Simple lattice model for biological gels

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We construct a three-dimensional lattice model for biological gels in which straight lines of bonds correspond to filamentous semi-flexible polymers and lattice sites, which are exactly four-fold coordinated, to crosslinks. With only stretching central forces between nearest neighbors, this lattice is sub-isostatic with an extensive number of zero modes; but all of its elastic constants are nonzero, and its elastic response is affine. Removal of bonds with probability $1 - p$ leads to a lattice with average coordination number less than four and a distribution of polymer lengths. When bending forces are added, the diluted lattice exhibits a rigidity threshold at $p = p_b < 1$ and crossover from bending-dominated nonaffine to stretching-dominated affine response between $p_b$ and $p = 1$.

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Biological gels [1–4] are elastic networks, formed by crosslinked semiflexible polymers, that play a critical role in determining and controlling the mechanical properties of eukaryotic cells. Here we introduce and analyze properties of a three-dimensional (3d) lattice model for these gels in which straight sequences of bonds correspond to polymers, and lattice sites, with a maximum coordination number of four, correspond to crosslinks.

Much of our intuition about filamentous networks comes from studies of two-dimensional (2d) Mikado models [5, 6] in which straight lines, representing semi-flexible polymers of length $L$ with stretching modulus $\mu$ and bending modulus $\kappa$, are laid down randomly on a plane and crosslinked at their crossing points. These studies show that there is a crossover from non-affine, bending dominated to affine, stretching dominated response as the number of crosslinks per polymer is increased [5–7]. The kagome lattice [Fig. 1a] with coordination number $z = 4$ is a periodic version of the infinite $L$ limit of the Mikado model, albeit with a monodisperse distribution of lengths between neighboring crosslinks (segment lengths). This lattice with nearest-neighbor springs only and no bending energy exhibits a nonvanishing shear modulus [8] and affine response even though it is just on the verge of mechanical instability: With $z = 2d$ (where $d$ is the spatial dimension) under periodic conditions, it is exactly isostatic [3, 10], but it has a number of zero modes that scales as its perimeter [8]. It provides a rigorous demonstration of the existence of a lattice with an $L \to \infty$ affine limit such as seen in simulations on the random lattice [8, 9]. A network of crosslinked semi-flexible polymers in 3d still has a maximum of only four neighbors per crosslink, and it is subisostatic in the absence of bending forces with a number of zero modes that scales with its volume. It is, therefore, not obvious that the affine, stretching-dominated shear-rigid limit found in 2d can exist in such networks even though models assuming affine response are in good agreement with experimental measurements [11]. Indeed, 3d computer-generated filamentous networks [12, 13] show bending but not stretching-dominated linear response.

By stacking and connecting kagome lattices, we construct a 3d model lattice with exact four-fold coordination that supports shear and compressional stress even in the absence of bending forces. Using analytical theory and numerical simulations, we study the elastic properties of this lattice as a function of the unitless measure $\tilde{\kappa} = \kappa/(\mu a^2)$, where $a$ is a length scale, of the relative strength of bending compared to stretching forces. We demonstrate analytically that our undiluted lattice does exhibit affine, bending-independent elastic moduli of order $\mu/a^2$ with that for pure shear in the $xy$ plane equal to $G_0 = 9\mu/a^2$. We use numerical simulations to study the elastic properties of our lattice when polymers are shortened by cutting bonds with probability $1 - p$. Figure 2 provides a phase diagram summarizing our results. For all $p_b < p_1$ stretching (bending) dominates response at large (small) $\tilde{\kappa}$. Near the rigidity percolation threshold
\[ p_h, G \sim (p - p_h)^f \] with \( f \approx 0.2 \) with amplitude proportional to \( G_0 \) for \( \kappa \gg 1 \) and to \( \kappa/a^4 \) for \( \kappa \ll 1 \). Near the dense limit \( p = 1 \), \( G/G_0 \) is well described by a critical-like scaling function of \( \tau \sim \kappa/(1 - p)^2 \sim \kappa L^2 \), where \( L = a(1 - p)^{-1} \) is the average polymer length, in which \( \frac{\kappa}{a^4} \) is the unit vector directed from site \( \alpha \) to \( \beta \) in the reference lattice. The summations run over all bonds and bond-pairs, respectively. \( \kappa_{\alpha \beta} = 2(1/(|\Delta x_{\alpha \beta}|) + |\Delta x_{\gamma \alpha}|) \) is a segment-length dependent bending constant derived from the worm-like-chain model. In the following, we treat \( \mu \) and \( \kappa \) as independent mechanical parameters; in real systems \( \mu \) is dominated by entropic stretching and is a function of temperature and \( \kappa \).

