The Mechanisms and Macroscopic Behavior of the Kagome Metamaterial

Robert V. Kohn
Courant Institute, NYU

Theory: Xuenan Li (Courant)
Numerics: Bolei Deng and Katia Bertoldi (Harvard)

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Mechanism-based mechanical metamaterials

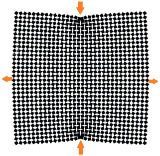
These mechanical systems take advantage of geometric nonlinearity and microstructural buckling to achieve novel mechanical response.

An easy-to-visualize example: the checkerboard (“rotating squares”) metamaterial, obtained by removing squares from a 2D elastic sheet. Its macroscopic stress-free deformations are isotropic compressions.

slightly compressed

very compressed

Its response to loading suggests that there’s an effective material.



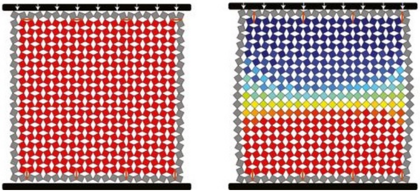
M Czajkowski et al, Nature Comm 2022

The rotating squares metamaterial

Some features of the rotating squares example:

- A continuum of energy-free states, parameterized by the amount of compression. (Reminiscent of a solid-solid phase transformation, but with a continuum of “phases.”)
- Created by making periodically-placed holes in a planar sheet. (Thus, basically just a porous elastic composite).
- Geometric nonlinearity is essential. (The energy-free patterns form by a process akin to buckling.)

Two symmetry-related compression patterns; domain walls are expensive.

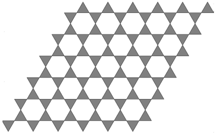


B Deng etal, PNAS 2020

The Kagome metamaterial

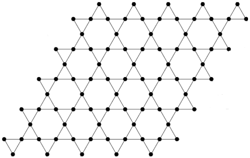
This metamaterial is like the rotating squares example, yet different.

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



Two slightly different versions of the Kagome metamaterial:

- A cutout-based model: hexagonal holes in a flexible sheet.
- A spring-based model: springs along edges of Kagome lattice (rotation at nodes is free).

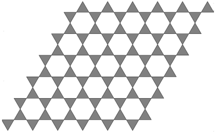


Either way: more or less a porous nonlinearly-elastic composite.

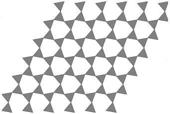
The Kagome metamaterial

A key similarity to rotating squares example: each can achieve isotropic (macroscopic) compression with zero elastic energy.

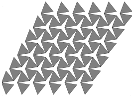
Kagome



reference lattice



one-periodic
small compression



one-periodic
large compression

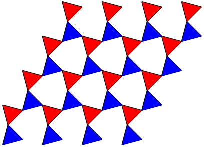
Rotating
Squares

slightly compressed

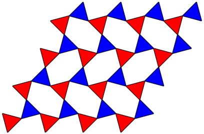
very compressed

The Kagome metamaterial

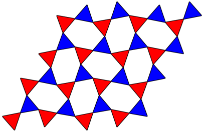
A key difference from rotating squares example: Kagome has a huge variety of energy-free compression patterns.



one-periodic

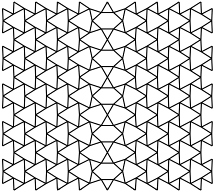


2×1 periodic



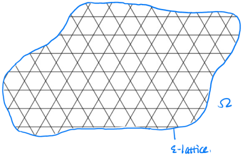
2×2 periodic (one of many)

Moreover, distinct energy-free compression patterns can meet at an energy-free wall.



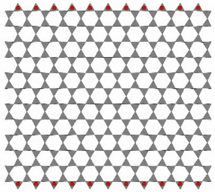
Effective behavior of the Kagome metamaterial

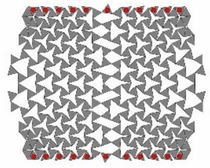
Does it make sense to call this a metamaterial? If so, what are its properties?



