Criticality and isostaticity in fiber networks

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The rigidity of elastic networks depends sensitively on their internal connectivity and the nature of the interactions between constituents. Particles interacting via central forces undergo a zero-temperature rigidity-percolation transition near the isostatic threshold, where the constraints and internal degrees of freedom are equal in number.¹² Fibrous networks, such as those that form the cellular cytoskeleton,¹³ become rigid at a lower threshold due to additional bending constraints. However, the degree to which bending governs network mechanics remains a subject of considerable debate.¹² We study disordered fibrous networks with variable coordination number, both above and below the central-force isostatic point. This point controls a broad crossover from stretching- to bending-dominated elasticity. Strikingly, this crossover exhibits an anomalous power-law dependence of the shear modulus on

\[ G \propto (z_c - \xi)^{-5} \]

equations near isostaticity with relatively stiff filaments (\( \kappa = 10^5 \)) in units of \( \mu \) (a) and floppy filaments (\( \kappa = 10^{-5} \)) (b). The deviation of the local deformation from a uniform deformation is indicated by color, where blue corresponds to a uniform or affine deformation and red corresponds to a highly non-affine deformation. (c) An example of a small section of the diluted FCC network at \( p = 0.7 \). To probe the mechanical properties of this network we shear the 111-plane (shown on top) along the direction of one of the bond angles in this plane.

\[ E_{\text{stretch}} = \frac{1}{2} \mu \sum_{ij} g_{ij} (\hat{u}_{ij} \cdot \hat{r}_{ij})^2 \]

(1)

\[ E_{\text{bend}} = \frac{1}{2} \kappa \sum_{ijk} g_{ijk} [(\hat{u}_{ijk} - \hat{u}_{ij}) \times \hat{r}_{ij}]^2 \]

(2)

where \( \ell_0 \) is the lattice spacing, \( \hat{u}_{ij} = \hat{u}_j - \hat{u}_i \), and \( \hat{r}_{ij} \) is the unit vector oriented along the \( ij \)-th bond in the undeformed reference state. Here, \( g_{ij} = 1 \) for present bonds and \( g_{ij} = 0 \) for removed bonds. The summation extends over neighboring pairs of vertices in the stretching term [Eq. (1)], and over coaxial neighboring bonds in the bending term [Eq. (2)]. Thus, in our networks the cross-links at each vertex are freely hinging.

To investigate the mechanical response of a network, we calculate its shear modulus \( G \) numerically. The diluted networks exhibit a finite shear modulus below the CF isostatic point (expected at \( p_c = 2/3 \) in 2D and \( p_c = 1/2 \) in 3D), as shown in Fig. 2b.\( ^{\text{a,b}} \) \( G \) vanishes at a \( k \)-independent rigidity percolation point located at \( p_b = 0.445 \pm 0.005 \) (2D triangular lattice) and \( p_b = 0.275 \pm 0.005 \) (3D FCC lattice), consistent with a
FIG. 2: Mechanics and non-affine strain fluctuations The shear modulus \( G \) in units of \( \mu /\ell_0^3 \) as a function of \( p \) for a range of filament bending rigidities \( \kappa \) for the 2D triangular lattice (a) and the 3D FCC lattice (b). The EMT calculations for the 2D triangular lattice are shown as solid lines. The non-affinity measure \( \Gamma \) is shown as a function of \( p \) for various values of \( \kappa \) for the 2D triangular lattice (c) and the 3D FCC lattice (d). The values of \( \kappa \) in units of \( \mu \ell_0^3 \) are \( 10^0 \) (green), \( 10^{-3} \) (cyan), \( 10^{-4} \) (red) and \( 10^{-6} \) (blue).

floppy mode counting argument that includes the bending constraints (suppl. info.). Plots of \( G \) versus \( p \) for different \( \kappa \) are shown for the triangular and FCC lattices in Figs. 2a,b. For \( p > p_c \), \( G \) approaches a nearly \( \kappa \)-independent stretching dominated limit with \( G \sim \mu \). In contrast, for \( p < p_c \), \( G \) falls off reaching a bending dominated limit with \( G \sim \kappa \) as \( p \to p_b \). The most interesting behavior occurs near \( p_c \) as a function of \( \kappa \). There is a stretched dominated regime at large \( \kappa \) and bending dominated one at small \( \kappa \) with a broad intermediate crossover regime with \( G \) depending on both \( \kappa \) and \( \mu \).

