Mechanics and dynamics of biopolymer networks
Broedersz, C.P.

2011

document version
Publisher's PDF, also known as Version of record

Link to publication in VU Research Portal

citation for published version (APA)

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

• Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
• You may not further distribute the material or use it for any profit-making activity or commercial gain
• You may freely distribute the URL identifying the publication in the public portal

Take down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

E-mail address: vuresearchportal.ub@vu.nl
Criticality and isostaticity in fiber networks

- C. P. Broedersz, X. Mao, T. C. Lubensky and F. C. MacKintosh
  *Criticality and isostaticity in fiber networks*,
  arXiv:1011.6535 (Submitted)

- C. P. Broedersz, M. Sheinman and F. C. MacKintosh
  *Elasticity of diluted super-isostatic lattices of stiff filaments in 2D and 3D*,
  (To be submitted)
CHAPTER 6. CRITICALITY AND ISOSTATICITY IN FIBER NETWORKS

Abstract

It has been known since Maxwell that collections of particles interacting via central forces only become rigid above the isostatic threshold, where the constraints and internal degrees of freedom just balance [1,2]. However, such networks can be stabilized below this threshold by additional interactions [3–5]. Here we elucidate the relative roles of bending versus central force interactions in stabilizing fibrous networks [6–16]. We study disordered networks with variable connectivity that exhibit both bending rigidity and central-force thresholds. Although the former determines the true onset of rigidity, the latter controls a cross-over between various mechanical regimes exhibiting rich critical behavior, including an anomalous power-law dependence of the shear modulus on both stretching and bending rigidities, as well as a breakdown of mean field theory. At the central force isostatic point, we also find divergent strain fluctuations together with a divergent correlation length $\xi$, implying a violation of continuum elasticity in this simple mechanical system. These results may apply to systems ranging from bond-bending network glasses [2,17–19] to the cellular cytoskeleton [21,22].

6.1 Introduction

Soft materials, such as foams and granular packings attain mechanical rigidity when the connectivity exceeds the isostatic point. This isostatic point is captured by a classical argument introduced by Maxwell [1], which balances the degrees of freedom in the system against the number of constraints due to connectivity. Interestingly, stiff fiber network form a distinct class of systems that exhibit solid-like behavior at connectivities well below the isostatic point. There are numerous examples of stiff-fiber networks, ranging from carbon nanotube gels at the small scale to felt and paper at the macroscopic scale [23–25]. In addition, critical biological components such as the intra-cellular cytoskeleton and extra-cellular matrices of collagen and fibrin are composed of such networks [26]. Biological systems largely employ network architectures with a coordination number $z \leq 4$, which is far below the central force (CF) isostatic point in 3D. The mechanical stability of such networks depends in large part on the considerable bending rigidity of the constituting filaments. Intriguingly, however, the elastic moduli of these systems can be either bend or stretch dominated. Both numerical and analytical approaches have demonstrated the existence
of these distinct elastic regimes for such stiff polymer networks [6–8, 12, 13, 16, 27]. In addition, experimental studies on reconstituted cross-linked actin networks provide evidence for the existence of both stretching dominated and bending dominated elastic regimes [9, 14, 15, 28]. However, the physical principles governing these elastic regimes remain poorly understood. In particular, the role of connectivity in the mechanics of semiflexible polymer networks is not known [4, 5].

Here we study the elasticity of disordered fiber networks composed of straight, stiff filaments organized on a triangular lattice in 2D and on a face centered cubic (FCC) lattice in 3D, as illustrated in Fig. 6.1. Undiluted, these networks have a coordination number \( z_m = 6 \) (triangular lattice) and \( z_m = 12 \) (FCC), placing them well above the CF isostatic point \( z_c = 2d \) in \( d \) dimensions [1]. There are physiological networks with such high connectivities, e.g. approximately 6-fold coordinated networks confined to 2D in the red blood cell [30], although most biological networks...
have lower connectivities. An important advantage of lattice based networks is their applications in various analytical effective medium approaches, which we will here compare to our numerical results [4,17,27,31–35]. We explore the effects of network connectivity—both above and below $z_c$—by removing filament segments between vertices with a probability $q = 1 - p$. In addition to lowering the connectivity, this also has the effect of introducing disorder in the networks. In the range of network connectivity spanning from the rigidity percolation point to the CF isostatic point, the average filament length remains approximately constant. Thus, in these networks we expect the network connectivity to be the major control parameter.