From simulations:

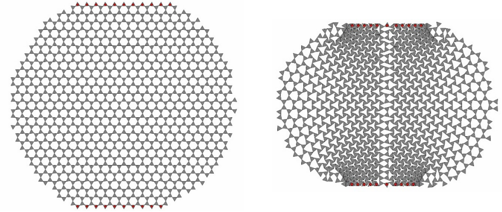
Uniaxial compression:
a Kagome-filled square with specified vertical displacement along top and bottom



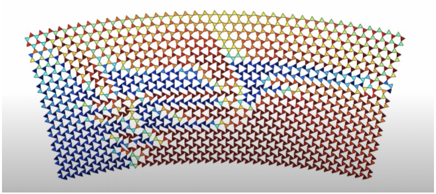


Effective behavior of the Kagome metamaterial

Uniaxial compression: another Kagome-filled region with specified vertical displacement along top and bottom



Bending: A Kagome-filled rectangle with well-chosen Dirichlet bdry condition



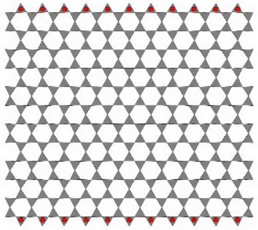
Simulation technique

Bolei Deng was already simulating the rotating squares metamaterial. He quickly adapted his code to the Kagome microstructure.

Degrees of freedom: for each triangle, position of center and orientation.

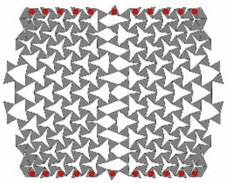
Forces: Triangles are rigid, so corners may not match up; linear springs (with rest length 0) penalize failure to match.

Different from treating edges springs, but energy-free states are the same.



Dynamics: Newton's law with damping.

Sometimes: additional forces introduced to avoid interpenetration.



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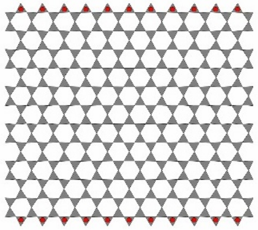

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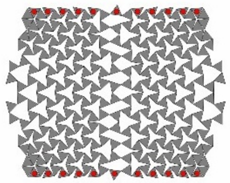
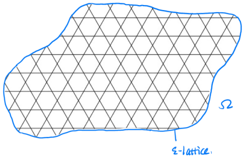


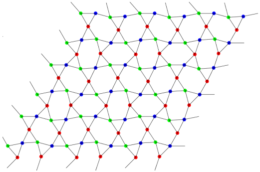
The microscopic elastic energy

Stable states of a mechanical system are local minima of its elastic energy.



$$E_\varepsilon[u^\varepsilon] = \varepsilon^2 \sum_{i\sim j} \left(\frac{|u^\varepsilon(x_i^\varepsilon) - u^\varepsilon(x_j^\varepsilon)|}{|x_i^\varepsilon - x_j^\varepsilon|} - 1 \right)^2$$

- x_i^ε are nodes of scaled lattice that lie in Ω
- $u^\varepsilon(x_i^\varepsilon)$ are locations of nodes after deformation
- sum is over arcs of scaled lattice ($|x_i^\varepsilon - x_j^\varepsilon| = \varepsilon$)
- physically linear (Hookean) springs but geometrically nonlinear
- rotation at nodes is free



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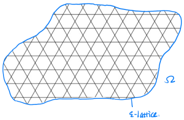

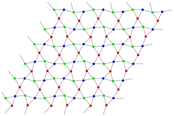

Local vs global min: E_ε may have many local minima. It is nevertheless meaningful consider deformations u^ε that achieve the *minimum energy* (exactly, or asymptotically in ε).

There is a mathematical framework, used eg to discuss composite materials. We say E_ε Gamma-converges to an effective energy E_{eff} if (for any bdry conds or loading) the minimizing u^ε converge to minimizers of E_{eff}.

Each u^ε is defined on nodes of a different lattice, but we can view it as a piecewise-linear function by triangulating the reference lattice. Then $u^\varepsilon(x)$ is defined everywhere, and one can show

$$\int_\Omega |\nabla u^\varepsilon|^2 \, dx \le C(1 + E_\varepsilon(u^\varepsilon)).$$

So the effective energy should be defined for u such that $\int_\Omega |\nabla u|^2 \, dx < \infty$.

