Statistical mechanics of a cat’s cradle

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Abstract. It is believed that, much like a cat’s cradle, the cytoskeleton can be thought of as a network of strings under tension. We show that both regular and random bond-disordered networks having bonds that buckle upon compression exhibit a variety of phase transitions as a function of temperature and extension. The results of self-consistent phonon calculations for the regular networks agree very well with computer simulations at finite temperature. The analytic theory also yields a rigidity onset (mechanical percolation) and the fraction of extended bonds for random networks. There is very good agreement with the simulations by Delaney et al (2005 Europhys. Lett. 72 990). The mean field theory reveals a nontranslationally invariant phase with self-generated heterogeneity of tautness, representing ‘antiferroelasticity’.

From simple hammocks to sophisticated modern architecture, tensional mechanical structures have always been fashionable. It is of great interest to study such mechanical assemblies generally. In fact, nature is thought to adopt a similar design for the cytoskeleton, the largest mechanical structure of the cell, which consists of a polymeric network maintained under tension [1]–[3], much like the child’s game made of strings known as a ‘cat’s cradle’. However, unlike a macroscopic ‘cat’s cradle’, the cytoskeleton has intrinsic disorder and is also subject to fluctuating forces from both thermal motions and the nonequilibrium noise due to motor proteins and constant (de)polymerization events [4]. Upon freezing, molecular fluids that resist compression undergo transitions to rigid solids. Here we show that a caricature of the cytoskeleton—a model of interconnecting ropes that easily buckle—also undergoes a variety of phase transitions. It is important to investigate the mechanical phases of the cytoskeleton as cells modulate their phases to realize various critical biological functions such as cell motion and cell division [5].

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We study networks of ropes that bear tension when they are stretched beyond a critical threshold, but otherwise buckle. While the model’s interactions contrast with the usual compression-bearing mechanical interaction between atoms or molecules, the ‘inverted’ nonlinearity of ropes still leads to an onset of rigidity like that in crystals or glasses, but when the system is expanded rather than compressed. Depending on where we set the baseline of environmental pressure or tension, we may also say the system buckles upon compression.

The cytoskeleton actually has both tension-bearing and compressional elements. The present theory can be extended to include both elements. Elsewhere we have discussed the nonequilibrium aspects [6] that are also needed to capture the essential features of the tensegrity model [2, 3] of cell mechanics [7], but here we limit ourselves to the effects of equilibrium fluctuations.

Delaney et al [8] pioneered the study of such buckling lattices with neighbouring sites that interact with an ‘inside-out’ potential $u(r; l) = \Theta(r - l) \cdot k/2 \cdot (r - l)^2$, where $\Theta(\cdot)$ is the Heaviside unit step function. The energy stored in a bond vanishes when the length of the bond $r$ is less than a critical value $l$, but increases quadratically beyond the cutoff $l$. This type of bond with buckling tendency directly contrasts with the interaction of objects with hardcore repulsion $u_{\text{hc}}(r; l) = \infty \times \Theta(-r + l)$. It also differs from nonlinear bonds that break beyond a cutoff length $u_{\text{nh}}(r; l) = \Theta(-r + l)k/2(r^2 - l^2)$. We investigate the statistical mechanics of a collection of particles connected by such buckling nonlinear bonds. The topology of the networks may be built on regular lattices such as 2D hexagonal, square, or triangular or 3D cubic, bcc, or fcc lattice (having coordination numbers $z = 3, 4, 6, 8, 12$ respectively). We assume that all of the nearest neighbours to any given particle are linked to it by bonds, but that there are no bonds between any particle with its next-nearest neighbours or beyond. Though the connectivity of the network is trivial, the nonlinear bonds and the possibility of bond-disorder in the network make the mechanical properties of the network nontrivial. An illustration of the system is shown in figure 1.

