Homogenization theory for Maxwell lattices

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May 29, 2020

Abstract

Maxwell lattices are a subcategory of the newly emergent field of mechanical metamaterials. Its special periodic construction leaves it some interesting mechanical behavior. Our main result consists of incorporating spatially-periodic homogenization theory into the Maxwell lattice system to understand its macroscopic and microscopic behavior.

1 Introduction

Mechanical metamaterials are artificial composite materials with mechanical properties which cannot be inherited from the single material they are composed of. A famous mechanical metamaterial is the artificial auxetic material, which has negative Poisson's ratio. Normally materials have positive Poisson's ratio. This means when we elongate such a material in one direction, it shrinks in other directions to maintain its volume. Although material with negative Poisson's ratio are not found in nature, people have creatively constructed auxetic material to get this property. These auxetic materials are greatly used in daily supplies, like packing bags, body armors and sponge mops. Another example is the lattice metamaterial. Scientists have found some special lattice metamaterials can sustain forces on one side, but cannot sustain forces on the other side [6].

Among the large family of mechanical metamaterials, we focus on the 2-dimensional Maxwell lattices. It is a periodic structure with each vertex connected by 4 bars. Maxwell lattices are interesting because they satisfy minimal rigidity requirements, thus the lattice has some mechanical instability. Physicists have discovered that Maxwell lattices have one more floppy mode other than translations in linear elasticity. This special floppy mode is referred as Guest-Hutchinson (GH) mode. With the GH mode, Maxwell lattices can be deformed in a nontrivial way without bars changing length to its first order in the amount of deformation. So far, there has been no complete mathematical explanation of why such GH mode arises.

How would a mathematician approach this issue of understanding the missing floppy mode? One tool that can be used to understand this GH mode mathematically is homogenization theory. This theory is often used to draw the connection between macroscopic and microscopic behavior of a periodically oscillatory system and it appears very often in analyzing the elastic behavior of composites

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and porous materials. The periodic structures of composites allow tremendous variations on the microscopic scale, for example the rapid oscillations. But if we take composites as a whole material, we get the macroscopic behavior of this new material by averaging out the rapid oscillations. The behavior of composites as a whole on the macroscopic scale is called the effective behavior. Homogenization connects the macroscopic and microscopic behavior of repetitive composites. A Maxwell lattice also has periodic structures, thus we believe formulating this lattice system in homogenization language can give a mathematical explanation for its interesting behavior. We also anticipate analyzing the macroscopic behavior of different Maxwell lattices after applying the homogenization theory.

The paper will be structured as follows. In section 2 and 3, we will give a brief introduction to Maxwell Lattice and a general introduction to homogenization theory for linear elasticity. We will view the homogenization theory on the lattice system as an optimization problem and give its primal and dual form. In section 4, we will incorporate homogenization theory into the Maxwell lattice system to see what effective behavior Maxwell lattice has. We will end the paper with several open questions we are working on.

2 Introduction to the Maxwell lattice and Guest-Hutchinson mode

In this section, we will briefly introduce the Maxwell lattice system and the Guest-Hutchinson mode, with an example of such mode in the Maxwell lattice system.

A Maxwell lattice is a special bar framework. A bar framework consists of vertices and bars. It is similar to a graph, but with edges replaced by bars, whose length cannot be changed. As you can imagine, if a bar framework has more bars in it, then it is harder for us to deform the framework without breaking any of these bars. If a bar framework can be deformed without breaking the bars, we call the framework non-rigid, and this special deformation is referred as a floppy mode. A 2-dimensional Maxwell lattice system has each vertex connected by 4 bars. Examples of Maxwell lattices are shown in Figure 1. Such systems are non-rigid and always have floppy modes.

