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Elasticity of randomly diluted central force networks under tension

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We study the rigidity of two-dimensional site-diluted central force triangular networks under tension. We calculate the shear modulus μ directly and fit it with a power law of the form $\mu \sim (p-p^*)^f$, where p is the concentration of sites, p^* its critical value, and f the critical exponent. We find that the critical behavior of μ is quite sensitive to tension. As the tension is increased there is at first a sharp drop in the values of both p^* and f, followed by a slower decrease towards the values of the diluted Gaussian spring network (or random resistor network). We find that the size of the critical region is also sensitive to tension. The tension-free system has a narrower critical regime with the power law failing for $p>0.8$. In contrast, a small tension is sufficient to extend the power law to near $p=1$. The physical basis for these behaviors is discussed.

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There has been considerable interest in the rigidity of random systems over the last few decades [1–21]. It has become clear that at zero temperature, the rigidity percolation of a tension-free diluted central force network has a different critical point from that of conductivity percolation, contrary to what de Gennes had suggested [1–10]. On the other hand, recent investigations [12,13,19] showed that at finite temperature the entropic component to the shear modulus of a central force system does follow de Gennes' conjecture. It sets in at the percolation point and has the same critical behavior as the macroscopic conductance σ of a randomly diluted network of resistors. The entropic component has its origin in the temperature driven entropic force whose effect on a network is similar to that of a finite stress. It is therefore natural to think that an elastic network under tension may have a different critical behavior from the tension-free one. In the limit of networks with zero equilibrium length springs [which are usually referred to as diluted Gaussian spring networks (DGSN's)] the nonvanishing stress-strain stiffnesses (or elastic stiffness coefficients) have exactly the same critical behavior as the conductance of the random resistor network [4,17,18]. This has been shown by Tang and Thorpe [4], and recently more rigorously by Zhou *et al.* [17] and Farago and Kantor [18]. It is therefore clear that the critical behavior of μ must be dependent on the tension. Tang and Thorpe examined the elasticity of random networks under tension [5] and showed how the critical point varied from the tension-free value to the DGSN limit, which is the infinite stress limit, but the behavior of the critical exponent is not yet clear. In this paper we present a systematic study of the elasticity of two-dimensional stressed random diluted networks near the onset of rigidity. This will help us to understand networks in real situations, where stresses are often present in materials either as applied or internal.

Here is a summary of our findings. The critical behavior of the shear modulus which characterizes the rigidity, $\mu \sim (p-p^*)^f$, is sensitive to tension; p^* is the critical value of the concentration p, and f the critical exponent. A small tension leads to a fairly large drop of p^* and f, followed by a slow decrease down to the DGSN values with increasing tension. This suggests that in practice the zero tension regime might be hard to access. Moreover, the stress itself has a different critical behavior than the shear modulus. We also find that the range of the critical regime, i.e., the regime where the power law is valid, is also sensitive to tension. The tension-free system is very special and has a narrower critical regime. A small tension extends the critical regime to $p=1$.

The system we studied consists of particles tethered to each other through the potential energy

$$\Phi(r_{ij}) = \frac{1}{2}\kappa[|\mathbf{r}_i - \mathbf{r}_j| - r_0]^2, \tag{1}$$

where, in the undiluted case with $p=1$, the vertices i, j label nearest neighbor sites on a triangular lattice with an equilibrium spacing of r_0 and where more distant neighbors are noninteracting. We begin with an undiluted triangular lattice of lattice constant d and randomly remove $(1-p)N$ sites, where N is the total number of sites in the undiluted lattice. Following Ref. [5], we refer to larger d's as higher tension cases, although for every d the stress also varies with p. The geometric or the conductance percolation of the system occurs at $p_c=0.5$. The DGSN with $p^*=p_c=0.5$ and $f=1.322$ [17,22] is the limiting case of $d/r_0=\infty$ or $r_0=0$.

To obtain μ, we first equilibrated the system with a molecular dynamics simulation at constant volume and constant

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temperature $T=0.005\kappa r_0^2/k_B$ to keep the system from falling into a metastable state. We then carried out a static relaxation. During the relaxation, each particle was displaced through a distance proportional to the force until the maximum force fell below a critical value of $F_c=10^{-7}\kappa r_0$. We have also tried $F_c=10^{-9}\kappa r_0$ and found that the two choices of F_c make no difference. We imposed a pure shear deformation $L_x d\rightarrow(1+\epsilon)Ld$, $L_y d\rightarrow L_y d/(1+\epsilon)$ on the computational box, where L_x and L_y are numbers of sites in the x and y directions, respectively. The geometry of our cells is such that $L_y d=(\sqrt{3}/2)L_x d=(\sqrt{3}/2)Ld$. For isotropic materials, the stress S and the shear modulus are given by

