Mechanism-Based Mechanical Metamaterials

Robert V. Kohn
Courant Institute, NYU

Aerospace & Mechanical Engineering Colloquium
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Mechanism-Based Mechanical Metamaterials

(1) Introduction

- the "rotating squares" metamaterial
- some research threads and issues

(2) The Kagome metamaterial

- explaining the question
- simulations and phenomenology
- macroscopic behavior

Analysis: joint with Xuenan Li (now at Columbia)

Simulations: also with Bolei Deng (now at Georgia Tech) and Katia Bertoldi (Harvard)

Different uses of “metamaterial”

The word metamaterial is used in many different ways:

- electromagnetics: designer materials modelled by Maxwell’s equations with exotic physical constants (e.g. negative index materials), usually harnessing some kind of resonance.
- linear elasticity: 3D printing lets us make almost anything; but what, exactly, to print? (Typical goal: high porosity and desired mechanical response.)
- mechanism-based mechanical metamaterials: systems with mechanisms, whose very structure changes in response to loading.

Today: only 3rd bullet. We’ll be using

- geometrically nonlinear elasticity, since mechanisms induce large deformations and especially large rotations;
- a variational perspective, since stable states of a mechanical system are (stable local) minima of its elastic energy.

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The rotating squares example

The "rotating squares" metamaterial can be obtained by patterning a 2D sheet like a checkerboard then cutting out the white squares.



slightly compressed



very compressed

It has a one-parameter family of mechanisms, which achieve macroscopic (isotropic) compression by rigidly rotating the black squares (bending the thin necks that join them).

The rotating squares example

Another version is obtained by making well-chosen slits in a 2D sheet. It has a one-parameter family of mechanisms, which achieve macroscopic (isotropic) expansion by expanding the slits.



a sheet with slits

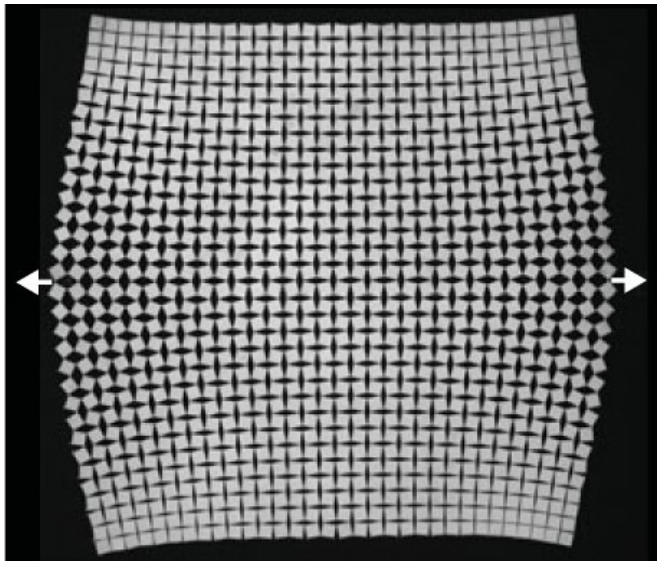


after expansion

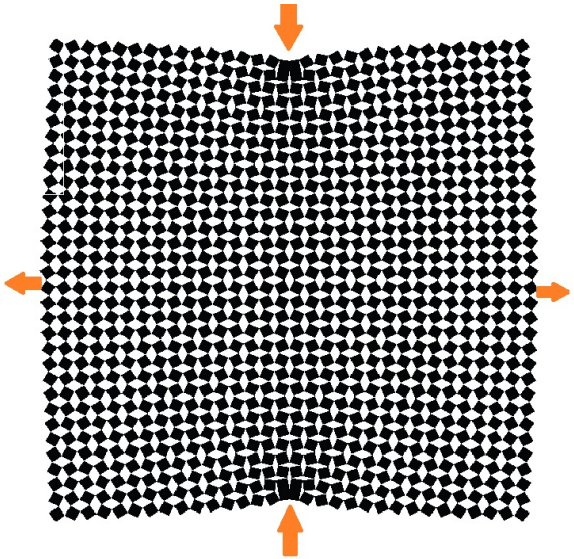
If we ignore the bending of the necks, its expanded states look like the checkerboard.

Soft modes

Nonuniform loading reveals soft modes via modulation of mechanism.



Y. Zheng et al, Proc R Soc A 2023



M. Czajkowski et al, Nature Comm 2022

This system has a single mechanism, and its soft modes are obtained by modulating it. But for systems with many mechanisms we need a more general viewpoint.

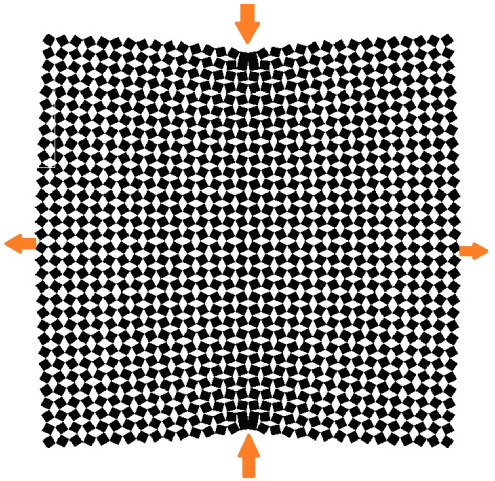
How to define a soft mode?

Which soft mode will be seen in a given experiment?