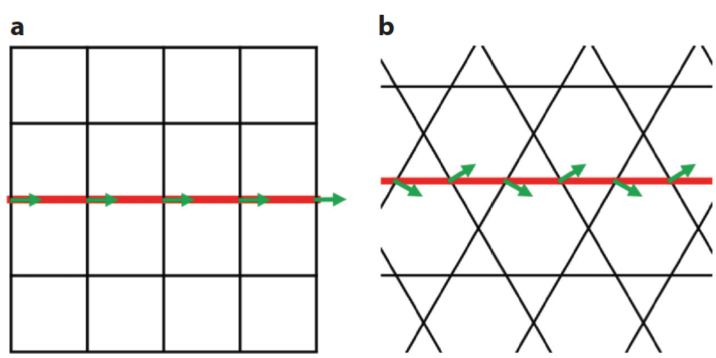

Figure 1: (Replotted from [5]) Figure a and b both have each vertex connecting 4 bars, thus they are Maxwell lattices. Figure a is a square lattice. It is non-rigid and we can deform every vertex with a same amount in the horizontal direction. Figure b is a standard kagome lattice. It is also non-rigid with a floppy mode shown in green arrows.

The Guest-Hutchinson(GH) mode is a special floppy mode in the first-order behavior of periodic lattice structures. When studying the first-order behavior of a lattice system, physicists usually relate deformation of vertices and bond extensions using linear algebra. Consider a Maxwell lattice with N vertices and $2N$ bars in the unit cell. For example, the square lattice has 1 vertex (any vertex) and 2 bars (one horizontal and one vertical bar) in the unit cell. We can write displacements of vertices as a vector $\vec{u} \in \mathbb{R}^{2N}$ and the first-order extensions of bars as another vector $\vec{e} \in \mathbb{R}^{2N}$. For the square lattice, elements in $\vec{u}$ are horizontal and vertical deformation of the only vertex in the unit cell. And $\vec{e}$ consists of the first-order extensions of the horizontal and vertical bars.

The linear algebra relationship between $\vec{u}$ and $\vec{e}$ is $\vec{e} = C\vec{u}$. The matrix C can always be determined by the geometry of each lattice system and is referred as the compatibility matrix. For the Maxwell lattice, this compatibility matrix C is always a square matrix, since $\vec{u}$ and $\vec{e}$ are both in $\mathbb{R}^{2N}$. We can also relate tensions $\vec{t} \in \mathbb{R}^{2N}$ on bonds and forces on vertices $\vec{f} \in \mathbb{R}^{2N}$ in a similar form $\vec{f} = Q\vec{t}$. The geometry of the lattice system will always give $C = Q^T$ [5].

The null space of the compatibility matrix C are the first-order floppy modes. Translations in horizontal and vertical directions are trivial floppy modes, so they are in the kernel space of the compatibility matrix C. Rigid rotations are ruled out because they are not periodic. However, Guest and Hutchinson [2] discovered that there is at least one floppy mode other than the two translations as a replacement of rotation in dimension 2. In matrix language, this tells that the compatibility matrix C always has a null vector other than horizontal and vertical translations. This null vector is named as Guest-Hutchinson (GH) mode. Figure 2 gives a non-trivial example of GH mode in the standard kagome lattice.

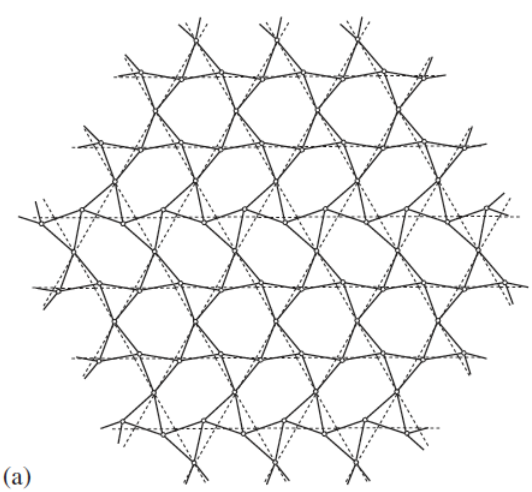

Figure 2: (Replotted from [3]) The dotted lines are the undeformed standard kagome lattice; the solid lines are the non-trivial Guest-Hutchinson mode for the standard kagome lattice. In the deformed lattice, there are some vertices still stay at the same position, while the others move with different displacements. And the GH mode is periodic with a different periodicity compared to the non-deformed standard kagome lattice.

The GH mode is important because it corresponds to non-trivial self-stress. Self-stresses are the null space of the equilibrium matrix Q. The relation $Q = C^T$ ensures every non-trivial GH mode will give a non-trivial self-stress. The existence of non-trivial self-stresses tells us that the bars are under tension or compression even though all vertices are at equilibrium. From an engineering perspective, self-stresses are dangerous because materials encounter abrasion without loads on them. Studying the GH mode gives a way to analyze these self-stresses.