The microscopic elastic energy

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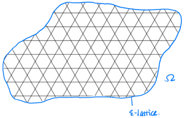

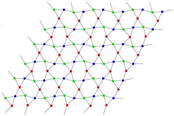

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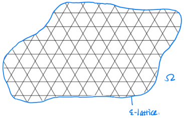

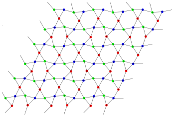

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So the effective energy should be defined for u such that $\int_\Omega |\nabla u|^2\, dx < \infty$.

The effective elastic energy

Theorem: The Gamma-limit exists. We view it as the macroscopic elastic energy. If u^ε asymptotically minimizes E_ε as $\varepsilon \to 0$ (subject to Dir bc on part or all of $\partial\Omega$), any limit u^* minimizes

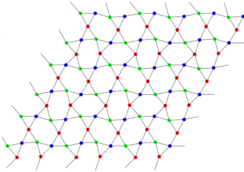
$$E_{\text{eff}}[u] = \int_{\partial\Omega} W_{\text{eff}}(Du)\, dx$$

(subject to the given Dirichlet bc). The effective energy density W_{eff} is nonnegative and frame indifferent:

$$W_{\text{eff}} \geq 0, \quad \text{and} \quad W_{\text{eff}}(F) = W_{\text{eff}}(QF) \text{ for any rotation } Q;$$

moreover it is independent of Ω, and is characterized by

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



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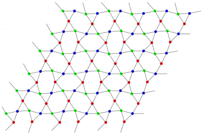


- Proof follows those of analogous results for
  - periodic nonlin-elastic composites (Braides 1985; Müller 1987)
  - less degenerate lattices of springs (Alicandro & Cicalese 2004)
- Effective energy describes *only* (asymptotic) energy minimizers.
  - If system gets stuck at local minimizers, the theory won't describe what is seen.
- This theory considers *only* the spatially-averaged energy.
  - It ignores the richness of the microscopic picture (for example domains separated by low-energy walls).

Estimating W_{eff}

W_{eff} vanishes only at isotropic compressions

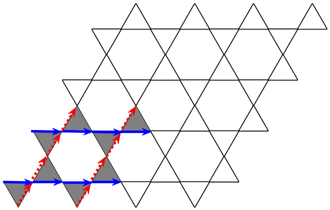
Recall: $W_{\text{eff}}(F)$ is min avg energy, among periodic patterns with macroscopic deformation $F \cdot x$ (with any periodicity $k = 1, 2, \ldots$).

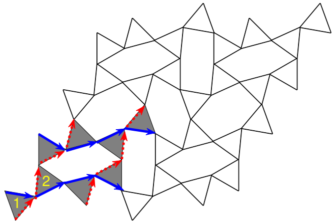
Examples of energy-free compression patterns show that $W_{\text{eff}}(F) = 0$ when F is an isotropic compression. But how to show it doesn't vanish elsewhere?

Capture idea using $k = 2$. Suppose $W_{\text{eff}}(F) = 0$. Let $e_1 = (1, 0)$ and $e_2 = R_{\pi/3} e_1$. Since $u = F \cdot x + \varphi(x)$ where φ is 2-periodic,

$$Fe_1 = \text{avg of blue vectors in right figure}$$

$$Fe_2 = \text{avg of red vectors in right figure}$$





Estimating W_{eff}

Recall: for $e_1 = (1, 0)$ and $e_2 = R_{\pi/3} e_1$,

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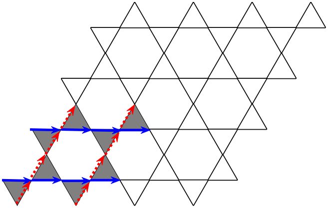
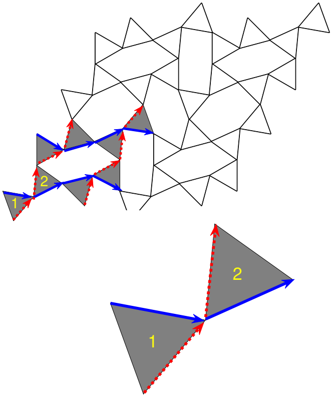




But $R_{\pi/3}$ (red vector) = orange vector along same triangle. So $R_{\pi/3} Fe_1 = Fe_2$.