A nonlinearly elastic perspective

As microstructural scale $\to 0$, macroscopic elastic energy of deformation u (taking x to $u(x)$) is $\int W_{\text{eff}}(Du)\,dx$, where

$$W_{\text{eff}}(F) = \begin{cases} \text{min energy per unit area} \\ \text{req'd for affine map } x \to Fx. \end{cases}$$



Since mechanisms achieve isotropic compression,

$$u \text{ is a soft mode} \Leftrightarrow W_{\text{eff}}(Du) = 0 \Leftrightarrow Du(x) = c(x)R(x)$$
$$\Leftrightarrow u \text{ is a conformal map.}$$

Which soft mode is selected in an expt? The one that minimizes energy assoc

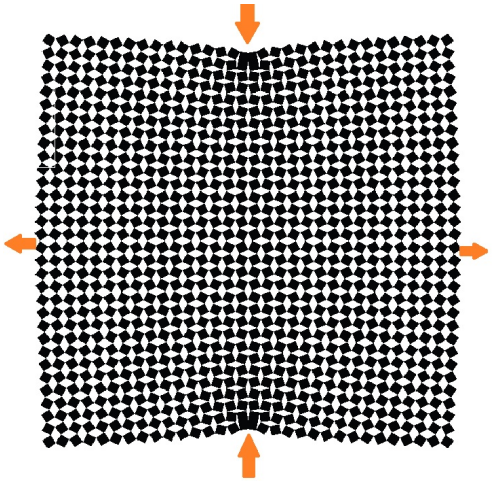
- bending of necks between (essentially rigid) squares
- cost of modulation

(leading-order corrections to the macroscopic energy).

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This viewpoint is powerful

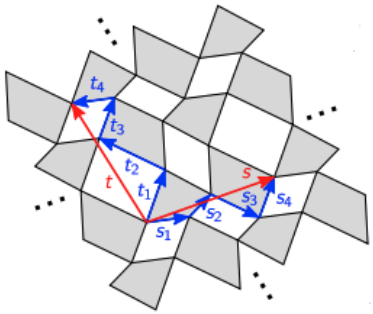
In the rotating squares setting

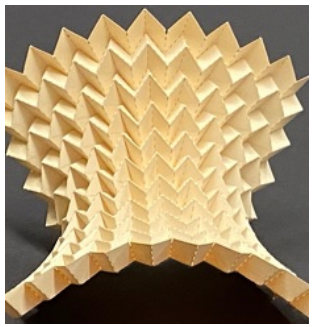
- there is a single mechanism;
- soft modes achieve vanishing energy per unit area in continuum limit, by modulating the mechanism.

Macroscopic deformation is selected among all soft modes, by minimizing the leading-order elastic energy (due to modulation, and to bending of thin necks).

A similar viewpoint is being applied (here at USC!) to other systems:

- Planar sheets with other cutouts (Y. Zheng et al, PRL 2022)
- An effective plate theory for origami-patterned sheets (H. Xu et al, JMPS 2024)





Two key issues

(1) Do these ideas work for all systems?

For example, do soft modes always use a modulated mechanism?

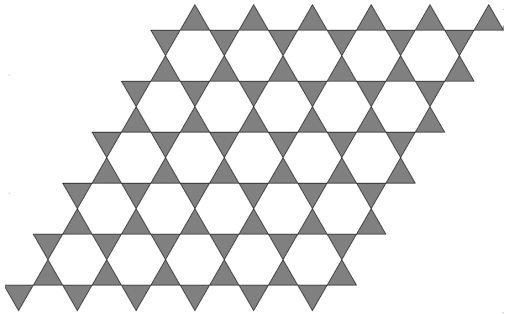
(2) What about systems with more mechanisms?

For example, what if we don't even know all mechanisms?

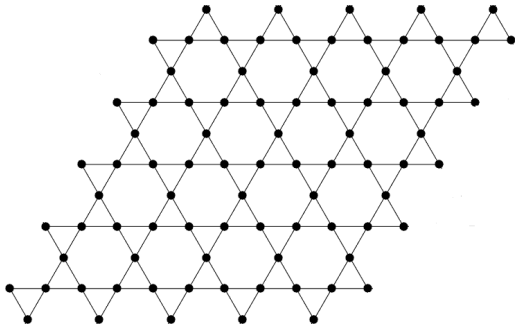
I'll address both questions by considering the Kagome metamaterial.

The Kagome metamaterial

The plane can be tiled periodically by equilateral triangles and regular hexagons.



The Kagome metamaterial has a (linear) spring at each edge. Rotation is free at nodes.



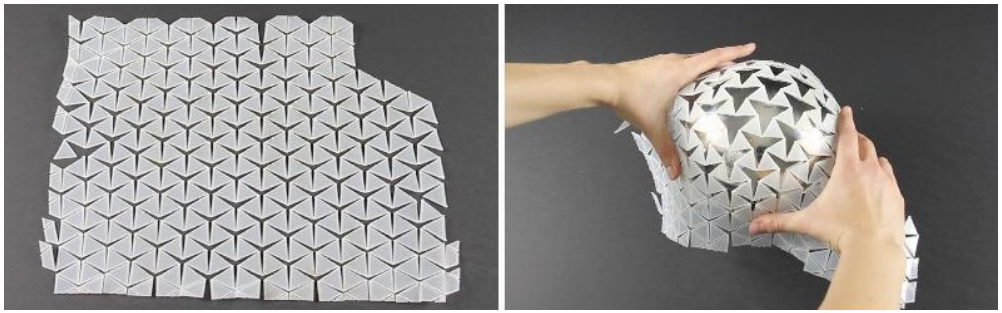
Like a porous elastic composite (thicken the springs, or revert to the cutout model).

Viewed as a linear elastic composite, its effective Hooke's law is nondegenerate. (Obvious: stretching costs energy.)

But: macroscopic compression is achieved without elastic energy, in many different ways.

Why focus on Kagome?

The Kagome structure arises in many settings. One application: mapping a flat (compressed) sheet to a curved (expanded) surface.



M. Konaković Luković thesis, EPFL, 2016

Others involve topological mechanics (X. Mao and T. Lubensky, Ann Rev Cond Matter Phys 2018) or how the mechanism affects band structure of elastic waves (M. Fruchart, Y. Zhou, and V. Vitelli, Nature 2020).

For me, Kagome is interesting because

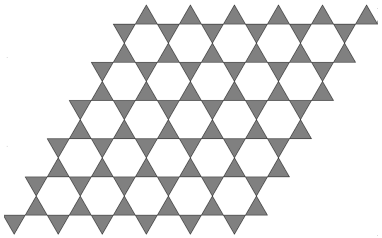
- it has many mechanisms; and yet
- it still has meaningful macroscopic behavior.

