

Predicting the mechanical properties of spring networks

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The elastic response of mechanical, chemical, and biological systems is often modeled using a discrete arrangement of Hookean springs, representing either finite material elements or even the molecular bonds of a system. However, to date, there is no direct derivation of the relation between a general discrete spring network, with arbitrary geometry, and its corresponding elastic continuum. Furthermore, understanding the network's mechanical response requires simulations that may be expensive computationally. Here, we report a method to derive the exact elastic continuum model of any discrete network of springs, requiring network geometry and topology only. We identify and calculate the so-called “nonaffine” displacements. Explicit comparison of our calculations to simulations of different crystalline and disordered configurations shows that we successfully capture the mechanics even of auxetic materials. Our method is valid for residually stressed systems with nontrivial geometries, and is an important step in generalizing active stresses on such discrete systems. It is easily generalizable to other discrete models, and opens the possibility of a rational design of elastic systems.

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I. INTRODUCTION

Since the 19th century [1,2], the theory of elasticity has mostly been phenomenological. First principles derivations of elasticity—derivations of continuum elastic properties from known microscopic characteristics—began to appear in the past 50 yr [3–13]. To date, past works have been focused on flat, compatible systems that do not exhibit residual stresses and are difficult to generalize. This includes works where rich nonlinearities are introduced such as those stemming from complex topology [13], singular defects in crystalline order [10], or active stresses [14,15]. Nevertheless, it is widely accepted that in essence, elasticity may be described using springlike interactions between constituents (e.g., first-order approximation of intermolecular forces around equilibrium). In fact, elasticity is often described using a spring network either for computational or analytical aspects [16–18] in a plethora of different systems and cases—from modeling the shape of self-assembled membranes [10,12,19–22], through biological systems [23,24], to modeling crack propagation [25] and various bioinspired and metamaterials [26–29]. Typically, calculation of the network's elastic response can only be done via direct simulation of a loading scheme (i.e., simulating a specific mechanical load and the response to it).

In this paper, we directly derive a generalized elastic continuum limit of any triangulated spring network, with arbitrary reference lengths and spring constants, in two and

three dimensions, within arbitrary geometry, including residually stressed systems. The resulting continuum limit depends solely on the network geometry and topology, as expressed by reference lengths, spring constants, and bonds. From this description, any macroscopic elastic quantity can be extracted, such as Poisson's ratio. We demonstrate the strength of this approach by calculating Poisson's ratios for different test cases, both ordered and disordered, recovering even auxetic behavior. We identify and directly calculate the so-called “nonaffine” displacement of every element. These are local deformations deviating from the local average deformation, and are responsible for the wide range of responses seen in disordered elastic media. The results are valid for residually stressed elastic systems by virtue of the mathematical formulation setting of the problem.

The continuum limit we derive is formulated within the theory of incompatible elasticity [30]. This is a modern formulation of elasticity that successfully describes residually stressed elastic systems [31–33]. In this formulation, an elastic material is described by a metric $\mathbf{g}$ with elements $g_{\mu\nu}$, describing actual distances between material elements, and a reference metric $\bar{\mathbf{g}}$ with elements $\bar{g}_{\mu\nu}$ describing ideal distances. The elastic energy then depends on the squared difference of $\mathbf{g} - \bar{\mathbf{g}}$, $E_{el} \propto \|\mathbf{g} - \bar{\mathbf{g}}\|^2$, for some proper choice (yet to be defined) of the norm $\|\cdot\|^2$, through the elastic (four-indexed) tensor $\bar{\bar{A}}$ (with elements $A^{\mu\nu\alpha\beta}$).

This description, via the use of metrics, is very similar in essence and form to the classical description of Hookean springs. It is independent of assumptions about the existence of a rest configuration, which enables the treatment of residual stresses, and distinguishes this framework from other approaches to elasticity. In the following, we consider a discrete network of springs and show how such formulation naturally arises. We then coarse grain the network, and will identify the nonaffine quantities, show how they contribute to the elastic

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continuum energy, and shortly discuss how this derivation relates to other methods found in the literature.

II. RESULTS

A. Framework

The theory of incompatible elasticity [30] is the framework to which the results of this paper are anchored. Within it, the elastic energy is given by

$$E_{el} = \int A^{\mu\nu\alpha\beta} (g_{\mu\nu} - \bar{g}_{\mu\nu}) (g_{\alpha\beta} - \bar{g}_{\alpha\beta}) dV_{\bar{g}}, \quad (1)$$

where $g_{\mu\nu}$ is the actual metric, describing distances between neighboring material points, and $\bar{g}_{\mu\nu}$ is the reference metric, describing ideal distances. $dV_{\bar{g}} = \sqrt{\bar{g}} d^M x$ is the volume element in M dimensions, $\bar{g} = \det \bar{\mathbf{g}}$. $A^{\mu\nu\alpha\beta}$ are the elements of the elastic tensor. Einstein summation is assumed for repeating upper and lower Greek indices. Greek indices refer to coordinates within the volume of the n -dimensional manifold.

In an isotropic material, $A^{\mu\nu\alpha\beta} = \frac{Y}{16(1-\nu^2)} [\frac{1}{2}(1-\nu)(\bar{g}^{\mu\alpha}\bar{g}^{\nu\beta} + \bar{g}^{\nu\alpha}\bar{g}^{\mu\beta}) + \nu\bar{g}^{\mu\nu}\bar{g}^{\alpha\beta}]$, where $\bar{g}^{\mu\nu}$ is the inverse reference metric, Y is Young's modulus, setting the rigidity scale of the system, and ν is Poisson's ratio, describing the amount a material contracts in one axis, when the other is stretched (negative values indicate expansion). In nonisotropic materials, Poisson's ratio is orientation dependent, and the expression of $A^{\mu\nu\alpha\beta}$ will typically depend on additional terms.

The elastic stress is given by the variation $\sigma^{\mu\nu} = \frac{\delta E_{el}}{\delta g_{\mu\nu}}$, and the material satisfies the usual force balance equation:

$$\bar{\nabla}_\mu \sigma^{\mu\nu} + \sigma^{\mu\alpha} (\Gamma_{\mu\alpha}^\nu - \bar{\Gamma}_{\mu\alpha}^\nu) = f_{\text{ext}}^\nu, \quad (2)$$

where f_{ext}^ν are the external forces acting on the system, $\sigma^{\mu\nu} = \frac{\delta E_{el}}{\delta g_{\mu\nu}}$ is the elastic stress, $\bar{\nabla}_\mu$ is the covariant derivative with respect to $\bar{g}_{\mu\nu}$, and $\Gamma_{\beta\gamma}^\alpha$, $\bar{\Gamma}_{\beta\gamma}^\alpha$ are the Christoffel symbols associated with the metrics $g_{\mu\nu}$ and $\bar{g}_{\mu\nu}$, respectively. The second term on the left-hand side of the equation corresponds to the contribution of residual stresses to the total stresses in the system.