Our main results are summarized in a phase diagram shown in Fig. 6.2. This diagram maps the mechanical response of the diluted superisostatic networks in terms of two key variables: the connectivity $z$ and the ratio of the bending rigidity $\kappa$ and the stretching modulus $\mu$ of the fibers. An important difference with most prior work on subisostatic off-lattice networks [6–8] is that we here characterize the system in terms of connectivity [5] instead of filament length or line density. Consistent with these prior studies we identify two distinct elastic regimes: A stretching governed regime and a bending governed regime. In addition however, we find an intermediate broad cross-over regime in which the shear modulus scales simultaneously with $\kappa$ and $\mu$, $G \sim \kappa^{f/\phi} \mu^{1-f/\phi}$ where $f/\phi \approx 0.50 \pm 0.01$ (2D) and $0.40 \pm 0.01$ (3D). This regime extends over a remarkably broad range of $z$ and $\kappa/\mu$. Such a regime—characterized by a strong coupling between stretch and bend modes—has not been observed in prior theoretical work on fiber networks. This cross-over regime is a direct consequence of the critical behavior close to the CF isostatic point and similar regimes appear in random resistor network [3] with good and bad conductors and mechanical models for a spring network with strong and weak springs [4,5].

In the bending dominated regime, we find that $G \sim \kappa |z - z_c|^{f-\phi}$ close to the CF isostatic point, where $f = 1.4 \pm 0.1$ (2D), $f = 1.6 \pm 0.2$ (3D) and and $\phi = 3 \pm 0.2$ (2D), $\phi = 3.6 \pm 0.3$ (3D). Above the CF isostatic point, the number of constraints on the lattice vertices provided by the stretching forces are sufficient to mechanically constrain the system. As a result, the system is necessarily dominated by stretching modes at superisostatic coordinations. This does not mean, however, that the bending rigidity does not play a role. For vanishing $\kappa/\mu$, we find that the mechanical response above the isostatic point becomes $G \sim \mu |z - z_c|^{f}$ close to the CF isostatic point. In contrast, in the limit of large $\kappa/\mu$ the shear modulus is approximately $G \sim \mu z$.

The stretching governed regime extends all the way down to the rigidity percolation point for large values of $\kappa/\mu$. This finding is in contrast with previous studies on off-lattice subisostatic networks that have reported that, upon dilution, the stretching governed regime crosses-over to a non-affine bending regime before losing rigidity [6,7]. It is important to note that, although the mechanics is governed by stretching modes in this regime, the shear modulus drops substantially below the
affine shear modulus, indicating that the deformation field contains a significant non-affine component.

The CF isostatic point plays a central role in determining the cross-over from the stretching dominated regime to the bending dominated regime \[3–5, 31\]. In the limit of vanishing \(\kappa/\mu\), the isostatic point is a true critical point. Indeed, we find for low \(\kappa/\mu\) that the fluctuations, in the form of non-affine deformations, become large around the isostatic point, reminiscent of a second order phase transition \[31\]. The finite bending rigidity, however, suppresses this divergence. From the perspective of critical phenomena, the bending rigidity may be thought of as an applied field or coupling constant that leads to a crossover from one critical system to another, such as from the Heisenberg model to the Ising model \[36\]. In such systems, there is a continuous evolution of the critical point. Interestingly, we find no such continuous evolution, but rather a discontinuous jump in the critical point as soon as \(\kappa\) becomes nonzero.

We show that we can express the mechanical response around the cross-over between the stretching and the bending regimes in terms of a scaling function, which allows us to collapse all the data on to a universal curve that exhibits distinct branches above and below the critical point. This provides further evidence that the physics of the isostatic point controls the cross-over from the stretching to the bending regime. These results are qualitatively consistent with the results of an effective medium theory (EMT) using the coherent potential approximation (CPA) by Mao and Lubensky \[31, 33\]. Importantly, however, the exponents governing the transition at the CF isostatic we obtain numerically differ significantly from the EMT predictions, indicating a breakdown of meanfield theory. By contrast, there is evidence that such a breakdown of meanfield theory does not occur in spring networks in jammed configurations \[5\].

### 6.2 Model

The networks consist of stiff filaments organized on a triangular lattice in 2D and an FCC lattice in 3D. In both cases, a perfect lattice consists of straight filaments spanning the system. At each lattice vertex, a cross-link is formed between all intersecting filaments. Thus, this results in cross-links between 3 (triangular) or 6 filaments (FCC). These cross-links hinge freely and do not introduce additional rigidity. To reduce network connectivity, we randomly remove filament segments between vertices with a probability \(q = 1 - p\). This procedure allows us to generate disordered lattice-based networks with a connectivity \(z \approx 6p\) in 2D and \(z \approx 12p\) in 3D. Cutting bonds also reduces the length of the polymer; the average filament length is given by \(\langle L \rangle = \ell_0/q\) \[31\].
Above the rigidity percolation point $z_b$ 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 $G \sim \mu^{1-x} \kappa^x$. Here $x$ is related to the critical exponents $x = f/\phi$. 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 $z_c$, which acts as a zero-temperature critical point.