Kagome vs rotating squares

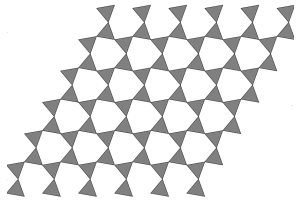
The Kagome metamaterial seems at first very similar to the rotating square example:

- It, too, can be achieved by cutting holes in a planar sheet (hexagonal holes, leaving triangles that meet at vertices).
- It, too, has a periodic mechanism that closes the holes, and the associated macroscopic deformation is isotropic compression.

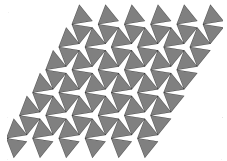
Kagome



reference structure



one-periodic
small compression



one-periodic
large compression

Rotating Squares



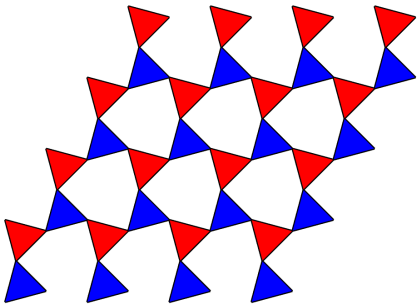
slightly compressed



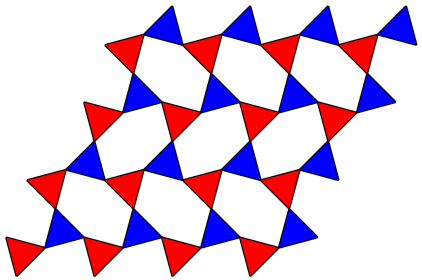
very compressed

Kagome vs rotating squares

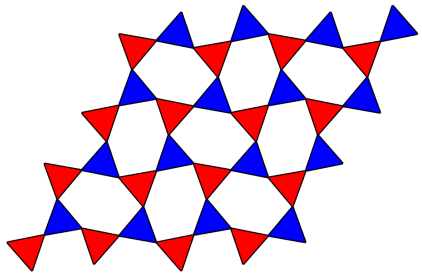
However, there's a big difference: the rotating squares structure has a single one-parameter family of mechanisms, while Kagome has a huge variety of mechanisms.



one-periodic



2×1 periodic



2×2 periodic
(a 3-parameter family)

Kagome has much more microstructural freedom than the rotating squares structure. Some questions:

(1) Can we investigate its mechanisms more systematically? What macroscopic deformations are possible?

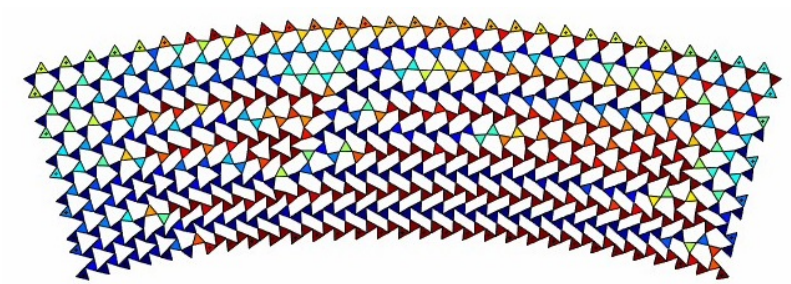
(2) Can we identify its soft modes, despite its microscopic floppiness?

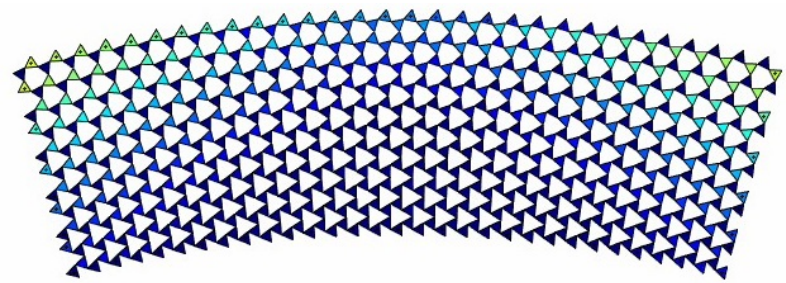
Looking ahead

I will address (and mostly answer) the questions just posed:

- Enumerating all mechanisms isn't feasible, but we can understand some features by considering their linearizations.
- Despite having no enumeration, we can show that the macroscopic effect of any mechanism is isotropic compression.
- Kagome is macroscopically a nonlinear elastic material, and its soft modes are (once again) compressive conformal maps.

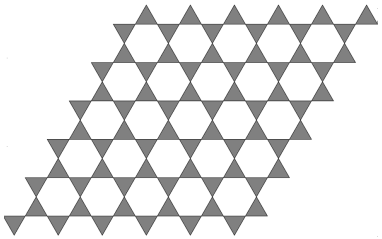
Macroscopic determinacy despite microscopic indeterminacy!





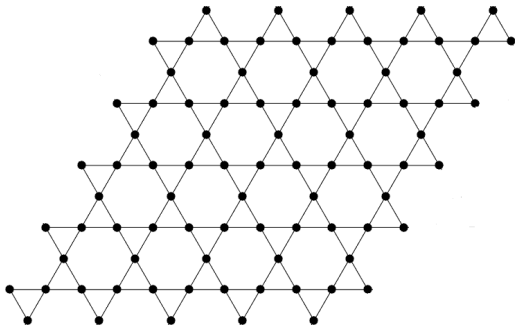
Getting started

As already noted: the plane can be tiled periodically by equilateral triangles and regular hexagons.



