Capillary statics, elasticity and liquid crystals

Elasticity

In this lecture we're going to look at how we can work out how elastic solids behave using energy minimisation. The key idea is that we can calculate the total elastic energy of a body by integrating its strain energy density W. W the strain energy per unit volume, and only depends upon the local strain of the solid: $W = W(\epsilon_{ij})$. Thus the total elastic energy of a solid body V is

$$E_{el} = \int_V W(\epsilon_{ij}) dV. \tag{4.43}$$

A key component of finite elasticity is selecting a suitable W to match the observed behaviour of the material that you are modelling. Neo-Hookean, and Mooney-Rivlin solids (that you saw examples of earlier) are specific examples of different models for W.

Elastic beams

Let's start by looking at the deformation of a thin elastic beam, that is initially flat, but which we bend to $y = h(x)$ by applying vertical forces. We assume that there is no stretching of the beam.

We need an expression for the strain energy density of the beam (i.e. the elastic energy per unit length). We will guess this by a bit of logical deduction. We know that the strain energy density depends on the strain, so it must be a function of h or its derivatives. First we notice that W cannot be a function of h, as otherwise the beam could increase its energy just by displacing it upwards or downwards. Second, we notice that W cannot be a function of h' otherwise a straight beam that was angled upwards at a constant angle would have a different elastic energy to a flat beam. Thus the lowest derivative that the energy can depend on is h''. However, the energy must depend on h''^2 so that the energy does not depend on whether the beam curves up or down.

Thus the simplest possible model for the strain energy density of a beam is $W = \frac{B}{2} h''^2$. This turns out to be exactly correct for a linear-elastic beam!

Let's now consider the problem where we put weights on a beam suspended between two points. Both ends of the beam are fixed with $h = h' = 0$. There is a distributed load $q(x)$ pushing upwards on the beam. Then the total energy consists of the elastic energy and the gravitational potential energy:

$$E = \int_0^L \frac{B}{2} (h'')^2 dx - \int_0^L q(x) h(x) dx. \tag{4.44}$$

We need to use the higher-dimensional Euler-Lagrange equation that you derived earlier (4.14), to minimise this expression:

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0. \tag{4.45}$$

Using this, we obtain

$$Bh'''' = q, \tag{4.46}$$

which is the static Euler-Lagrange beam equation.

For example, we can consider the case where the beam has an evenly distributed, constant pressure $q(x) = p$ pushing upwards along its surface. Solving the beam equation, we find

$$h = p\frac{x^2(L-x)^2}{24B}. \tag{4.47}$$

Stretching vs bending energy

We have just seen that the bending energy density of a thin sheet is $W_b = Bh''^2/2$. This is energy per unit length and width of the sheet and thus has units of $\mathrm{J/m^2}$. B can only depend on Young's modulus of the material, E (units of pressure), and the thickness of the beam t. From dimensional analysis we find that:

$$\frac{\mathrm{J}}{\mathrm{m}^2} \sim \frac{[B]}{\mathrm{m}^2}, \tag{4.48}$$

and so B has units of energy, and we must have $B \propto Et^3$. We can also consider the stretching energy density of a thin sheet. By analogy with a linear spring, $W_s = k\epsilon^2/2$, where ϵ is the local extensional strain. This time, from dimensional analysis, we find that $k \propto Et$. Thus we see that the energy to stretch (or compress) a sheet is proportional to t, but the energy to bend a sheet is proportional to t^3.

This is an important result. As t becomes small, bending energy will always be much smaller than stretching energy. Thus if you compress a sheet, it will prefer to bend rather than compress, as this results in a much lower stored energy. You can see this by putting a piece of paper on a table, and sliding the two ends towards each other. The paper does not compress, but instead rapidly buckles out of plane. Another example is what happens when you crumple up a ball of paper. In this case, there is no configuration the paper can take which only involves bending. It has to do a little bit of stretching, but it minimises this by confining the stretching to ridges and points. In between these, the paper bends as expected. This gives a scrunched up ball of paper its characteristic shape.

The elastica

The idea that an elastic sheet will bend and not stretch is the key principle of Euler's elastica. We have already seen that linear-elastic beams have a strain energy density of $W_b = Bh''^2/2$. In fact Euler showed that for large deformations, this can be generalised to $W_b = B\mathcal{K}^2/2$, where $\mathcal{K}$ is the local curvature of the beam.