To gain insight into the mechanical behavior of our models, we developed a new effective medium theory (EMT) or coherent potential approximation (CPA) for lattices with bending forces, which we discuss in more detail in the methods section, whose results for \( G \) for different \( \kappa \) are shown in Fig. 2. These results overestimate the rigidity percolation point \( p_b \). Nonetheless, this model captures the essential features of the simulations well, including the crossover between stretching and bending dominated regimes close to \( p_c \). Our EMT theory predicts that when \( \kappa /\mu \ll \Delta p \), \( G \) can be expressed in the vicinity of \( p_c \) in the scaling form

\[
G = \mu |\Delta p|^f G_f \left( \frac{\kappa}{\mu} |\Delta p|^{-\phi} \right),
\]

where \( f = f_{\text{EMT}} = 1 \) and \( \phi = \phi_{\text{EMT}} = 2 \) are, respectively, the rigidity and crossover critical exponents. This scaling form is analogous to that for the conductivity of a random resistor network with bonds occupied with resistors of conductance \( \sigma_+ \) and \( \sigma_- \) with respective probabilities \( p \) and \( 1-p \). When \( y \ll 1 \), \( G_+(y) \sim \text{const.} \) and \( G_-(y) \sim y \) implying \( G \sim \mu |\Delta p|^f \) for \( \Delta p > 0 \) and \( G \sim \kappa |\Delta p|^{-\phi} \) for \( \Delta p < 0 \). In the opposite limit \( (\kappa /\mu) \gg |\Delta p|^\phi \), \( G \) must become independent of \( \Delta p \) since it is neither zero nor infinite at \( \Delta p = 0 \). Equation (3) predicts \( G \sim \kappa^{1/\phi} \mu^{1-(f/\phi)} \), which reduces of \( G \sim \kappa^{1/\phi} \mu^{1-(f/\phi)} \) in the EMT theory. The full EMT results for \( G \) along with the scaling form valid at \( \kappa /\mu \ll |\Delta p|^\phi \) are shown in Fig. 2.

Our simulation data for both 2D and 3D networks are well described by the scaling hypothesis in Eq. (3), consistent with a second-order transition for \( \kappa = 0 \) in both cases. Fig. 3 shows the results for both the triangular case and FCC cases (inset). As expected from previous simulation work, we find a bending-dominated regime at small \( \kappa \) and a stretching-dominated regime at large \( \kappa \). Consistent with the EMT prediction above, we find a previously unexpected intermediate regime with \( G \sim \kappa^{x} \mu^{-1} \) where \( x = f/\phi \approx 0.50 \pm 0.01 \) (2D) and \( f/\phi \approx 0.40 \pm 0.01 \) (3D). These results are consistent with our exponents obtained above (Table 1, suppl. info.). While the extent of this intermediate regime is bounded from above by the affine modulus, it can extend to arbitrarily small \( \kappa > 0 \) as the system is brought closer to CF.
isostaticity.

To investigate the nature of the various mechanical regimes, we examine the local deformation field in our simulations. Several methods have been proposed to quantify the deviation from a uniform (affine) strain field. Here we utilize a measure for this non-affinity given by

$$\Gamma = \frac{1}{N\gamma^2} \sum_i [u_i - u_i^{(aff)}]^2,$$

where $u_i^{(aff)}$ is the affine displacement of vertex $i$ and $N$ is the number of vertices. This quantity varies over eight orders of magnitude, indicating non-affine fluctuations that depend strongly on both $\kappa$ and $p$, as shown in Figs. 2c,d. For stretch-dominated networks (high $\kappa$), we find a monotonic increase in non-affine fluctuations with decreasing $p$, which appear to diverge at $p_c$. Remarkably, for smaller values of $\kappa$, a second peak in $\Gamma$ develops at $p_c$. Importantly, the development of this peak coincides with the appearance of a crossover between the stretching and bending regimes (Figs. 2c,d).

The critical behavior we observe suggests both a divergence of the non-affine fluctuations according to $\Gamma \sim |\Delta p|^{-\nu}$ and the existence of a divergent length-scale $\xi = \xi_p |\Delta p|^{-\nu}$ near the critical point $P_c$ for vanishing $\kappa$. However, the divergence of $\xi$ is limited by the system size $W$, which should suppress the divergence of $\Gamma$. Consistent with this picture, we find that the location of the cusp in the local fluctuations $\Gamma$ shift towards higher $p$ with increasing $W$ according to $p_c(W) = p_c + 6W^{-1/\nu}$, with $\nu = 1.4 \pm 0.2$ and $p_c = 0.659 \pm 0.002$ (suppl. info.); these values consist with previous reports on generic CF networks. In addition, the amplitude of $\Gamma$ increases with system size (Fig. 3), in quantitative accord with the expected finite-size scaling. Specifically, we find a good collapse of the simulation data with $\Gamma = W^{\lambda/\nu} f(xW^{1/\nu})$ over a range of system sizes, with $\lambda/\nu = 1.6 \pm 0.2$ and $\mu/\nu = 1.4 \pm 0.2$, as shown in Fig. 3. Similarly, the shear modulus exhibits finite-size scaling (Suppl. info.) according to $G = W^{-f/\nu} f_G(xW^{1/\nu})$, as shown in Fig. 3. We obtain a good collapse of the elasticity data using $f/\nu = 0.9 \pm 0.1$, along with $\mu$ determined from the finite-size scaling of $\Gamma$ (Fig. 3) and suppl. info., consistent with the value of $f$ obtained from the scaling in Fig. 3.

