Fluid lipid membranes – a primer

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Contents

1 Self assembly

Lipid membranes are quasi-two-dimensional structures which form by spontaneous aggregation of lipid molecules in aqueous solution. Such a process is an example of what is termed *self-assembly*. It can be found frequently in nature, whenever a large number of molecules form a condensed aggregate of some nontrivial structure, driven by the possibility to lower the free energy in doing so. Strictly speaking, even the formation of a sodium-chloride crystal may thus be viewed as a self-assembly process, but the terminology is usually restricted to cases in which supramolecular aggregates of somewhat more complicated structure are being formed – in particular, when due to

Box 1 *(Hydrophobic effect)*

The insertion of a molecule into water occurs spontaneously when it leads to a lowering of the overall free energy. Recall that this involves not only the question whether there exists a favorable interaction *energy* (say, of van der Waals or electrostatic type), but also whether the process is *entropically* favorable. Liquid water has a great deal of entropy, related to the translational or rotational degrees of freedom of water. However, particularly the latter are restricted by the fact that water just *loves* to form hydrogen bonds with itself, *i. e.*, point an H-atom of one H_2O molecule towards the O-atom of another. The resulting network of hydrogen bonds is a delicate balance between energy and entropy, and the insertion of other molecules might locally disturb this network, thereby also influencing the water entropy. A good rule of thumb is that if a molecule is also able to efficiently take part in hydrogen bonding (such as glucose or sucrose), it will tend to dissolve easier than a molecule which is unable to do this (such as oil). Generally, polar molecules (*i. e.*, molecules with local electrical dipole moments) blend more readily into the hydrogen bond network. Around the very non-polar surface of a hydrocarbon chain water molecules can only form hydrogen bonds with themselves, but since these molecules have fewer neighbors, they have *fewer possibilities* to do so, leading thereby to lower entropy in the water layer adjacent to a non-polar surface, which in turn works against solubilization. What may sound intuitively appealing, is in fact much more complicated and remains partially disputed even today. The difficulty is that certain energy-entropy compensation effects make it impossible to “attribute” certain effects in an unambiguous way to either energy or entropy. The interested reader will find some useful material in Refs. [10, 18, 22, 23].

the aggregation process entities appear which are characterized by the emergence of new length scales. Self-assembly is thus a classical route by which hierarchically structured materials form, and it is thus of great interest to physicists and engineers alike. And since Nature has the well-deserved reputation of having engineered the best machines literally walking this planet, self-assembly is indeed one of its close allies, and it is thus of great interest for biologists, too. Fluid lipid bilayers of course belong to the class of systems which hold an obvious biological relevance. In this introductory section we first want to familiarize ourselves a bit with some of the idiosyncrasies of lipid self assembly, before we turn to properties of the structures which form in this process – lipid membranes.

1.1 Lipids

Lipids are Nature’s sophisticated version of surfactants. They are amphiphilic molecules which consist of one part, called the *head*, which is hydrophilic – “in love with water”, and another part, termed *tail*, which is hydrophobic – “afraid of water”. Whether a molecular structure or a part of it likes or dislikes water depends on its detailed chemical buildup, and it is closely related to the question of whether this structure could be solubilized in water. Sugar for instance dissolves readily in water, oil doesn’t — see also Box 1

Lipids come in many different kinds in nature, and this is not the place to classify them (the reader will find a bit more detail in Ref. [16, Chap. 1]. I only want to say a bit more about the most common ones – glycerophospholipids. Their hydrophobic part consists of (normally) two simple hydrocarbon chains, having a (typically even) number of C-atoms (typically between 12 and 24) and maybe some (typically cis-) double bonds. These chains previously belonged to the corresponding fatty acid, for instance palmitic acid, and two such chains are linked via ester bonds to two of the OH groups of a molecule of glycerol. Its third OH group is esterified to a phosphate group, which carries the terminal head group of the lipid, for which again there exist many possibilities, for instance a choline group. A sophisticated (and partly intimidating) terminology has been developed to communicate the relevant details of this architecture. For instance, palmitoyloleoylphosphatidylcholine – abbreviated POPC – is a lipid which has one hydrocarbon chain derived from palmitic acid (a saturated fatty acid with 16 carbons and no double bond), another chain coming from oleic acid (an unsaturated fatty acid with one cis double bond at position 9 and 18 carbons), and a phosphate link to a choline group. Or dimyristoylphosphatidylserine – abbreviated DMPS – has two chains stemming from myristic acid (a saturated fatty acid with 14 carbon atoms and no double bond) – linked again via a phosphate to the amino acid serine. Some more on structure and naming conventions can be found in the Boxes 2 and 3. As physicists we can permit ourselves to neglect much of the detail, but some key points are worth paying attention to:

- The length of the fatty acids. The longer they are, the more hydrophobic is the lipid (and the thicker will the membrane be later).
- Are there double bonds? If yes, the tails tend to be more disordered, and this increases the fluidity of the forming membranes (more precisely, it increases the temperature of the "main transition" between "fluid" and "gel" phase) [16, Chap. 5].
- Is the head group charged? Note that the phosphate itself already carries one negative charge. For neutral lipids the group attached to the phosphate must thus carry a positive counter charge (as choline does, but for instance not serine).

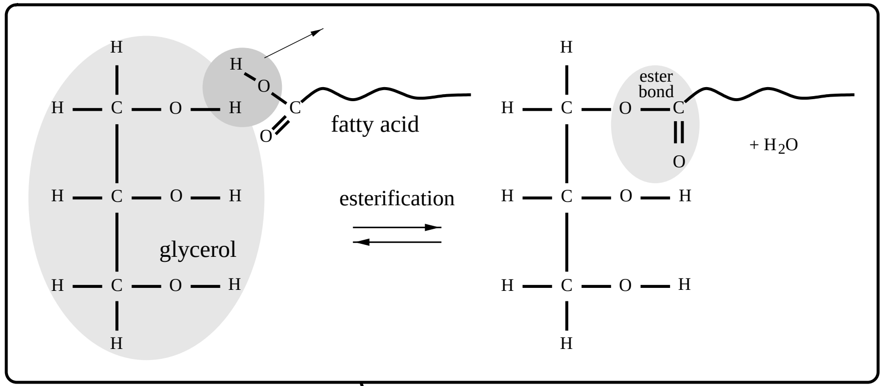
1.2 The morphology of surfactant aggregates

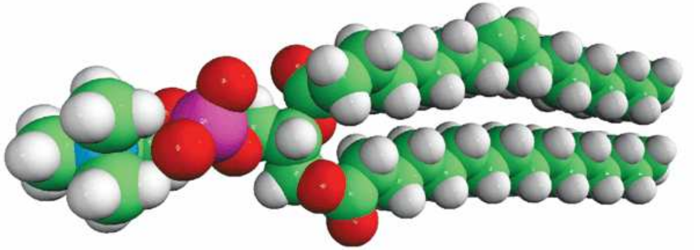
The hydrophobic parts of amphiphilic molecules do not like to dissolve in water. But what if they have to, because we put them in water anyways? The trick is that they can develop a cooperative strategy in which many of them combine to an aggregate which shields its hydrophobic part against the surrounding water by using the hydrophilic part. Morphologically such aggregates can for instance be spheres, with all the tails in the inside and the heads on the surface. Such objects are called (spherical) "micelles" (from the Latin word "mica", *grain*). One could also imagine cylindrical aggregates with the hydrophobic tails in the inside and the heads again on the surface; these are called cylindrical or wormlike micelles. And finally one can also imagine a double-layer in which the hydrophobic tails are sandwiched between two planes of hydrophilic head groups. This is the lipid bilayer membrane that will keep us busy later. But before we look at it in any greater detail, we would like to understand what aspect of the amphiphile determines the morphology that is spontaneously being formed.

Possibly the simplest answer to this question has been given by Israelachvili, Mitchell, and Ninham in a famous paper from 1976, and it is a wonderful example of a simple geometry argument [13]. Here's how it goes: Assume that the particular amphiphilic molecule has a head that needs an area a inside an aggregate, and that it has a volume v and a tail length ℓ. Let's try to form a spherical aggregate of radius R out of N such molecules. Of course, we then must have $4\pi R^2 = Na$ and $\frac{4}{3}\pi R^3 = Nv$. By forming the ratio of these two equations the aggregate number N drops out and we find for the radius

$$R_{\text{sphere}} = \frac{3v}{a} . \tag{1}$$

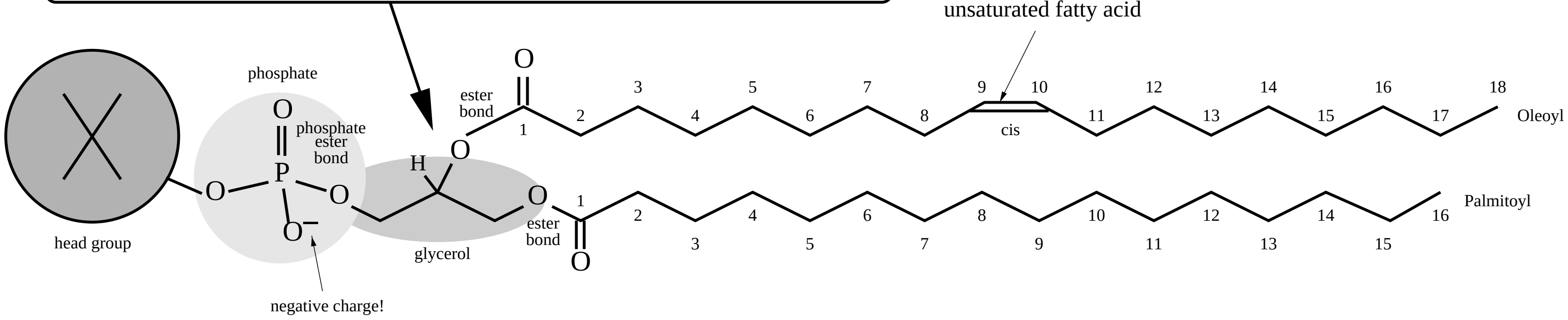
Box 2 *(Lipid structure and head-groups)*

