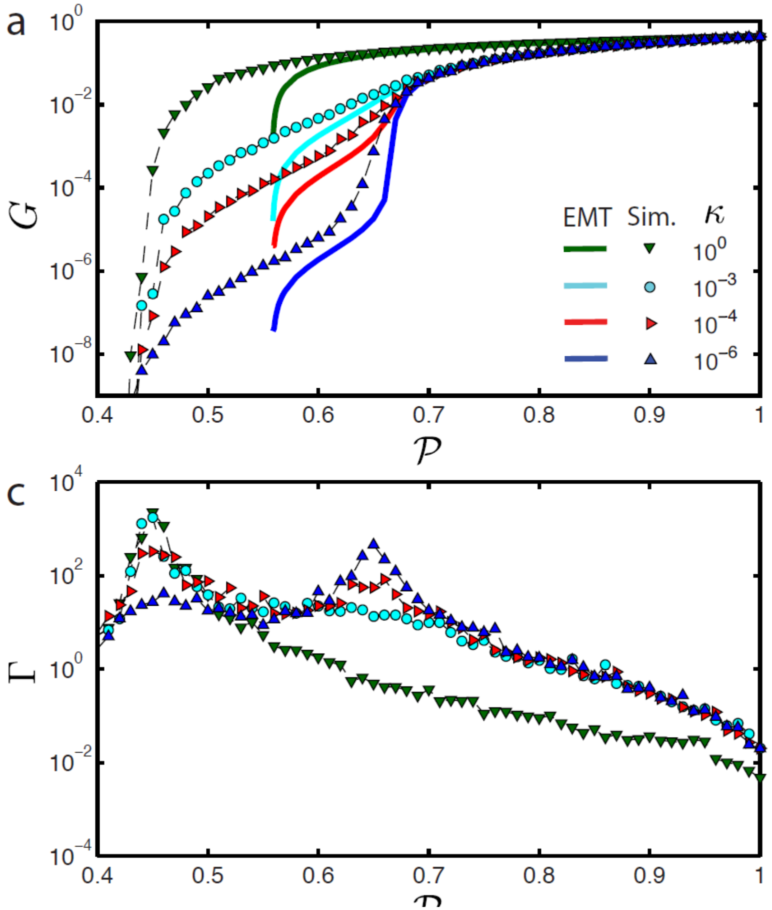
$t = 1.0; \quad \phi = 2.0$

Broedersz, X. Mao, TCL, MacKintosh, Nature Physics **7** (12), 983-988 (2011).

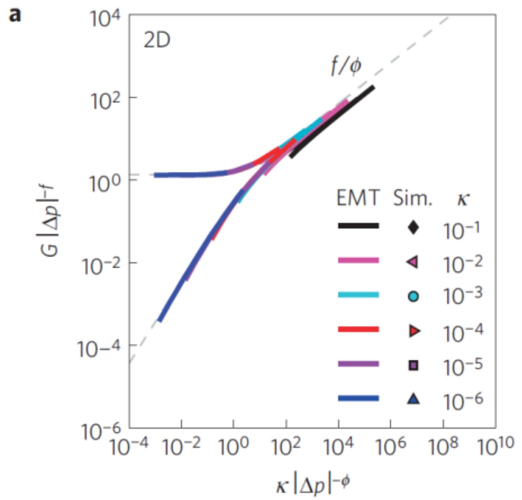
$$G \sim k(\Delta p)^t f[y)]$$
$$\sim k(\Delta p)^t \tfrac{3}{2}(\mp 1 + \sqrt{1 + 4Ay/9})$$
$$\sim k^{1-(t/\phi)} \kappa_b^{t/\phi}; \quad \Delta p \to 0$$
$$\Delta p = p - p_c; \quad t_{EMT} = 1, \phi_{EMT} = 2$$
$$t_{2d} = 1.4; \phi_{2d} = 3.0; t_{3d} = 1.6; \phi_{3d} = 3.6$$
$$y = (\kappa_b / k) / (\Delta p)^\phi)$$
$$p_c = \text{ threshold at } \kappa_b = 0$$
$$\Gamma = \langle (\mathbf{u}(\mathbf{x}) - \mathbf{u}_{\text{affine}})^2 \rangle$$

Analogy with resistor network with $\sigma_>$ and $\sigma_<$ (Straley); Jamming with extra bonds (M. Wyart, H. Liang, A. Kabla and L. Mahadevan)

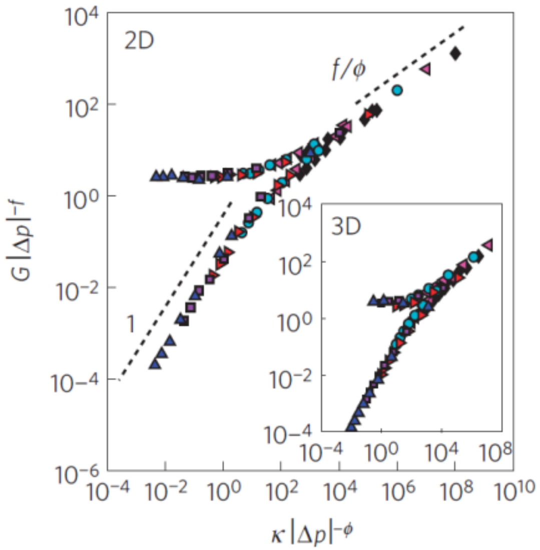
Scaling Results



Note increase in G at both the central-force and bending
Rigidity percolation thresholds.



2D EMT and simulations



3D simulations

Review and Conclusions

- Periodic lattices provide good models for filamentous networks
- Effective medium theories provide excellent descriptions of the elasticity of beam models near p=1
- Beam models have special features that are not necessarily shared by real filamentous networks
- Under-coordination of z=4 3d models with bending is not an important factor in determining their elastic response.