Under imposed external strain, individual lattice sites undergo displacements \( u_{\alpha,i} = \eta_{ij} x_{\alpha,i} + \delta u_{\alpha,i} \) for \( i = x, y, z \), where \( \eta_{ij} \) is the imposed macroscopic deformation. When the equilibrium value of \( \delta u_{\alpha} \) is zero, each displacement follows the macroscopic strain, and response is affine; when it is nonzero, response is nonaffine. In both the affine and nonaffine cases, the elastic energy \( \mathcal{E} = E/(Na^3) \) per crosslink per volume \( a^3 \) of our model obtains the form appropriate to tetragonal symmetry with 6 independent elastic constants:

\[
\mathcal{E} = \frac{1}{2} C_{xxxx} u_{xx}^2 + \frac{1}{2} C_{yyyy} [u_{yy}^2 + u_{zz}^2] + \frac{1}{2} C_{xxyz} [u_{xy}^2 + u_{xz}^2] + \frac{1}{2} C_{yyzz} u_{yz}^2 + C_{xyy} u_{xy} u_{yz} + C_{yyyy} u_{yy} u_{zz} + C_{yyzz} u_{yy} u_{zz} \tag{3}
\]

where \( u_{ij} = \frac{1}{2}(\eta_{ij} + \eta_{ji}) \) is the usual, linearized symmetric Lagrange strain tensor \[ 16 \] and \( N \) is the number of sites in the lattice.

We consider first the undiluted model with \( \kappa = 0 \). In this case, a straightforward symbolic solution for all \( u_{\alpha} \) in terms of \( \eta_{ij} \) yields \( \delta u_{\alpha} = 0 \) for all \( \alpha \), i.e., response is purely affine. This implies that all filaments remain straight under elastic distortion, and, as a result, the elastic energy is independent of \( \kappa \). Our model thus provides a proof of principal of the existence of 3d central-force, subisostatic lattices with purely affine response. The elastic constants of the undiluted lattice in units of \( \mu/a^2 \) read \( C_{xxxx} = \frac{25}{32}, C_{yyyy} = \frac{49}{32} \), \( G \equiv C_{xxyz} = 9, C_{yzyz} = \frac{31}{2}, C_{xyy} = \frac{3}{2}, \) and \( C_{yyzz} = 9 \).

The polymers forming biological gels have finite length and they are polydisperse. Furthermore, the topology of their networks is that of a random solid rather than of a crystalline solid with a well defined point group symmetry. To study the influence of randomness and network
We focus on the response to shear in the unit cells as a function of configurations with nonvanishing \( p_0 \), indicating that response for physical dense networks can be nearly affine. For all \( \kappa > 0 \), \( \mathcal{G} \) vanishes at a rigidity percolation threshold \( p_0(\kappa) \). For \( \kappa = 0 \), however, \( \mathcal{G} \) vanishes at a much larger threshold \( p_c(S) \). Both \( p_0(\kappa) \) and \( p_c(S) \) decrease as the system-size decreases, with \( S \to \infty \) values of \( p_c \approx 1 \) and \( p_0 \approx 0.602 \), the latter in good agreement with the Maxwell counting arguments of Ref. 13. The fraction \( n \) reaches unity, its upper limit, for \( \kappa > 0 \) at \( p \to 0.6 \), a value that changes little with \( S \). For smaller \( p \), it drops down to zero with steepness that increases with \( S \) and that approaches a unit-step function for \( S \to \infty \). The values of \( n \) between 0 and 1 below \( p \to 0.6 \) are a finite size effect. The corresponding conformations are the ones that lead to nonzero values of \( \mathcal{G} \) in Fig. 3 below \( p \to 0.6 \). For \( \kappa = 0 \), \( n \) approaches a unit-step function at \( p = 1 \) for \( S \to \infty \). The nonaffinity parameter \( \Gamma \), shown in Fig. 3, has a peak at \( p \to 0.6 \) for all \( \kappa \) and vanishes as required for \( p = 1 \); for \( p \) just below 1, however, it increases substantially for small \( \kappa \). The location of the peak changes little with \( S \).