Two slightly different versions of the Kagome metamaterial:

- Hexagonal holes in a sheet (easier to make)
- A lattice of springs rotating freely at nodes (easier to analyze)



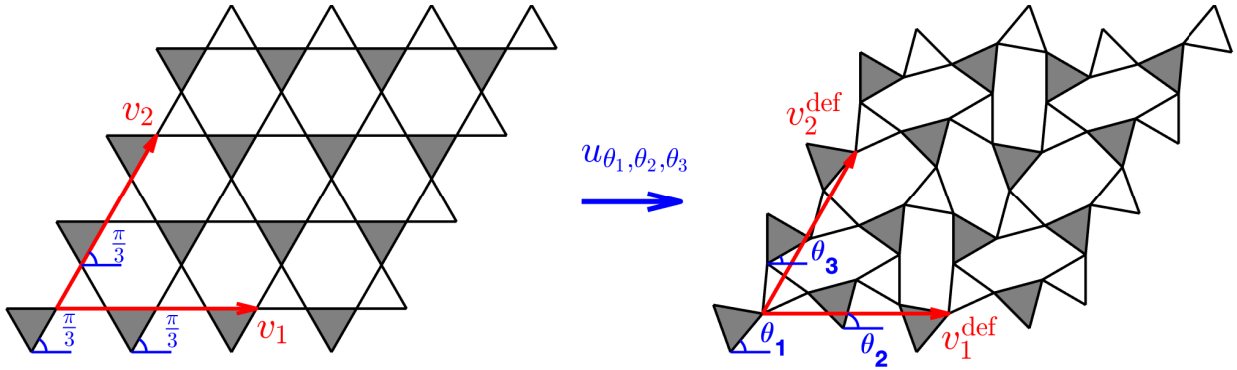
Completely equivalent, for discussion of mechanisms; very similar, for discussion of elastic behavior. Elastic energy of spring network:

$$E[u] = \frac{1}{\#\,\text{springs}} \sum_{i \sim j} \left(\frac{|u(x_i) - u(x_j)|}{|x_i - x_j|} - 1 \right)^2$$

Thinking about periodic mechanisms

By definition, a periodic deformation of a lattice has the form

$u(x) = F \cdot x + \psi(x)$
with F constant and
ψ periodic.



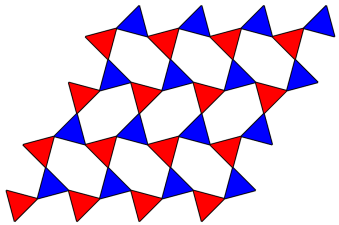
It takes a reference lattice (periods v_1, v_2) to a new, deformed lattice (periods $v_i^{\text{def}} = Fv_i$). The assoc macroscopic deformation is affine, with gradient F.

For a mechanism, we need $|u(x_j) - u(x_i)| = |x_j - x_i|$ when $i \sim j$.

Thinking about periodic mechanisms

But really, our mechanisms are parameterized families of energy-free deformations, starting from the identity at $t = 0$:

$$u_t(x) = F_t \cdot x + \psi_t(x)$$
with $u_0(x) = x$.



If $\dot{F} = \frac{dF}{dt}|_{t=0} \neq 0$, the linear Hooke's law of the lattice is degenerate ($\dot{F}$ is in its kernel). (The deformed Kagome lattices are like this.)

For standard Kagome, mechanisms have $\dot{F} = 0$, so $\dot{u} = \frac{du}{dt}|_{t=0}$ is periodic. Since

$$|u(x_j) - u(x_i)|^2 = |x_j - x_i|^2 + 2t\,(\dot{u}(x_j) - \dot{u}(x_i)) \cdot (x_j - x_i) + O(t^2)$$

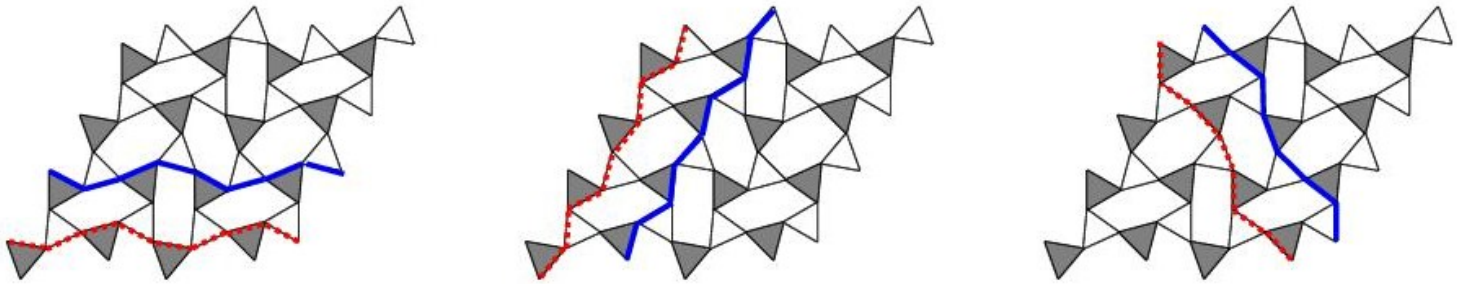
an infinitesimal mechanism must satisfy:

$$(\dot{u}(x_j) - \dot{u}(x_i)) \cdot (x_j - x_i) = 0 \quad \text{for } i \sim j.$$

When $\dot{F} = 0$, this gives a linear space of periodic linearly elastic defs ("Guest-Hutchinson modes") which could be incipient mechanisms.

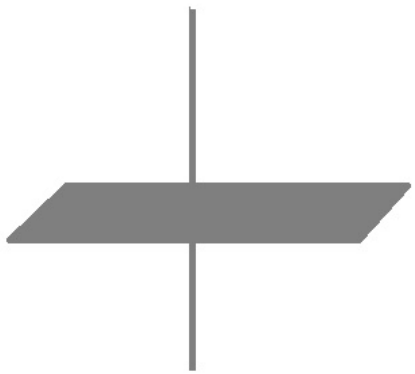
Thinking about periodic mechanisms

But not every Guest-Hutchinson mode comes from a mechanism. There is a quadratic necessary condition: the lines in each parallel family must experience the same macroscopic compression.