Thus, we find a scale-dependence of the shear modulus that is consistent with critical behavior governed by the CF isostatic critical point. Furthermore, the critical behavior in these purely mechanical networks is accompanied by shear-induced divergent non-affine fluctuations. These results imply a breakdown of continuum elasticity below the divergent length-scale $\xi$.

The undiluted triangular and FCC lattices we study have an average coordination number greater than $2d$ and thus are above the Maxwell central-force isostatic threshold. These networks also consist of infinitely long filaments. Cutting bonds as we do introduces both finite length polymers, as well as lower connectivity, down to the CF threshold and below. Cytoskeletal and extracel-
lular networks can have $z$ as low as 3 (e.g., in branched networks) and as high as 6 (in the case of actin-spectrin networks), although they typically have a local connectivity $\gamma \simeq 4$, where two filaments are connected by a cross-link. As a consequence, the CF isostatic point is expected to occur for high molecular weight in 2D. We conjecture that there is an analogous crossover behavior for such networks, including the anomalous scaling behavior for the elasticity. In addition, we expect that our results for the crossover behavior will apply to bond-bending models on similar lattices to ours\cite{24,25,26} for rigidity percolation and network glasses that include bending forces between bonds pairs at each network node. Finally, from the perspective of critical phenomena more generally, the kind of crossover behavior we find here is in contrast to most thermal systems, where a field or coupling constant leads to a crossover from one critical system to another, such as from the Heisenberg model to the Ising model\cite{20}. In such systems, there is a continuous evolution of the critical point that is governed by the crossover exponent $\phi$. Interestingly, we find no such continuous evolution, but rather a discontinuous jump in the critical point $p_c$ as soon as $\kappa$ becomes nonzero.

I. METHODS

Simulations

The mechanical response of the network is determined in our simulations by applying a shear deformation with a strain $\gamma$. This is realized by translating the horizontal boundaries to which the filaments are attached, after which the internal degrees of freedom are relaxed by minimizing the energy using a conjugate gradient algorithm\cite{20}. To reduce edge effects in our simulation, periodic boundary conditions are employed at all boundaries. The shear modulus of the network is related to the elastic energy through $G = \frac{E}{V} = \frac{\gamma^2}{W} \frac{E}{V_{\text{cell}}}$ for a small strain $\gamma$, where $V_0$ is the area/volume of a unit cell. Here $W^d$ is the system size, which in our simulations is $W^2 \approx 40000$ (2D) and $W^3 \approx 30000$ (3D), and we used strains no larger than $\gamma = 0.05$.

EMT

The EMT maps the diluted random network to an undiluted uniform effective medium (EM) with respective stretching modulus $\mu$ and bending rigidity $\kappa$, which are determined self-consistently as follows. In our theory, $\kappa$ is as a property of the filament connecting neighboring sites rather than as a site-associated rigidity that connects next-nearest neighbor sites. Following standard EM procedures, an arbitrary bond is either replaced with probability $p$ by a bond of stretching modulus $\mu$ and bending rigidity $\kappa$ or removed with probability $1 - p$. The phonon Green’s function after this replacement is calculated as a perturbation with respect to the uniform effective medium, treating the replaced bond as a scattering potential $V$ on the EM Hamiltonian. The EMT self-consistency condition requires that the disorder-averaged Green’s function equals that of the unperturbed EM, i.e., that the average $T$-matrix arising from the perturbed bond vanishes, giving us equations determining $\mu_m$ and $\kappa_m$ for given $p$.

In the EMT scattering potential $V$, the stretching term is simply proportional to $\mu - \mu_m$ if the bond is occupied and $-\mu_m$ if it is removed. The bending terms must, however, be treated differently because replacing a bond generates two bending terms, both of which involve second-neighbor interactions. This can be understood by considering 4 sites $ijkl$ along a filament. If one replaces bond $jk$, two bending terms involving second-neighbors $ijk$ and $jkl$ are generated in $V$. The coefficients of these two bending terms can be found by considering a composite filament connecting $ijkl$ that is composed of rods with bending rigidity $\kappa_s$ between sites $jk$ and $\kappa_m$ between