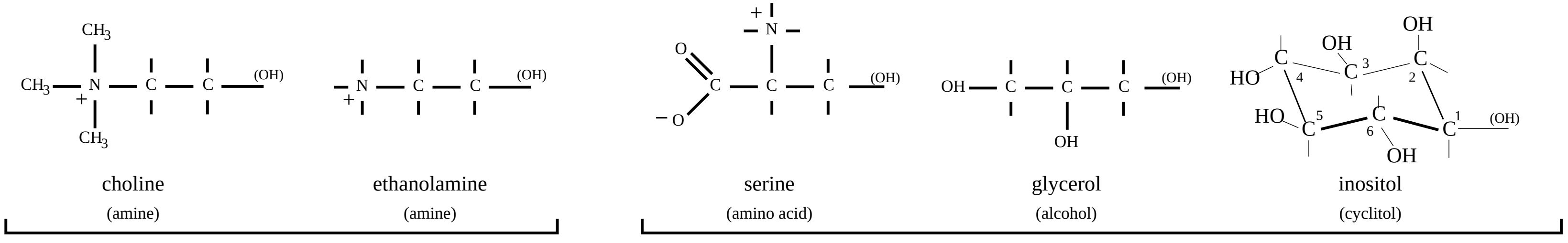




Example: 1−Palmitoyl−2−Oleoyl−sn−Glycero−3−Phosphocholine (POPC)

phosphatidylcholin = "Lecithin"





positively charged
→ gives neutral lipid

neutral
→ gives negative lipid

Box 3 *(Naming conventions for simple fatty-acid lipid-tails)*

# carbon	saturated	1-fold unsaturated	2-fold unsaturated	4-fold unsaturated	6-fold unsaturated
12	**Lauroyl**				
13	Tridecanoyl				
14	**Myristoyl**	Myristoleoyl (9-cis) Myristelaidoyl (9-trans)			
15	Pentadecanoyl				
16	**Palmitoyl**	Palmitoleoyl (9-cis) Palmitelaidoyl (9-trans)			
17	Heptadecanoyl				
18	**Stearoyl**	Petroselinoyl (6-cis) **Oleoyl** (9-cis) Elaidoyl (9-trans)	**Linoleoyl** ((9,12)-cis)		
19	Nonadecanoyl				
20	Arachidoyl	Eicosenoyl (11-cis)		Arachidonoyl ((5,8,11,14)-cis)	
21	Heniecosanoyl				
22	Behenoyl	Erucoyl (13-cis)			Docosahexaenoyl ((4,7,10,13,16,19)-cis)
24	Lignoceroyl	Nervonoyl (15-cis)			

This is the "famous"
Omega−3 fatty acid

Symmetric Fatty Acid lipids: 1,2-Diacyl-*sn*-Glycero-3-Phosphocholine
e.g. 1,2-Dipalmitoyl-*sn*-Glycero-3-Phosphocholine (16:0-PC, DPPC)

Asymmetric Fatty Acid lipids: 1-Acyl-2-Acyl-*sn*-Glycero-3-Phosphocholine
e.g. 1-Palmitoyl-2-Oleoyl-*sn*-Glycero-3-Phosphocholine (16:0-18:1-PC, POPC)

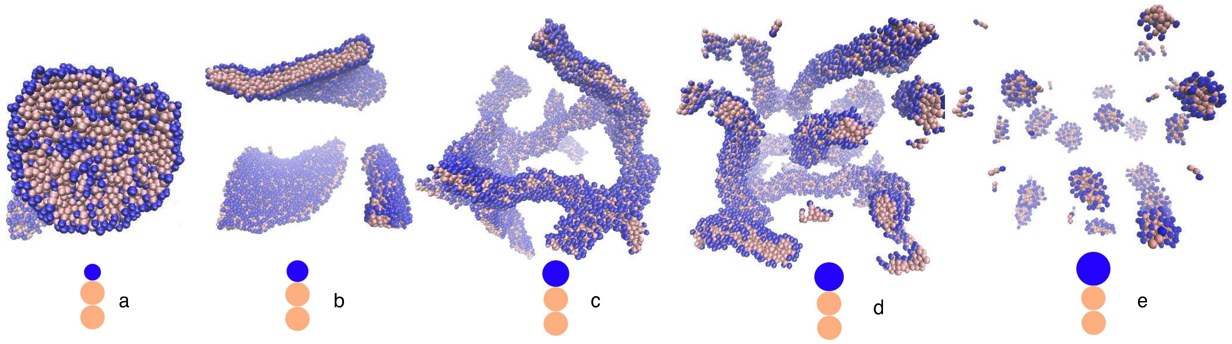


Figure 1: A sequence of aggregate shapes driven by the aspect ratio of a simplified model amphiphile. a) three-dimensional droplet, b) bilayer, c) branched cylindrical micelles, d) unbranched cylindrical micelles, e) spherical micelles. Taken from Ref. [4].

Since we don't want to leave a hole in the inner bit of the micelle, the tail length has to be at least as big as this value, *i. e.* $\ell \geq R_{\text{sphere}}$, which we can write as

$$P := \frac{v}{\ell a} \leq \frac{1}{3} \qquad \text{(spherical aggregates)}\ , \tag{2}$$

where the dimensionless combination P is referred to as the *packing parameter*. This condition says that spherical aggregates form if the packing parameter is smaller than $\frac{1}{3}$.

Let's repeat the same argument with *cylindrical* aggregates of (average) length L. Let's assume that they are long enough such that we can ignore end effects, *i. e.*, $L \gg R$. Now, N amphiphiles forming an aggregate have to satisfy the two conditions $2\pi RL = Na$ and $\pi R^2 L = Nv$, implying by again taking the ratio

$$R_{\text{cylinder}} = \frac{2v}{a}\ . \tag{3}$$

Since again $\ell \geq R_{\text{cylinder}}$ must hold, we find that cylinders form if $P \leq \frac{1}{2}$. But wait, if $P \leq \frac{1}{3}$ we know that spheres form. This tells us that the proper condition for cylindrical aggregates is

$$\frac{1}{3} \leq P \leq \frac{1}{2} \qquad \text{(cylindrical aggregates)}\ . \tag{4}$$

Doing all this again for planar structures, we finally find

$$\frac{1}{2} \leq P \leq 1 \qquad \text{(planar aggregates)}\ . \tag{5}$$

Notice that the packing parameter essentially tells us something about the *aspect ratio* of the amphiphile. A small packing parameter corresponds to "lots of head with little tail", comparable to an ice-cone, where the ball of ice cream is the head and the cone is the tail. Unsurprisingly such amphiphiles would aggregate into spheres. In contrast, large values of the packing parameter look more cylindrical, and it makes sense that such amphiphiles indeed pack in two-dimensional planar aggregates. A sequence of self-assembled aggregate shapes is illustrated in Fig. 1 Notice that lipids typically look cylindrical – and they owe a fair amount of this property to the fact that they have *two* tails.

While the argument sounds irresistibly nice at first sight, it is upon closer inspection not as predictive as it might seem. Suppose you get ambushed by some sinister looking guy in some dark alley at midnight, who forces you at gun-point to tell him the tail volume of, say, DOTAP – what would you say? Getting actual numbers in order to *calculate* P and thus predict the structure is a whole different question, and it shall not be addressed here. However, it should be pointed out that this almost obscenely naive scenario can nevertheless be mapped quantitatively to model lipids for which one would never believe that a simplistic ansatz such as this would lead to anything. The sceptical reader is encouraged to peek into Ref. [4], where it is shown how the sequence from Fig. 1 can be related to P.

2 Membrane elasticity

A physical description of a membrane requires us to know how its *energy* changes when we do something to it. But what can we do that would change the energy? For obvious reasons, overall translations and rotations of a piece of bilayer don't change the energy at all – unless of course there exist external (possibly position dependent) fields that couple to the membrane, and we will assume that this is not the case.

2.1 Stretching and shearing

Classical elasticity theory studies energy changes due to *stretching* or *shearing*, so let's look at such deformations, but *restricted to the membrane plane*.

Stretching does indeed cost energy. Assume that we have a piece of membrane which at zero external stress has an area A_0, and we now stretch it to a size $A > A_0$. To lowest order we can write the energy change as

$$E_{\text{stretch}} = \frac{1}{2} K_{\text{stretch}} \frac{(A - A_0)^2}{A_0} \ , \tag{6}$$

where the modulus K_{stretch} enters as the proportionality constant between a quadratic deviation of the area from its unstressed state and the respective energy. The additional $1/A_0$ is a convention.[1]

What is the lateral stress, the *tension* Σ, under which the membrane is when we subject it to such a strain? Per definition, it is the derivative of energy with respect to area:

$$\Sigma := \frac{\partial E_{\text{stretch}}}{\partial A} = K_{\text{stretch}} \frac{A - A_0}{A_0} =: K_{\text{stretch}} u \ , \tag{7}$$

where we have defined the dimensionless *strain* $u = A/A_0 - 1$. What we have thus recovered is Hooke's law for membrane stretching: Stress is proportional to strain, and the constant of proportionality is the stretching modulus K_{stretch}.