Based on these observations, we expect the following scenario for the infinite-size limit: For \( \kappa = 0 \), \( \mathcal{G} \) displays a discontinuous jump from zero to its affine value at \( p = p_c = 1 \) reminiscent of a first-order phase transition. For all \( \kappa > 0 \), \( \mathcal{G} \) undergoes a rigidity percolation transition at \( p_0 \sim 0.6 \). The behavior for both \( \kappa = 0 \) and \( \kappa > 0 \) is in qualitative agreement with the 2d kagome lattice, where the shear modulus displays a first-order jump at \( p = 1 \) for \( \kappa = 0 \) and a rigidity percolation transition at \( p_0 \sim 0.6 \) for \( \kappa > 0 \) 19. Guided by effective medium theory (EMT) for the 2d kagome lattice 19, we fit \( \mathcal{G} \) near \( p_0 \) to the scaling form

\[
\mathcal{G}(\kappa, p) = g(\kappa)|\Delta p|^{f},
\]

where \( \Delta p = p - p_c \) and \( g(\kappa) = c_1 \kappa/(c_2 + \kappa) \). As shown in Fig. 3 data-collapse is obtained for \( p_0 = 0.602, c_1 = 0.08, c_2 = 0.1 \) and \( f = 0.2 \), but we cannot rule out somewhat different functions \( g(\kappa) \) and values of \( f \) as small as zero, which leaves open the possibility of a weak first-order transition. Interestingly, the exponent \( f = 0.2 \) is not far from the exponent \( \beta = 0.175 \) for the size of the percolating rigid cluster in simulations of the transition to a rigid but unstressed state in models of network glasses 20. Near \( p = 1 \), the kagome EMT suggests the scaling form

\[
\mathcal{G}(\kappa, p) = \tau^{-1} (1 + \sqrt{1 + \tau})^{2},
\]

as long as the scaling variable \( \tau = A\kappa/(1 - p)^2 \) is greater than \( 10^5 \kappa \). With \( A = 0.7 \), this form provides a excellent fit to our data for \( \tau > 10^4 \kappa \) as shown in Fig. 4. The EMT scaling form crosses over from \( \mathcal{G} = \mathcal{G}_0 \) for \( \tau \gg 1 \) to \( \mathcal{G} = \frac{4}{3} \mathcal{G}_0 \tau \sim (\kappa/\kappa_0)^{2}(1 - p)^{-2} \sim (\kappa/\kappa_0) L^2 \) for \( \tau \ll 1 \), and we expect our model network to show the same crossover for \( S \to \infty \), although further simulations with larger system-sizes and smaller values of \( \kappa \) are necessary.
needed to corroborate this conjecture which is consistent with the findings for the 3d phantom lattice [14]. Over all, the EMT predictions for the 2d kagome lattice work remarkably well for our 3d kagome based lattice. The likely explanation is that bending forces are quite effective at restoring rigidity, and in the end, the important thing is that both the 2d and 3d lattices have nonvanishing bulk and shear moduli at \( p = 1 \) and \( \kappa = 0 \) and both exhibit a first-order rigidity transition at \( p = 1 \) when \( \kappa = 0 \).

In our network, all filaments are straight. In real networks of semi-flexible polymers, filaments are in general not straight, and as a result, like the 4-coordinated diamond lattice [21], they may not have nonvanishing shear and bulk moduli [13] when \( \kappa = 0 \) even in the limit \( p = 1 \) (\( L \rightarrow \infty \)). If unit cells in the kagome lattice are twisted through an angle \( \psi \) so that filaments are no longer straight, the lattice no longer resists compression when \( \kappa = 0 \), but it does resist shear [22]. These examples make it clear that network geometry can play a roles as important as coordination number in determining elastic response. Further research on lattices with different bend geometries is clearly of interest. We have begun studying a twisted version of our 3d lattice, and our preliminary results indicate that at \( p = 1 \) and \( \kappa = 0 \) as in the twisted kagome lattice, compression moduli vanish for all \( \psi > 0 \) but contrary to the kagome lattice, shear moduli remain nonzero only up to a small critical value \( \psi_c \) of \( \psi \). Thus for \( \psi > \psi_c \), shear moduli at \( p = 1 \) vanish with \( \kappa \) as they do in the diamond [21] and computer generated network lattices [12, 13].

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