B. Analytical derivation

We begin by considering a triangulated mesh of springs, each with reference length $\bar{\ell}_e$, spring constant k_e , and an actual length ℓ_e , where the index e enumerates the springs. The elastic energy of the system is exactly given by

$$E_{el} = \sum_e \frac{1}{2} k_e (\ell_e - \bar{\ell}_e)^2. \quad (3)$$

A triangulated network is easily divided into a sum of specific simplices (cells). In three dimensions, these are tetrahedra, and in two dimensions these are simple triangles. The energy can then be rewritten as a sum over simplices, and taking care not to count the same edge twice

$$E_{el} = \frac{1}{2} \sum_s \sum_{e \in s} \frac{1}{2} k_e (\ell_e - \bar{\ell}_e)^2. \quad (4)$$

Here, the index s enumerates simplices, and $e \in s$ means summation over all the springs associated with the simplex s . When left to relax, the network assumes some configuration

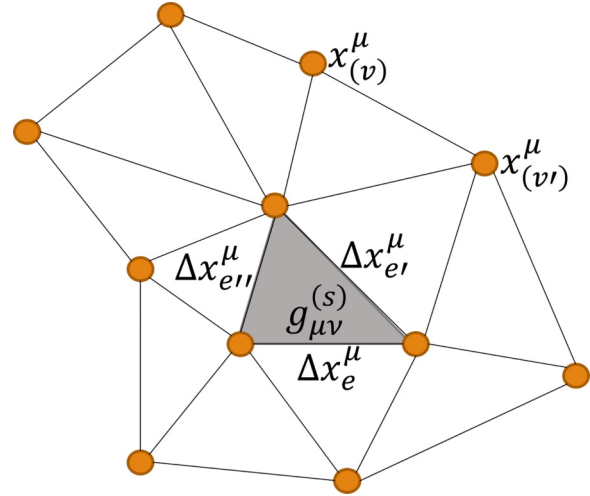


FIG. 1. Depiction of a small portion of a spring network. Showing the coordinates of different vertices (x^μ), the edge vectors Δx^μ of the edges $\{e, e', e''\}$ associated with triangle (s) , and the local metric $g_{\mu\nu}^{(s)}$ (shaded triangle).

(not necessarily unique) $\{\tilde{f}_v\}$ in $\mathbb{R}^n$ for every vertex v . By setting coordinates x_v^μ to each vertex v (μ is the coordinate component), given actual lengths $\{\ell_e\}$, we may uniquely define a “local metric” $g_{\mu\nu}^{(s)}$ associated with a cell s , so that

$$\ell_e^2 = g_{\mu\nu}^{(s)} \Delta x_e^\mu \Delta x_e^\nu \forall e \in s, \quad (5)$$

where $\Delta x_{(1,2)}^\mu = x_2^\mu - x_1^\mu$ is the “coordinate difference” of the edge $e = (1, 2)$ connecting vertices 1 and 2. Equation (5) is not an approximation, rather it is an exact definition of the local quantity $g_{\mu\nu}^{(s)}$, over the whole simplex (see Fig. 1).

Hence, a given simplex uniquely defines a local metric $g_{\mu\nu}^{(s)}$ associated with it. A physical system is constrained such that any two local metrics $\mathbf{g}^{(i)}$ and $\mathbf{g}^{(j)}$ with a shared edge Δx_e agree on its length $\ell_e[\mathbf{g}^{(i)}] = \ell_e[\mathbf{g}^{(j)}]$, where $\ell_e[\mathbf{g}]$ is the edge's length, as measured using the metric $\mathbf{g}$. We can now rewrite the energy

$$E_{el} = \frac{1}{4} \sum_s \sum_{e \in s} k_e (\sqrt{g_{\mu\nu}^{(s)} \Delta x_e^\mu \Delta x_e^\nu} - \bar{\ell}_e)^2. \quad (6)$$

To proceed, we introduce three assumptions. First, we assume that the reference lengths $\{\bar{\ell}_e\}$ are compatible, so that a single simplex can assume the shape described by the lengths $\bar{\ell}_e$. This assumption definitely holds in any nonresidually stressed system, curved or not, but in fact also most residually stressed systems. It might fail in certain glasses (see Sec. III for more details). This assumption means that the reference lengths locally define a reference metric $\bar{g}_{\mu\nu}^{(s)}$. We can therefore write $\bar{\ell}_e = \sqrt{\bar{g}_{\mu\nu}^{(s)} \Delta x_e^\mu \Delta x_e^\nu}$.

Second, we assume that in an equilibrium configuration (again, not necessarily unique), deviations of actual lengths from the reference lengths are small. This is true even for most residually stressed systems. As the curvatures are typically of a much larger scale than the elements' scale (i.e.,

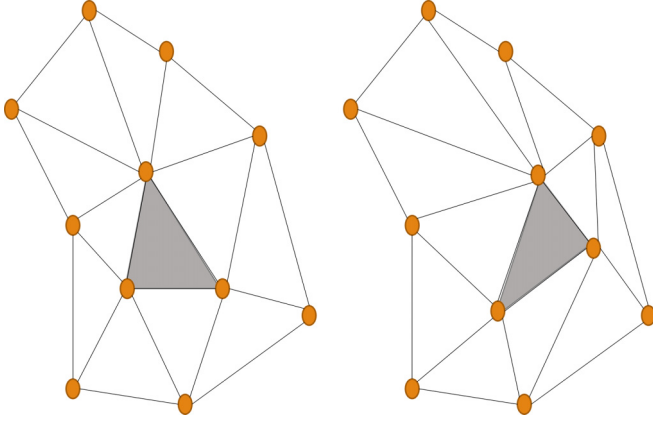


FIG. 2. Schematic (exaggerated) of nonaffine deformations. The same network from Fig. 1 stretched along the y axis. Left: the network when only affine deformations are allowed; every element is elongated by the same ratio. Right: a response with non-affine deformations. Different elements may respond differently to the stretch. The shaded triangle is for visualization only.

atomic/molecular or even mesoscopic),

$$l_e - \bar{l}_e = \frac{l_e^2 - \bar{l}_e^2}{l_e + \bar{l}_e} \simeq \frac{1}{2\bar{l}_e} (l_e^2 - \bar{l}_e^2) + \dots \quad (7)$$

where the ellipse (...) marks higher-order terms of $l_e^2 - \bar{l}_e^2$. Thus, exchanging the expressions for l_e and $\bar{l}_e$ with their g

and $\bar{g}$ expressions, we get

$$E_{el} = \sum_s \sum_{e \in s} \frac{k_e}{16\bar{\ell}_e^2} (g_{\mu\nu}^{(s)} \Delta x_e^\mu \Delta x_e^\nu - \bar{g}_{\mu\nu}^{(s)} \Delta x_e^\mu \Delta x_e^\nu)^2 + \dots \quad (8)$$

We expand the energy

$$E_{el} = \sum_s (g_{\mu\nu}^{(s)} - \bar{g}_{\mu\nu}^{(s)}) (g_{\alpha\beta}^{(s)} - \bar{g}_{\alpha\beta}^{(s)}) \sum_{e \in s} \frac{k_e \Delta x_e^\mu \Delta x_e^\nu \Delta x_e^\alpha \Delta x_e^\beta}{16\bar{\ell}_e^2}. \quad (9)$$

Marking the local elastic tensor

$$A_{(s)}^{\mu\nu\alpha\beta} = \sum_{e \in s} \frac{k_e \Delta x_e^\mu \Delta x_e^\nu \Delta x_e^\alpha \Delta x_e^\beta}{16\bar{\ell}_e^2}, \quad (10)$$

we write

$$E_{el} = \sum_s A_{(s)}^{\mu\nu\alpha\beta} (g_{\mu\nu}^{(s)} - \bar{g}_{\mu\nu}^{(s)}) (g_{\alpha\beta}^{(s)} - \bar{g}_{\alpha\beta}^{(s)}). \quad (11)$$

This equation is very similar to Eq. (1) and may be considered as a discrete version of that equation.