The stretching modulus K_{stretch} can be measured experimentally, for instance in micropipette experiments [8, 19]. There, part of the surface of giant unilamellar vesicles ("lipid-bilayer bubbles in water") is being sucked into much smaller micropipettes, such that the vesicle gets under tension.

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[1] How can physics be a convention? Well, we have not yet specified what exactly we mean by the stretching modulus! You could define your own stretching modulus $K_{\text{alternative}} = K_{\text{stretch}}/A_0$, and end up with an alternative stretching energy $E_{\text{stretch}} = \frac{1}{2} K_{\text{alternative}} (A - A_0)^2$ which of course describes exactly the same physics. However, Eqn. (6) is preferable for reasons that will become clear in a second.

The area change can be measured quite accurately by the amount of membrane which ends up in the micropipette, the tension can be inferred from the vesicle radius and the suction pressure.[2] A linear stress-strain relation is indeed confirmed, and for phospholipid membranes one typically finds values of K_{stretch} around 250 mN/m [19]. Once the membrane stress Σ exceeds a few mN/m, the lipid bilayer suddenly fails and ruptures without much premonition. Using Eqn. (7) we see that the corresponding rupture strain is only of the order of a few percent. So, in that respect membranes are not particularly stretchable.

What about shear? In order to have a relation analogous to Eqn. (7) relating a shear stress with a shear strain, the membrane would of course need to be able to support a shear strain in the first place. However, the fluid lipid bilayers which we will be concerned with here are unable to do this, precisely *because* they are fluid. For the same reason that water does not have a shear modulus, fluid lipid membranes don't.[3] Hence, static shear is no deformation which costs a fluid membrane energy; in fact, it cannot even be *defined*.

2.2 Bending

In a three-dimensional chunk of material small elastic stresses always give rise to small *overall* deformations of the material. This is markedly different if the material is not ‘really” three-dimensional, because it is “thin” in one direction (a plate) or even two directions (a rod). Plates and rods can be *bent* in the directions away from the dimension in which they are extended, and these deformations lead to substantial overall changes in material shape without requiring excessive stresses. We have seen this already for polymers in the context of the wormlike-chain model. The same is true for membranes. On sufficiently large length scales membranes can be considered as essentially two-dimensional surfaces that can be bent into the third dimension.

Characteristically, weak bending is a deformation which costs significantly less energy than stretching. Think of a sheet of paper. Its stretching modulus is extremely high, so you will have a hard time rupturing it by *stretching* rather than *tearing*.[4] Yet, *bending* is something that we can do very easily, because the concomitant local volume strain is very small. Let's see how this works out quantitatively. (The subsequent calculation is a bit simplified, in particular since it neglects issues such as the Poisson ratio, which is defined in Box. 4. The reader will find a more careful treatment in Ref. [15].)

Take a quadratic sheet of paper of side length L and curve it in one direction such that it has a radius of curvature R (see Fig. 2). The outside of the paper is stretched a little bit, while the inside is compressed a little bit. In the middle of the paper will be a region which is not strained at all, the so called *neutral surface*. What is the total stretching energy? If we assume that *locally* the paper material follows a simple elastic relation in analogy to Eqn. (6), namely

$$E_{\text{stretch}} = \frac{1}{2} Y \frac{(V-V_0)^2}{V_0} \qquad \text{(three dimensions, uniaxial extension)}\ , \tag{9}$$

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[2] A spherical surface of radius R and surface tension Σ must have an excess internal pressure P. It can easily be worked out to be $P = 2\Sigma/R$ – a relation known as the Young-Laplace law.

[3] Water has a shear *viscosity*, though, telling us how much stress results from a given shear *rate*. The analogue of this also exists for membranes, but we will not worry about such dynamical phenomena here.

[4] In the paper industry the tensile strength of paper is sometimes quantified by the *breaking length*, which is the maximum length a hanging sheet of paper can have without rupturing under its own weight. Good paper has a breaking length in the range of many *kilometers*. This corresponds to a tensile strength in excess of 10^4 N/m.

Box 4 *(Poisson ratio)*

The Poisson ratio ν quantifies how a uniaxial strain of some material gives rise to a change in sample dimensions *perpendicular* to the direction of strain. For instance, think of a bar of length L and width w which is stretched (or compressed) to a length L' and changes its thickness accordingly to w'. Define $\Delta w = w' - w$, $\Delta L = L' - L$ and the dimensional strain $e = \Delta L/L$. Then the Poisson ratio ν is defined from the equation

$$\frac{\Delta w}{w} = -\nu e \; . \tag{8}$$

For instance, for a perfectly incompressible material we would have $Lw^2 = L'w'^2$, or $Lw^2 = (L+\Delta L)(w+\Delta w)^2$, which up to lowest order in the changes implies $2Lw\Delta w + w^2\Delta L = 0$, from which we readily find $\nu = \frac{1}{2}$, which is indeed the largest value possible.

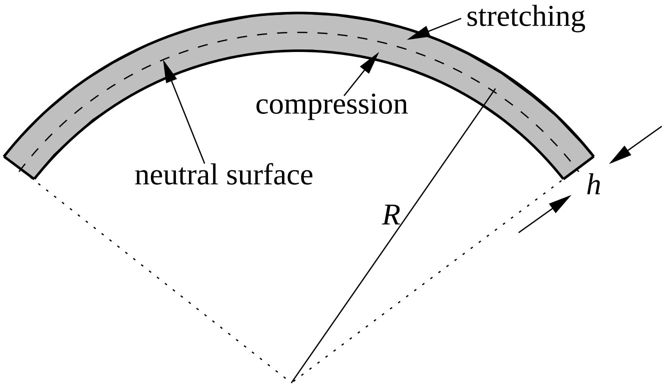

Figure 2: When a piece of material is bent, the outer side is stretched, while the inner side is compressed. Using our knowledge of the elastic behavior, we can thus predict its resistance to *bending*.

where Y is referred to as the *Young modulus* of uniaxial extension (or compression), and when we assume that the paper has a thickness h, then we find the *bending energy per area*

$$\begin{aligned} e_{\text{bend}} &= \frac{E_{\text{bend}}}{L^2} = \frac{1}{L^2}\int_0^L\int_0^L\int_{-h/2}^{h/2}\frac{1}{2}Y\frac{\big((1+\frac{z}{R})\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z - \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z\big)^2}{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z} \\ &= \frac{1}{2}Y\int_{-h/2}^{h/2}\mathrm{d}z\left(\frac{z}{R}\right)^2 = \underline{\underline{\frac{1}{24}Y\frac{h^3}{R^2}}} \; . \end{aligned} \tag{10}$$

Notice the very strong cubic dependence of the bending energy on thickness. If we make our membrane thinner, the bending energy goes down *very* rapidly.

Since bending thus only leads to uniaxial extension (or compression) of the little volume elements within the membrane plane, the three-dimensional modulus Y of uniaxial extension can be re-expressed using the two-dimensional stretching modulus K_{stretch} defined in Eqn. (6), namely by

$$K_{\text{stretch}} = Yh \; , \tag{11}$$

leading to

$$e_{\text{bend}} = \frac{1}{24}K_{\text{stretch}}\left(\frac{h}{R}\right)^2 \; . \tag{12}$$

Now, the ratio h/L can be *very* small indeed, even for significant deformations. A noticeable bending of a piece of paper would have an R of, say, $10\,\text{cm}$, while the thickness h is on the order of $0.1\,$mm, hence $(h/R)^2 \sim 10^{-6}$! Even if the stretching modulus K_{stretch} is very large, this factor reduces the concomitant bending energy down to much smaller values. If you think about it, this is in fact how every spring made out of metal or some other material with a very high Young modulus works.[5]

There is yet a different way in which Eqn. (12) can be written, that makes it look even more similar to expressions such as Eqn. (6). Let us define the *bending modulus* κ according to

$$\kappa := \frac{1}{12} K_{\text{stretch}} h^2 \qquad \text{(single elastic sheet)}\ . \tag{13}$$

Then we can write the bending energy per area as

$$e_{\text{bend}} \ = \ \frac{1}{2}\,\kappa\,\frac{1}{R^2}\ . \tag{14}$$

This looks very much like the bending energy density for a wormlike chain, only that in this case it's meant per area and not per length, and thus the modulus κ has the dimension of an energy and not of an energy times a length. But the spirit is the same: The energy, per area, is locally proportional to the square of the curvature. Quadratic curvature elasticity, again.

It must be pointed out that the relation (14) expresses a level of universality which does *not* hold for the connection between Young modulus and bending modulus, Eqn. (13). The latter ought not to be taken too seriously due to the approximations that went into our calculations (neglect of the Poisson-ratio, certain implicit assumptions about how the stress distributes along the paper cross-section, etc.). Yet, there is one correction to Eqn. (13) that we should still make, since it goes back to a quite fundamental difference between an elastic sheet and a lipid bilayer, namely the fact that the latter of course consists of *two* sheets. If these sheets can laterally move with respect to each other, something which is not too hard to imagine, this has quite dramatic consequences for their extent to resist bending. Technically speaking, a bent elastic sheet has to support shear across its thickness, which is of course how stretching and compression are communicated between outer and inner side. However, if we slice the elastic sheet into two stacked sheets that can slide past each other, no shear can be transmitted between them. Hence, for all intents and purposes bending them is equivalent to independently bend *two* sheets of half the thickness.[6] Let's now look first at Eqn. (10) and ask how the energy changes if we bend two sheets of half the original thickness. First, bending two sheets gives a prefactor of 2. Next, the Young modulus Y is of course independent of sheet thickness, since it is simply a material property. And h would change to $h/2$, so the term h^3 is reduced in magnitude by a factor of 8. All in all we thus see that the bending energy of the double layer is reduced by a factor of 4 compared to a single elastic sheet of the same thickness. Finally, there is no change in Eqn. (11), since stretching involves no sliding. Combining these insights, we arrive at the modified relation between stretching and bending modulus, as it should more likely apply to bilayers:

$$\kappa := \frac{1}{48} K_{\text{stretch}} h^2 \qquad \text{(two uncoupled elastic sheets)}\ . \tag{15}$$

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[5] Steel has a Young modulus of about $10^{10}\,$N/m^2. The bending energy density for a thin steel plate of $0.5\,$mm thickness bent to a radius of curvature of 10 cm is thus $e_{\text{bend}} = \frac{1}{24} \times 10^{10}\,\text{N/m}^2 \times (0.0005\,\text{m})^3/(0.1\,\text{m})^2 = 5.2\,\text{J/m}^2$. This means that we can easily bend samples which are not too large.