**Figure 6.2** – (Color online) **Phase diagram** The phase diagram for diluted super-isostatic networks. Above the rigidity percolation point $z_b$ 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 $G \sim \mu^{1-x} \kappa^x$. Here $x$ is related to the critical exponents $x = f/\phi$. 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 $z_c$, which acts as a zero-temperature critical point.
6.2. MODEL

Semiflexible polymers are well described by the wormlike chain model. At finite temperature \( T \), bending fluctuations are excited; such fluctuations generate small undulations in the polymer that are characterized by the persistence length \( \ell_p = \kappa/k_B T \). This length scale represents the decay length in tangent vector correlations along the polymer backbone. These thermal bending undulations contract the polymer longitudinally, and result in an entropic or thermal modulus \( \mu_{th} = 90\ell_p^2k_B T/\ell^3 \) for a polymer segment of length \( \ell \) \[37\]. In addition, the polymer exhibits an enthalpic or mechanical stretch modulus \( \mu_{mech} \). For simple elastic cylinders, this stretch modulus is related to \( \kappa \) through the radius \( r \), by \( \mu_{mech} = 4\kappa/r^2 \). Biopolymers typically have a large aspect ratio, in which \( r \) is much smaller than the other length-scales \( \ell_c \) and \( \ell_p \). Thus, it is usually the case that \( \mu_{th} \ll \mu_{mech} \), and the entropic stretch mode dominates the response to a longitudinal force, even when the network scale \( \ell_0 \) is small compared to the persistence length \[7\].

Here we aim to capture the zero-frequency behavior of semiflexible polymer networks. On such timescales the polymer bending dynamics does not play a role. This allows us to integrate out these degrees of freedom. The resulting coarse grained Hamiltonian describes a discretized extensible worm like chain,

\[
\mathcal{H} = \frac{\kappa}{2\ell_0} \sum_i |\Delta \mathbf{t}_i|^2 + \frac{\mu}{2\ell_0} \sum_i \Delta \ell_i^2
\]  

(6.1)

where \( \Delta \mathbf{t}_i \) is the change in the tangent vector between nodes \( i \) and \( i-1 \), and \( \Delta \ell_i \) represents the change in length with respect to the restlength \( \ell_0 \) between nodes \( i \) and \( i-1 \). The mechanical and thermal moduli add as springs in series and the full longitudinal compliance is given by \( \mu^{-1} = \mu_{mech}^{-1} + \mu_{th}^{-1} \). With this, we have reduced the approach to a purely mechanical model in which the stretch modulus \( \mu \) captures the entropic compliance. This model also captures the athermal limit in which the fibers can be considered to be simple elastic beams for which \( \mu = \mu_{mech} \).

The relative importance of the bending and the stretching term in Eq. 6.1 is captured by the length scale \( \ell_b = \sqrt{\kappa/\mu} \), which forms one of the key control parameters for the network mechanics. For simple mechanical beams of radius \( r \), \( \ell_b = r/2 \), while for a thermally excited semiflexible polymer of length \( \ell \), \( \ell_b = \ell/\sqrt{90\ell_p} \) \[7\]. For our networks, the characteristic polymer length is \( \ell_0 \), and the most relevant values of \( \ell_b/\ell_0 \) for biopolymer systems are in the range \( 10^{-2} - 10^{-1} \), corresponding to systems ranging from actin filaments to the more flexible intermediate filaments; in systems where actin forms tightly coupled stiff bundles even lower values of \( \ell_b/\ell_0 \) may be reached. It is, however, instructive to explore limits of the model outside this range.

The mechanical response of the fibers in the network is determined by their bending rigidity \( \kappa \) and stretching modulus \( \mu \). For small deformations, the stretching and bending energy of the network can be expanded to quadratic order in the displace-
CHAPTER 6. CRITICALITY AND ISOSTATICITY IN FIBER NETWORKS

ments $u_i$ from the undeformed reference state at each vertex $i$,

\begin{align}
E_{\text{stretch}} &= \frac{1}{2} \mu \sum_{(ij)} g_{ij} (u_{ij} \cdot \hat{r}_{ij})^2 \tag{6.2} \\
E_{\text{bend}} &= \frac{1}{2} \kappa \sum_{(ijk)} g_{ij} g_{jk} \left[ (u_{jk} - u_{ij}) \times \hat{r}_{ij} \right]^2, \tag{6.3}
\end{align}

where $\ell_0$ is the lattice spacing, $u_{ij} = u_j - u_i$ 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. (6.2)], and over coaxial neighboring bonds in the bending term [Eq. (6.3)]. Thus, unlike bond-bending [20] and network glass models [2, 17–19], here the crosslinks at each vertex are freely hinged. In contrast to our model, network glasses and most prior models for stiff-fiber networks [6, 8, 11, 12] have maximum coordination number 4. In this paper, all lengths are expressed in units of the lattice spacing $\ell_0$, and all energies and moduli are measured in units of $\mu/\ell_0$. Thus, the bending rigidity $\kappa$ is given in units of $\mu\ell_0^2$.

The mechanical response of the network is determined numerically 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 [38]. 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 $G = \frac{2}{V_0 W^2} \frac{E}{\gamma^2}$ for a small strain $\gamma$, where $V_0$ is the area/volume of a unitcell. 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 use strains no larger than $\gamma = 0.05$.