The third and last assumption introduced is that $\bar{g}_s$ varies slowly on some large enough region. Without this assumption, the continuum limit cannot hold (though an effective continuum may be derived in principle). As before, this is very common in continuous media, where the actual elements are very small relative to almost any other quantity (see Sec. III for more details).

Defining an average metric, $g_{\mu\nu}$, on some neighborhood Ω , we may expand $g_{\mu\nu}^{(s)} = g_{\mu\nu} + \delta g_{\mu\nu}^{(s)}$. Formally, $\delta g_{\mu\nu}^{(s)}$ describes the “nonaffine” deformations (see Fig. 2). The energy then reads

$$E_{el} = \sum_{\Omega} \left(\sum_{s \in \Omega} A_{(s)}^{\mu\nu\alpha\beta} \Delta g_{\mu\nu} \Delta g_{\alpha\beta} + \sum_{s \in \Omega} A_{(s)}^{\mu\nu\alpha\beta} \Delta g_{\mu\nu} \delta g_{\alpha\beta}^{(s)} + \sum_{s \in \Omega} A_{(s)}^{\mu\nu\alpha\beta} \delta g_{\mu\nu} \Delta g_{\alpha\beta} + \sum_{s \in \Omega} A_{(s)}^{\mu\nu\alpha\beta} \delta g_{\mu\nu} \delta g_{\alpha\beta}^{(s)} \right), \quad (12)$$

where $\Delta g_{\mu\nu} = g_{\mu\nu} - \bar{g}_{\mu\nu}$ and $\sum_{\Omega}$ is the sum over all the neighborhoods in which $\mathbf{g}$ and $\bar{\mathbf{g}}$ may be regarded as constant. Since, under our assumptions, if $g_{\mu\nu} = \bar{g}_{\mu\nu}$, $\delta g_{\mu\nu}^{(s)} = 0 \forall s$, then for small deviations from $\bar{g}_{\mu\nu}$, $\delta g_{\mu\nu}^{(s)} = W_{(s)\mu\nu}^{\alpha\beta} \Delta g_{\alpha\beta}$. The proportion tensors $W_{(s)\mu\nu}^{\alpha\beta}$ describe how the local metric (basically the shape) of a triangle changes under a general deformation (prescribed by the metric difference $\Delta g_{\mu\nu}$), with respect to the average metric $g_{\mu\nu}$. While mathematically different, we identify the proportion tensors $W_{(s)\mu\nu}^{\alpha\beta}$ with the “non-affine” deformations of each simplex, which are yet unknown. Note that this linear expression does not assume that a situation where $g_{\mu\nu} = \bar{g}_{\mu\nu}$ is indeed achievable (i.e., the system may be residually stressed [30]) and is only dependent on the assumption of small deformation.

The elastic energy E_{el}^{Ω} within a single neighborhood ($E_{el} = \sum_{\Omega} E_{el}^{\Omega}$) then reads

$$E_{el}^{\Omega} = \sum_s (A_{(s)}^{\mu\nu\alpha\beta} + A_{(s)}^{\mu\nu\rho\sigma} W_{(s)\rho\sigma}^{\alpha\beta} + A_{(s)}^{\alpha\beta\rho\sigma} W_{(s)\rho\sigma}^{\mu\nu} + A_{(s)}^{\tau\lambda\rho\sigma} W_{(s)\rho\sigma}^{\alpha\beta} W_{(s)\tau\lambda}^{\mu\nu}) \Delta g_{\mu\nu} \Delta g_{\alpha\beta} + \chi^{\alpha\beta} \sum_s W_{(s)\alpha\beta}^{\mu\nu} \Delta g_{\mu\nu}. \quad (13)$$

The last term of Eq. (13) is a Lagrange term forcing the requirement that $\sum_s \delta g_{\mu\nu}^{(s)} = 0$. We note that as $g_{\mu\nu}$ is an average metric $\sum_s \delta g_{\mu\nu}^{(s)} = 0$. This translates to $\sum_s W_{(s)\mu\nu}^{\alpha\beta} = 0$. Note that this is a simplified requirement, enough to calculate the geometrical response of the system as is used throughout this paper. However, when calculating the energetic (rigidity) response of the system, a different approximation is required or else the exact constraints, see Sec. IID. Given

that in many applications we are interested in the geometric response, we continue with this approximation. For exactness, the complete constraints include the χ term above and the requirement that neighboring “local metrics” agree on the same edge length. In other words, one must add the constraint $l_e[\mathbf{g}^{(i)}] = l_e[\mathbf{g}^{(j)}]$.

We now seek to find the elastic response of the system, that is to find both $g_{\mu\nu}$ and all $W_{(s)\mu\nu}^{\alpha\beta}$. To this end, we take the

functional derivative of the energy with respect to $g_{\mu\nu}$, $W_{(s)\mu\nu}^{\alpha\beta}$, and $\chi^{\alpha\beta}$ and find

$$\begin{aligned} \bar{\nabla}_\mu \sigma^{\mu\nu} + \sigma^{\mu\alpha} (\Gamma_{\mu\alpha}^\nu - \bar{\Gamma}_{\mu\alpha}^\nu) &= f_{\text{ext}}^\nu, \\ (A_{(s)}^{\mu\nu\alpha\beta} + A_{(s)}^{\lambda\tau\alpha\beta} W_{(s)\lambda\tau}^{\mu\nu}) \Delta g_{\mu\nu} + \frac{1}{2} \chi^{\alpha\beta} &= 0. \end{aligned} \quad (14)$$

The first line is actually the elastic equation (2), derived from the variation of the energy [Eq. (13)] with respect to the metric [30], and the second line was obtained through variation of $\{W_{(s)\alpha\beta}^{\mu\nu}\}$. At this point, it is enough to note that the elastic stress tensor $\sigma^{\mu\nu} = \frac{\delta E_{\text{el}}}{\delta g_{\mu\nu}}$, where E_{el} is given by Eq. (13), that $\Gamma_{\beta\gamma}^\alpha$ and $\bar{\Gamma}_{\beta\gamma}^\alpha$ are the Christoffel symbols associated with the metrics $\mathbf{g}$ and $\bar{\mathbf{g}}$, and $\bar{\nabla}_\mu$ is the covariant derivative associated with the metric $\bar{\mathbf{g}}$.

Simplifying further, by summing the second line of Eq. (14) over all triangles, we find that

$$\frac{1}{2} \chi^{\alpha\beta} = -\frac{1}{n} \sum_s (A_{(s)}^{\mu\nu\alpha\beta} + A_{(s)}^{\lambda\tau\alpha\beta} W_{(s)\lambda\tau}^{\mu\nu}) \Delta g_{\mu\nu},$$

where n is the number of simplices in the neighborhood Ω . We can now rewrite the second equation in Eq. (14), by defining the naive elastic tensor $A^{\mu\nu\alpha\beta}$ (describing the “bare” elastic response without the nonaffine displacements), the true elastic tensor $\tilde{A}^{\mu\nu\alpha\beta}$ (describing the actual response when nonaffine displacements are present), and the local deviation from the naive elastic tensor $\delta A_{(s)}^{\mu\nu\alpha\beta}$:

$$A^{\mu\nu\alpha\beta} = \frac{1}{n} \sum_s A_{(s)}^{\mu\nu\alpha\beta}, \quad (15)$$