[6] Just imagine the following experiment: Take two sheets of paper on top of each other and bend them together, but permit sliding. Now do the same experiment again but this time glue the sheets together at several points. You will readily see that the second arrangement will display a noticeably different bending resistance.

This relation can indeed be found in the literature quite often, and it it sometimes even used to determine the bending modulus by way of measuring K_{stretch}. Yet, we have seen that the derivation of Eqn. (15) still relies on some continuum approximations which may not be very appropriate for actual lipid bilayers. For instance, the regular arrangement of lipids perpendicular to the bilayer plane very vividly illustrates that the "material" is *not* isotropic. Moreover, doing the elastic calculation leading to Eqn. (10) properly [15] shows that there will be an additional factor $1-\nu^2$ in the denominator, where ν is the *Poisson ratio* (see Box 4). The thermodynamically permitted values for the Poisson ratio are $-1 \leq \nu \leq 0.5$, but materials having a negative value (so called "auxetics") are extremely rare. For perfectly incompressible substances $\nu = 0.5$, and most "ordinary" materials have $\nu = 0.3 \ldots 0.5$.[7] Hence, assuming perfect incompressibility, the factor 48 in the denominator is reduced to $48(1-0.5^2) = 36$. Finally, it ought not to be overlooked that it is not entirely obvious which value for h should be used when calculating κ from Eqn. (15) – is it the phosphate-phosphate distance in phospholipids, for instance, or merely the width of the hydrophobic region? Since h enters quadratically, small differences may well matter. We thus see that Eqn. (15) may serve as a reasonable *estimate* for the bending rigidity of a lipid membrane, but ought not to be trusted to within, say, a factor of 2. More reliable experimental approaches avoid the somewhat tricky relation between Young modulus and bending modulus and either directly measure the energy required to impose some bending, or monitor thermal fluctuations opposed by the bending rigidity.

Let us finally ask the question: How big is the bending modulus of membranes? Without even doing a single measurement we can readily determine the order of magnitude: κ has the units of energy. What is the characteristic energy for a structure which emerged from self-assembly? Answer: the thermal energy $k_{\mathrm{B}}T$! In fact, since the structure should have some stability, we expect the modulus to be somewhat bigger than thermal energy. Here's yet a different consideration: The core of lipid membranes consists of dense hydrocarbon chains, and the characteristic length scale is about $5\,\text{nm}$ (the bilayer thickness). This reminds us strongly of typical polymer materials, and we thus expect the Young modulus to be somewhere between rubber and plastic – say $10^7\,\text{N/m}^2$. Using Eqn. (15) with $h = 5\,\text{nm}$, we end up at $\kappa \approx \frac{1}{48} \times 10^7\,\text{N/m}^2 \times (5\,\text{nm})^3 \approx 10^{-19}\,\text{J} \approx 6\,k_{\mathrm{B}}T$. Quite remarkably, this is again fairly close (maybe a bit low) to typical values for phospholipid membranes [16, Chap. 8]. A good rule of thumb is a few tens of $k_{\mathrm{B}}T$, and $20\,k_{\mathrm{B}}T$ usually appears as an agreeable value if one needs to put in some numbers.

Notice that a few tens of $k_{\mathrm{B}}T$ is a very remarkable energy: It is big enough such that the bilayer will not fluctuate into pieces when it is "flapping in the thermal breeze"[8]. Yet it is not outrageously bigger than thermal energy, hence nanoscopic sources of energy (such as ATP molecules, or the energy released by some other self-assembly process of proteins) will be enough to deform the bilayer. Lipid membranes are therefore an *ideal material for nanotechnology*. This sometimes appears not to be fully appreciated by nano-scientists, at least not the ones who haunt us with glossy illustrations that picture shiny stuff made out of metal. However, this wonderful mixture of properties cannot be achieved with metal. Just take Eqn. (13) and turn it around: Require a modulus of $25\,k_{\mathrm{B}}T$, but this time make the material of steel, $Y = 10^{10}\,\text{N/m}^2$. You find a thickness $h = 0.5\,\text{nm}$, and such a thin metal sheet will basically fall apart. One is almost inclined to conclude that nanotechnology is invariably soft matter physics. Well, at least the nanotechnology which

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[7] Cork has a value close to zero, which means that upon lateral extension or compression it does not change its dimensions in the perpendicular direction. This is of course what makes it a useful material to close bottles with.

[8] A phrase coined by David Needham.

Nature has been perfecting since more than 4 billion years is based on soft matter physics.

3 Surface curvature

While we have committed a few crimes of sloppiness that are considered venial sins (at least from the point of view of a soft matter physicist), there is one delicate aspect we have glossed over fairly quickly that really requires a more careful treatment. This is the notion of curvature. While a semiflexible polymer is locally sufficiently well characterized by a single radius of curvature, the same is not true for a membrane. Being a two-dimensional surface, there is an awful lot of weird bending that could be going on at a single point, and we need to look at this in a bit more detail.

Unsurprisingly, the mathematical language in which this is properly discussed is *differential geometry*. Sadly, though, there is a certain "activation barrier" to be overcome before one can really see the elegance and beauty that goes along with such a description, and we do not have the time to master it now. Instead, we will only have a qualitative look at a few general aspects, and then use a specific surface parametrization to write down a few quantitative formulas. A more advanced treatment can be found elsewhere [5, 6, 7, 14].

3.1 Directional curvature and principal curvatures

What is the difference between the curvature of a curve and that of a surface? Consider, for instance, some curved surface, and a curve winding on it. For the sake of a picture, think of it as the path of an all-terrain vehicle in a mountainous environment.[9] The path will not be a straight line. Why? There are two fundamentally different reasons for that. First, the terrain is hilly, so the vehicle will go up and down, and may also get deflected sideways[10] by the curved underground. This is something the driver cannot do anything about, he or she has to live with the terrain that is given. However, the driver could also actively turn the steering wheel, which will give his or her path a curvature that has nothing to do with the local ground conditions. Specifically, it could even lead to a curved path on a completely flat terrain. Hence, when looking at a curve on a surface, one cannot readily identify the curvature of the curve with the curvature of the surface. First one has to disentangle these two different contributions. How does that work?

The trick is to look at two (unit) vectors: One is the local normal vector $\hat{\boldsymbol{n}}$ of the surface, and the other is the principal normal $\hat{\boldsymbol{p}}$ of the curve, *i. e.*, the direction in which the curve locally curves. The key point is that these vectors need not coincide – see Fig. 3 for the following. Think on the one hand of a vehicle driving along the equator of a sphere. The local normal vector of the sphere points locally upward[11], while the principal normal of the curve points towards the center of the sphere. Hence, both vectors are collinear. Indeed, in this situation the driver drives as straight as possible, the steering wheel is not turned at all. Now think on the other hand of a driver driving in a circle on a flat ground. The local normal of the underground points upward, while the principal normal of the driver's path points horizontally towards the center of the circle; the two vectors now make an angle of 90°. In this case the curvature of the driver's path is 100% due to the fact that the steering wheel is turned and has nothing to do with surface curvature (which in this case

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[9] No trees, though. We want a smooth surface!

[10] You don't see how a sideways deviation can occur without turning the wheel? Then think for a minute what the path of the vehicle would look like if it crosses a valley which is deeper to the right than to the left.

[11] Whether it points "upward" or "downward" is a convention we're free to choose for every (orientable) surface.

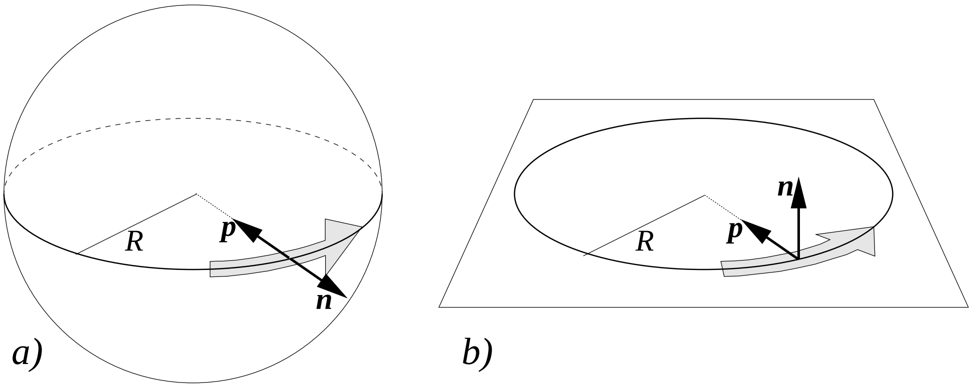

Figure 3: Disentanglement of the curvature of a curve and that of the underlying surface by the angle between the principal normal $\hat{\boldsymbol{p}}$ and the surface normal $\hat{\boldsymbol{n}}$. Both Figures show a circle of radius R and curvature $1/R$. However, in a) this curvature is entirely due to the surface the circle rests on (a car on this path would not have to turn its steering wheel), while in b) the curvature is entirely due to the curve (the driver would have to turn the steering wheel to the left).