$\mathcal{K}$ can be calculated from the normal vector to the beam from $\mathcal{K} = \nabla.\mathbf{n}$. If the position of the beam is $y = h(x)$, $\mathbf{n} = \nabla(y - h(x))/|\nabla(y - h(x))|$, so

$$\mathbf{n} = \frac{(-h', 1, 0)}{\sqrt{1 + h'^2}} \tag{4.49}$$

and

$$\mathcal{K} = \frac{-h''}{(1 + h'^2)^{3/2}}. \tag{4.50}$$

Alternatively, if s is arclength and θ is the angle from horizontal, then

$$\mathcal{K} = \frac{d\theta}{ds} \tag{4.51}$$

Let's use this to calculate the shape of a "ruck in a rug". We lay an elastic of length L on a flat surface, and bring the ends together with a force F, so that they are now a distance $L - \Delta L$ apart. The ends are clamped with $h = h' = 0$. What is the final shape?

In this case, the energy consists of three parts: the bending energy, the gravitational potential energy, and the energy done in compressing the ends together:

$$E = \int_0^L \frac{B}{2}\frac{d\theta}{ds}^2 ds + \int_0^L (\rho g t) h ds - F\Delta L \tag{4.52}$$

We note

$$\Delta L = L - \int_0^L \frac{dx}{ds} ds = \int_0^L (1 - \cos\theta) ds, \tag{4.53}$$

and that by integrating by parts,

$$\int_0^L (\rho g t) h ds = [\rho g t s h]_0^L - \int_0^L \rho g t s h_s ds = -\int_0^L \rho g t s \sin\theta ds \tag{4.54}$$

Thus

$$E = \int_0^L \left(\frac{B}{2}\frac{d\theta}{ds}^2 - \rho g t s \sin\theta - F(1 - \cos\theta) \right) ds \tag{4.55}$$

Using the Euler-Lagrange equation, we finally obtain the heavy elastica equation:

$$B\theta'' = -\rho g t s \cos\theta - F \sin\theta. \tag{4.56}$$

This is a surprisingly simple equation, given that we have to deal with curvatures, which normally bring in many nasty derivatives. It can be solved numerically, as you'll see in the Problems.

General elastic equations

Finally, let's derive the general elastostatic equations for a given strain energy density function. Suppose that we prescribe the stresses over the surface of an elastic body.

In this case, the elastic energy of the body is

$$E_{el} = \int_V W(\epsilon_{ij})dV - \int_S \mathbf{u}.\sigma.\mathbf{n}dS \tag{4.57}$$

where $\mathbf{n}$ is the normal to the body, S is the surface of the body, and $\mathbf{u}$ is the displacement at its surface. Recall that the strain is given by

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{4.58}$$

We minimise the energy by letting $u \to u + \delta u$. Then

$$\delta E = \int_V \frac{\partial W}{\partial \epsilon_{ij}} \delta\epsilon_{ij} dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n}dS \tag{4.59}$$

and using equation (4.58)

$$\delta E = \frac{1}{2}\int_V \frac{\partial W}{\partial \epsilon_{ij}}\left(\frac{\partial \delta u_i}{\partial x_j} + \frac{\partial \delta u_i}{\partial x_j}\right) dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n}dS \tag{4.60}$$

ϵ_{ij} is symmetric, which gives

$$\delta E = \int_V \frac{\partial W}{\partial \epsilon_{ij}} \frac{\partial \delta u_i}{\partial x_j} dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n}dS \tag{4.61}$$

and we can rewrite this as

$$\delta E = \int_V \left[\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\delta u_i\right) - \delta u_i \frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right)\right] dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n}dS. \tag{4.62}$$

Using the divergence theorem, we obtain

$$\delta E = -\int_V \delta u_i \frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right) dV + \int_S \left[\delta u_i \frac{\partial W}{\partial \epsilon_{ij}} n_j - \delta u_i \sigma_{ij} n_j\right] dS. \tag{4.63}$$

The only way that this can always be minimised is if

$$\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right) = 0 \tag{4.64}$$

in the bulk of the solid, while

$$\frac{\partial W}{\partial \epsilon_{ij}} = \sigma_{ij} \tag{4.65}$$

on the boundaries. If we compare equation (4.64) to the elastostatic equation $\nabla.\sigma = 0$, we see that these equations are satisfied if $\partial W/\partial \epsilon_{ij} = \sigma_{ij}$ everywhere. This demonstrates the importance of the choice of the strain energy density function W: it contains all the information to give us both the strains and the stresses in an elastic body.

Although this section is a little abstract, the other main point is to show you how we can generalise the Calculus of Variations to higher dimensions. In this case, we have to use the divergence theorem instead of integrating by parts. However otherwise, the procedure is completely analogous. Note also, that as before we cannot throw away automatically throw away surface terms - here they add an extra boundary constraint.