$$\begin{aligned} \tilde{A}^{\mu\nu\alpha\beta} &= \frac{1}{n} \sum_s (A_{(s)}^{\mu\nu\alpha\beta} + A_{(s)}^{\mu\nu\rho\sigma} W_{(s)\rho\sigma}^{\alpha\beta} + A_{(s)}^{\alpha\beta\rho\sigma} W_{(s)\rho\sigma}^{\mu\nu} \\ &\quad + A_{(s)}^{\tau\lambda\rho\sigma} W_{(s)\rho\sigma}^{\alpha\beta} W_{(s)\tau\lambda}^{\mu\nu}), \end{aligned} \quad (16)$$

$$\delta A_{(s)}^{\mu\nu\alpha\beta} = A_{(s)}^{\mu\nu\alpha\beta} - A^{\mu\nu\alpha\beta}, \quad (17)$$

marking $\langle A_{(s)} W_{(s)} \rangle^{\mu\nu\alpha\beta} = \frac{1}{n} \sum_s A_{(s)}^{\lambda\tau\alpha\beta} W_{(s)\lambda\tau}^{\mu\nu}$, and using $\langle A_{(s)} W_{(s)} \rangle^{\mu\nu\alpha\beta} = \langle \delta A_{(s)} W_{(s)} \rangle^{\mu\nu\alpha\beta}$, we may rewrite the second line of Eq. (14), after a little algebra

$$\delta A_{(s)}^{\mu\nu\alpha\beta} + A_{(s)}^{\lambda\tau\alpha\beta} W_{(s)\lambda\tau}^{\mu\nu} - \langle \delta A_{(s)} W_{(s)} \rangle^{\mu\nu\alpha\beta} = 0. \quad (18)$$

This is a linear equation for the nonaffine deformation terms $\{W_{(s)\lambda\tau}^{\mu\nu}\}$. It is solved by mapping the tensor components and indices into a multi-index notation and using the symmetries of the tensors (in two dimensions $W_{(s)\mu\nu}^{\alpha\beta}$ has only 9 independent entries, while in three dimensions, it has 36):

$$\delta A_S + \sum_{S'} (A_{SS'} - B_{SS'}) W_{S'} = 0, \quad (19)$$

where δA_S , $A_{SS'}$, and $B_{SS'}$ are reorganizations of the elements of $\{A_s^{\mu\nu\alpha\beta}\}$ and $\{\delta A_s^{\mu\nu\alpha\beta}\}$ into matrices compatible with the multi-index (see Appendix A in the Supplemental Material [34]). The solution is given by inversion of the coefficient matrix

$$W_S = - \sum_{S'} [A - B]^{-1}_{SS'} \delta A_{S'}. \quad (20)$$

We may now write the elastic energy

$$E_{\text{el}} = \sum_\Omega n \tilde{A}^{\mu\nu\alpha\beta} (g_{\mu\nu} - \bar{g}_{\mu\nu}) (g_{\alpha\beta} - \bar{g}_{\alpha\beta}). \quad (21)$$

This equation is essentially already coarse-grained

$$\begin{aligned} E_{\text{el}} &= \sum_\Omega n \tilde{A}^{\mu\nu\alpha\beta} (g_{\mu\nu} - \bar{g}_{\mu\nu}) (g_{\alpha\beta} - \bar{g}_{\alpha\beta}) \frac{V_\Omega^\Omega}{V_\Omega} \\ &= \sum_\Omega \rho_\Omega \tilde{A}^{\mu\nu\alpha\beta} (g_{\mu\nu} - \bar{g}_{\mu\nu}) (g_{\alpha\beta} - \bar{g}_{\alpha\beta}) \int_\Omega dV_{\bar{\mathbf{g}}} \\ &= \int \tilde{A}^{\mu\nu\alpha\beta} (g_{\mu\nu} - \bar{g}_{\mu\nu}) (g_{\alpha\beta} - \bar{g}_{\alpha\beta}) dV_{\bar{\mathbf{g}}}, \end{aligned} \quad (22)$$

where V_Ω^Ω is the volume of the neighborhood Ω , $\rho_\Omega = n/V_\Omega^\Omega$ is the local density (which we absorb into the definition of $\tilde{A}^{\mu\nu\alpha\beta}$), $\int_\Omega dV_{\bar{\mathbf{g}}}$ is an integral over the region Ω , and we use the fact that $\sum_\Omega \int_\Omega dV_{\bar{\mathbf{g}}} = \int dV_{\bar{\mathbf{g}}}$ over all the network.

Equations (20) and (22) form the central result of this work. Together with the definitions of $A^{\mu\nu\alpha\beta}$, $\tilde{A}^{\mu\nu\alpha\beta}$, $W_{(s)\lambda\tau}^{\mu\nu}$, they fully describe the response of the network and offer a way of computing it directly from the network geometry, without the need to consider any specific load. Under this view, the metric $\mathbf{g}$ is the actual, coarse-grained metric of the system, $\bar{\mathbf{g}}$ describes the reference geometry of the system, and $\tilde{A}^{\mu\nu\alpha\beta}$ is the coarse-grained elastic tensor, governing the mechanical response (as opposed to the local or “bare” term $A_{(s)}^{\mu\nu\alpha\beta}$). $W_{(s)\alpha\beta}^{\mu\nu}$ describe the nonaffine displacements.

C. Comparison to simulation

Results were validated numerically by comparing the expected Poisson’s ratio and Young’s modulus using the above scheme, to that of simulated two-dimensional (2D) triangulated spring networks. The (possibly orientation dependent) Poisson’s ratio was chosen as a measure for comparison, as this is the quantity describing the complex response of the system. In isotropic materials, there is only one other independent quantity—Young’s modulus. In general, we find a very good agreement between theory and simulation, the details of which are described in Sec. V. We considered three cases—ordered, foamlike, and honeycomb networks.

We simulated ribbons with a 4:1 aspect ratio and a given element geometry. We then minimized their elastic energy after clamping their far ends and stretching them slightly (see Sec. V for exact details). The 4:1 ratio was chosen to eliminate boundary effects that result from the clamping. Energy was minimized using a simple gradient descent algorithm (from the SCIPY Python package) over the position of each vertex. Width measurement was done at the middle of the ribbon as far from both clamped edges as possible.

1. Ordered networks

In the ordered case, we simulated a triangular lattice of varying unit cells’ shapes and computed the angle dependence of Poisson’s ratio. A unit cell’s shape was quantified using two parameters—the shear factor ϕ and elongation factor ψ to describe the deviation from an equilateral triangle (when $\phi = \psi = 1$), see Fig. 3. In this case, all of the nonaffine tensors

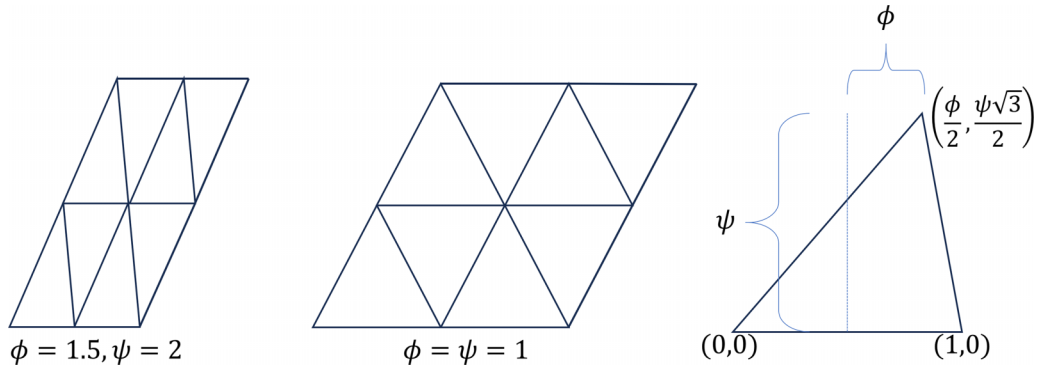


FIG. 3. Quantifying the shape of unit cell, using the shear (ϕ) and elongation (ψ) factors, as described in the right pictures. Coordinates are used to demonstrate how to create the triangle, up to scaling. Left: demonstration of two possible lattices as indicated.