3 Introduction to homogenization theory

In this section, we give a general introduction to homogenization theory to see how it connects the microscopic and macroscopic behavior of some composite materials. In linear elasticity theory, we would like to solve the corresponding deformation $u : \Omega \to \mathbb{R}^n$ of a specific material given a body force $f : \Omega \to \mathbb{R}$ on some domain $\Omega \subset \mathbb{R}^n$. The governing equation is

$$\nabla \cdot (a(x)e(u)) = f(x) \qquad u \in H^1(\Omega) \tag{3.1}$$

with some proper boundary conditions. The symmetric gradient $e(u)$ is defined as $1/2 \left(\nabla u + (\nabla u)^T\right)$. We refer $a(x)$ as the Hooke's coefficient and it is a 4-tensor. In a spring system, the Hooke's coefficient times deformation gives tension. Similarly in linear elasticity, $a(x)e(u)$ is the stress at point x. Usually $a(x)$ is spatially dependent. So for composites, $a(x)$ can take different values on different regions. For example, in Figure 3, we consider a 2d composite made by one material in square M and filled in with another material in the remaining part F. The whole domain is $\Omega = (0, 1) \times (0, 1)$. A simple choice of $a(x)$ with different constants on M and F is

$$a(x) = \begin{cases} a_1 I & x \in M \\ a_2 I & x \in F \end{cases} \tag{3.2}$$

where I is the identity 4-tensor.

Figure 3 gives a concrete example of this choice of $a(x)$. We can always solve (3.1) on Ω if a_1, a_2 are both positive. More interestingly, we can use Ω as a building block and assemble it periodically to get a $N \times N$ block material Ω_N. We care about the behavior as $N \to \infty$ when Ω_N is given a boundary load, and the study of this kind of limit behavior is called homogenization theory. Each small block in Ω_N has its own microscopic displacement to sustain the overall boundary force. For large N, the microscopic displacement of every block averages to some macroscopic displacement. We can now view Ω_N as a whole piece with some new Hooke's constant a^*, and it sustains the boundary force with the averaged macroscopic displacement. Homogenization theory gives a way to find this new Hooke's constant a^*.

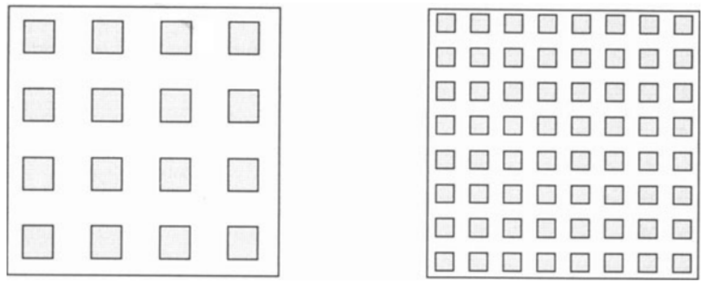

Figure 1.1. The case $N = 16$. Figure 1.2. The case $N = 64$.

Figure 3: (Figure 1.1 and 1.2 are replotted from [1]) The left plot has 4×4 unit cells and the right plot has 8×8 unit cells. Squares in Figure 1.1 and Figure 1.2 has Hooke's coefficient $a(x) = a_1$. The rest part has Hooke's coefficient $a(x) = a_2$. As N gets larger, $a(x)$ quickly oscillates between a_1 and a_2. And the corresponding solution to (3.1) has rapid oscillation.

As $N \to \infty$, this $N \times N$ block looks very similar to a periodic lattice. So we believe homogenization is a promising tool to explain the mysteries in Maxwell lattice.