A two (three) dimensional network of bonds is thermodynamically characterized by its tension (negative pressure), as a function of its area (volume) $-p_2 = \partial F/\partial s$ ($-p_3 = \partial F/\partial v$). In the low temperature limit, the entropy term can be ignored and elementary statics suffices to describe regular networks. The square network, for example, has a tension as a function of the low temperature limit, the entropy term can be ignored and elementary statics suffices to describe regular networks. The square network, for example, has a tension as a function of the area expansion given by $-p_2^{sq}(s/s_0) = k(1 - \sqrt{s_0/s})\Theta(s/s_0 - 1)$. Rigidity only occurs for areas exceeding $s_0$. Tensions for other lattices can also be computed $p_2^{tri} = 2\sqrt{3}p_2^{sq}$ and $p_2^{hex} = p_2^{tri}/3$ for the triangular and the hexagonal network respectively. For the 3D cubic network one finds at $T = 0$, $-p_3^{cu}(v/v_0) = 2k(1 - \sqrt{v_0/v})\sqrt{v_0/v}\Theta(v/v_0 - 1)$ yielding a rigidity threshold at $v_0$. We have set $s_0$ (or $v_0$) as the area (or the volume) of the corresponding network constructed from all bonds at the unit length. The tension of 3D networks has a maximum as a function of volume, because at large volume the energy density of the system decreases as $v^{-1/3}$.

At high temperature or equivalently for soft springs, even without disorder, static models are insufficient and one always needs a statistical mechanical description. If the network is disordered, i.e., having a broad distribution of onset length $l$, finding the tension is a nontrivial statistical problem even in the limit of low temperature [8]. To analytically treat statistical cat’s cradles, we adopt the self-consistent phonon (SCP) technique, initially developed for anharmonic lattice solids with compression bearing interactions [9, 10]. In this approach one replaces the pairwise interaction in the equilibrium density matrix exp$[-\beta \sum_{ij}u_{ij}(\vec{r}_i - \vec{r}_j)]$ by a nearly equivalent effective single-body term as $\Pi_i \exp[-\tilde{u}_i(\vec{r}_i - \vec{R}_i)]$. Decoupling the
Figure 1. An illustration of 2D square network with bond-disorder. During expansion, more bonds are changing from tension-free (green) to force-bearing (red).

many-body effects can be carried out by assuming a self-consistent one-body potential $\tilde{u}$ has a quadratic form $\alpha(\vec{r} - \vec{R})^2$.

The SCP method has not only been applied to crystals but also to noncrystalline solids [11], network glasses [12], and to problems of nonequilibrium structural assembly [13]. The SCP method can be made the beginning of a systematic expansion [9], but already has been shown to work very well for systems made up of compressive elements.

We study both 2D and 3D systems. Long wavelength phonons lead to a diverging mean square displacement (MSD) with increasing system size for 2D systems, in a strict sense. However this divergence is weak (logarithmic) and there is still a crossover reflecting rather rapid decrease in fluctuations of the mean square nearest-neighbour distance upon extension. In fact, the SCP method, when used for the 2D system predicts the correct onset of rigidity for the random 2D network at $T = 0$ as we shall see.

In the SCP theory the partition function $z(\xi) = \int d\vec{r} \exp(-\epsilon(\xi) - \alpha(\xi)\vec{r}^2)$ is evaluated as a function of expansion ratio $\xi = s/s_0$ or $v/v_0$. Both the on-site free energy $\epsilon$ and the phonon frequency $\alpha$ depend on the ratio of the mean neighbour distance $R$ to the critical extension $l$, $R/l = \sqrt{\xi}$. We can use the chain rule to calculate tension, e.g., $-p_2 = \frac{\partial f}{\partial s} = -\frac{\partial}{\partial s} \ln z(\xi(R))/\beta \partial s(R)$.