We probe mechanical the properties of diluted fiber networks on an FCC lattice by applying a shear on the 111-plane along one of the bond directions in the plane. An example of a small portion of the network is shown in Fig. 6.1. From this viewing angle the 111-plane lies on top. At $p = 1$, the cubic symmetry of the lattice allows us to express the mechanical response in terms of three components $C_{11}$, $C_{12}$ and $C_{44}$. With a shear of the 111-plane we probe a combination of these components $G_{111} = (4C_{11} - 4C_{12} + C_{44})/12$.

6.3 Results

6.3.1 Elastic response

An example of a small portion of a diluted triangular lattice, to which a shear deformation is applied, is shown in Fig. 6.1. When the bending rigidity is high ($\kappa = 10$) the
Figure 6.3 – (Color online) Mechanics and non-affine strain fluctuations in a triangular lattice a) The shear modulus \( G \) in units of \( \mu/\ell_0 \) as a function of \( p \) for a range of filament bending rigidities \( \kappa \) for the 2D triangular lattice The EMT calculations for the 2D triangular lattice are shown as solid lines for various values of \( \kappa \). b) The non-affinity measure \( \Gamma \) is shown as a function of \( p \) for various values of \( \kappa \) for the 2D triangular lattice.
Figure 6.4 – (Color online) Mechanics and non-affine strain fluctuations in an FCC lattice a) The shear modulus $G_{111}$ in units of $\mu/\ell_0$ as a function of $p$ for a range of filament bending rigidities $\kappa$ for the 3D FCC lattice. b) The non-affinity measure $\Gamma$ is shown as a function of $p$ for various values of $\kappa$ for the 3D FCC lattice.
6.3. RESULTS

Figure 6.5 – (Color online) Various elastic regimes in lattice-based fiber networks
The shear modulus $G$ scaled by $\kappa$ as a function of $\kappa$ for various values of $p$ for (a) the triangular lattice ($p = 0.5$ blue circles, 0.65 green squares, 0.8 red triangles) and (b) the FCC lattice ($p = 0.35$ blue circles, 0.47 green squares, 0.65 red triangles). The horizontal line indicates a bending dominated regime ($G \sim \kappa$) and a line with a slope of -1 indicates a stretching dominated regime ($G \sim \mu$).

deformation field is uniform or affine (Fig. 6.1a). In contrast, for low bending rigidity ($\kappa = 10^{-5}$), the deformation field is highly non-affine (Fig. 6.1b). This non-affine deformation field is clearly sensitive to the local disorder in the network; regions with a locally high connectivity appear to behave much more affinely in comparison with regions with a low connectivity. The deformation of the rigid network is clearly dominated by filament stretching. In comparison, large bending deformations are evident in the sheared floppy network.

To investigate the mechanical response of a network, we calculate its shear modulus $G$ numerically. Plots of $G$ versus $p$ for different $\kappa$ are shown for the triangular and FCC lattices in Figs. 6.3a and 6.4a, respectively. The diluted networks exhibit a finite shear modulus well below the CF isostatic point (expected at $p_c = 2/3$ in 2D and $p_c = 1/2$ in 3D); $G$ vanishes at a $\kappa$-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 floppy mode counting argument that includes the bending constraints [31,33] (See section 6.5). For $p > p_c$, $G$ approaches a nearly $\kappa$-independent stretching dominated limit with $G \sim \mu$. In contrast, between the rigidity percolation threshold and the isostatic point ($p_b < p < p_c$), we identify distinct stretching and bending dominated regimes. At high $\kappa$ the shear modulus converges to a $\kappa$-independent curve, indicating that the stretching regime extends down to $p_b$ for large
bending rigidities. However, when the bending rigidity is reduced, the shear modulus adopts a strong $\kappa$ dependence, indicating a bending governed regime. In this bending regime, the shear modulus scales directly with the bending rigidity $G_{\text{bend}} \sim \kappa$. To resolve the bending regime we plot the shear modulus scaled by $\kappa$ as a function of $\kappa$ for various values of $p$, as shown in Fig. 6.5. The bending dominated regions appear in this plot as horizontal lines, while a pure stretch region appears as a line with a slope of $-1$. The most interesting behavior occurs near $p_c$ as a function of $\kappa$; close to the critical point the shear modulus scales as $G \sim \kappa^x$ with $x < 1$, suggesting a broad crossover regime with $G$ depending simultaneously on both $\kappa$ and $\mu$.

To gain further insight into the mechanical behavior of our models, we compare our results with a new effective medium theory (EMT) or coherent potential approximation (CPA) \cite{27, 35, 39} for lattices with bending forces developed by Mao and Lubensky \cite{31, 32}, whose results for $G$ for different $\kappa$ are shown in Fig. 6.3a. These results overestimate the rigidity percolation point $p_b$. Although the EMT overestimates the rigidity percolation point $p_b$, it does capture the essential features of the mechanical behavior, including the existence of separate bending and CF rigidity thresholds and the crossover between stretching and bending dominated regimes close to $p_c$.