$W_{(s)\mu\nu}^{\alpha\beta} = 0$ identically vanish, leading to a simple calculation using Eq. (10) (detailed analysis is given in Appendix C in the Supplemental Material [34]). In Fig. 4, we see a comparison between the analytical solution and the numerical

estimation. Insets show the lattice structure at an arbitrary orientation chosen as $\theta = 0$. In general, good agreement is seen between theory and simulation. Some systematic errors might be seen near graph minima and maxima. This is especially

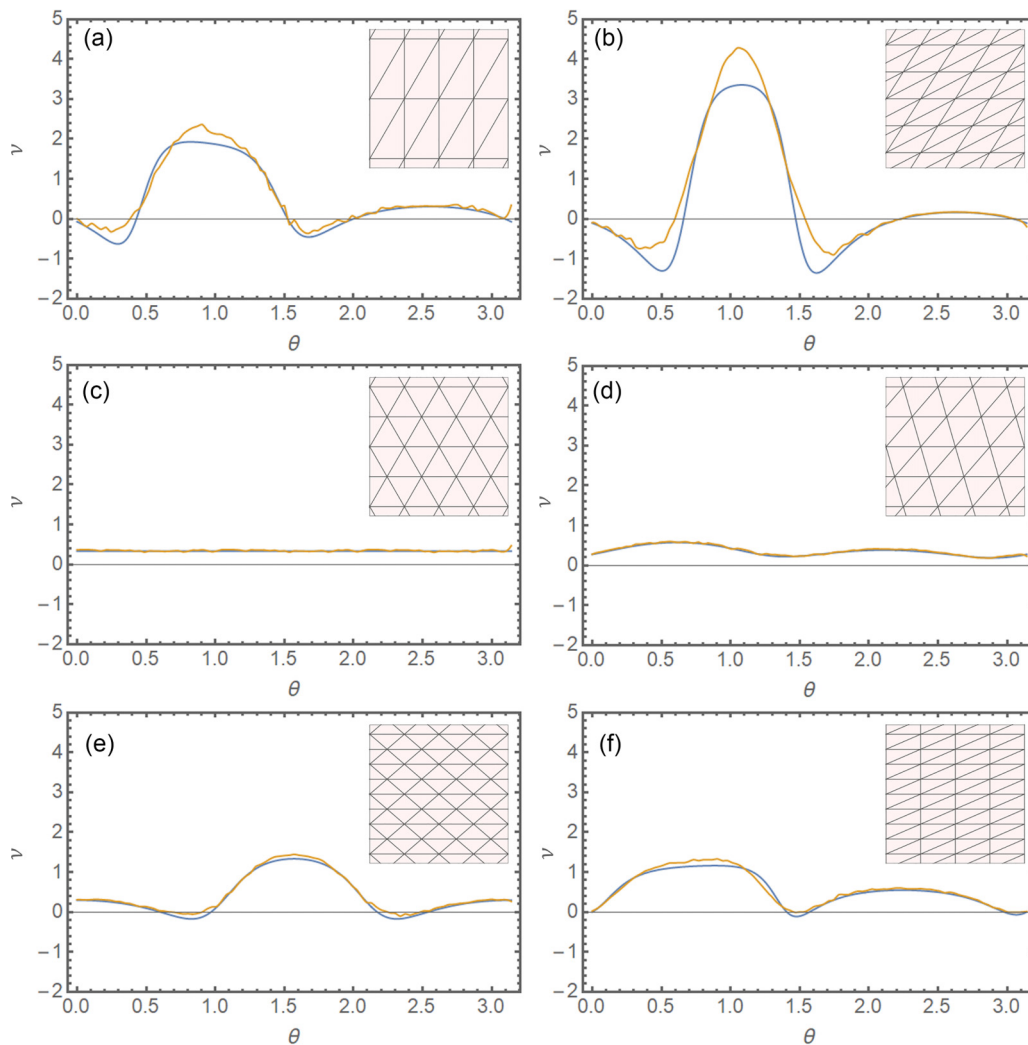


FIG. 4. Ordered networks. Simulation (yellow) vs analytical estimation (blue) of Poisson's ratio as a function of the angle depending on different shape parameters (ϕ, ψ) . (a) $(\phi = 2, \psi = 2)$, (b) $(3, 0.9)$, (c) $(1, 1)$, (d) $(1.5, 1)$, (e) $(1, 0.5)$, and (f) $(2, 0.5)$. Insets—the spring network shape at the initial orientation $\theta = 0$. Other orientations are created by rotating the pattern, while keeping the ribbon orientation fixed.

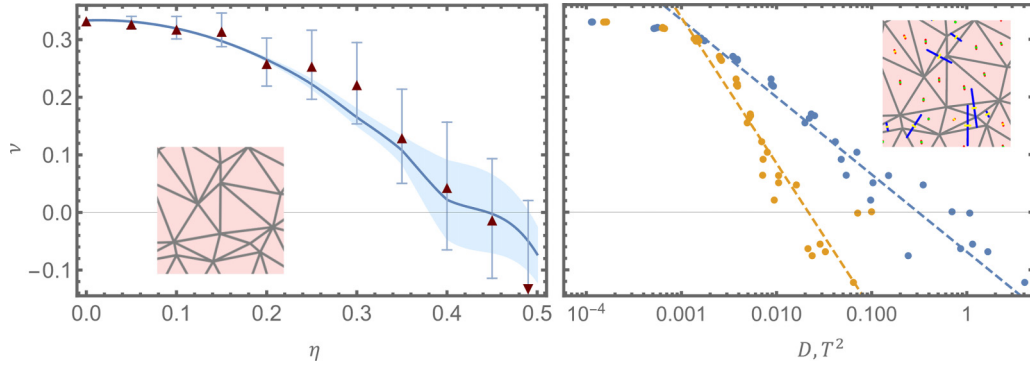


FIG. 5. Random foamlike networks. Left—comparison between theoretical calculation (solid line) and numerical simulation (triangles). Solid line represents the average of seven different realizations of about 150 vertices each (shaded region is typical deviation). Numerical simulations were done over 10 realizations of 676 vertices each, error bars mark the deviations. Note that the last triangle is pointing down, indicating the average is beyond plot boundaries. Inset—an example of a $\eta = 0.3$ realization. Right—relation between Poisson's ratio, to the response averages D (yellow) and T^2 (blue) (see text for description) quantifying the network response. Points are the calculated results for different realizations, dashed lines—trend indicators. Inset—same inset as in left, this time with principal components of $\frac{\delta g_{\mu\nu}}{\epsilon}$. Blue and red—elongation or contraction of the major principal direction (respectively). Yellow and green—out-of-phase or in-phase response of minor principal direction relative to the major direction. Size of lines—relative size of principal response coefficients.

true for subfigure (b). These systematic decreases on higher resolution and are related to finite size effects.