This implies, by simple algebra, that F is isotropic ($F = cQ$ where Q is some rotation).

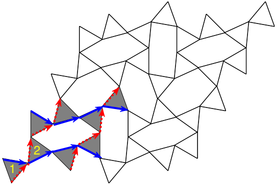
Estimating W_{eff}

Thus far: $W_{\text{eff}}(F) = 0 \Rightarrow F = cQ$ for some rotation Q, using that triangles are rigid under energy-free deformations. Still need $c \leq 1$.

If energy is small, then triangles are almost rigid. Arguing much as before, we get

$$W_{\text{eff}}(F) \geq C(\lambda_1 - \lambda_2)^2$$

for any F, where λ_1, λ_2 are the principal stretches (eigenvalues of $(F^T F)^{1/2}$).



The reference lattice has springs in straight lines. It costs energy to stretch those lines. This leads to the estimate

$$W_{\text{eff}} \geq C[(\lambda_1 - 1)_+^2 + (\lambda_2 - 1)_+^2].$$

These results combine to give the desired result: W_{eff} vanishes only at isotropic compressions.

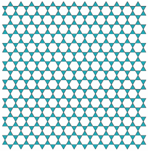
Energy-free maps are conformal

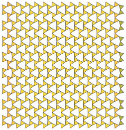
$W_{\text{eff}}(Du) \equiv 0$ when $Du = c(x)Q(x)$ with $c(x) \leq 1$ and $Q^T Q = I$.

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 $|f'(z)| \leq 1$.

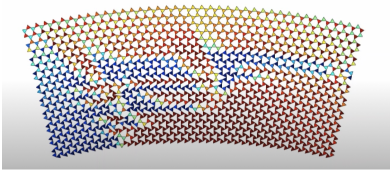
Simulations with Dirichlet bdry data from compressive conformal maps:

Biaxial compression produces a uniform one-periodic pattern.



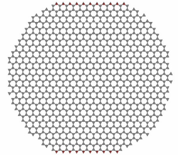


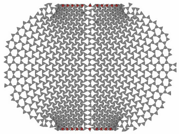
Bending is more interesting. Here the conformal map is $f = u_1 + iu_2 = e^{iz} = e^{ix_1} e^{-x_2}$. The compression factor is $c = 1$ at the top edge.



Energy-free maps are conformal

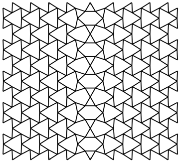
Uniaxial compression: flattened circle with vert displ specified along top and bottom





Why is the deformation nonuniform? Specifying only u_2 along flattened segments doesn't determine a unique conformal map. Our dynamics (Newton's law with damping) made a choice.

Energy-free domain wall: The simulations show low-energy walls separating domains with mirror-image patterns. As noted earlier, such walls can even be energy-free!



Mathematical essence of the relaxed problem

Elastic energy sees the principal strains

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

When $\lambda_1, \lambda_2 < 1$ we have $W_{\text{eff}}(Du) \sim (\lambda_1 - \lambda_2)^2$. 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 $\lambda_1 \lambda_2 = \det E = \det Du$
- $\left| \nabla u_1 - (\nabla u_2)^\perp \right|^2 = |Du|^2 - 2 \det Du$

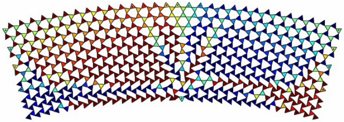
A paradox

Kagome lattice is far from rigid – it has huge variety of mechanisms.

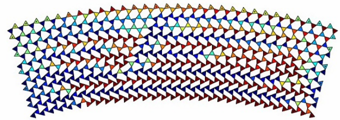
But its macroscopic energy still makes sense (if we accept that the observed u^ε have energy comparable to the global min of E_ε).

Not surprisingly: a small bias can change the microstructure change a lot.