To investigate the role of the CF isostatic point in the cross-over between stretching and bending regimes we perform a scaling analysis. We motivate this analysis by drawing an analogy with second order phase transitions in thermal systems. In this analogy the shear modulus may be thought of as the order parameter in the system, which vanishes continuously as the system undergoes a critical phase transition at the CF isostatic point in the limit $\kappa \to 0$. Thus, in this zero-$\kappa$ limit we expect a behavior $G \sim \mu|\Delta p|^f$ in the vicinity of the CF isostatic point, where $\Delta p = p - p_c$ and $f$ is the rigidity exponent. However, when bending interactions are included, rigidity is restored below the CF isostatic point. Thus $\kappa$ may be thought of as an effective applied field or a coupling parameter that brings the system away from criticality, resulting in a cross-over to a different elastic regime governed by bending interactions. To capture this cross-over we can express the shear modulus in terms of $\frac{\kappa}{\mu} |\Delta p|^{-\phi}$ when $\kappa/\mu \ll \Delta p$, where $\phi$ is the cross-over exponent. Taken together, these arguments suggest the following scaling ansatz,

$$G = \mu|\Delta p|^f \mathcal{G}_\pm \left( \frac{\kappa}{\mu} |\Delta p|^{-\phi} \right),$$

(6.4)

where $\mathcal{G}_\pm$ is a universal function where the two branches apply above and below the transition. When the argument of $\mathcal{G}_\pm(y)$, $y \ll 1$, $\mathcal{G}_+(y) \sim \text{const.}$ and $\mathcal{G}_-(y) \sim y$ such that $G \sim \mu|\Delta p|^f$ for $\Delta p > 0$ and $G \sim \kappa|\Delta p|^{f-\phi}$ 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 (6.4) predicts $G \sim \kappa^{f/\phi} \mu^{1-(f/\phi)}$. The scaling form in Eq. 6.4 is analogous to that for the conductivity of a random resistor network \cite{3} with bonds occupied with resistors of conductance $\sigma_>$ and $\sigma_<$ with respective probabilities $p$ and
Figure 6.6 – Scaling analysis of the mechanics in the triangular lattice. Scaling of the shear modulus in the vicinity of the isostatic point with the scaling form $G|\Delta p|^{-f} = \mathcal{G}_\pm (\kappa|\Delta p|^{-\phi})$, with $G$ in units of $\mu/\ell_0$, for the mechanical properties of the diluted triangular lattice for the EMT calculations (a) and the simulations (b) for a broad range of filament bending rigidities ($\kappa$ in units of $\mu\ell_0^2$: $10^{-1}$ black, $10^{-2}$ magenta, $10^{-3}$ cyan, $10^{-4}$ red, $10^{-5}$ purple and $10^{-6}$ blue). The asymptotic form of the scaling function for low $\kappa$ is shown as a dashed grey line in (a). The EMT exponents are $f_{\text{EMT}} = 1$, $\phi_{\text{EMT}} = 2$. In contrast, for the numerical data we obtain $f = 1.4 \pm 0.1$, $\phi = 3.0 \pm 0.2$ (2D). The scaling for the numerical data is performed with respect to the isostatic point of the finite system for which we find $p_c(W) \approx 0.651$ (2D, $W=200$).
Scaling analysis of the mechanics in the FCC lattice

Scaling of the shear modulus in the vicinity of the isostatic point with the scaling form \(G|\Delta p|^{-f} = \mathcal{G}_\pm(\kappa|\Delta p|^{-\phi})\), with \(G\) in units of \(\mu/\ell_0\), for the mechanical properties of the FCC lattice for a broad range of filament bending rigidities (\(\kappa\) in units of \(\mu\ell_0^2\): \(10^{-1}\) black, \(10^{-2}\) magenta, \(10^{-3}\) cyan, \(10^{-4}\) red, \(10^{-5}\) purple and \(10^{-6}\) blue). we obtain the exponents \(f = 1.6 \pm 0.2\) and \(\phi = 3.6 \pm 0.3\) (3D). The scaling for the numerical data is performed with respect to the isostatic point of the finite system for which we find \(p_c(W) \approx 0.473\) (3D, \(W=30\)).