is even zero). Indeed, it may be shown that the local *curvature of the curve* multiplied by the *scalar product between the two normal vectors,* $\hat{\boldsymbol{p}} \cdot \hat{\boldsymbol{n}}$*,* is a curvature that no longer depends on any property of the curve, *except its direction* [14].[12] This resulting curvature is called the *directional curvature* or *normal curvature* into the local direction of the curve, and we may write this formally as

$$c_{\text{surface, direction of }\gamma} \;=\; c_{\text{curve }\gamma}\,\hat{\boldsymbol{p}}\cdot\hat{\boldsymbol{n}} \;=\; c_{\text{curve }\gamma}\;\cos\vartheta\;, \tag{16}$$

where ϑ is the angle between $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{n}}$. Incidentally, the combination $c_{\text{curve }\gamma}\;\sin\vartheta$ can be identified as the counterpart of the directional curvature. It is the amount of curvature which is exclusively due to the curve alone, *i. e.*, due to the turning of the steering wheel. It is called the *geodesic curvature*. This completes the disentanglement we have sought for.[13]

At every point a surface thus has a directional curvature in each direction. Since there are infinitely many directions, there may also be infinitely many curvatures. But don't fret, the situation is much less unpleasant than it might initially seem. It turns out that there are always two directions, and they are even orthogonal (but not necessarily unique), in which the directional curvatures are *extremal*. These directions are called *principal directions*, and the corresponding curvatures are called *principal curvatures*. Once we know these directions and the corresponding curvatures, we can calculate *every* directional curvature by means of a formula derived first by Euler [14]:

$$c(\alpha) = c_1 \cos^2\alpha + c_2 \sin^2\alpha\;, \tag{17}$$

where α is the angle between the chosen direction and the principal direction belonging to curvature c_1. It thus suffices to know only two curvatures and maybe some directional information.

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[12] Incidentally, this curvature coincides with the local curvature of the cross-cut curve which originates when we intersect our surface with a plane spanned by the local surface normal and the surface direction in question.

[13] As a side note: Curves on a surface whose geodesic curvature vanishes everywhere are called *geodesics*. These are the generalization of what straight lines are on a plane. On a sphere they are for instance great circles. Fig. 3 also illustrates, how a circle of radius R, which has a simple curvature $1/R$ when viewed as a curve embedded in $\mathbb{R}^3$, can have anything between geodesic curvature 0 – if viewed as a curve on a sphere of radius R (a great circle) – or geodesic curvature $1/R$ – if lying in a flat plane. Geodesics play a fundamental role in General Relativity, since the paths of all particles as well as of light rays are geodesics in spacetime.

Let us finally define two more quantities:

$$\begin{aligned} \text{extrinsic curvature:} \qquad K \;&:=\; c_1 + c_2 \;, && \text{(18a)} \\ \text{Gaussian curvature:} \qquad K_{\rm G} \;&:=\; c_1\, c_2 \;. && \text{(18b)} \end{aligned}$$

Sometimes one also finds $H := K/2$, the so-called *mean curvature*, and in more differential geometry flavored texts one finds $R := 2K_{\rm G}$, the so-called *Ricci scalar curvature*.

3.2 Monge parametrization

It is all well to talk in geometrical terms about surface curvatures. However, what if we want to actually *calculate* them? Well, in this case we first have to solve a more fundamental problem, namely: How do we describe the surface to begin with?

There are many answers to the question of how to describe a surface embedded in three-dimensional space. Some more sophisticated, some less. Some particularly adapted to special symmetries, some not. We will not go into any deeper detail here and rather pick only one particular surface description, the so-called *Monge parametrization*. It is not the most general one, and it is not even the most convenient one for many applications. But it is fair to say that it is the one which one encounters most frequently in the literature. It is suitable for surfaces which on average are horizontal and which don't have any "overhangs". In such a case the surface can evidently be described by specifying its height h above some arbitrarily chosen horizontal reference plane. If $\boldsymbol{r}$ is the two-dimensional position vector in that plane, then $h(\boldsymbol{r})$ is the corresponding height.

We now want to calculate the curvature K within Monge gauge. Box 5 shows a very elementary way for how this is done in one dimension. The calculation for a surface is a fair bit more involved, and it is advisable to use proper differential geometric techniques for its derivation which we do not want to introduce here (see Ref. [6] for more details). However, it turns out that the final formula can be expressed very compactly in a way which resembles the second expression in Eqn. (19). It is given by

$$K = \boldsymbol{\nabla} \cdot \left(\frac{\boldsymbol{\nabla} h(\boldsymbol{r})}{\sqrt{1 + (\boldsymbol{\nabla} h(\boldsymbol{r}))^2}} \right) \overset{|\boldsymbol{\nabla} h| \ll 1}{\approx} \Delta h(\boldsymbol{r}) \;, \tag{20}$$

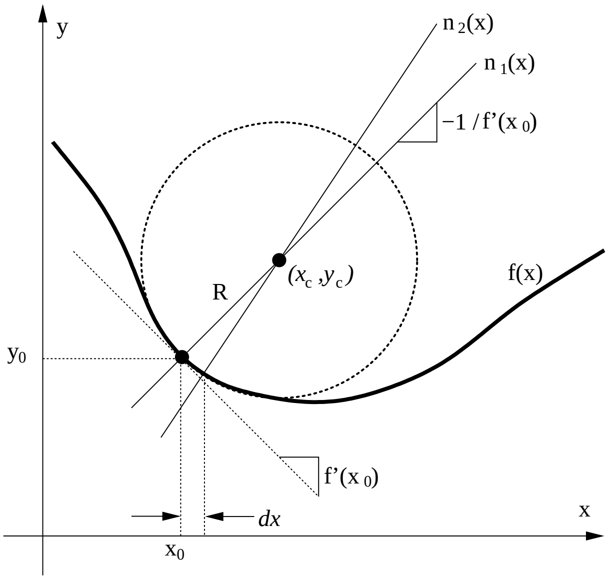
where $\boldsymbol{\nabla}$ and Δ are the nabla- and Laplace-operator *on the base plane*, respectively. The approximation in the second step is evidently good when the gradient term $\boldsymbol{\nabla} h$ has a magnitude small compared to one, and it is thus referred to as the *small gradient approximation*.

It should be remembered, once more, that the *sign* of K is a matter of convention. In the present choice a surface bending "up" has a positive curvature.

4 Helfrich theory

It is time to finally come back to membranes and their curvature elasticity. In this section we want to study the complete version of curvature elasticity, of which we have already seen a preliminary version in the form of Eqn. (14). We then want to look at a few simple consequences that can be derived from this theory.

Box 5 *(Curvature of a planar curve given in Monge parametrization)*



Given a function $f(x)$, we want to determine the local curvature at the point $P = (x_0, f(x_0))$. Let's first find the center of the circle of curvature touching at P. It must lie somewhere on the normal $n_1(x)$ through the point P, which has the equation

$$n_1(x) = f(x_0) - \frac{x - x_0}{f'(x_0)} \equiv f_0 - \frac{x - x_0}{f'_0} \; .$$

If we deviate a tiny bit $\mathrm{d}x$ away from x_0, we can construct a slightly different normal $n_2(x)$. Since we are interested in the touching curvature circle, *all* neighboring normals should to first order in $\mathrm{d}x$ go through the center of the curvature circle touching at P. The equation for such a neighboring normal $n_2(x)$ is

$$n_2(x) \;=\; f(x_0 + \mathrm{d}x) - \frac{x - x_0 - \mathrm{d}x}{f'(x_0 + \mathrm{d}x)} \;\approx\; f_0 + f'_0 \mathrm{d}x - \frac{x - x_0 - \mathrm{d}x}{f'_0 + f''_0 \mathrm{d}x} \; .$$

The x-position x_c of the curvature circle must thus satisfy $n_1(x_\mathrm{c}) = n_2(x_\mathrm{c})$ up to first order in $\mathrm{d}x$. Solving this equation readily leads to the center coordinates

$$x_\mathrm{c} \;=\; x_0 - \frac{f'_0(1 + f'^2_0)}{f''_0} \qquad \text{and} \qquad y_\mathrm{c} \;=\; n(x_\mathrm{c}) \;=\; f_0 + \frac{1 + f'^2_0}{f''_0} \; .$$

Hence, the radius of curvature ρ of the touching curvature circle satisfies

$$\rho^2 = (x_\mathrm{c} - x_0)^2 + (y_\mathrm{c} - f_0)^2 = \frac{(1 + f'^2_0)^3}{f''^2_0} \; ,$$

and the local curvature K at any point with horizontal coordinate x is thus given by

$$K = \frac{1}{\rho} = \frac{f''(x)}{(1 + f'(x)^2)^{3/2}} = \left(\frac{f'(x)}{\sqrt{1 + f'(x)^2}} \right)' \overset{|f'| \ll 1}{\approx} f''(x) \; . \tag{19}$$

4.1 The Helfrich Hamiltonian

We have seen in Sec. 2.2 that the curvature energy density can be written as a bending modulus times the local curvature squared. Since then we have learned a fair bit more about curvature. In which way does this help us to write down a complete energy functional – a Hamiltonian?