Liquid Crystals

Liquid crystals are an important tool that have found use in the majority of modern visual technologies. Most computer and TV screens incorporate liquid crystals, as does everything from your digital watch to a calculator screen. As you will be aware, in each of these cases, liquid crystals are use to alter the opacity of a small pixel on the screen, allowing the screen to display complex pictures. Liquid crystals are often found in many other places - the tobacco mosaic virus is a famous virus that shows liquid crystalline properties.

So what is a liquid crystal? The key is that the molecules or particles that make up the liquid crystal have some sort of directionality to them - these could be rod-like, disk-like, or more asymmetric. In certain temperature regimes, this directionality will make the molecules want to line up in a certain orientation. The temperature is important: when the temperature is too low, the molecules will form a rigid crystal lattice When the temperature is too high, the molecules have so much thermal energy that they align themselves randomly. However, in between these two phases, the molecules want to align themselves, but have too much energy to form a crystal lattice. This means they have long-ranged *directional order*, but no long-ranged *positional order*.

We will focus our attention from hereon on a specific type of liquid crystal - the nematic liquid crystal. These consist of rod-like molecules or particles that want to line up parallel to each other (I'll refer to them as rods from now onwards). You can think of them as long, thin cylinders floating in a liquid phase. As we shall see, these have useful properties that make them ideal for liquid-crystal devices.

The potential energy density of a liquid crystal

As with the elasticity results that we derived in the previous lecture, we will model liquid crystals by defining a local potential energy density of the liquid crystal that depends on some local property of the individual particles. As mentioned above, the rods preferentially line up parallel to each other, so therefore the energy should be minimal when the particles are locally aligned. On the other hand, if the rods fan out from each other at a point, then the energy should be increased locally.

In fact we can separate the different ways that energy can be locally increased into three different categories: *Splay, twist*, and *bend*. Splay can be thought of as the rods all fanning out from a point in a plane. Twist is like a helix, with the rods twisting around as you move downwards through a sample. Bend is where the rods circle around a point.

The most natural way of characterising the local energy density is by using the local *director*, $\mathbf{n}$, of the rods. This is the unit vector that points along the long axis of the rod. Then

$$\nabla.\mathbf{n} \neq 0 \tag{4.66}$$

corresponds to splay.

$$\mathbf{n}.(\nabla \wedge \mathbf{n}) \neq 0 \tag{4.67}$$

corresponds to twist, and

$$\mathbf{n} \wedge (\nabla \wedge \mathbf{n}) \neq 0 \tag{4.68}$$

corresponds to bend.

The simplest model describing liquid crystal behaviour is given by the Frank distortion energy density:

$$W(\mathbf{n}) = \frac{K_1}{2}|\nabla.\mathbf{n}|^2 + \frac{K_2}{2}|\mathbf{n}.(\nabla \wedge \mathbf{n})|^2 + \frac{K_3}{2}|\mathbf{n} \wedge (\nabla \wedge \mathbf{n})|^2 \tag{4.69}$$

2D liquid crystals

Let's start by considering a 2D liquid crystal, as this will significantly simplify the energy density. To do this, we assume that

$$\mathbf{n} = (\cos\theta, \sin\theta, 0), \tag{4.70}$$

with $\theta = \theta(x, y)$. Then we find

$$\nabla.\mathbf{n} = -\sin\theta\frac{\partial\theta}{\partial x} + \cos\theta\frac{\partial\theta}{\partial y}, \tag{4.71}$$

$$\nabla\wedge\mathbf{n} = \left(\cos\theta\frac{\partial\theta}{\partial x} + \sin\theta\frac{\partial\theta}{\partial y}\right)\mathbf{k} \tag{4.72}$$

where $\mathbf{k}$ is the unit vector in the z direction. From this, we see that $\mathbf{n}.(\nabla\wedge\mathbf{n}) = 0$, and there is no twist.

If we continue to churn the handle, we eventually obtain that the distortion energy density reduces to:

$$W = \frac{K_1}{2}(\theta_x^2\sin^2\theta - 2\theta_x\theta_y\sin\theta\cos\theta + \theta_y^2\cos^2\theta) + \frac{K_3}{2}(\theta_x^2\cos^2\theta + 2\theta_x\theta_y\sin\theta\cos\theta + \theta_y^2\sin^2 \tag{4.73}$$

This is still rather messy, but if we make the simplifying assumption that $K_1 = K_3 = K$, we find

$$W = \frac{K}{2}(\theta_x^2 + \theta_y^2) = \frac{K}{2}|\nabla\theta|^2. \tag{4.74}$$

So the local potential energy density only depends on the change in the angle of the rods in the liquid crystal. The assumption that $K_1 = K_3 = K$ is known as the one-constant approximation.