In three dimensions the Mayer $f$-bond $v(R; l, \alpha)$ for the interaction $u(r; l)$ when averaged over the Gaussian fluctuation of a neighbouring particle around its mean position $\vec{R}$ having its own spring constant $\alpha$ gives

$$\exp[-\beta v(R)] \equiv \left(\frac{\pi}{\alpha}\right)^{-3/2} \int r^2 d\Omega e^{-\alpha(R - \vec{R})^2 - \beta u(r)}.$$ 

This can be expressed using the error function erf(). The 2D averaged Mayer $f$-bond can be expressed as a numerical integral of modified Bessel function $I_0$.

An interesting property that can be calculated within the SCP theory is the fraction of the bonds bearing force (that are taut), i.e., having a length larger than the intrinsic cutoff $l$. These are functions of $\alpha$ and $R$: $q_2 = 2\alpha e^{-\alpha R^2} \int_{\sqrt{\alpha}}^{\infty} r^2 dr I_0(2\alpha R r) e^{-\alpha r^2}$ and $q_3 = 1 + 1/2 \text{erf}[(R - l)/\sqrt{\alpha}] - 1/2 \text{erf}[(R + l)/\sqrt{\alpha}] + e^{-\alpha(R - l)^2 - \beta u(\vec{R})}$ for 2D and 3D cases.

The SCP frequency $\alpha$ for several different regular networks is shown in the left panels of figure 2. Unlike the situation for the systems made of hard-spheres [6], there is always some nonzero self-consistent solution $\alpha$. Entropy always leads to some rigidity. There is, however, a
Figure 2. The phonon frequencies $\alpha$ are shown in the left panels as functions of the area (a) or volume (b) of networks for various $b = \beta k / 2$, and as functions of the linear expansion parameter with constant $b = 1$ for various types of networks (c). The fractions of free bonds $1 - q$ of corresponding setups are shown in the right panels (d)–(f). Note that (a), (b), (d), and (e) share a legend while (c) and (f) share the other legend.

rapid crossover from low $\alpha$ to high $\alpha$ accompanying the expansion of the system. Generally either high coordination number $z$ or larger microscopic rigidity-temperature ratio $b(= k\beta / 2)$ lead to a larger $\alpha$. The fraction of ‘loose’ bonds, $(1 - q)$ predicted from the phonon theory is plotted in the right panels of figure 2. This fraction decreases as the network expands.

We have shown there is a distinct bifurcation of $\alpha$ that also occurs when the volume ratio $\xi$ becomes small enough for 3D networks with high rigidity-temperature ratio $b$. This bifurcation appears in all three types of 3D networks studied here. The fcc networks most clearly display this bifurcation, followed by the bcc, and then the sc networks at smaller $\xi$ and higher $b$. As shown in figure 3, usually there is only one stable solution of the self-consistent equation $\alpha_{\text{tagged}} = f(\alpha_{\text{neighbour}})$. However, under certain conditions (small volume and large rigidity-temperature ratio, or pictorially, when the slope at the intercept is not in the range of between −1 and 1), the self-consistent solution becomes unstable, and another pair of solutions
\(\alpha_l\) and \(\alpha_h\) satisfying \(\alpha_l = f(\alpha_h)\) and \(\alpha_h = f(\alpha_l)\) emerges as the stable solution. This stable pair solution indicates the possibility of having a nontranslationally invariant solution, in which a low \(\alpha\) particle is surrounded by high \(\alpha\) neighbours and vice versa. The resulting spatial heterogeneity is self-generated. In the bcc and sc networks, this solution can be easily interpreted physically: there is a symmetry-broken phase of bcc or sc networks that can be thought as an ‘antiferromagnetic’ (AF) one with the underlying lattice being split to two subnetworks (sc \(\rightarrow\) fcc or bcc \(\rightarrow\) sc): one of the two equal subnetworks bears more tension than the other. We call this the ‘antiferroelastic’ phase. In the fcc case, since there are four particles in the unit cell, one high \(\alpha\) particle cannot be completely surrounded by low \(\alpha\) particles. Nevertheless one can have two possible ordered AF ground states similar to the crystal structures of AuCu and AuCu3. To test this possibility, we set up a more elaborate self-consistent solution having four values of \(\alpha = (\alpha_0, \alpha_x, \alpha_y, \alpha_z)\) at (000), (011), (101), (110) respectively, \(\alpha_0 = f(\alpha_x, \alpha_y, \alpha_z)\), \(\alpha_x = f(\alpha_0, \alpha_z, \alpha_y)\), \(\alpha_y = f(\alpha_z, \alpha_0, \alpha_x)\), \(\alpha_z = f(\alpha_y, \alpha_x, \alpha_0)\). By explicitly labelling all four particles in a unit cell (as done similarly in the AF Ising fcc system [14]), we searched but failed to find these explicit symmetry-broken solutions. Thus we believe this frustration of fcc network would lead to a random phase which is analogous to a self-generated glass. This possibility may potentially be resolved using a replica calculation [15, 16].