In 1970 Canham [3] proposed that we should generalize Eqn. (14) in the following way: $E_\text{bend} = \frac{1}{2}\kappa_1 c_1^2 + \frac{1}{2}\kappa_2 c_2^2$, where the c_i are the principal curvatures and the κ_i the corresponding elastic moduli. However, if the material is *isotropic*, κ_1 and κ_2 should be identical, since bending in the two different directions should not be observable as an energy difference. Canham thus proposed the bending energy density [3]

$$\begin{aligned} e_{\text{bend,Canham}} &= \frac{1}{2}\kappa(c_1^2 + c_2^2) && \text{(21a)} \\ &= \frac{1}{2}\kappa(K^2 - 2K_{\text{G}}) && \text{(21b)} \end{aligned}$$

Still, we clearly have two independent curvatures, wouldn't we also expect two moduli?
In 1973 Helfrich [12] proposed a slightly different energy density:

$$\begin{aligned} e_{\text{bend,Helfrich}} &= \frac{1}{2}\kappa(c_1 + c_2 - c_0)^2 + \bar{\kappa}c_1c_2 && \text{(22a)} \\ &= \frac{1}{2}\kappa(K - c_0)^2 + \bar{\kappa}K_{\text{G}}\ . && \text{(22b)} \end{aligned}$$

It features two moduli, κ and $\bar{\kappa}$, termed the "bending modulus" and the "saddle splay modulus", respectively. It also contains a characteristic curvature c_0, called the "spontaneous curvature". If it is nonzero, this means that the membrane would like to be spontaneously curved into one direction, which is of course only possible if the membrane is not up-down symmetric, *i. e.*, if it has two different sides. This, for instance, occurs when the lipid compositions in the two leaflets is different, as it is frequently the case in biology [16, Chap. 1]. However, in the following we will only look at the simpler cases in which $c_0 = 0$.

We now have two expressions for the energy density. Which one is right? As it turns out, the answer is that in most cases *both are right*. How can that be – they clearly look different! The answer is that there exists a subtle and beautiful theorem from differential geometry – called the Gauss-Bonnet-Theorem – which states that the surface integral over the Gaussian curvature K_{G} can be written as a boundary term[14] and a topological constant [5, 7, 14]. But since the total membrane energy of course involves a surface integral over (21) or (22), the K_{G} terms in these equations will both only lead to constants which don't influence the subsequent physics. And what remains – in the case $c_0 = 0$ – is in both cases $\frac{1}{2}\kappa K^2$. So modulo boundary terms both Hamiltonians agree – and indeed only one relevant[15] elastic constant appears. However, the Helfrich expression is usually preferred over Canham's equation, because it nicely singles out the Gaussian curvature – which, as we have just seen, has this Gauss-Bonnet specialty.

So, let us for completeness write down the total bending energy of a symmetric membrane in the Helfrich picture:

$$E_{\text{bend}} = \int_{\text{membrane}} \mathrm{d}A \left\{ \frac{1}{2}\kappa K^2 + \bar{\kappa}K_{\text{G}} \right\}\ . \tag{23}$$

The integral extends over the entire membrane, and $\mathrm{d}A$ is the area element *on the membrane*. Box 6 explains that in Monge parametrization it is given by $\mathrm{d}A = \mathrm{d}x\,\mathrm{d}y\sqrt{1 + (\boldsymbol{\nabla}h)^2}$.

In small gradient approximation $\mathrm{d}A = (1 + \frac{1}{2}(\boldsymbol{\nabla}h)^2)\mathrm{d}x\,\mathrm{d}y$. Hence, if we also want to add a term which penalizes *area increase* due to the curving of the surface, it would enter in small gradient approximation by a density $\frac{1}{2}\Sigma(\boldsymbol{\nabla}h)^2$, where Σ is the surface tension. Hence, in this approximation the Helfrich Hamiltonian – including bending and tension, and excluding the Gaussian term – can

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[14] This boundary term involves the *geodesic curvature*.

[15] This is really a bit simplified. There are of course instances where boundary and/or topology changes occur, and then $\bar{\kappa}$ also plays a role. For a nice example, see Ref. [1].

Box 6 *(Area element in Monge parametrization)*

Take some point P on a surface with coordinates $(x, y, h(x, y))$. A point P_x a distance $\mathrm{d}x$ in x-direction has the coordinates $(x + \mathrm{d}x, y, h(x + \mathrm{d}x, y)) \approx (x + \mathrm{d}x, y, h(x, y) + h_x(x, y)\mathrm{d}x)$, where $h_x = \partial h/\partial x$. So the vector $\overrightarrow{PP_x}$ from P to P_x is approximately $(1, 0, h_x)\mathrm{d}x$. We can do the same consideration for a point P_y a distance $\mathrm{d}y$ in y direction. The vectors $\overrightarrow{PP_x}$ and $\overrightarrow{PP_y}$ span a little parallelogram, whose area is equal to the modulus of the cross product between these vectors. Since

$$\begin{pmatrix} 1 \\ 0 \\ h_x \end{pmatrix} \mathrm{d}x \;\times\; \begin{pmatrix} 0 \\ 1 \\ h_y \end{pmatrix} \mathrm{d}y \;=\; \begin{pmatrix} -h_x \\ -h_y \\ 1 \end{pmatrix} \mathrm{d}x\,\mathrm{d}y \;,$$

we thus obviously get

$$\mathrm{d}A \;=\; \left|\overrightarrow{PP_x} \times \overrightarrow{PP_y}\right| \;=\; \sqrt{1 + h_x^2 + h_y^2}\,\mathrm{d}x\,\mathrm{d}y \;=\; \sqrt{1 + (\boldsymbol{\nabla} h)^2}\,\mathrm{d}x\,\mathrm{d}y \;.$$

be written as

$$\underline{\underline{E_{\text{bend}} \;=\; \frac{1}{2}\int_{\text{base plane}} \mathrm{d}x\,\mathrm{d}y \left\{\kappa(\Delta h)^2 + \Sigma(\boldsymbol{\nabla} h)^2\right\}}} \;. \tag{24}$$

It is this form in which one probably finds the Helfrich Hamiltonian most often. But recall that in this version it is already a small gradient approximation.

4.2 The shape equation of linear theory

Assume that we have an essentially flat membrane, which is here or there perturbed in such a way that it slightly deviates from its flat state, in which it evidently would have the lowest energy – namely zero. The membrane will try to assume a shape in which the resulting energy, even though not zero, is at least as small as possible. Which shape does the membrane therefore have to assume?

4.2.1 Variation of the energy functional

The question we just encountered is a classical problem from the *calculus of variations*. Given a (scalar) expression – here the energy E – which depends on a whole function – here some integral over differentiated terms of the shape function h – find that function which minimizes the scalar expression. This is not nearly as complicated as it seems, one only has to proceed patiently.

Let's assume we perform a small variation of the height function, according to

$$h(x, y) \longrightarrow h(x, y) + \delta h(x, y) \;. \tag{25}$$

What is the concomitant change in the bending energy? Using Eqn. (24), and working only in first order of the small quantity δh, we can calculate

$$\begin{aligned} \delta E_{\text{bend}} &= \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\,\Big\{\kappa(\Delta h + \Delta\delta h)^2 + \Sigma(\boldsymbol{\nabla} h + \boldsymbol{\nabla}\delta h)^2\Big\} - \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\,\Big\{\kappa(\Delta h)^2 + \Sigma(\boldsymbol{\nabla} h)^2\Big\} \\ &= \int \mathrm{d}x\,\mathrm{d}y\,\Big\{\kappa\Delta h\,\Delta\delta h + \Sigma\boldsymbol{\nabla} h\cdot\boldsymbol{\nabla}\delta h\Big\} \\ &= \int \mathrm{d}x\,\mathrm{d}y\,\Big\{\kappa\Big[\boldsymbol{\nabla}\cdot(\Delta h\boldsymbol{\nabla}\delta h) - (\boldsymbol{\nabla}\Delta h)\cdot\boldsymbol{\nabla}\delta h\Big] + \Sigma\Big[\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla} h\delta h) - (\Delta h)\delta h\Big]\Big\}\,. \end{aligned} \tag{26}$$

In the last step we have created two divergence terms, $\boldsymbol{\nabla}\cdot(\text{some vector})$. We will later turn them into boundary terms with the help of the divergence theorem. The whole point of this exercise is to get rid of terms which contain derivatives of δh in the integral. (As we'll see soon, we don't mind these derivatives in the boundary terms). Since there is one more none-divergence-term containing a derivative of δh, let's repeat this trick once more:

$$\begin{aligned} \delta E_{\text{bend}} &= \int \mathrm{d}x\,\mathrm{d}y\,\Big\{-\kappa(\boldsymbol{\nabla}\Delta h)\cdot\boldsymbol{\nabla}\delta h - \Sigma(\Delta h)\delta h \;+\; \boldsymbol{\nabla}\cdot\Big[\kappa\Delta h\boldsymbol{\nabla}\delta h + \Sigma\boldsymbol{\nabla} h\delta h\Big]\Big\} \\ &= \int \mathrm{d}x\,\mathrm{d}y\,\Big\{-\kappa\Big[\boldsymbol{\nabla}\cdot\big((\boldsymbol{\nabla}\Delta h)\cdot\delta h\big) - (\Delta\Delta h)\,\delta h\Big] - \Sigma(\Delta h)\delta h \\ &\qquad\qquad + \boldsymbol{\nabla}\cdot\Big[\kappa\Delta h\boldsymbol{\nabla}\delta h + \Sigma\boldsymbol{\nabla} h\delta h\Big]\Big\} \\ &= \int \mathrm{d}x\,\mathrm{d}y\,\Big\{\Big[\kappa\,\Delta\Delta h - \Sigma\,\Delta h\Big]\,\delta h \;+\; \boldsymbol{\nabla}\cdot\Big[\Big(\kappa\Delta h\Big)\boldsymbol{\nabla}\delta h + \Big(\Sigma\boldsymbol{\nabla} h - \kappa\boldsymbol{\nabla}\Delta h\Big)\delta h\Big]\Big\} \\ &= \int \mathrm{d}x\,\mathrm{d}y\,\Big[\kappa\,\Delta\Delta h - \Sigma\,\Delta h\Big]\,\delta h \\ &\qquad + \oint \mathrm{d}s\,\boldsymbol{l}\cdot\Big[\Big(\kappa\Delta h\Big)\boldsymbol{\nabla}\delta h + \Big(\Sigma\boldsymbol{\nabla} h - \kappa\boldsymbol{\nabla}\Delta h\Big)\delta h\Big]\,. \end{aligned} \tag{27}$$

In the last step we finally used the divergence theorem and rewrote the area integral over $\boldsymbol{\nabla}\cdot(\text{some vector})$ as a closed line integral along the curve surrounding the area we originally integrated over. With $\boldsymbol{l}$ we denote the unit vector which lies in the x-y-plane and locally points *perpendicular* to the curve encircling the (projected) membrane area and is directed *outward*[16].