As a result, the infinitesimal mechanisms of standard Kagome do not form a linear space. For example, while the space of 2-periodic GH modes is 4-dimensional, the infinitesimal mechanisms are limited to

- a 3-dimensional subspace, tangent to the 3-parameter family of mechanisms
- a line, tangent to the one-periodic mechanism



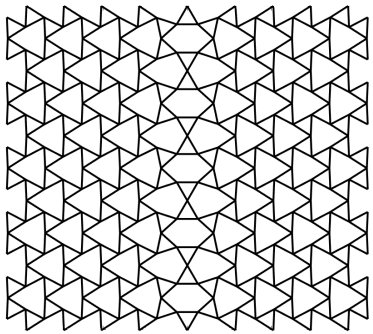
Enumerating mechanisms seems hopeless

The (standard) Kagome lattice has plenty of periodic mechanisms, but they are not easy to enumerate:

- the space of k-periodic GH modes gets larger as k increases;
- the set where our necessary condition holds gets larger too;
- for more examples & results: Li & Kohn, JMPS 2023.

In addition, there are also non-periodic mechanisms, for example:

an energy-free wall between two symmetry-related versions of the one-periodic mechanism



Thus, to make statements about all mechanisms, we must make do without explicit formulas.

Periodic mechanisms are isotropic compressions

For every periodic mechanism, the associated macroscopic deformation is an isotropic compression.

Theorem

Let $u = F \cdot x + \psi(x)$ be a k-periodic mechanism, in the sense that

- *F is a constant matrix with $\det F \geq 0$*
- *ψ is defined on the nodes of the Kagome lattice, with any periodicity $k \geq 1$*
- *u preserves the length of each spring, and the orientation of each equilateral triangle.*

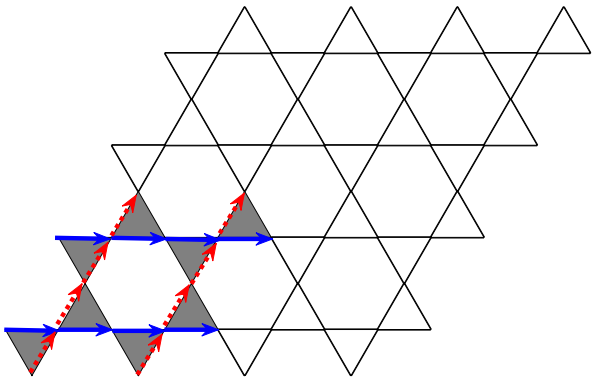
Then $F = c\,R$ for some real number $c \in [0, 1]$ and orientation-preserving rotation $R \in SO(2)$.

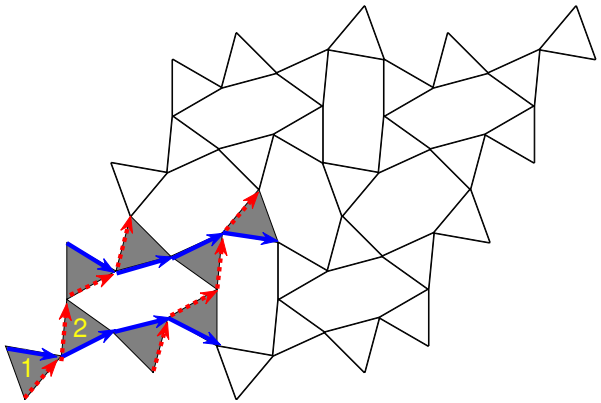
Note: $F = 0$ is possible, even using the one-periodic mechanism, since we have not imposed a non-interpenetration condition. (If interpenetration is prohibited then $c \in [1/2, 1]$.)

Periodic mechanisms are isotropic compressions

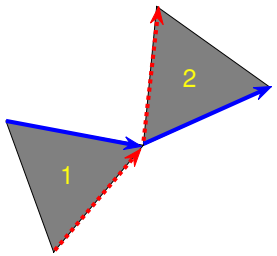
Capture the idea using $k = 2$. Let $v_1 = (4, 0)$ and $v_2 = R_{\pi/3} v_1$, and let $u = F \cdot x + \psi(x)$ be a 2-periodic mechanism.

Periods of image are $\begin{cases} v_1^{\text{def}} = Fv_1 = \text{sum of blue vectors in right figure} \\ v_2^{\text{def}} = Fv_2 = \text{sum of red vectors in right figure} \end{cases}$





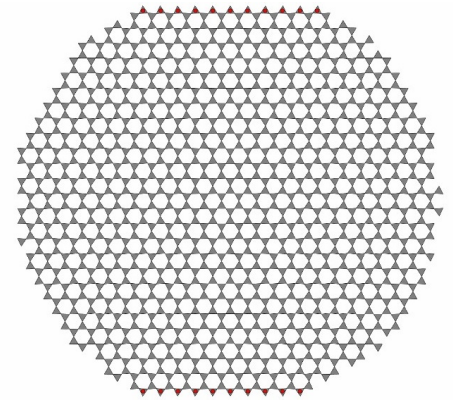
Now observe:
$R_{\pi/3}$ (blue vector) = red vector along same triangle. So
$R_{\pi/3} F v_1 = F v_2$.

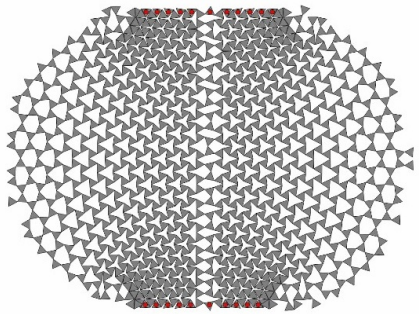


This implies F is isotropic ($F = cR$ with $R \in SO(2)$). Clearly $0 \le c \le 1$, since reference lattice has springs in straight lines.