Now we give the formal math formulation of homogenization theory. We would like to solve the problem

$$\nabla \cdot (a(x/\epsilon) \nabla u^\epsilon(x)) = f(x) \qquad u^\epsilon \in H^1(\Omega) \tag{3.3}$$

with some proper boundary conditions. We assume $a(y)$ is periodic in $\mathbb{R}^d$, and Q is the smallest period. Q is usually a cube, like the above unit cell Ω. Thus for small ϵ, $a(x/\epsilon)$ oscillates rapidly with period ϵ. The limit N to infinity becomes the limit ϵ to 0^+. Each ϵ gives a solution u^ϵ. As $\epsilon \to 0^+$, solutions u^ϵ converges weakly to some $u^*(x)$ in $H^1(\Omega)$, where $u^*(x)$ solves

$$\nabla \cdot (a^* \nabla u^*(x)) = f(x) \tag{3.4}$$

with the same boundary condition as in (3.3). We refer a^* as the effective tensor and it is a constant 4-tensor. Finding this effective tensor a^* is the so-called cell problem.

The fact that a^* is a constant is not easy to see. We know that given deformation u, the stored elastic energy on Q can be viewed as

$$E[u] = \int_Q \langle a(y) \nabla u(y), \nabla u(y) \rangle dy. \tag{3.5}$$

The gradient ∇u has rapid oscillations in it, and on the macroscopic scale, we only see its average $\xi = \fint_Q \nabla u(y) dy$. We refer this ξ as the average strain, which characterizes the average deformation over Q. The effective energy with respect to this average strain ξ is $\langle a^* \xi, \xi \rangle$, and this energy can be written as a minimization problem of the elastic energy $E[u]$ over all deformations u with average strain ξ.

$$E_{\text{eff}}(\xi) = \langle a^*\xi, \xi\rangle = \inf_{\xi = \fint_Q \nabla u} \fint_Q \langle a(y)\nabla u(y), \nabla u(y)\rangle dy \tag{3.6}$$

$$= \inf_{\phi \text{ periodic on } Q} \fint_Q \langle a(y)(\xi + \nabla\phi(y)), \xi + \nabla\phi(y)\rangle dy. \tag{3.7}$$

As an optimization problem, it also has its dual form, given by Kohn and Milton[4]

$$E_{\text{eff}}(\xi) = \langle (a^*)^{-1}\bar{\sigma}, \bar{\sigma}\rangle = \inf_{\substack{\nabla\cdot\sigma = 0 \\ \fint_Q \sigma = \bar{\sigma}}} \fint_Q \langle a(y)^{-1}\sigma(y), \sigma(y)\rangle dy \tag{3.8}$$

with strong duality holds when $\bar{\sigma} = a^*\xi$. We refer $\bar{\sigma}$ as the average stress.

Equation (3.8) draws the connection between stress and strain. In a spring system, if the deformation is Δx, then the force on this spring is $k\Delta x$. In homogenization theory, average strain ξ and average stress $\bar{\sigma}$ play the role of deformation and force, in the sense that average stress in the material is $\bar{\sigma} = a^*\xi$, when the deformation achieves average strain ξ. The optimization part in (3.8) tells us that the effective energy can also be viewed as the minimum elastic energy of all stress $\sigma(y)$ with average $\fint_Q \sigma = \bar{\sigma}$.

4 Our framework of a discrete lattice system

In this section, we will apply homogenization theory to the Maxwell lattice and formulate the linearized effective energy E_{eff} of the lattice system as an optimization problem in both primal and dual form.

In a periodic lattice system, we only care about the behavior of vertices and bonds in the unit cell. For example, in a 2-dimensional lattice with 3 vertices in the unit cell, given a deformation u, we only consider its deformation at the three vertices x_1, x_2 and x_3. The deformation at each vertex is in $\mathbb{R}^2$, thus this reduces the deformation function u to a 6-vector. The reduction makes the periodic lattice setting to a linear algebra problem and simplifies the calculation in the optimization problem.

The effective energy E_{eff} with a given average strain ξ is $\langle A_{\text{eff}}\xi, \xi\rangle$, where A_{eff} is the effective tensor. The effective tensor A_{eff} plays the role of a^* in section 3. Every deformation u with average strain ξ can be written as $u = \xi x + \phi$, and ϕ is periodic on the unit cell. In the periodic lattice setting, u and ϕ are both vectors. Since we are formulating the linearized effective energy, we only consider the bond extension to its first order. After some calculation, the effective energy E_{eff} can be written as

$$E_{\text{eff}} = \langle A_{\text{eff}}\xi, \xi\rangle = \min_{\phi} \sum_{i\sim j} \left[\sqrt{A_{ij} l_{ij}} \left(\hat{b}_{ij}^T \xi \hat{b}_{ij} + \frac{\phi(x_j) - \phi(x_i)}{l_{ij}} \cdot \hat{b}_{ij}\right)\right]^2, \tag{4.1}$$

where $\hat{b}_{ij} \in \mathbb{R}^2$ as the unit vector indicating the direction of ijth bond, A_{ij} as the Hooke's constant of ijth bond and l_{ij} as the length of ijth bond.