Figure 6.7 – (Color online) Scaling analysis of the mechanics in the FCC lattice

Scaling of the shear modulus in the vicinity of the isostatic point with the scaling form \(G|\Delta p|^{-f} = \mathcal{G}_\pm(\kappa|\Delta p|^{-\phi})\), with \(G\) in units of \(\mu/\ell_0\), for the mechanical properties of the FCC lattice for a broad range of filament bending rigidities (\(\kappa\) in units of \(\mu\ell_0^2\): \(10^{-1}\) black, \(10^{-2}\) magenta, \(10^{-3}\) cyan, \(10^{-4}\) red, \(10^{-5}\) purple and \(10^{-6}\) blue). we obtain the exponents \(f = 1.6 \pm 0.2\) and \(\phi = 3.6 \pm 0.3\) (3D). The scaling for the numerical data is performed with respect to the isostatic point of the finite system for which we find \(p_c(W) \approx 0.473\) (3D, \(W=30\)).
Table 6.1 – Critical exponents

<table>
<thead>
<tr>
<th>exponent</th>
<th>2D sim</th>
<th>2D EMT</th>
<th>3D sim</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f$</td>
<td>$1.4 \pm 0.1$</td>
<td>1</td>
<td>$1.6 \pm 0.2$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>$3.0 \pm 0.2$</td>
<td>2</td>
<td>$3.6 \pm 0.3$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>$1.4 \pm 0.2$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda$</td>
<td>$2.2 \pm 0.4$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(1 − $p$), as well as random spring networks with floppy and stiff springs [4, 5]. This scaling form is also predicted by the EMT theory when $\kappa/\mu \ll \Delta p$, with

$$G_{\pm}(y) \simeq \frac{3}{2} \left( \pm 1 + \sqrt{1 + 4\mathcal{A}y/9} \right)$$

(6.5)

where $\mathcal{A} \simeq 2.413$, $f_{\text{EMT}} = 1$ and $\phi_{\text{EMT}} = 2$. Interestingly, these MF exponents are identical to those found in central-force networks with two types of springs [4, 5], which have been used to describe [5] bending models such as ours.

The full EMT results for $G$ along with the scaling form valid at $\kappa/\mu \ll |\Delta p|^{\phi}$ are shown in Fig. 6.6a. Our simulation data for both 2D (Fig. 6.6b) and 3D networks (Fig. 6.7) are well described by the scaling hypothesis in Eq. (6.4), consistent with a second-order transition for $\kappa = 0$ in both cases [41]. Remarkably, however, the obtained numerical exponents ($f = 1.4\pm0.1$, $\phi = 3.0\pm0.2$) are significantly different from the EMT predictions, suggesting a breakdown of meanfield theory close to the CF isostatic point, in distinct contrast with the meanfield exponents observed for the jamming transition [5]. Importantly, we find that the bending stiffness $\kappa$ is a relevant perturbation at $p_c$, which is reflected as a broad crossover regime with an anomalous scaling $G \sim \kappa^{x} \mu^{1-x}$ with $x = f/\phi$ (Fig. 6.8 where $x = 0.50 \pm 0.01$ (2D), consistent with the EMT prediction above, and $x = 0.40 \pm 0.01$ (3D). However, the precise nature of the interaction, such as the three-body bending interaction in our case, is expected to be irrelevant at $p_c$. Furthermore, our results for $f$ are consistent with previous work on diluted periodic [40] and generic [41] lattices when $\kappa = 0$.

6.3.2 Non-affine deformations

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 [6,28,42]. Here we utilize a measure
Figure 6.8 – (Color online) **Anomalous elasticity** The shear modulus as a function of \( \kappa \) close to the isostatic point for the triangular lattice \((p = 0.643, \text{blue circles})\) and the FCC lattice \((p = 0.47, \text{red squares})\). At low \( \kappa \) there is a bending dominated regime \( G_{\text{bend}} \sim \kappa \), at intermediate \( \kappa \) there is a regime in which stretching and bending modes couple strongly with \( G \sim \mu^{1-x} \kappa^x \), where \( x = 0.50 \pm 0.01 \) (2D) and \( x \approx 0.40 \pm 0.01 \) (3D). The EMT calculation for \( \kappa/\mu \gg |\Delta p|^{\phi_{\text{EMT}}} \) is shown as a solid blue line.
for the non-affinity given by

\[ \Gamma = \frac{1}{N \gamma^2} \sum_i \left[ u_i - u_i^{(aff)} \right]^2, \] (6.6)

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. 6.3b and 6.4b. For stretch-dominated networks (high \( \kappa \)), we find a monotonic increase in non-affine fluctuations with decreasing \( p \), which appear to diverge at \( p_b \). In addition, for smaller values of \( \kappa \), a second peak in \( \Gamma \) develops at \( p_c \). The amplitude of the non-affine fluctuations at \( p_c \) scales with \( \kappa \) as \( \Gamma_{\max} \sim \kappa^{\beta} \), with \( \beta \approx 0.5 \), as shown in Fig. 6.9. The development of the peak in \( \Gamma \) around \( p_c \) coincides with the appearance of a crossover between the stretching and bending regimes (Figs. 6.3 and 6.4).