We checked our SCP theory using explicit computer simulations of the network with thermal noise. We show the results for the bcc case in figure 4. The simulations were performed with stochastic dynamics on \(n^3\) unit cells with periodic boundary condition for various rigidity-temperature ratios \(b\) and nonlinearity parameters \(l\) for various values of \(n\). We see the SCP theory agrees quite well with the simulation. For the simulation of size \(5^3\), the errors for the MSD of the particle position between theory and simulation are only about 1%. We extrapolated to the thermodynamic limit based on a series of simulation of different sizes of networks. The predicted slope differ from the extrapolation of simulation to infinite size by 20% but the correlation coefficient is 0.9995. The larger slope in the thermodynamic limit indicates that the SCP method underestimates the fluctuations. This is understandable since this method at lowest order only considers the local environment and ignores long wavelength phonons. A similar good agreement is achieved for 2D networks when the MSD of relative neighbour positions from simulation is compared with theory.

To check the prediction of spontaneous symmetry breaking of neighbouring \(\alpha\) values requires a large ratio of \(l/R \sim 10\) necessitating simulation using a very large system at a very
Figure 4. The comparison of the MSD of bcc networks between theory and simulation for various parameters $R \equiv \sqrt{3}/2 \times A$, $b$, and $l$. The corresponding results for square networks are shown in the inset ($R \equiv A$).

We plot the tension versus extension in figures 5(a) and (b). Above a critical tension, there are two solutions for $p(s/s_0) = p$. The solution with $\partial p/\partial s < 0$ is thermodynamically stable for a constant pressure ensemble. The system always appears to be stable in two dimensions. For 3D networks, as shown in figure 5(b), there is single (unstable) solution at high temperature for constant $p_3$; but there are three (one stable and two unstable) solutions at low temperature. The values of the critical rigidity-temperature ratio for this transition are $b^* = 1.04$, 0.76, and 0.48 for sc, bcc, and fcc networks respectively. Thus the network is intrinsically unstable for the constant $p$ ensemble for high temperature or low spring constant, i.e. $b < b^*$, regardless of supplied tension $-p$. For $b > b^*$, there is a critical tension $-p^*$ above which the system is no longer stable. Generally a larger $b$ implies a larger stable region.

In the large $s/s_0$ or $v/v_0$ limit, the Dulong–Petit law provides pressure that can be based on dimension counting alone, giving $p_2 - p^o = Nk_BT/(2S)$ and $p_3 - p^o = Nk_BT/(2V)$. Here $p^o = p(T = 0)$ is the pressure from the mechanical static calculations at zero temperature. The factor $1/2$ arises because only the potential energy is counted here, the kinetic energy counts the other half. Thus for large expansion ratios, $p_2 \to$ const. and $p_3 \to 0$, which are consistent with the tension curves shown in figures 5(a) and (b). The aforementioned critical rigidity-temperature ratio $b^*$ for 3D networks (demonstrated in figure 5(b)) is analogous to the phase transition of the van der Waals gas. The pressure of the van der Waals gas is analogous to the tension of the network while the microscopic hard sphere repulsion parameter of the gas is analogous to the microscopic onset rigidity parameter of the bonds.