The minimization problem over vector ϕ in (4.1) is the primal problem. It plays the role of (3.7) as minimizing the effective energy over all deformations with average strain ξ. After some manipulations, we can reformulate its dual problem as:

$$E_{\text{eff}} = \max_{\substack{t_{ij} \\ C^T t=0}} 2\sum_{i\sim j} t_{ij}\hat{b}_{ij}^T\xi\hat{b}_{ij} - \sum_{i\sim j}\frac{1}{A_{ij}l_{ij}}t_{ij}^2 \tag{4.2}$$

with the optimal ϕ^* and t_{ij}^* satisfying strong duality

$$t_{ij}^* = A_{ij}l_{ij}\langle\hat{b}_{ij}\otimes\hat{b}_{ij},\xi\rangle + A_{ij}l_{ij}\frac{\vec{\phi}^*(x_j)-\vec{\phi}^*(x_i)}{l_{ij}}\cdot\hat{b}_{ij}. \tag{4.3}$$

The dual problem (4.2) maximizes over the tension vector t, with its element t_{ij} as the tension on ijth bond. But not all tensions are allowed, the legal ones should keep all vertices at equilibrium. Thus we have the constraint $C^T t = 0$.

The above formulation (4.1) and (4.2) incorporates homogenization theory into our lattice type problem. Now we can use it to analyze the macroscopic behavior of Maxwell lattice.

Theorem 4.1. *The effective energy (4.1) can also be written with the average stress $\bar{\sigma}$*

$$E_{\mathit{eff}} = \langle A_{\mathit{eff}}\xi,\xi\rangle = \min_{\substack{t_{ij}\ C^T t=0 \\ \sigma_{ij}=t_{ij}\hat{b}_{ij}\otimes\hat{b}_{ij} \\ \bar{\sigma}=\sum_{i\sim j}\sigma_{ij}=\sum_{i\sim j}t_{ij}^*\hat{b}_{ij}\otimes\hat{b}_{ij}}} \frac{1}{A_{ij}l_{ij}}\langle\sigma_{ij},\sigma_{ij}\rangle = \langle Q_{\mathit{eff}}\bar{\sigma},\bar{\sigma}\rangle, \tag{4.4}$$

where Q_{eff} is another 4-tensor and plays the role as $(a^*)^{-1}$ in section 3.

The proof resembles Kohn and Milton's paper [4]. So here we omit the proof.

Theorem 4.1 writes the effective energy E_{eff} as the smallest energy over all admissible stresses $\sigma(y)$ with its average as the optimal stress $\sum_{i\sim j} t_{ij}^*\hat{b}_{ij}\otimes\hat{b}_{ij}$. This theorem is important because it gives a way to compute the average stress $\bar{\sigma}$ on the lattice when we are given a deformation with average strain ξ. For a given ξ, the optimal microscopic oscillation $\vec{\phi}$ in (4.1) gives the optimal tension $\vec{t}$ in (4.3). The optimal tension then uncovers the effective stress $\bar{\sigma}$ in (4.4).

5 Conclusion and open disucssion

Our main work focuses on formulating the lattice system using the homogenization language and finding its dual form in terms of stress σ. The discrete lattice setting makes this formulation as an accessible linear algebra problem. The subsequent work will apply this homogenization idea on some Maxwell lattice to see the effective tensor directly. There are still many interesting questions to be considered.

(1) What are the macroscopic behavior of different Maxwell lattices? Do they share similarities?

(2) What kind of Maxwell lattices have their effective tensors A_{eff} positive-definite?

(3) If the effective tensor is degenerate, meaning if the effective tensor A_{eff} has a nonzero null direction, then there should be some stresses that cannot be held by the lattice. And how does this affect our duality theory?

(4) In section 2, we introduced the Guest-Hutchinson mode. How does it manifest itself in the homogenization theory?

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