Strong anchoring

As you can imagine, rod-like liquid crystals will also have a preferential orientation when they meet a flat boundary. This can be controlled very specifically. For instance if you rub a piece of glass, the electrostatic charge will make the rods line up along the rubbing direction, parallel to the glass. The rods can also be force to line up perpendicular to, or at a fixed angle to the wall.

If the interaction is sufficiently strong that the rods take a fixed orientation at a boundary, then we can use this as a fixed boundary condition. For example, let's consider the case where the liquid crystal is placed between two walls: one at $y = 0$, and one at $y = d$. At the bottom wall, $\theta = 0$ (rods parallel to the wall), while at the top wall, $\theta = \pi/2$ (rods perpendicular to the wall).

θ is only a function of y, so the total distortion energy of the sample per unit length in the x direction is

$$\int_0^d \frac{K}{2}\theta_y^2 dy, \tag{4.75}$$

and from the Euler-Lagrange equation, we find that $\theta_{yy} = 0$, so we find the solution

$$\theta = \frac{\pi y}{2d}. \tag{4.76}$$

Note the subtlety that $\theta = -\frac{\pi y}{2d}$ is also a valid solution - the rods are assumed symmetrical, and so this will also satisfy the boundary conditions. The difference is that in the first solution, the rods rotate anticlockwise by a quarter turn as they move upwards towards the top boundary. In the second solution, the rods rotate clockwise by a quarter turn.

Weak anchoring

If the rods are not strongly anchored onto the wall, then we need to use a surface energy term to describe the energy of the interaction of the rod with the wall. The most well known of these is the Rapini-Papoular expression for the surface energy density:

$$w_s = \mathcal{W}\sin^2(\theta - \theta_p), \tag{4.77}$$

where θ_p is the preferred binding angle at the wall.

Let's return to the previous example (see Figure ??), and assume that the preferred binding angle at the bottom is θ_b, and the preferred binding angle at the top is θ_t. Then the energy per unit length in the x direction becomes

$$E = \int_0^d \frac{K}{2}\theta_y^2 dy + \mathcal{W}\sin^2[\theta(0) - \theta_b] + \mathcal{W}\sin^2[\theta(d) - \theta_t], \tag{4.78}$$

then from equation (4.8), we have that

$$\delta E = \left[\delta\theta\frac{\partial f}{\partial \theta'}\right]_0^d + \int_0^d \delta\theta\left[-\frac{d}{dx}\left(\frac{\partial f}{\partial \theta'}\right)\right]dx + \mathcal{W}\sin^2[\theta(0) + \delta\theta(0) - \theta_b] + \mathcal{W}\sin^2[\theta(d) + \delta\theta(d) - \theta_t]$$
$$-\mathcal{W}\sin^2[\theta(0) - \theta_b] - \mathcal{W}\sin^2[\theta(d) - \theta_t] = 0 \tag{4.79}$$

We Taylor expand the last four terms to find

$$\left[\delta\theta K\frac{\partial \theta}{\partial y}\right]_0^d - \int_0^d \delta\theta K\theta_{yy}dy + \frac{\mathcal{W}\delta\theta(0)}{2}\sin[2(\theta(0) - \theta_b)] + \frac{\mathcal{W}\delta\theta(d)}{2}\sin[2(\theta(d) - \theta_t)] = 0. \tag{4.80}$$

Finally we see that the only way that this can always be zero is if

$$\theta_{yy} = 0 \tag{4.81}$$

in the bulk, while we have boundary conditions

$$K\theta_y(0) + \frac{\mathcal{W}}{2}\sin[2(\theta(0) - \theta_b)] \tag{4.82}$$

$$K\theta_y(d) + \frac{\mathcal{W}}{2}\sin[2(\theta(d) - \theta_t)]. \tag{4.83}$$

You can solve these. Here, I will just mention that there is a natural lengthscale in the equations $K/\mathcal{W}$. When the gap thickness d is much larger than this lengthscale, the anchoring is strong enough that it rotates all the rods to be at their preferred orientation at both boundaries. When $d \ll K/\mathcal{W}$, the anchoring is not strong enough to rotate the rods. Then all the rods will be at a constant, intermediate angle.