### 6.3.3 Finite size scaling

The critical phenomena we observe in the mechanical behavior suggests a divergence of the non-affine fluctuations according to \( \Gamma = \Gamma_{\pm} |\Delta p|^{-\lambda} \), in a manner similar to that of spring networks in a jammed configuration [5], but with a non mean-field exponent. Moreover, we anticipate an associated divergent length-scale \( \xi = \xi_{\pm} |\Delta p|^{-\nu} \) 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
CHAPTER 6. CRITICALITY AND ISOSTATICITY IN FIBER NETWORKS

Figure 6.10 – (Color online) Finite size scaling of the CF isostatic point The finite size dependence of the central force isostatic point $p_c$. We performed a least square fit of the expected dependence $p_c(W) = p_c + bW^{-1/\nu}$, to the $p_c$ determined from our simulations for a range of system sizes $W$. From this we obtain $p_c = 0.659 \pm 0.002$, $\nu = 1.4 \pm 0.2$ and $b = -0.3 \pm 0.1$.

In addition, the amplitude of $\Gamma$ increases with system size (Fig. 6.11a), in quan-
6.3. RESULTS

titative accord with the expected finite-size scaling. Specifically, we find a good
collapse of the simulation data with \( \Gamma = W^{\lambda/\nu} \mathcal{F}_{R,\pm}(|\Delta p|W^{1/\nu}) \) over a range of
system sizes, with \( \lambda/\nu = 1.6 \pm 0.2 \) and \( \nu = 1.4 \pm 0.2 \), as shown in Fig. 6.11b. Similarly,
the shear modulus exhibits finite-size scaling (Fig. 6.12a) according to
\( G = W^{-f/\nu} \mathcal{F}_{G,\pm}(|\Delta p|W^{1/\nu}) \), as shown in Fig. 6.12b. We obtain a good collapse
of the elasticity data using \( f/\nu = 0.9 \pm 0.1 \), along with \( \nu \) determined from the finite-
size scaling of \( \Gamma \) (Fig. 6.11 and Fig. 6.10), consistent with the value of
\( f \) obtained from the scaling in Fig. 6.6. In addition to a divergent \( \Gamma \) and \( \xi \) at \( p_c \), we also find sim-
ilar critical behavior at \( p_b \), with \( \lambda = 1.8 \), \( \nu = 1.3 \), and rigidity exponent \( f = 3.2 \) for
small \( \kappa \). (This places our fiber model, along with Mikado models [6,8] in a different
universality class than bond-bending models, where \( f = 3.97 \) [20]). Thus, at both
central-force and bending thresholds, we find critical behavior that is accompanied
by divergent non-affine fluctuations and a scale-dependent shear modulus, implying
a breakdown of continuum elasticity below the divergent length-scale \( \xi \).

Finally, from the finite size scaling of the non-affine fluctuations at \( \kappa = 0 \) (Fig. 6.11)
and the scaling of the elasticity data (Fig. 6.6), we can now predict the \( \kappa \)-dependence
of \( \Gamma_{\text{max}} \), which is shown in Fig. 6.9. Close to the CF isostatic point we expect a scaling behavior,

\[
\Gamma \sim W^{\lambda/\nu} (|\Delta p|W^{1/\nu})^{x'} \left( \frac{\kappa}{\mu|\Delta p|^{-\phi}} \right)^{y'}.
\]  

(6.8)

From this, we can determine the unknown exponents \( x' \) and \( y' \), by requiring that
the \( W \) and \( \Delta p \) dependences cancel out. This leads to the prediction \( \Gamma_{\text{max}} \sim \kappa^{-(\lambda/\phi)} \),
similarly, \( \xi \sim \kappa^{-(\nu/\phi)} \) at finite \( \kappa \) as \( \Delta p \to 0 \). Based on the exponents determined above
(Table 1) we expect \( \lambda/\phi = 0.7 \pm 0.2 \), consistent with the observed scaling behavior
\( \lambda/\phi \approx 0.5 \) for \( \Gamma_{\text{max}} \) in Fig. 6.9.

The simple one-point non-affinity measure we use here quantifies the average
local deviation from the global shear profile. If we assume that the non-affine defor-
mations associated to bending deformations in the filaments follow the same scaling
dependence as \( \Gamma \) for \( \kappa \to 0 \), we expect a scaling for the shear modulus in the bending
regime \( < p_c \) of the form \( G \sim \kappa \Gamma \sim \kappa |\Delta p|^{-\lambda} \) [5], implying \( \lambda/\phi = 1 - f/\phi \). The most
accurate and direct determinations of the ratios \( \lambda/\phi \) and \( f/\phi \) for the 2D triangular
lattice are obtained from Figs. 6.9 and 6.8, \( \lambda/\phi \approx 0.5 \) and \( f/\phi \approx 0.5 \), consistent
with the prediction of the scaling argument that relate these two ratios. This scaling
argument also predicts the cross-over regime with anomalous elasticity. In this regime
\( \Gamma \sim \kappa^{-\lambda/\nu} \) and, thus \( G \sim \kappa \Gamma \sim \kappa^{1-\lambda/\phi} \) consistent with our earlier results.
CHAPTER 6. CRITICALITY AND ISOSTATICITY IN FIBER NETWORKS

Figure 6.11 – Finite size scaling of the non-affine fluctuations (a) The non-affinity measure $\Gamma$ for the 2D triangular lattice at $\kappa = 0$ for various systems sizes $W$ (25 blue, 50 green, 100 red, 150 cyan and 200 purple). (b) Finite size scaling of the non-affinity measure $\Gamma$ according to the scaling form $\Gamma = W^{\lambda/\nu} F_{\Gamma,\pm}(\Delta p W^{1/\nu})$. The exponents we obtain are $\lambda/\nu = 1.6 \pm 0.2$, $\nu = 1.4 \pm 0.2$.