FIG. 4: Finite size scaling (a) The non-affinity measure $\Gamma$ for the 2D triangular lattice at $\kappa = 0$ for various system sizes $W$ (25 blue, 50 green, 100 red, 150 cyan and 200 purple). Finite size scaling of the non-affinity measure $\Gamma$ according to the scaling form $\Gamma = W^\lambda/\nu \mathcal{F}_{\Gamma,\pm}(\Delta p W^{1/\nu})$ (b) and of the shear modulus with the scaling form $G = W^{-1/\nu} \mathcal{F}_G(|\Delta p| W^{1/\nu})$ (c). Here $\Delta p = p - p_c$, where $p_c = 0.659 \pm 0.002$. The exponents we obtain are $\lambda/\nu = 1.6 \pm 0.2$, $\nu = 1.4 \pm 0.2$ and $f/\nu = 0.9 \pm 0.1$. 


sites $ij$ and $jk$, respectively, where $\kappa_s = \kappa$ if the bond is occupied and $\kappa_s = 0$ if it is removed. A direct calculation of the minimum bending energy yields the effective bending rigidity

$$\kappa_c = 2\left(\frac{1}{\kappa_s} + \frac{1}{\kappa_m}\right)^{-1}, \quad (5)$$

and thus the coefficients of the two bending terms involving $ijk$ and $jkl$ in $V$ is given by $\kappa_c - \kappa_m$.

To close the EMT self-consistency equation,

$$p\mathbf{T}(\mu, \kappa) + (1 - p)\mathbf{T}(0, 0) = 0, \quad (6)$$

where $\mathbf{T}$ is the $\mathbf{T}$-matrix constructed from the perturbation of the scattering potential $V$, a third-neighbor coupling $\lambda_m$

$$\frac{1}{2} \lambda_m \sum_{(ijkl)} [(\mathbf{u}_{jk} - \mathbf{u}_{ij}) \times \hat{\mathbf{r}}_{ij}] [(\mathbf{u}_{kl} - \mathbf{u}_{jk}) \times \hat{\mathbf{r}}_{kl}] \quad (7)$$

must be introduced to the EM and to $V$ accordingly. Thus the EM is characterized by 3 parameters ($\mu_m$, $\kappa_m$, $\lambda_m$), determined by the self-consistency equation [(9)]. We obtained asymptotic solutions to the this equation for small $\kappa$ in the vicinity of the CF isostatic point, in which $\mu_m$ can be written into a scaling form same as that of Eq. (8) by identifying that the shear modulus $G = \sqrt{3}\mu_m/4$, and the scaling function is

$$\hat{G}(\mu) \sim \frac{3}{2} \left(1 + \sqrt{1 + 4\hat{A}\mu/9}\right) \quad (8)$$

with $\hat{A} \simeq 2.413$.

For $\kappa/\mu \ll |\Delta p|^{\phi_{EMT}}$, to leading order, the value for $\mu_m$ reduces to $3\mu |\Delta p|$ for $|\Delta p| > 0$, and $|\Delta p|^{\phi_{EMT}}$ for $|\Delta p| < 0$. For $\kappa/\mu \gg |\Delta p|^{\phi_{EMT}}$ we get $\mu_m \simeq \sqrt{A}\mu^{1/2}\kappa^{1/2}$. These three scaling regimes correspond to three different slopes 0, 1, 1/2 in the $G|\Delta p|^{-f}$ vs $\kappa|\Delta p|^{-\phi}$ plot, as shown in Fig. 5.

Effective medium theories for bond-diluted lattices with central-force springs are straightforward because the springs reside on an individual bond. In contrast, EMTs for lattices with bending forces are less so because bending forces reside on two bonds and dilution removes only a single bond at a time. Our solution is to treat a given bond as a filament segment with bending modulus $\kappa_s$. The effective lattice bending modulus for neighboring bonds with respective bending moduli $\kappa_s$ and $\kappa_m$ is given by Eq. (5). This treatment allows us to unambiguously remove one bond at a time. The resultant effective theory necessarily includes bend-stretch coupling. A previous EMT theory treated the bending problem by removing two bonds at a time. The result was a theory that lacks bend-stretch coupling and predicted separate thresholds for the development of non-vanishing $\mu_m$ and $\kappa_m$, which is inconsistent with both the numerical and analytical EMT results presented here.

FIG. 5: Phase diagram The phase diagram for diluted super-isostatic networks. Above the rigidity percolation point $z_0$ there are three distinct mechanical regimes: a stretching dominated regime with $G \sim \mu$, a bending dominated regime with $G \sim \kappa$ and a regime in which bend and stretch modes couple with $G \sim \mu^{1-\nu} \kappa^\nu$. Here $x$ is related to the critical exponents $f = f/\phi$. We find here that $x = 0.50 \pm 0.01$ (2D triangular lattice) and $x = 0.40 \pm 0.01$ (3D FCC). The mechanical regimes are controlled by the isostatic point $z_i$, which acts as a zero-temperature critical point.

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CPB and FCM designed the simulation model, which was developed and executed by CPB, XM and TCL developed and executed the EMT. All authors contributed to the writing of the paper.

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