Recall that for a stationary solution we want $\delta E_{\text{bend}} = 0$. This means that *both* the area integral as well as the line integral have to vanish. Let's look at the area integral first. Since the variation $\delta h(x,y)$ was a completely arbitrary function (well, small and differentiable, but arbitrary otherwise), the above calculation tells us that the term in square brackets has to vanish. This gives us a *differential equation* – the so-called Euler-Lagrange equation – which h has to satisfy in the lowest energy state:

$$\kappa\,\Delta\Delta h - \Sigma\,\Delta h \;=\; 0\,. \tag{28a}$$

This is a fourth order linear partial differential equation. It is called the *shape equation*. By introducing the length $\lambda := \sqrt{\kappa/\Sigma}$, we can also rewrite it as

$$\Delta(\Delta - \lambda^{-2})\,h \;=\; 0\,. \tag{28b}$$

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[16] We assume orientability here, which is not trivial. However, we do not want to potter around with technicalities.

	“direct” boundary condition	“alternative” boundary condition
first condition	fix h	require $(\Delta - \lambda^{-2})\nabla_\perp h = 0$
second condition	fix $\nabla_\perp h$	require $\Delta h = 0$

Table 1: Possible choices of boundary conditions for the differential equation (28). For each of the two rows *one* condition needs to be fulfilled. Recall the definition of the normal derivative at the boundary, $\nabla_\perp = \boldsymbol{l} \cdot \boldsymbol{\nabla}$.

Since the operators Δ and $\Delta - \lambda^{-2}$ evidently commute, the differential equation (28) is solved by their eigenfunctions to the eigenvalue 0. This is a neat little insight, because it means that we only have to look for solutions of *two second order* differential equations. But finding these functions is only a part of the problem, often the easier one. What may turn out to be a real pain is getting the *boundary conditions* right.

4.2.2 Boundary conditions

Speaking of boundary conditions – where do they come from? Well, we still have the boundary integral which has to vanish, too! How can we make sure that this happens? Looking at the boundary term in Eqn. (27) we see that one way is for instance to demand that both the variation δh as well as the normal component of its gradient, $\boldsymbol{l} \cdot \boldsymbol{\nabla}\delta h =: \nabla_\perp \delta h$, vanishes everywhere on the boundary. If we do not permit these two to vary, this basically means that we want them to always have specific values for all possible surfaces we “test out” in the functional variation. In other words, *we fix h and $\nabla_\perp h$ at the boundary* and have thus found a permissible set of boundary conditions! However, this recipe is not the *only* possibility by which we can ensure that the boundary integral vanishes. For instance, we might alternatively decide not to fix the value of $\nabla_\perp h$ and can still make the boundary integral vanish if we instead demand that the expression by which it is multiplied, namely Δh, vanishes everywhere on the boundary. Or we might permit the height h to vary and rather set its prefactor to zero, giving the condition $\Sigma \nabla_\perp h = \kappa \nabla_\perp \Delta h$. These possibilities are summarized in Table 1.

If you have never encountered this line of reasoning, you might be a bit shocked here. Regrettably often the treatment of variational problems (which you may or may not have come across before) blissfully ignores the boundary terms. One typically finds either the statement “we push the boundaries to infinity” (as if it’s always clear that they would not pick up some contribution there) or the disarmingly honest phrase “we assume the boundary terms to vanish”. What is missed in this sloppy way is the quite beautiful insight that *the requirement of vanishing boundary terms gives us the appropriate boundary conditions*! Since there are indeed cases where it is not at all clear what the correct conditions would be, this formal route may even be extremely valuable.

4.2.3 A few worked out examples

Before things get too abstract it is recommendable to take a step back and look, what we have accomplished and what we can do with it. This section works out a few examples of shape determination that illustrate how the shape equation (28) and the corresponding boundary conditions from Table 1 are used. Not all examples are directly related to fluid membranes. However, now

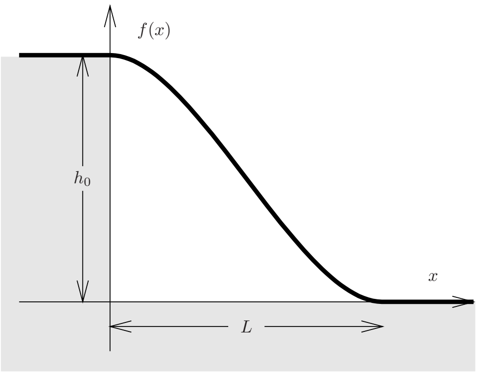

Figure 4: A fluid membrane is laid over a step edge of height h_0 and attaches a distance L away from the edge to the lower-level substrate. What is the shape the membrane will assume?

that we have understood how to handle bending problems, we might just as well have a bit more fun with it.

1. Membrane spread over a step-edge

Assume we want to calculate the shape of a membrane that smoothly covers a step-edge of height h_0 and touches the lower level a distance L away, as illustrated in Fig. 4. Since the membrane shape changes only in x-direction, we have a one-dimensional problem, *i. e.*, a function $f(x)$ to find, and the Laplacian Δ is simply equal to the second derivative $\mathrm{d}^2/\mathrm{d}x^2$. Two independent eigenfunctions belonging to the eigenvalue 0 are 1 and x, and for the eigenvalue λ^{-2} we conveniently take $\cosh(x/\lambda)$ and $\sinh(x/\lambda)$. The shape equation (28) becomes $f''''(x) - f''(x)/\lambda^2 = 0$, and defining the scaled variables $\tilde{x} := x/\lambda$ and $\ell := L/\lambda$, we can write its general solution as

$$f(x) = A + B\tilde{x} + C\,\cosh(\tilde{x}) + D\,\sinh(\tilde{x})\ , \tag{29}$$

where the integration constants $A \ldots D$ are determined by the four obvious boundary conditions

$$\begin{aligned} h_0 &= \quad f(0) = A + C\ , && (30a)\\ 0 &= \quad f'(0) = B + D\ , && (30b)\\ 0 &= \quad f(L) = A + B\ell + C\,\cosh(\ell) + D\,\sinh(\ell)\ , && (30c)\\ \text{and}\qquad 0 &= \lambda\, f'(L) = B + C\,\sinh(\ell) + D\,\cosh(\ell)\ . && (30d)\end{aligned}$$

From Eqn. (30a) follows $A = h_0 - C$, and from Eqn. (30b) follows $B = -D$. Inserting this into the remaining two equations (30c) and (30d) yields a simple matrix equation for C and D,

$$\begin{pmatrix} \cosh(\ell) - 1 & \sinh(\ell) - \ell \\ \sinh(\ell) & \cosh(\ell) - 1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} -h_0 \\ 0 \end{pmatrix}\ , \tag{31}$$

which can be readily solved by matrix inversion. We thus find the solution of our shape problem. It can be expressed in the following way – not fully simplified, but this way it's a bit more revealing:

$$\begin{aligned} \frac{f(x)}{h_0} &= 1 - \frac{\big[\cosh(\ell) - 1\big]\big[\cosh(\tilde{x}) - 1\big] - \sinh(\ell)\big[\sinh(\tilde{x}) - \tilde{x}\big]}{\big[\cosh(\ell) - 1\big]\big[\cosh(\ell) - 1\big] - \sinh(\ell)\big[\sinh(\ell) - \ell\big]} && (32a)\\ &\overset{\Sigma\to 0}{=} 1 - 3\left(\frac{x}{L}\right)^2 + 2\left(\frac{x}{L}\right)^3\ . && (32b)\end{aligned}$$

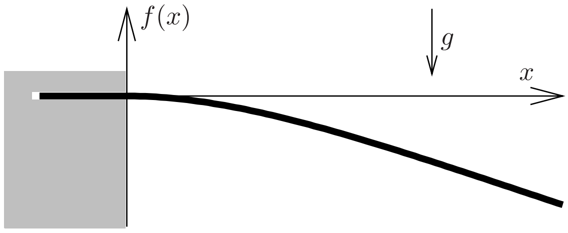

Figure 5: Illustration of the shape of an elastic sheet which is clamped horizontally at one end and hangs under its own weight.

For $\Sigma > 0$ there are two characteristic length scales in the problem: λ and L, and the shape looks qualitatively different depending on which of these two is the bigger one, *i. e.*, depending on whether ℓ is small or large compared to 1, as the interested reader might want to check.