So far we have focused on the effects of thermal disorder alone. We now discuss the effects of bond disorder. The bond disorder accounts for the quenched randomness due to the random cross-linking between the fibres of the cytoskeleton. For illustration, we concentrate on the 2D random network, especially in the $\beta k \to \infty$ limit. Following Delaney et al [8], we studied a ‘flat’ random distribution of string lengths. More general distributions present no new challenges to our method.
Figure 5. The applied tensions as functions of area expansion of 2D triangular network for various $b$ are shown in (a) with the zoom-in at the small $s/s_0$ region shown as an inset. We show the tensions of 3D networks in (b). The random bond 2D triangular network results are shown in (c)–(e). The effects of the random bond distribution $w$ on the phonon frequency $\alpha$ are shown in (c) with the inversion $1/\alpha$ shown in the inset of (c) to better illustrate the critical area for onset of rigidity. The portion of vertices with $n$ bonds tauted $P_n$ and the mean taut ratio $q$ are shown in (d) and (e) respectively. We show the inversion $1/\alpha$ as functions of volume for various 3D random networks in (f).

As shown in figure 5(c) for the triangular network, phonon frequencies $\alpha$ rise quickly with expansion at zero temperature when $b = \infty$. The smallest area $s^*/s_0$ satisfying $\alpha^{-1}(s/s_0) = 0$ is the critical value for the onset of macroscopic rigidity (mechanical percolation). Since the spring constant $k$ and temperature are always bundled together in the treatment, once the system is taut, $\alpha \to \infty$ for $1/b = 0$. For finite temperature, $\alpha$ is always finite. The rigidity onset $s^*/s_0$ calculated here quantitatively agrees with the simulation results in [8] as a function of width of distribution of string length $w$. As expected, a larger $w$ means a lower $\alpha$ generally. We also display in figure 5 the fraction of vertices with given number of taut bonds $P_n$ (d) and the mean fraction of taut bonds $q$ (e). These properties have also been obtained by the simulations of Delaney et al. We can only make a qualitative comparison for these two properties since our calculations were performed with finite $b$, corresponding to $T \neq 0$ while the simulations were strictly done at $T = 0$. Our theory does not allow us to calculate the loose bond fraction at $T = 0$ due to the bundling of $\beta$ and $k$. An approximation was made for the calculation of $p(n)$, the fraction of vertices with given number $n$ bonds taut based on the mean fraction of taut bonds $q$, i.e., $p(n) = Z^n/(Z-n)!q^n(1-q)^{Z-n}$. Here $Z$ is the coordination number. As shown in figure 5(f), for bond-disordered 3D networks, again there is a rigidity onset, which is similar to those of 2D networks. Among the cases studied only the $w = 1$ fcc network showed the antiferroelastic structural inhomogeneity bifurcation. The SCP method suggests random bond-disorder destroys antiferroelasticity.

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In summary, we have examined the properties of a class of novel mechanical networks using the SCP method. The method sheds light on the generic properties of tensional assemblies including cellular structures. We studied how both 2D and 3D regular and bond-disordered networks respond to the expansion of the volume. The results of computer simulation of regular networks with thermal noise are consistent with the SCP calculation. The previous results of simulation of 2D bond-disordered at $T = 0$ are also recovered by the present approximation.

Overall, lower temperatures increase the macroscopic rigidity of the network. The nonlinear bonds characterizing the onset of microscopic rigidity result in several interesting phase transitions in the parameter space of volume and tension. The model suggests that there may exist a new antiferroelastic phase at low temperature and high connectivity for 3D networks.

Admittedly, the detailed Hamiltonian described in this study is quite far from a biologically specific model that can give quantitative predictions for cells. In our view, cell mechanics remains at an early stage of development. More detailed modelling will continue to be developed, but we feel this model provides a generic understanding of a key aspect of the physics of cellular matter.

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