Module 4 : Nonlinear elasticity

Lecture 39 : Network with six-fold symmetry at non-zero temperature (contd...)

The Lecture Contains

“Mechanics of the Cell” by David Boal, Cambridge University Press, 2002, Cambridge, UK

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Network with six-fold symmetry at non-zero temperature (contd from lecture 38)

In other word, the fluctuation of the spring increases with temperature. It is not however clear how the network would appear at non-zero temperature as the length of the springs and the area of the plaquette would have considerable variations. Molecular dynamic simulation computes many such configurations. Interestingly it predicts that the area of the network $\frac{A_v}{A_0}$ decreases in the temperature range $\frac{k_B T}{k_{sp} s_0^2}$ 0 to 0.2, implying that the network has a negative coefficient of thermal expansion at this temperature range. At higher temperature $\frac{A_v}{A_0}$ increases linearly with temperature $\frac{k_B T}{k_{sp} s_0^2}$ with slope equal to $\frac{1}{2}$. In contrast to area, the elastic modulii of the network vary weakly with temperature from their temperature value.

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Network with four-fold symmetry

The free energy density of deformation of a network with four-fold symmetry has already been derived as

$$\Delta\Pi = \frac{K_A}{2}\left(u_{xx}+u_{yy}\right)^2 + \frac{\mu_p}{2}\left(u_{xx}-u_{yy}\right)^2 + 2\mu_s u_{xy}^2 \qquad (39.1)$$

This equation suggests that when $u_{yy} = -u_{xx}$ and $u_{xy} = 0$, $\Delta\Pi = 2\mu_p u_{xx}^2$, which is called pure shear. Similarly, we can have $u_{yy} = u_{xx} = 0$, so that $\Delta\Pi = 2\mu_s u_{xy}^2$, which is called simple shear. We can have also $u_{yy} = u_{xx}$ and $u_{xy} = 0$, leading to $\Delta\Pi = 2K_A u_{xx}^2$ which is known as area compression. Thus, it is possible that for same $\Delta\Pi$, the network can deform in either of all these three different ways. In other words, without any other constraint, the network can have degenerate states. Notice that the network has 2 springs and 1 vertex per rectangular unit called plaquette, so that when each spring stretches by equal amount from unstressed length s_0 to s, the enthalpy per vertex is obtained as

$$H_v = k_{sp}\left(s-s_0\right)^2 - \tau^2 \qquad (39.2)$$

The spring length s_τ that minimizes H_v is obtained as

$$s_\tau = \frac{s_0}{1-\frac{\tau}{k_{sp}}} \qquad (39.3)$$

Equation 39.3 suggests that the spring length and the area per vertex of the plaquette diverges for

$$\tau_{eq} = k_{sp} \qquad (39.4)$$

because beyond this critical value the tension term dominates. Under positive pressure, the fourfold network collapses because all plaquettes have the same energy $\tau_{coll} < 0$

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Network with four-fold symmetry (contd...)

Following the procedure described earlier, the area modulus of the network can be related to the stresses network as,

$$K_A = (k_{sy} - \tau)/2\,, \quad \mu = (k_{sy} + \tau)/2 \qquad \mu_s = \tau \tag{39.5}$$

Notice that μ_s vanishes at zero τ implying that the spring energy of the network under simple shear deformation vanishes under zero tension. That is the plaquette is not stable under simple shear mode of deformation.

The square plaquette approximation also implies that the area of the plaquette at zero temperature is $A_v = s_0^2$ at $\tau = 0$. However, in practice this estimation does not appear to be correct, in fact, in molecular simulation too this value is calculated to be $0.62 s_0^2$. Further difference is observed with the elastic modulii of the network. This difference is actually linked to the degeneracy of the system at low stress. The square form is the largest area of the plaquette while the system can explore many other configurations. An estimation of the area per vertex can be made at low temperature condition in which the springs can be assumed to have lengths very close to s_0:

$$\langle A_v \rangle = \frac{s_0^2 \int \sin\theta \, d\theta}{\int d\theta} = \frac{2}{\pi} s_0^2 \tag{39.6}$$

Here the plaquette is in the form of a parallelogram with the angle between adjacent sides θ which varies from 0 to $\frac{\pi}{2}$. The mean area is estimated to be $0.65 s_0^2$ which corroborates very well with that calculated from rigorous MD simulation.

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Network with four-fold symmetry (contd...)

Question is can we now extend these ideas for non-zero temperature. More relevant question is can we sample the configurations of any one plaquette in such a manner that it resembles the average configuration of the whole network.

The approach to do this is the following: We consider that the plaquettes assume shapes of parallelograms with one side fixed at zero temperature length s_0. Thus the parallelogram assumes different shapes as one vertex as it samples different co-ordinates in two dimensional space. In essence we are talking about a mean field model in which the behavior of plaquettes are identical to each other and also to that of the network. In reality the plaquettes are not independent, rather correlated locally, something which is missing in our approach. Furthermore, the following approach will not consider the more general quadrilateral shapes that would appear with rise in temperature, nor the length of the fixed side will remain constant.

In any case, our network consists of N plaquettes, N vertices and $2N$ springs, so that each plaquette consists of 1 vertex, and 2 springs, one of length s_0 and the other one of length s. Then the potential energy of the plaquette is written as,

$$E = \frac{k_{sp}}{2}(s - s_0)^2 \tag{39.7}$$

Then the corresponding Boltzmann factor can be written as

$$\exp(-\beta E) = \exp\left(-\frac{\beta k_{sp}[s - s_0]^2}{2}\right) = \exp\left(-\alpha[\sigma - 1]^2\right) \tag{39.8}$$

Where, we have introduced two variables, $\alpha = \frac{\beta k_{sp} s_0^2}{2}$ and $\sigma = \frac{s}{s_0}$. Then the probability of finding the chain at a length between s and s_0 and orientation between angles θ and $\theta + d\theta$ can be written as $\wp(s)s\,d\theta\,ds \equiv \wp(\sigma)\sigma\,d\theta\,d\sigma$. However, energy does not depend on θ, hence, the probability distribution is,

$$\wp(\sigma)\alpha d\sigma = \frac{\exp\left(-\alpha[\sigma - 1]^2\right)\alpha d\sigma}{\int \exp\left(-\alpha[\sigma - 1]^2\right)\alpha d\sigma} \tag{39.9}$$

The ensemble average $\langle A_v \rangle$ of the plaquette can be estimated from the sides of the parallelogram as $\langle A_v \rangle = s_0 \langle s \rangle \langle \sin\theta \rangle = \frac{2}{\pi} s_0^2 \langle \sigma \rangle$, where,

$$\langle \sigma \rangle = \int \sigma \wp(\sigma) \alpha d\sigma = \frac{\int \sigma^2 \exp\left(-\alpha[\sigma - 1]^2\right) d\sigma}{\int \exp\left(-\alpha[\sigma - 1]^2\right)\alpha d\sigma} \tag{39.10}$$

The final value of the integration can be obtained as

$$\langle \sigma \rangle = 1 + \frac{1}{2\alpha} \tag{39.11}$$

The average area per vertex is obtained as,

$$\langle A_v \rangle = \frac{2}{\pi} s_0^2 \left(1 + \frac{k_B T}{k_{sp} s_0^2} \right) \tag{39.12}$$

This estimation of $\langle A_v \rangle$ from mean field approach corroborates very well with the MD simulation results.

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