$$S_{\alpha\beta}=\frac{1}{A}\sum_{i<j} r_\alpha(ij)r_\beta(ij)\frac{\Phi'}{r_{ij}},$$

$$\mu=\frac{S_{xx}(\epsilon)-S_{yy}(\epsilon)}{4\epsilon}, \tag{2}$$

where A is the area of the system, and $r_\alpha(ij)=r_{i\alpha}-r_{j\alpha}$. In practice, we have taken $\epsilon=\pm 0.001$ for each sample and averaged the results over both calculations to eliminate the frozen initial stress caused by finite size effects. Periodic boundary conditions were used throughout to provide the tension. The bulk of these calculations were carried out for pL^2 particles with L ranging from 16 to 144. For a given p, the fluctuations from sample to sample are very substantial and it is necessary to average over a large number of different samples to obtain well-converged results, especially in the critical region. For the smallest samples ($L=16$), close to p^*, over 300 realizations were used. For lattices of dimension $L=144$, 15–30 samples are enough. The exact results for S, μ, and energy E for an isotropic undiluted lattice are given by [23]

$$S_0=\sqrt{3}\left(1-\frac{r_0}{d}\right)\kappa, \quad \mu_0=\frac{\sqrt{3}}{4}\left(4-3\frac{r_0}{d}\right)\kappa,$$

$$E_0=\frac{3}{2}(d-r_0)^2\kappa. \tag{3}$$

In Figs. 1, 3, and 4, normalized quantities are given, that is, we plot μ/μ_0, S/S_0, and E/E_0.

The results of the normalized shear modulus as a function of p for diluted lattices of size $L=16$, 32, 64, 96, and 144 at an initial lattice constant $d=1.0r_0$ are displayed in Fig. 1. We performed a least-square fit to find the $p^*(L)$ and $f(L)$ for each size L. We then plotted the $p^*(L)$ and $f(L)$ vs $1/L$ and found that they fall on a straight line, especially the $p^*(L)$, so we made a linear extrapolation to $1/L=0$ to find p^* and f. We should mention that $p^*(144)$ and $f(144)$ are already very close to the asymptotic values p^* and f for all d's, so we use $|p^*-p^*(144)|$ and $|f-f(144)|$ as error bars.

In this way, we find p^*, and f for the systems with $d=r_0$, $1.05r_0$, $1.3r_0$, $1.5r_0$, and $3.0r_0$. The results are listed in Table I and displayed in Fig. 2. As expected, at large d we obtain values very close to that of the DGSN. From Fig. 2 and Table I we find that both p^* and f decrease smoothly to

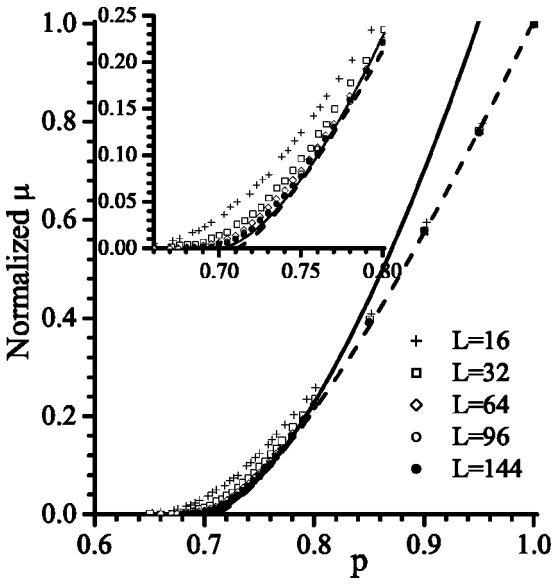

FIG. 1. The normalized shear modulus μ/μ_0 plotted as a function of concentration p of particles for lattices of size $L=16$, 32, 64, 96, and 144 at $d=1.0r_0$. The lines represent the $L\rightarrow\infty$ distributions. The solid line is a plot of $(p-0.7000)^{1.619}$ (a fit till $p=0.8$). The dashed line is a plot of $(p-0.7101)^{1.327}$(a fit for all p values). The inset is a blowup of the region near the critical density p^*.

$p_c=0.5$ with increasing d. However, the critical behavior is quite sensitive to tension. For the tension-free system, with $d=1.0r_0$, we find that $p^*=0.7000$ and $f=1.62$. But at $d=1.05r_0$, p^* and f have dropped to $p^*=0.6009$ and $f=1.52$. With increasing tension there is a slower decrease of p^* and f, towards the DSGN values.