Figure 6.12 – Finite size scaling of the elasticity (a) The shear modulus $G$ in units of $\mu/l_0$ as a function of $|\Delta p|$ of a 2D triangular network at $\kappa = 0$ for various systems sizes $W$ (25 blue, 50 green, 100 red, 150 cyan and 200 purple). Finite size scaling of the shear modulus with the scaling form $G = W^{-f/\nu} F_{G,\pm}(|\Delta p| W^{1/\nu})$. Here $\Delta p = p - p_c$, where $p_c = 0.659 \pm 0.002$. The exponents we obtain are $\nu = 1.4 \pm 0.2$ and $f/\nu = 0.9 \pm 0.1$. 
6.4 Discussion and implications

In this chapter we studied the cross-over between bending and stretching behavior in lattice-based fiber networks. This cross-over is governed by the CF isostatic point, analogous to the behavior in multicomponent random resistor or spring networks [3–5], and bond bending networks [2,17–19]. Interestingly, the critical behavior of weak-spring stabilized isostatic jammed packings is consistent with mean field predictions, while we observe a clear breakdown of mean field theory. It is interesting to compare the lattice based networks studied here with off-lattice random networks, also referred to as the mikado model. Prior studies [6–8] on that model have also identified both a stretching and a bending governed regime, consistent with our results. However, in the mikado model the cross-over between the two regimes has been argued to be governed by the filament length compared to a non-affinity length scale [6,7]. This is in contrast with our results on superisostatic lattices. The range of \( p \) values between the rigidity percolation threshold and the isostatic point only result in a roughly 2-fold change in filament length. Therefore, we attribute the behavior we observe mostly to a change in the local coordination number.

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. As a result, the networks in our model exhibit two thresholds at \( p_c \) and \( p_b \), in contrast to, e.g. the Mikado model in 2D [6,8,12] and network glass models [18] with only the bending rigidity threshold. Cytoskeletal and extracellular 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 \( z \approx 4 \), 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 [2,17–19] for rigidity percolation and network glasses that include bending forces between bond pairs at each network node.

Interestingly, 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 [36]. 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.
6.5 Appendix: Counting argument for rigidity threshold

The bend isostatic point $p_b$ of lattice-based fibrous networks can be calculated using Maxwell counting and mean-field arguments. Isostatic conditions imply that the total number of the network constrains due to both stretching and bending are equal to the total number of degrees of freedom. In $d$ dimension, the total number of the network degrees of freedom is equal to $dN_c$, where $N_c$ is the number of network crosslinks. The number of the network constrains due to the stretching modulus of network filaments is $N_b p$, where $N_b$ is the number of bonds in the undiluted network ($p = 1$). In addition, the bending rigidity contributes $d - 1$ constraints at any pair of present neighboring coaxial bonds. The total number of such bonds is $N_b^2$.

Thus, the rigidity percolation transition occurs when

$$dN_c = N_b \left( p + (d - 1) p^2 \right)$$

or

$$p_b = \frac{\sqrt{1 + \frac{4dN_c}{N_b} (d - 1) - 1}}{2(d - 1)}.$$

We now compute the rigidity percolation point for various cases. For the triangular and FCC networks we obtain values that are in reasonable agreement with our numerical results.

**Triangular lattice**

$$d = 2$$

$$\frac{N_c}{N_b} = \frac{1}{3}$$

$$p_b = \frac{\sqrt{\frac{11}{3}} - 1}{2} \approx 0.4574$$

**Kagome and square lattices**

$$d = 2$$

$$\frac{N_c}{N_b} = \frac{1}{2}$$

$$p_b = \frac{\sqrt{5} - 1}{2} \approx 0.618$$

142
FCC lattice

\[
d = 3
\]
\[
\frac{N_c}{N_b} = \frac{1}{6}
\]
\[
p_b = \frac{\sqrt{5} - 1}{4} \approx 0.309
\]

6.6 Acknowledgments

This work was performed in collaboration with X. Mao, T.C. Lubensky and M. Sheinman. X.M. and T.C.L. developed and executed the EMT and M.S. developed the counting argument. We thank M. Das and L. Jawerth for useful discussions.
Bibliography


[33] X. Mao and T. C. Lubensky (to be published).