2. Foamlike

Following Ref. [27], we simulate a random, foamlike network, exhibiting auxetic behavior at a certain parameter range. Network is produced by shifting each vertex position of a regular triangular lattice in a random direction by a fixed amount $0 < \eta < 0.5$. Calculation was performed several times to average the results. Our results are consistent with those in [27]— ν decreases as a function of η reaching $\nu = 0$ at $\eta \simeq 0.46$ and reaching $\nu = -0.1$ when $\eta \rightarrow 0.5$. On the left side of Fig. 5, we compare the simulation (discrete triangles) and the semianalytical computation described in this paper (smooth line). All the springs are assumed to have the same spring constant in this case (which was conveniently chosen as 1). As described in Sec. V, simulation was done over a “strip” with about 680 vertices and an aspect ratio of 4:1, mimicking a real experiment (a large aspect ratio is required in order to eliminate boundary effects). On the other hand, the calculation introduced in this paper was performed using a geometrical mean field (see Sec. V and also Appendix B in the Supplemental Material [34]), which naturally eliminated the boundary effects expected in an exact solution. As a direct result of this choice, there was no need of a large network, and a square network with about 150 vertices proved enough. The fact that such very different methods of calculation produce similar results points at the strength of our method.

Additionally, the network response can be computed and visualized. Ideally, we would like to quantify the elements of $W_{(s)}^{\mu\nu\alpha\beta}$ as they are the basic quantities. However, for simplicity, we opted for quantifying the “local metric” response $\delta g_{\mu\nu} = W_{\mu\nu}^{\alpha\beta} \Delta g_{\alpha\beta}$. An example of the visualization may be found in the inset of the right image in Fig. 5 for the case of $\eta = 0.3$. Most notably, it is clear that the change in Poisson's ratio is related to the response of high aspect-ratio triangles that occur randomly via the process described. In these

triangles, one of the edges is exceptionally short. Since all the springs have the same spring constant, this translates to lower local rigidity value, which intuitively means a stronger response. To quantify the total response of a network, we calculated the eigenvalues of the response coefficients $\frac{\delta g_{\mu\nu}}{\epsilon}$ of each triangle, and then averaged the determinant $D = \det \frac{\delta g_{\mu\nu}}{\epsilon}$ and the square of the trace $T^2 = (\text{Tr} \frac{\delta g_{\mu\nu}}{\epsilon})^2$ (as the average of the trace by definition vanishes over the whole network). These are plotted on the right side of Fig. 5.

3. Hexagonal (honeycomb) network

Finally, we consider a honeycomb network, in which the basic hexagonal unit can vary between regular and a re-entrant hexagon continuously with a diameter (distance between two opposing vertices) of $2\bar{\ell}$, where $0 < \bar{\ell} < 1$ (see inset in Fig. 6).

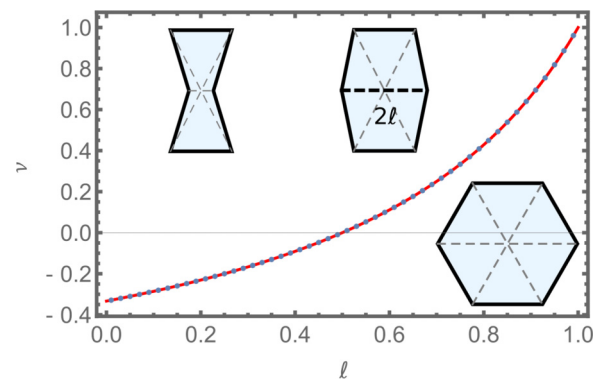


FIG. 6. Hexagonal networks. Theoretical (solid line) and computational (points) results for a honeycomb made of uniform hexagons with diameter $2\bar{\ell}$. To avoid singular expressions, each hexagon was divided into triangles (as indicated by dashed lines). Added edges had negligible but finite rigidity ($k_{\text{dashed}} = 10^{-3}k_{\text{solid}}$), insets (from left to right)—re-entrant hexagon, general hexagon, and regular hexagon.

In such a case, Poisson's ratio is analytically given [35]

$$\nu(\bar{\ell}) = -\frac{(2 - 4\bar{\ell})(\bar{\ell} + 1/2)}{3 + 4\bar{\ell} - 4\bar{\ell}^2}. \quad (23)$$

In order to calculate the elastic response, we use a triangularized hexagon, with a vertex at the center, and set the spring constant of the radial springs connecting the center with each corner of the hexagon to a very small value (1/1000th of the peripheral springs). Without this, the original formulation becomes singular when the spring constant vanishes completely. Results are shown in Fig. 6 with a very high degree of agreement between the analytical result and our formulation, despite the use of a large difference between spring constants, strengthening our approach.

D. Young's modulus

In the previous sections, we used a simplified requirement over the nonaffine deformations $\delta g_{\mu\nu}^{(s)}$. In fact, it is a single constraint for the N simplices. However, the following simple consideration reveals that this constraint is not enough, as it leaves too many degrees of freedom compared to the original problem.

Originally, in d dimensions, we have n_V vertices, each with d degrees of freedom (total of $d \times n_V$ degrees of freedom). In this formulation, we have n_s simplices, each with a local metric of its own, which contains $d(d+1)/2$ independent components. Typically, $\frac{d(d+1)}{2}n_s > dn_V$. We thus require more constraints, which are found in the requirement that the length of an edge must be agreed upon by all adjacent local metrics (in two dimensions, there are only two simplices adjacent to each edge, but in higher dimension, there are more, depending on the coordination number). Additionally, we require that whatever the total volume of the deformed system is, it must be the same regardless of the use of the local metric $g_{\mu\nu}^{(s)}$ or the average $g_{\mu\nu}$. In other words,

$$\begin{aligned} V_{\text{tot}} &= \sum_s \sqrt{\frac{\det g}{\det \bar{g}}} V_s = \sum_s \sqrt{\frac{\det [g + \delta g_{(s)}]}{\det \bar{g}}} V_s \\ &\simeq \sum_s V_s \sqrt{\frac{\det g}{\det \bar{g}}} (1 + \text{Tr}[\bar{g}^{-1} \delta g_{(s)}]) \\ &\simeq \sum_s V_s \sqrt{\frac{\det g}{\det \bar{g}}} (1 + \text{Tr}[\bar{g}^{-1} \delta g_{(s)}]), \end{aligned}$$

where V_s is the original volume of the simplex. This means that we have an additional requirement that

$$\text{Tr}[\bar{g}^{-1} \delta g_{(s)}] = 0$$

to leading order. Using these constraints, while formally more accurate, is rather cumbersome and difficult to implement. However, as shown in this and previous sections, these can be successfully replaced with $\sum_s \delta g_{(s)\mu\nu} = 0$ for the geometrical response, and that for the energy response we require the weighted sum $\sum_s \frac{V_s}{\sqrt{\bar{g}}} \delta g_{(s)\mu\nu} = 0$. The first requirement works for the geometrical response since less-rigid regions contribute significantly to the total response (easier to deform) and are important (at least as evident by analysis in previous

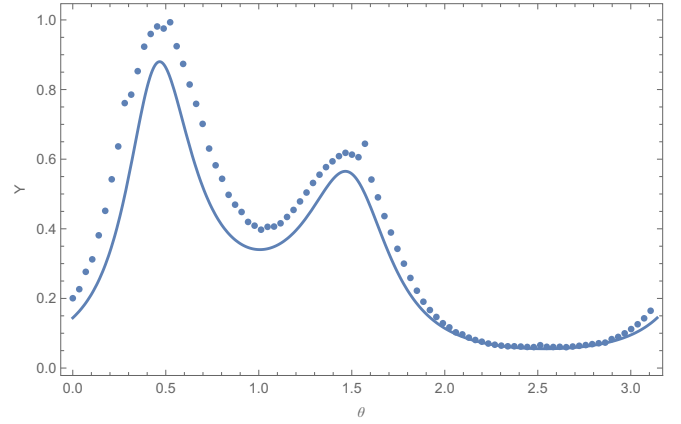


FIG. 7. Angle-dependent Young's modulus as a function of angle for triangular lattice with parameters $\phi = 3$, $\psi = 2$. Simulation results in dots, calculation in a solid line.

sections). However, since we have too many degrees of freedom, we are bound to reach an energy minimum, which is unattainable physically. The second constraint, however, gives a better approximation of the energetic contribution (smaller, softer regions contribute less to the total), at the price of giving those regions insufficient weight and therefore miscalculating the correct geometric response. For practical use, we follow the exact same derivation as in the previous section, replacing the constraint and sums are turned to volume-weighted sums, the expression looks formally the same.