Moreover, our results also show that the range of the critical regime is sensitive to tension. For the tension-free system, if we fit μ up to $p=1$, we obtain $p^*=0.7101$ and $f=1.326$. The p^* so obtained is very close to results of earlier work which solved the force equations directly and reported a $p^*=p_r=0.713$ [3,6]. However, if we fit up to $p=0.8$ only, we obtain $p^*=0.7000$ and $f=1.62$, a value very close to that obtained by counting rigid modes for the same system up to $L=1024$ [7,8], $p^*=p_r=0.697\,55$, and $f\approx 1.68$. From Fig. 1, we see that $(p-0.7000)^{1.62}$ provides a very good fit in the critical regime but is poor for $p>0.8$ (for $p=0.715$, $\mu(L\rightarrow\infty)=0.010\,96$, to be compared with $\mu=9.5^*(p$

TABLE I. Critical concentrations and critical exponents for different d.

d/r_0	p^*	f
1.0	0.7000 ± 0.0006	1.62 ± 0.01
1.05	0.6009 ± 0.0006	1.52 ± 0.015
1.1	0.5703 ± 0.005	1.50 ± 0.02
1.3	0.5296 ± 0.0016	1.45 ± 0.010
1.5	0.5185 ± 0.002	1.43 ± 0.02
3.0	0.5031 ± 0.003	1.37 ± 0.02
∞	0.5	1.322

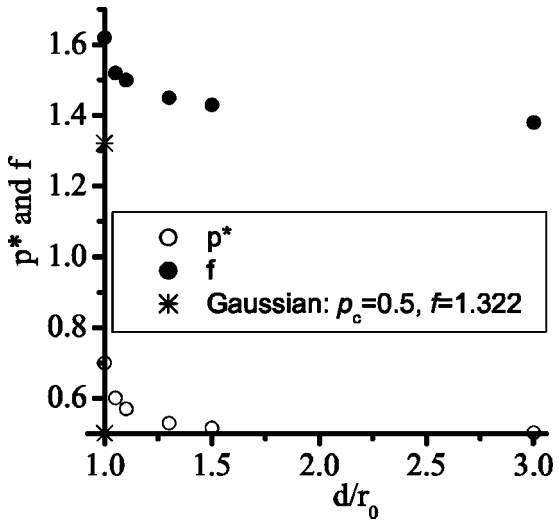

FIG. 2. The critical concentration p^* and the critical exponents f of the shear modulus plotted as function of the initial lattice constant d.

$-0.7000)^{1.62}=0.010\,554$). The remaining discrepancy between our results and those of Refs. [7,8] should be due to our smaller system sizes. In other words, our results suggest that the tension-free system has a narrower critical regime so the power law fails for $p>0.8$. However, a small tension alters the picture and extends the power law so that it works well up to about $p=1$, as we can see from Fig. 3 for the system with $d=1.05r_0$. For this system, with $L=144$, with a fit up to $p=1$ we got $p^*(144)=0.5947$ and $f(144)=1.546$, and a fit up to $p=0.7$ we got $p^*(144)=0.5951$ and $f(144)=1.557$, and therefore the power law works well for all p. These results suggest that the tension-free system is very special in both critical behavior and critical regime.

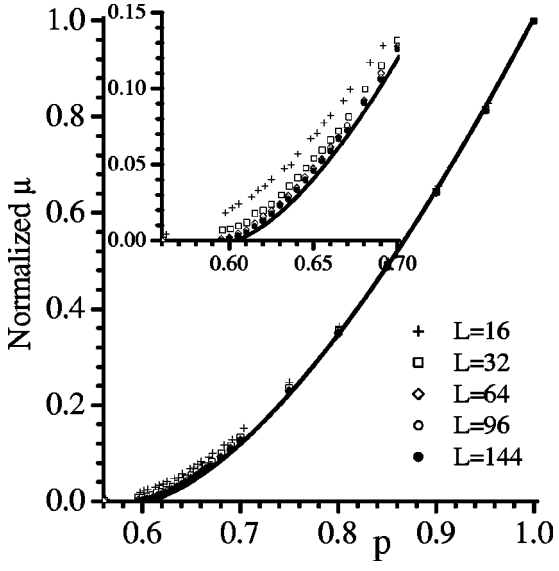

FIG. 3. The normalized shear modulus μ/μ_0 plotted as a function of concentration p of particles for lattices of size $L=16$, 32, 64, 96, and 144 at $d=1.05r_0$. The solid line is the function $(p-0.6009)^{1.521}$, a fit to the $L\to\infty$ values. The inset is a blowup of the region near the critical density p^*.