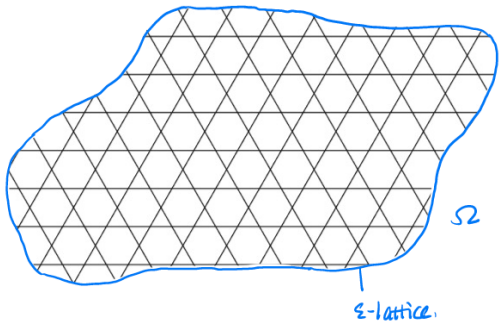
Macroscopic behavior

A numerical experiment: a Kagome-filled region with specified vertical displacement along flat parts of top & bottom





Question: Is Kagome (viewed as a lattice of springs) a numerical approximation of some 2D nonlinear elastic material?

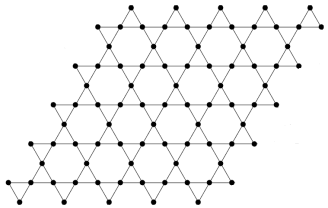


$$E_\varepsilon[u^\varepsilon,\Omega] = \varepsilon^2 \sum_{\text{springs in } \Omega} \left(\frac{|u^\varepsilon(x_i^\varepsilon) - u^\varepsilon(x_j^\varepsilon)|}{|x_i^\varepsilon - x_j^\varepsilon|} - 1 \right)^2 \xrightarrow[u^\varepsilon \to u]{??} \int_\Omega W_{\text{eff}}(Du)$$

A familiar idea: square lattice with diagonal springs approximates continuum 2D elasticity (with a particular elastic law).

Penalizing change of orientation

But using only the spring energies gives a nonphysical result, since the lattice can fold on itself while preserving lengths of all springs.





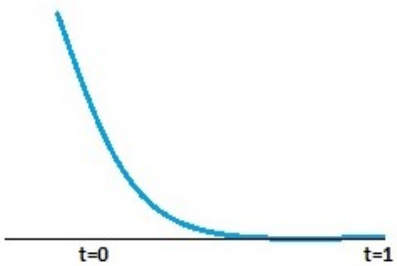


The fix: introduce an additional term that penalizes change of orientation of the equilateral triangles

$$E_\varepsilon^{\text{pen}}[u^\varepsilon, \Omega] = \varepsilon^2 \left[\sum_{\text{springs in } \Omega} \left(\frac{|u^\varepsilon(x_i^\varepsilon) - u^\varepsilon(x_j^\varepsilon)|}{|x_i^\varepsilon - x_j^\varepsilon|} - 1 \right)^2 + \sum_{\text{triangles in } \Omega} g(\det Du^\varepsilon) \right]$$

choosing a penalization g for example s.t.

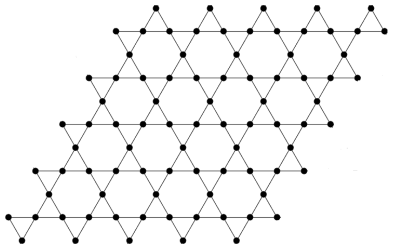
- $g(t) = 0$ for $t \geq 1/4$
- $g(0)$ is sufficiently large

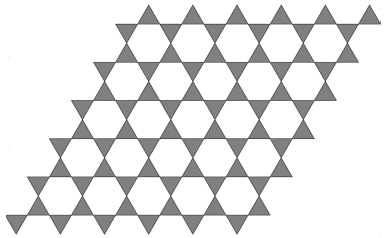


Penalization has no effect on moderately-deformed triangles that keep their orientations, but makes change of orientation expensive.

Intuition

Viewed as a cutout, Kagome consists of equilateral triangles that meet at corners.





Using just the spring energy, a triangle is stress-free if

(a) it experiences rigid motion, or

(b) it gets reflected then experiences rigid motion.

Our penalization leaves the energy unchanged near (a), while assigning large energy to (b).



$$E_\varepsilon^{\text{pen}}[u^\varepsilon, \Omega] = \varepsilon^2 \left[\sum_{\text{springs in } \Omega} \left(\frac{|u^\varepsilon(x_i^\varepsilon) - u^\varepsilon(x_j^\varepsilon)|}{|x_i^\varepsilon - x_j^\varepsilon|} - 1 \right)^2 + \sum_{\text{triangles in } \Omega} g(\det Du^\varepsilon) \right]$$

Macroscopic behavior

The sum of spring energy + penalization does describe, in the limit $\varepsilon \to 0$, a 2D nonlinear elastic solid:

$$E_\varepsilon^{\text{pen}}[u^\varepsilon, \Omega] \quad \xrightarrow[u^\varepsilon \to u]{} \quad \int_\Omega W_*(Du) \qquad \text{(Gamma-convergence)}$$

Its elastic energy density $W_*(F)$ is nonnegative, and satisfies

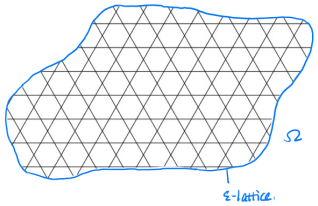
$$W_*(F) \geq \begin{cases} C\left[(\lambda_1 - \lambda_2)^2 + (\lambda_1 - 1)_+^2 + (\lambda_2 - 1)_+^2\right] & \text{if } \det(F) \geq 0 \\ C\left[(\lambda_1 + \lambda_2)^2 + (\lambda_1 - 1)_+^2 + (\lambda_2 - 1)_+^2\right] & \text{if } \det(F) \leq 0 \end{cases}$$

where λ_1, λ_2 are principal stretches of F (eigenvalues of $(F^T F)^{1/2}$). In particular, $W_*(F) = 0$ exactly when F is an isotropic compression ($F = c\,R$ for $0 \leq c \leq 1$ and $R \in SO(2)$).

Gamma-convergence implies convergence of (global) minimizers: Suppose u^ε asymptotically minimizes $E_\varepsilon^{\text{pen}}$ subject to displacement bc on part of $\partial\Omega$, and suppose further that $u^\varepsilon \to u$. Then u minimizes $\int_\Omega W_*(Du)$ subject to the same displacement bc.