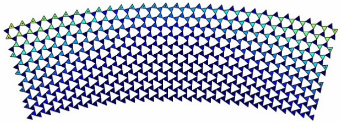
Local min obtained by gradually "bending a rectangle" (using Dir bc).



Local min obtained by gradual bending with a bias favoring 2×1-periodic patterns.

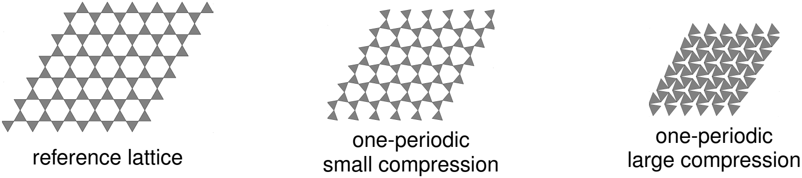


Local min starting from ansatz based on one-periodic mechanism.



Now a word about those compression patterns

By a mechanism, we mean a one-parameter family of deformations whose energy is exactly zero.



Q: A mechanism looks like progressive buckling. Is there a linear elastic calculation that predicts its onset and explains its geometry?

A: For Kagome, the linearization of a periodic mechanism is a linear displacement with linear-elastic energy zero. These are called Guest-Hutchinson modes. They form a linear space.

Definition: a periodic u is a GH mode if $\langle u(x_i) - u(x_j), x_i - x_j \rangle = 0$ whenever x_i and x_j are connected by a spring. Such a displacement deforms each line of springs to an (infinitesimally) zig-zag line.

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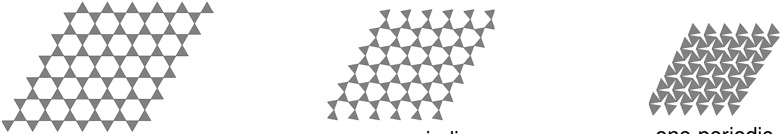

reference lattice

one-periodic small compression

one-periodic large compression

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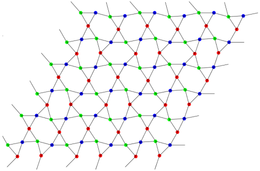
Guest-Hutchinson modes vs mechanisms

However, finding periodic mechanisms is not a bifurcation problem.

Not every k-periodic Guest-Hutchinson mode comes from a mechanism when $k > 1$.

For a k-periodic mechanism, there are k distinct horizontal lines that go to zigzag lines.

Each must experience the same overall compression.

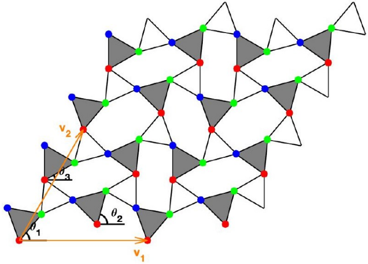


This places a quadratic condition on a GH mode, if it is to come from a mechanism.

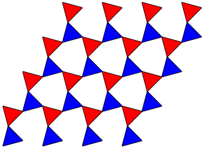
The 2 periodic case

We have explicit formulas for all periodic mechanisms with period at most twice that of the Kagome lattice.

There is a three-parameter family of 2-periodic mechanisms, parameterized by the angles $\theta_1, \theta_2, \theta_3$ as shown. (The compression ratio is an explicit function of the angles.)



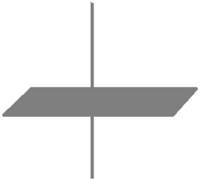
The one-periodic mechanism can also be viewed as a two-periodic one.



The 2 periodic case

The space of 2-periodic GH modes is 4-dimensional. But the only ones that come from mechanisms are

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



Other GH modes don't come from mechanisms (they violate the necessary condition).

Stepping back

- The Kagome metamaterial has a lot of microstructural freedom. Many energy-free patterns. Walls btwn them can be energy-free.
- The macroscopic energy of the Kagome metamaterial is nevertheless well-defined.
- We understand where W_{eff} vanishes. The macroscopically energy-free deformations are compressive conformal maps.
- Just one example, but an interesting one. Paul Plucinsky will discuss other mechanism-based mechanical metamaterials tomorrow.