In any case, these considerations are relevant only for the disordered case. For an ordered lattice, the calculation yields an exact result. The results for an ordered case are shown in Fig. 7, and for foamlike in Figs. 8 and 9. Additionally, especially in numerical calculations, rigidity is oftentimes of lesser importance, as it can always be chosen or normalized to whatever value is needed. However, the exact geometric response (i.e., ratios between different components) cannot be normalized and is harder to reproduce.

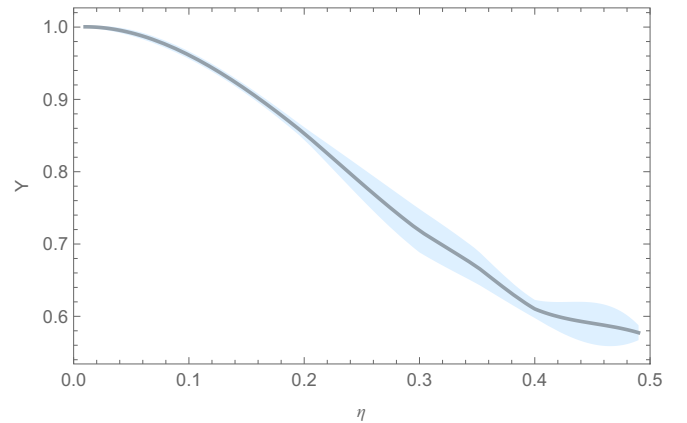


FIG. 8. Young's modulus, correctly weighted. Solid lines are the average values over 10 different realizations for each η , shaded regions indicate the spread of those values.

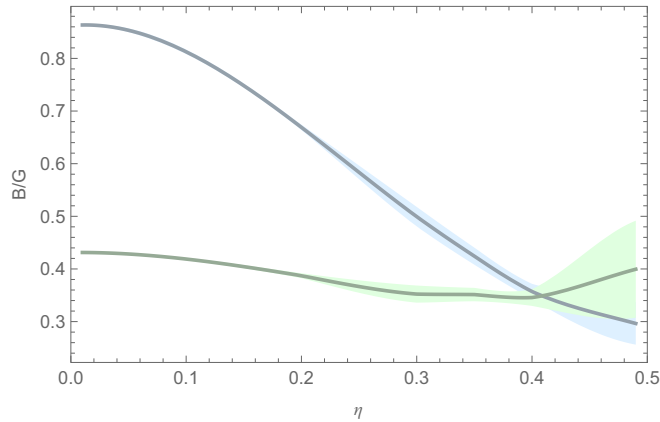


FIG. 9. Bulk modulus (B , blue) and shear modulus (G , green), derived from the corrected Young's modulus, and Poisson's ratio as derived in the text. Correctly recovering results from Ref. [27]. Solid lines are the average values over 10 different realizations for each η , shaded regions indicate the spread of those values.

III. DISCUSSION

Here, we discuss the relevancy of assumptions made and the implications of their breakage on the coarse-graining process and the calculations made here. Additionally, we will exemplify why, under these assumptions, there is no need to consider other nonflat geometries.

A. Assumptions

(1) The first assumption we made is that the reference lengths satisfy the triangle inequality. Mathematically speaking, if this is not satisfied, then the geometry cannot be described by a reference metric, as any metric space must satisfy this inequality. Physically, such a system will be highly frustrated, with residual stresses that are very large relative to the system and typically cannot occur in nature. This is because typical geometry is of system-size scale, rather than element size—e.g., consider the shape of a leaf, the cells are much smaller than its typical curvature. Possibly, certain glassy systems may exhibit a few of such regions, but this remains to be tested. Theoretically, unless this assumption breaks in some small manner, the derivation presented here cannot continue beyond Eq.(6), and a different treatment is required.

(2) The second assumption made is that actual lengths are close to reference lengths. Given that our first assumption is valid, this assumption breaks when deformations are very localized and very large. This is not a typical realistic case (materials tend to break on such scales). Considering a theoretical hyperelastic material, in which this assumption cannot be made, is an interesting problem in and of itself, especially from the mathematical point of view, as it involves averaging nontrivial functions of tensors.

(3) Finally, the last assumption made is essentially the continuum limit. That is—there are many elements within a region enough to *self-average* so that $\bar{g}$ is well defined on the region. If variations of $\bar{g}$ occur on finite regions, then (as often the case is) finite-size effects cannot be neglected. It is known [36] that disordered systems converge only slowly to

this limit, and as such finite-size effects may become important even at relatively large scales (with respect to element size). The treatment of finite-size effects is kept to a later opportunity, and is beyond the scope of this work.

Note that for every point on a continuous medium, we may choose what are known as “normal coordinates” around that point. In these coordinates, the reference metric can be written as

$$\bar{g}_{\mu\nu} = \delta_{\mu\nu} - \frac{1}{3}\bar{R}_{\mu\nu\rho\sigma}x^\rho x^\sigma + \dots, \quad (24)$$

where $\bar{R}_{\mu\nu\rho\sigma}$ is the completely contravariant form of the Riemann curvature tensor of the reference metric and $\delta_{\mu\nu}$ is the flat Euclidean metric (represented as a Kronecker delta). Equation (24) means that the deviation of the metric from Euclidean one is quadratic around this point and heavily depends on the (intrinsic) curvature. In a continuous material, we can always choose a small enough region so that this correction is arbitrarily small. Hence, as long as we work with expressions, which are covariant, it is enough to prove them locally, and general covariance will “take care of the rest.”

In our case, though, we do not deal with a continuum. However, this is exactly the meaning of our last assumption: that elements are small enough and multitude, so that we may still work in a small enough region such that the correction term in Eq. (24) is negligible.

B. Context and relation to past works

In the past, works have been focused on compatible and flat geometries, or close to such (aside from finite discrete points). In that sense, they represent a family of measure zero among all possible elastic models, especially in relation to residually stressed systems. In this aspect, the formulation presented here encompasses a significantly more general result, which can be further generalized to include active stresses (such as in Refs. [14,15]), which will likely couple nontrivially to curvature and residual stresses. One way to study the coupling of active stresses in nontrivial geometry is to derive the three-dimensional (3D) description of active systems, and then dimensionally reduce the 3D model to an effective 2D or even quasi-1D as was done in [30,32,37].