Electric and magnetic fields

The most useful property of liquid crystals stems from their ability to align with electric and magnetic fields (**E** and **B** respectively). For the case of an electric field, we can see that it's natural to construct a potential energy that depends on $\mathbf{E}.\mathbf{n}$. In fact the potential energy of a liquid crystal in an electric field is given by

$$E_{\text{elec}} = -\int_V \frac{1}{2}\epsilon_0 \Delta\epsilon (\mathbf{E}.\mathbf{n})^2 dV, \tag{4.84}$$

where ϵ_0 is the vacuum permittivity and $\Delta\epsilon$ is the electric dipole moment of the rods. Similarly the potential energy of a liquid crystal in an magnetic field is given by

$$E_{\text{mag}} = -\int_V \frac{1}{2}\mu_0^{-1}\Delta\chi(\mathbf{B}.\mathbf{n})^2 dV, \tag{4.85}$$

where μ_0 is the magnetic permeability of vacuum, and $\Delta\chi$ is the diamagnetic anisotropy of the rods.

Fréedericksz transitions

We can use these expressions to study a very useful property of liquid crystals: the fact that they will suddenly jump between orientations when an electric or magnetic field is applied that is above a certain strength. Depending on their orientation, the rods will either block, or allow polarised light to pass. Thus we can use these fields to control the brightness of a liquid crystal pixel on a screen very accurately and quickly.

Let's go back to the strong anchoring geometry, but now assume that $\theta(0) = \theta(d) = 0$. i.e. the rods are constrained to lie parallel to the bottom and top plates. However, now we add an electric field that points in the y direction. In this case, $\mathbf{E} = (0, E, 0)$ and $\mathbf{n} = (\cos\theta, \sin\theta, 0)$ so that $\mathbf{E}.\mathbf{n} = E\sin\theta$.

Again we utilise the one-constant approximation, so that the total potential energy is:

$$\int_0^d \left[\frac{K}{2}\theta_y^2 - \frac{1}{2}\epsilon_0 \Delta\epsilon E^2 \sin^2\theta\right] dy. \tag{4.86}$$

We can use the Euler-Lagrange equation to then establish that

$$\epsilon_0 \Delta\epsilon E^2 \sin\theta\cos\theta + K\theta_{yy} = 0. \tag{4.87}$$

This has an obvious solution $\theta = 0$. However we want to know what the non-zero solution is when the electric field is strong enough to distort the rods. Multiply by θ_y and integrate once to obtain

$$K\theta_y^2 + \epsilon_0 \Delta\epsilon E^2 \sin^2\theta = c. \tag{4.88}$$

To determine the constant, note that the solution is expected to be symmetric about $y = d/2$. Therefore $\theta_y(d/2) = 0$, and $\theta(d/2) = \theta_m$, so

$$K\theta_y^2 + \epsilon_0 \Delta\epsilon E^2(\sin^2\theta - \sin^2\theta_m) = 0. \tag{4.89}$$

We nondimensionalise by setting $d\hat{y} = y$, and $\xi_d = \sqrt{K/(\epsilon_0 \Delta\epsilon E^2 d^2)}$ to obtain

$$\xi_d^2 \theta_{\hat{y}}^2 + (\sin^2\theta - \sin^2\theta_m) = 0, \tag{4.90}$$

which we wish to solve with boundary conditions $\theta(0) = 0$ and $\theta(1/2) = \theta_m$.

Now let $k = \sin\theta_m$ and $t = \sin\theta/\sin\theta_m$ and after some rearrangement this becomes

$$\frac{\partial t}{\partial \hat{y}} = \frac{1}{\xi_d}\sqrt{1-t^2}\sqrt{1-k^2t^2}. \tag{4.91}$$

Separate and integrate from $\hat{y} = 0$ to $1/2$ (which corresponds to integrating t from 0 to 1):

$$\int_0^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-k^2t^2}} = \int_0^{1/2} \frac{d\hat{y}}{\xi_d} = \frac{1}{2\xi_d} = \frac{1}{2}\sqrt{\frac{\epsilon_0 \Delta\epsilon E^2 d^2}{K}}. \tag{4.92}$$

The left hand side is the complete elliptic integral of the first kind $K(k)$. It has its smallest value when $k = 0$, where $K(0) = \pi/2$. Thus there is only a non-zero solution when

$$\sqrt{\frac{\epsilon_0 \Delta\epsilon E^2 d^2}{K}} > \pi. \tag{4.93}$$

In other words, the electric field has to exceed the critical strength

$$E_c = \frac{\pi}{d}\sqrt{\frac{K}{\epsilon_0 \Delta\epsilon}}, \tag{4.94}$$

and then the liquid crystal rods will start to rotate. Note that, from measuring E_c, we have a technique for measuring K.

References and further readings

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