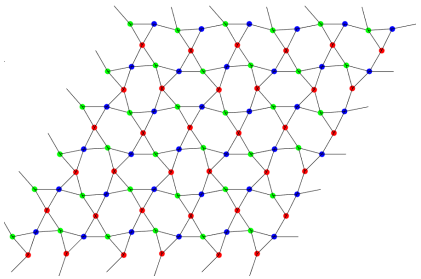
A hint about the proof

$$\varepsilon^2 \left[\sum_{\text{springs in } \Omega} \left(\frac{|u^\varepsilon(x_i^\varepsilon) - u^\varepsilon(x_j^\varepsilon)|}{|x_i^\varepsilon - x_j^\varepsilon|} - 1 \right)^2 + \sum_{\text{triangles in } \Omega} g(\det Du^\varepsilon) \right]$$



(1) Use general tools from calculus of variations to get existence of a limiting variational problem $\int_\Omega W_*(Du)$, with

$$W_*(F) = \min_{k=1,2,\ldots} \min_{\substack{u(x)=F\cdot x+\psi(x) \\ \text{where } \psi \text{ is } k\text{-periodic}}} \left\{ \begin{array}{l} \text{spatially-averaged} \\ \text{microscopic energy} \end{array} \right\}$$



(2) Use Kagome-specific tools to get properties of W_*

The arguments build on our proof that periodic mechanisms are isotropic compressions.

Additional ideas beyond those used for mechanisms

The lower bound says

$$W_*(F) \geq \begin{cases} C\left[(\lambda_1-\lambda_2)^2+(\lambda_1-1)_+^2+(\lambda_2-1)_+^2\right] & \text{if } \det(F)\geq 0 \\ C\left[(\lambda_1+\lambda_2)^2+(\lambda_1-1)_+^2+(\lambda_2-1)_+^2\right] & \text{if } \det(F)\leq 0 \end{cases}$$

The argument used for mechanisms was quite flexible:

- If F is a 2×2 matrix F and $v_1=(1,0)$, then

$$|(FR_{\pi/3}-R_{\pi/3}F)v_1| = \begin{cases} \frac{\sqrt{3}}{2}|\lambda_2-\lambda_1| & \text{if } \det F\geq 0 \\ \frac{\sqrt{3}}{2}|\lambda_2+\lambda_1| & \text{if } \det F\leq 0 \end{cases}$$

- If a triangle is deformed then its contribution to $(FR_{\pi/3}-R_{\pi/3}F)v_1$ is nonzero, but its spring energy is also nonzero – unless it is flipped.
- If a triangle is flipped then its contribution to $(FR_{\pi/3}-R_{\pi/3}F)v_1$ is large, but its penalization energy is also large.

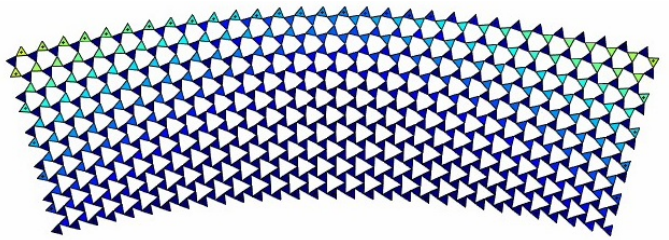
The soft modes are compressive conformal maps

$$W_*(Du) \equiv 0 \text{ when } Du = c(x)R(x) \text{ with } c(x) \leq 1 \text{ and } R \in SO(2).$$

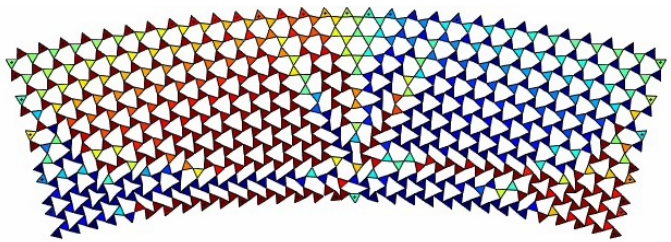
Such maps are conformal. There are many examples: $f = u_1 + iu_2$ should be a complex analytic function of $z = x_1 + ix_2$, with $|f'(z)| \leq 1$.

A convenient class of examples involves bending a rectangle, for example using the conformal map $f = u_1 + iu_2 = e^{iz} = e^{ix_1} e^{-x_2}$.

By modulating a mechanism, one easily gets u^ε such that each spring has strain $\sim \varepsilon$, so $E_\varepsilon^{\text{pen}} \sim \varepsilon^2$. (By being careful, energy can actually be made much smaller.)



Any mechanism can be used. In simulations, domains using different mechanisms can coexist.



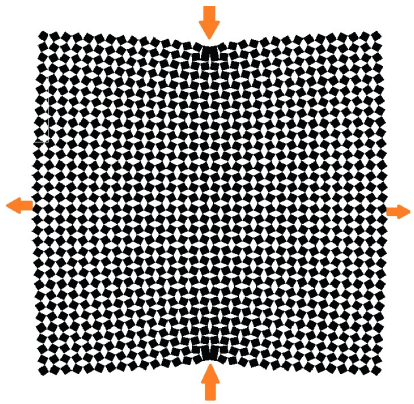
Rotating squares vs Kagome, revisited

Both systems have the same soft modes: compressive conformal maps. There are many soft modes, though the class is quite rigid:

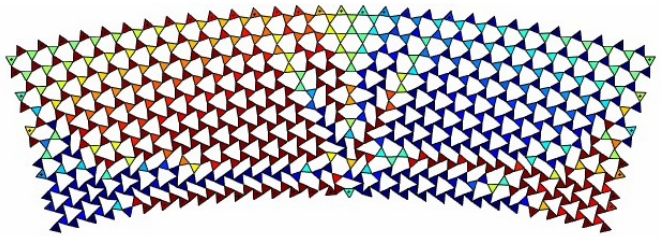
$$Du(x) = c(x)R(x) \Leftrightarrow u = (u_1, u_2) \text{ is a conformal map}$$
$$\Leftrightarrow u_1 + iu_2 = \text{complex analytic fn of } x_1 + ix_2$$

And yet, the two systems are very different.

For rotating squares, the leading-order energy required for modulation of the mechanism is well-understood, and has been used to model experiments.