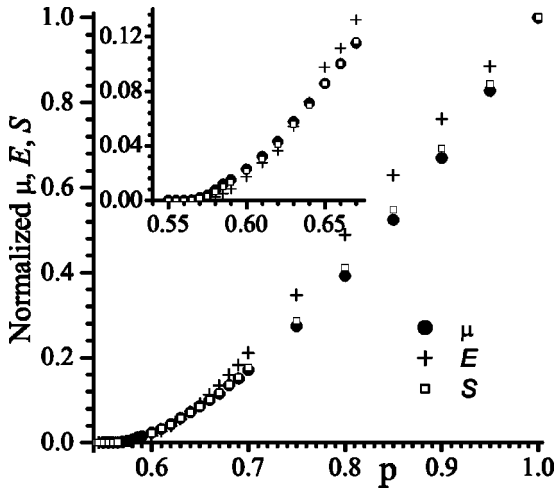

FIG. 4. The normalized shear modulus μ/μ_0, stress S/S_0, and energy E/E_0 plotted as a function of concentration p of particles for lattices of size $L=144$ and $d=1.05r_0$. The inset is the blowup of the critical regime.

It would also be interesting to know whether the different ''elastic constants'' [17,24,25] have the same critical behavior. One indication as to whether they do is to compare the critical behavior of S and μ. As one expects, at $d\sim r_0$, the effects of a very small stress on the different ''elastic constants'' can be ignored. However, for a moderate d we have to consider their effects. Our results show that for $d>1.05r_0$, the values of S become comparable to μ in the critical regime. Moreover, as can be seen from Fig. 4, there is a crossover between μ/μ_0 and S/S_0 at about $p=0.64$ for the system with $d=1.1r_0$. Such crossovers are found for all system sizes and for $1.05r_0\leqslant d\leqslant 1.30r_0$. It follows that μ and S have clearly and systematically different critical behaviors for these $d's$. For $d\geqslant 1.5r_0$, their behaviors become similar though their values are still different. This is in fact a must since a tension-free system has always vanishing S and E but may have a nonvanishing μ, but for an infinitely stressed system (DGSN), S and μ must have the same behavior. It follows that in the intermediate case, the critical point of μ should be lower, but gradually closer to that of S and E with increasing d, as is confirmed by our data. This in turn supports the conclusion that care is required in establishing the difference in behavior of the ''elastic constants'' [24,25] in the study of critical elasticity.

We do not have enough data to calculate the critical exponents, ν, of the correlation length. However, assuming that $\Delta p^*=p^*(L)-p^*\sim L^{-1/\nu}$ [7], we found that ν should be close to 1.0, since the variation of $p^*(L)$ with $1/L$ is consistent with a linear behavior for all systems. In fact, trying to fit the data to $p^*(L)-p^*\sim L^{-1/\nu}$ with $0.9<\nu<1.3$, we found almost the same results for p^*'s. But for $\nu>1.5$, the linearity becomes visibly poor. This is also consistent with the result that $\nu=1.21$ for the tension-free system [7] and $\nu=t=1.322$ [22] for the DGSN.

It is well known that $p_r>p_c$ because at p_c, the percolating cluster can still pivot freely at some nodes [2,7,8]. This is similar to the case of an equilibrium length chain which cannot resist shear. However, this analogy is not sufficient to

account for the behavior of the central force system under tension, since such a straight chain will resist shear once subject to tension. In fact, our system near p_c is more like a loose curved chain, a small tension would not be enough to straighten it out fully so it is still soft. More exactly, in our system, for those p in the range of $p^* > p > p_c$, the percolating cluster may contain some pieces of *simple* meandering paths, defined as paths on which every node connects to others with only two nonparallel bonds. Without tension, these *simple* meandering paths cannot resist any shear. With increasing d, the meandering paths straighten and hence gradually become more rigid, leading to the decrease of p^* and f. Near p_r, at $d = r_0$, there are few *simple* paths, and the tension is zero. The rigidity is caused by the bonds added to the *simple* paths only. With the application of tension, the meandering paths are straightened, lowering the onset of rigidity. The rigidity is enhanced and its rate of increase is larger (f drops). By a certain tension ($1.05 r_0 \lesssim d$), most of the meandering paths are straightened, and increasing tension has a diminishing effect on rigidity. The rate of increase of rigidity with tension is reduced and this leads to a smaller change in p^* and f. Temperature has a more immediate effect. It gives rigidity to the meandering paths because strands want to crumple to increase the entropy. At any finite temperature the system has rigidity above p_c and it is Gaussian for p's up to p^* [12,13].

In conclusion, our results suggest that the effect of tension is significant and cannot therefore be neglected when studying rigidity. The idealized situation of zero tension may be hard to probe with the usual combined effects of temperature and tension. Systems have a bias towards the Gaussian behavior. While we carried out this study for a two-dimensional system, we expect similar results in three dimensions. A real material is usually subject to tension, so our results should be helpful in understanding critical rigidity. Our results may be instructive for a biopolymer network, such as the cytoskeleton, a partially crosslinked network which governs the elasticity of cells, since it is in general subject to relatively strong tensions *in vivo* [26]. Another example of systems are the amorphous and disordered semiconductors. Their rigidity transition has attracted considerable interest [27]. As disordered systems often have internal stresses [28], their effects need to be considered.

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