The coarse-graining approach introduced here diverges from standard coarse-graining approaches [9,10,14] or effective medium (EM) approaches [13] in several important ways, despite some similarities. First, the metric approach is inherently nonlinear. Strain in this formulation is not a deformation gradient—it is a metric difference. This allows for treatment of relatively large geometric differences, even when a reference configuration cannot be defined (and therefore a deformation relative to it cannot be defined). In this aspect, the derivation here diverges significantly from Bohr's approach and more standard ways to coarse grain elasticity. Additionally, it is this nonlinearity, which allows treatment of nontrivial and residually stressed geometries, as explained in the discussion of our assumptions.

Second, in contrast to effective medium approaches, here we do not make analogies to ordered media (which is inherently flat and compatible), nor do we limit the calculation to a single mode of deformation. Similarities arise due to similar-looking expansions of nonaffine terms relative to the

affine terms, but unlike EM methods, here, we calculate explicitly, the response of every element in the network, to every possible deformation. It would be very interesting to see how EM approaches might be used to derive completely analytic expressions, but these require some prior knowledge of the distribution of possible nonaffine response, or otherwise, some self-consistent condition.

IV. CONCLUSIONS

In this work we give, to our knowledge, the first analytical derivation of the effective, coarse grained, elastic description of a general spring network. This work generalizes a large body of work in different fields regarding the mechanical response of spring networks [3–12,18,22,38]. It expands this work in its generality, as it encompasses a much wider range of possible reference geometries, which are not necessarily flat and indeed may not be even attainable within the confines of three-dimensional Euclidean space. Such systems are residually stressed (as there is no stress-free rest configuration) and are common in man made and especially biological systems that can grow and move.

Among the important aspects of this paper is the formal derivation of the continuum limit of the formulation of incompatible elasticity, which was derived originally from a phenomenological aspect [30].

Comparison of computational results stemming from this derivation to known/numerical results shows a high degree of agreement. Additionally, we identified and quantified the “nonaffine” deformations, and have shown how they affect the resulting continuum elastic model, and related them to network structure. In systems such as granular media, these quantities play a role in local stress release by means of plastic deformations [36].

While derived over a spring network, the results’ derivation shown is relevant to many fields and systems in two ways. First, the interaction between elements is often approximated as that of a simple spring, especially at small deformations. This is true for mechanical systems such as metamaterials [26–28] and coarse grained mechanical models [25], chemical systems such as self-assemblies [10,19–21], and many biological systems as well [23,24]. As such, the resulting theory, as is, is relevant to engineers, physicists, chemists, and biologists, and opens the possibility of rational design of materials.

Second, the coarse-graining process described here can be generalized to other, more complicated interactions, and is not limited to point masses connected by linear springs. Nonlinearities can be addressed by using higher-order terms (shape-related nonlinearities are already addressed by the use of a metric description). Adding angle-preferring interaction is also a relatively simple generalization that may be relevant even in polygonal networks (see Appendix D, for example). Formulated correctly, it could also apply to complex molecules, cell-cell interactions, and to polymer networks. Activity may be involved in it as well. It would be very interesting to see how the activity [14,15], or nontrivial network topology [13], may couple to geometry, possibly giving rise to additional geometrical terms, resulting in a richer and more complex theory.

Finally, the introduction of the W quantities invites further investigation as to the nature of the solutions of Eq. (20), both analytically (possible through effective medium [13] approaches), and numerically. It is known, for example, that nonaffine deformations become substantially less significant at large scales (though strictly scale independent) [36], this formulation may allow further insight into their scale dependence, and possible interaction with curvature. Other uses would involve intelligent design—relating the required mechanical behavior to the nonaffine deformations, and from that to the network structure.

V. METHODS

We used our assumptions that $\bar{\mathbf{g}}$ is well defined on a large enough region to limit our numerical and analytical solution for the case $\bar{g}_{\mu\nu} = \delta_{\mu\nu}$, since we can always work in a locally flat frame. This condition is sufficient as we want to isolate the effects of the nontrivial structure of the network itself, not the full (nonuniform) mechanical response of a complex, possibly residually stressed structure. We compared the results of three test cases, ordered (nonisotropic), foamlike (following the procedure in Ref. [27]), and a honeycomb, despite the latter being strictly nontriangulated. The latter can be calculated analytically, rather than simulated.

In parallel to simulation, for every network architecture we calculated $\tilde{A}^{\mu\nu\alpha\beta}$ and, using it, we calculated the response to a hypothetical small strain ϵ by setting $g_{yy} = 1 + \epsilon$. Using the elastic Eq. (14), and working in a geometric mean-field approximation, we solved the other terms g_{xx} and g_{xy} , and calculated Poisson’s ratio $\nu = -\frac{g_{xx}-1}{\epsilon}$ (see Appendix B in the Supplemental Material for details [34]).

A. Simulation

The simulation was created for the purpose of this research. In each run, we simulated a strip with length-to-width ratio of 4:1. A total of about $13 \times 13 \times 4 = 676$ vertices, corresponding to about 1000 edges, depending on the exact details of each simulation. Energy minimization was done using a simple gradient descent, implemented as the `SciPy.Optimize.Minimize()` class in Python.

When creating a lattice, vertices were positioned using the base vectors

$$\begin{aligned} v_1 &= (1, 0), \\ v_2 &= \left(\phi \frac{1}{2}, \psi \frac{\sqrt{3}}{2} \right), \end{aligned} \quad (25)$$

where $0 < \phi, \psi$ are the shear and elongation parameters, respectively, and are used to control the shape of the triangles. $\psi = \phi = 1$ corresponds to an equilateral triangle, and any $\phi = 1$ is an isosceles triangle. The strip was created by keeping all vertices whose coordinates satisfy $0 \leq x \leq 13$ and $0 \leq y \leq 52$ (“trimming”). Different orientations lattices were created by rotating the base vectors before trimming, so that the strip orientation remains constant, but the orientation of triangles relative to it changes.

The set of vertices was then used to create the list of edges via triangulation and extracting the list of neighbors. The

energy of each edge was directly calculated from the positions of its vertices, using a simple spring energy. In the simulation, the positions of the top and bottom vertices are held constant, and all other vertices are allowed to move in order to minimize the total energy.

The two vertices initially closest to $x = 0$, $y = 26$ and $x = 13$, $y = 26$ were identified to measure the strain between them $\delta = \frac{\Delta x_{\text{final}}}{\Delta x_{\text{initial}}}$, where Δx_{final} is the final x coordinate difference between the two vertices and $\Delta x_{\text{initial}}$ is the initial difference. After setting the top vertices at $y = 52(1 + \epsilon)$ ($\epsilon = 0.01$), and letting the system relax elastically, Poisson's ratio was calculated via $\nu = -\delta/\epsilon$. And averaged over several simulations, if required (in the more stochastic simulations).

Simulating the foamlike structure is stochastic in essence. We used the same initialization process, with the following differences. After generating a triangular lattice strip with $\phi = \psi = 1$ and triangulation, we changed the position of each vertex by an amount $0 < \eta < 0.5$ in a random direction, and used the resulting distances as the reference lengths of each vertex. We then followed the regular procedure by stretching the strip, and letting the system relax (with the reference lengths calculated just a moment before).

B. Calculation through Eq. (20)

A square patch was generated, independently of the simulation. Generation of the network itself was done similar to the way described in the simulation. However, once that calculated, instead of stretching the network, we calculate $A^{\mu\nu\alpha\beta}$ using the $\{W_{(s)\lambda\tau}^{\mu\nu}\}$, which are calculated using Eq. (20). Poisson's ratio is calculated in the mean field approximation as described in Appendix B in the Supplemental Material [34].

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DATA AVAILABILITY

The simulation code and computation code are available at request.

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