Kagome has much greater microscopic freedom. Conjecture: energy of soft modes can be very small, maybe even 0.



Mathematical essence of the effective energy

For orientation-preserving maps,

$$W_*(Du) \sim (\lambda_1 - \lambda_2)^2 + (\lambda_1 - 1)_+^2 + (\lambda_2 - 1)_+^2$$

where

$$\lambda_1, \lambda_2 = \begin{cases} \text{eigenvalues of } E = (Du^T Du)^{1/2}, \\ \text{so that } Du(x) = R(x)E(x) \end{cases}$$

When $\lambda_1, \lambda_2 < 1$ we have $W_*(Du) \sim (\lambda_1 - \lambda_2)^2$. So for compressive maps, the relaxed energy is like

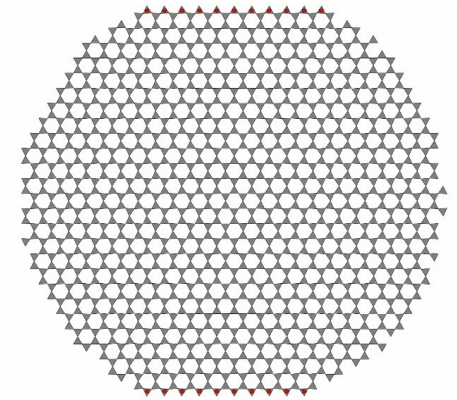
$$\int_\Omega (\lambda_1 - \lambda_2)^2 \, dx = \int_\Omega |Du|^2 - 2 \det Du \, dx.$$

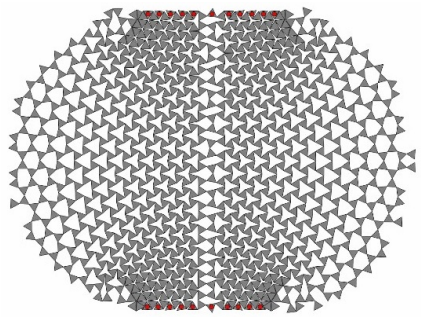
A very simple variational problem; nonnegative, vanishing only at conformal maps!

- $\lambda_1^2 + \lambda_2^2 = |E|^2 = |Du|^2$ and $\lambda_1 \lambda_2 = \det E = \det Du$
- $\left|\nabla u_1 - (\nabla u_2)^\perp\right|^2 = |Du|^2 - 2 \det Du$

What about the flattened circle?

A numerical experiment:
a Kagome-filled region with specified vertical displacement along flat parts of top & bottom



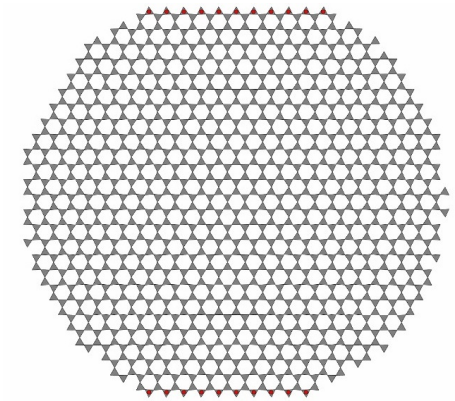


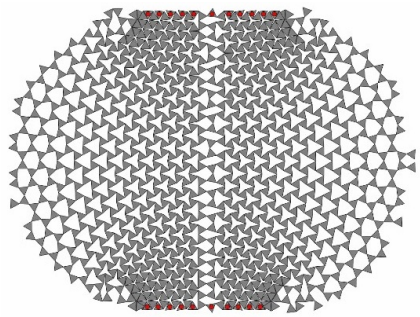
Our boundary condition didn't determine a unique conformal map. The simulation made a choice. Presence of the wall is permitted energetically, but not required.

- Bdry cond was fixed *vertical* displacement along flattened parts of $\partial\Omega$.
- Numerical method used viscoelastodynamics (change of bdry cond adds energy to system, viscosity removes it).
- Discretization was not what we use for theory. Instead, triangles were rigid, so their corners don't quite meet. The energy in the simulation measured this discrepancy.

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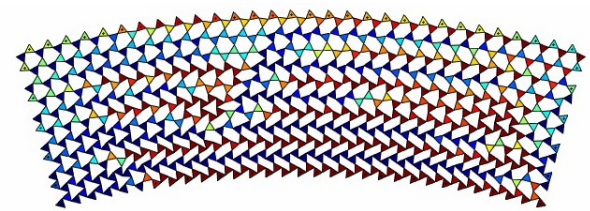


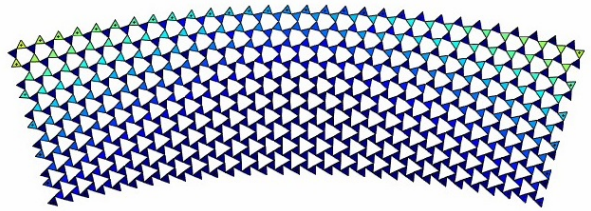


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Why is this interesting?





(1) Nonlinear elastic structures can buckle. Usually the details of buckling matter, and predicting post-buckling behavior is hard.

In Kagome, the mechanisms amount to buckling patterns. Surprisingly, the *macroscopic elastic behavior doesn't seem to care which mechanisms are used.*

(2) In computing, we discretize continuous problems to solve them numerically. In mechanics we often do the opposite – modeling discrete systems using continous methods. Success usually relies on a detailed understanding of the discrete system.

In Kagome, we don't have a full list of mechanisms, nor an understanding which will occur in a given setting. Surprisingly, *the macroscopic elastic behavior doesn't need such details.*

Stepping back

- Mechanism based mechanical metamaterials are geometrically nonlinear systems which often admit simple (discrete) models.
- Soft modes are macroscopic deformations whose energy/unit area vanishes (in the continuum limit). We have identified these for Kagome, despite not knowing all its mechanisms.
- Matching expts requires more than knowing soft modes – it seems to need the leading-order energy. Well-understood in some examples, but not for Kagome.