What determines L? In the simplest case the substrate becomes "sticky" a distance L away from the step and pins the membrane there. A more complicated situation arises when the substrate has a uniform adhesion energy w per area, and the membrane can *decide* at which distance L to detach. For small L much adhesion energy will be gained, but the membrane has to bend a lot. Conversely, if L is chosen very large, bending will be weak, but a lot of adhesion energy is sacrificed. At some optimal distance the energy is minimal. It can be shown [15, §12, prob. 6] that this leads to another boundary condition – this time for the *moving boundary* L – that in the present situation reads $f''(L) = 1/\rho_{\rm c}$, where $\rho_{\rm c} = \sqrt{\kappa/2w}$ is the contact radius of curvature. Using Eqn. (32b) this results in the transcendental equation $\ell \coth\frac{\ell}{2} - 2 = h_0\rho_{\rm c}/\lambda^2$ for ℓ, whose solution is easily determined numerically. For $\Sigma \to 0$ (*i. e.* $\lambda \to \infty$) it can be solved exactly: $L = \sqrt{6h_0\rho_{\rm c}}$.

2. Paper bending under its own weight

Assume you have a strip of paper which you hold horizontally. Under its own weight it will bend down, as illustrated in Fig. 5. Which shape will the paper take?

Since the strip only bends because its weight pulls it down, gravity must somehow be included. How is that done? The easiest way is to again start with the functional. Let's say the strip has a width w, a length L, and a mass per unit area of ρ. Describe its location by the function $f(x)$. Then the energy of the bent piece of paper is given by

$$E \;=\; w\int_0^L {\rm d}x\,\left\{\frac{1}{2}\kappa\big(f''(x)\big)^2 + \rho g f(x)\right\}\,. \tag{33}$$

Notice that we have cheated slightly: If the projected length of the strip is L, then its actual length is generally longer. In other words, the integral shouldn't really go up to L. However, for small bending this is an effect of higher order which we will ignore here.[17]

We first need to do the variation of this functional. Now, the first term we know how to deal with, and the second term is extremely easy: The variation of $f(x)$ is $\delta f(x)$ and that's that. Hence, we end up at the shape equation $\kappa f''''(x) + \rho g = 0$, or in a nicer way:

$$f''''(x) + \ell^{-3} \;=\; 0 \qquad \text{with} \quad \ell^3 = \frac{\kappa}{\rho g}\,, \tag{34}$$

where we introduced the length ℓ for convenience. This is a fourth order linear inhomogeneous differential equation. The solution of the homogeneous equation $f''''(x) = 0$ can be written as

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[17] One has to be careful with such approximations, though: For the case of Euler buckling, to be discussed in Example 3, this difference between total length and projected length makes all the difference in the world.

$a + bx + cx^2 + dx^3$, and an obvious particular solution is $f(x) = -x^4/(24\ell^3)$. Hence, the general solution is

$$f(x) = a + bx + cx^2 + dx^3 - \frac{1}{24\ell^3}x^4 \ . \tag{35}$$

Two boundary conditions are obvious, namely $f(0) = 0$ (from which follows $a = 0$) and $f'(0) = 0$ (from which follows $b = 0$). However, neither f nor f' have any obvious values at the other end of the strip. But peaking at Table 1, we see that since these values are unspecified, we rather have to demand $f''(L) = 0$ and $f'''(L) = 0$ (recall that $\Sigma = 0$ here).[18] The latter condition gives $d = L/(6\ell^3)$, which together with the former leads to $c = -L^2/(4\ell^3)$. If we define the scaled variables $\tilde{f} = f/L$, $\tilde{\ell} = \ell/L$, and $\tilde{x} = x/L$, we see that the final solution can be written as

$$\tilde{f}(\tilde{x}) \ = \ -\frac{\tilde{x}^4 - 4\tilde{x}^3 + 6\tilde{x}^2}{24\tilde{\ell}^3} \ . \tag{36}$$

Up to a scaling prefactor the shape of the solution is thus always the same, unlike in the case of the membrane spreading over a step edge in Example 1, where a second length scale existed, λ, and its relation to the length L mattered beyond a simple amplitude scaling.
The solution (36) in particular shows that the total sag of the strip is $\tilde{f}(1) = -(2\tilde{\ell})^{-3}$, or

$$|f(L)| \ = \ \frac{L^4}{8\ell^3} \ = \ \frac{\rho g L^4}{8\kappa} \ . \tag{37}$$

This relation is quite interesting, since it permits the determination of the bending modulus of paper from a fairly simple measurement. Moreover, using the relation between stretching modulus K_{stretch} and bending modulus κ of an isotropic elastic sheet, as worked out earlier, we obtain an estimate of the stretching modulus of paper:

$$K_{\text{stretch}} \ \overset{(13)}{=} \ \frac{12\kappa}{h^2} \ = \ \frac{3\rho g L^4}{2|f(L)|h^2} \ , \tag{38}$$

where h is the thickness of the paper. Let's think of a typical paper with $\rho = 80\,\text{g/m}^2$ and $h = 0.1\,\text{mm}$. If we let a strip of $L = 10\,\text{cm}$ hang over the edge of a table, it would droop down by maybe $2\,\text{cm}$. Hence, the stretching modulus is

$$K_{\text{stretch}} \ \approx \ \frac{3 \times 0.08\,\frac{\text{kg}}{\text{m}^2} \times 10\,\frac{\text{N}}{\text{kg}} \times (0.1\,\text{m})^4}{2 \times 0.02\,\text{m} \times (0.0001\,\text{m})^2} \ \approx \ 0.6 \times 10^6\,\frac{\text{N}}{\text{m}} \ . \tag{39}$$

3. Euler buckling

Take a slender elastic rod. Under which compressional force will it buckle?
Assuming that such a rod is again described by curvature elasticity (just as the strip of paper in the previous problem was), we will approach the problem in two steps. We first ask ourselves: What is the bending energy of such a rod of length L, if its ends are forced to a separation $L' = L - \Delta L < L$ (see Fig. 6). In a second step we will then change to an ensemble where this compression is achieved by an externally applied force.

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[18] Notice that this is a perfect example for the occurrence of the less-than-obvious boundary conditions which nevertheless follow easily from the boundary terms of the full variation.

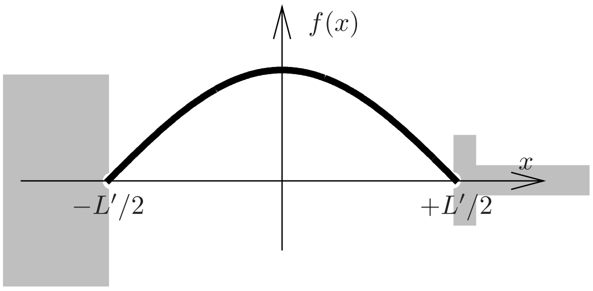

Figure 6: An elastic rod of length L is compressed such that its end-to-end distance shrinks to $L' = L - \Delta L < L$ and consequently buckles perpendicular to the direction of compression. Notice that the rod ends are fixed, but their terminal direction is not (*i. e.*, the ends are *not* clamped). The compression in the picture is $\delta = \Delta L/L = 0.2$.

For the energy we may thus use the curvature elastic formula we've gotten used to by now:[19]

$$E \;=\; \int_{-L'/2}^{L'/2} \mathrm{d}x \, \frac{1}{2}\kappa\big(f''(x)\big)^2 \, . \tag{40}$$

We would like to minimize this functional, subject to the constraint that the *total length* of the rod has the fixed value L, or in other words, that the amount of compression, ΔL, is given. As usual, this constraint can be fixed by a Lagrange multiplier, say Σ, and so we have to minimize the constrained functional

$$E' \;=\; \int_{-L'/2}^{L'/2} \mathrm{d}x \, \left\{ \frac{1}{2}\kappa\big(f''(x)\big)^2 - \Sigma\Big[\frac{1}{2}\big(f'(x)\big)^2 - \frac{\Delta L}{L'}\Big] \right\} . \tag{41}$$

This expression looks basically like our shape functional from Eqn. (24), with two apparent differences: First, there is one more constant term in the functional. This of course we need not worry about (who cares about a constant in the energy?). And second, the sign in front of the $\big(f'(x)\big)^2$-term is *negative*. Why is that so? The boring answer is: There is absolutely no physical significance to this sign! The entire term is multiplied by the Lagrange multiplier Σ, whose value – and thus sign! – needs to be determined later from the constraint. Here we write it with a minus sign as this will turn out to be more "convenient". Had we chosen a positive sign instead, the final result would follow identically, albeit with one more twist in thinking, as we will see soon.

Minimizing E at constant L means minimizing E', *i. e.* solving the Euler-Lagrange-equation belonging to the functional (41). With a glance at Eqn. (28) we see that this equation will be

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{\lambda^2}\right) f(x) \;=\; 0 \, , \tag{42}$$

where we again introduced $\lambda = \sqrt{\kappa/\Sigma}$ and where the plus-sign stems from the sign difference just mentioned. Once more, the general solution is given by the eigenfunctions of the two commuting second order operators belonging to the eigenvalue 0, into which the above fourth order differential operator conveniently factorizes, so we can readily write it down:

$$f(x) \;=\; a + bx + c\cos\frac{x}{\lambda} + d\sin\frac{x}{\lambda} \, . \tag{43}$$

Guessing (correctly) that the (lowest order) buckling will lead to a symmetric situation as depicted in Fig. 6, we see that b and d have to be zero. Making $h(L'/2) = 0$ then leads to

$$f(x) \;=\; c\left(\cos\frac{x}{\lambda} - \cos\frac{L'}{2\lambda}\right) . \tag{44}$$

---

[19] Notice that in this case κ is a bending energy per unit *length* rather than per unit *area* for obtaining a certain radius of curvature. Therefore, κ has units of *energy times length* here.

What is the second boundary condition? As Fig. 6 suggests, we imagine a situation in which the ends of the rod are merely compressed but *not* clamped, *i. e.*, we don't hold them at some particular angle. Hence, $h'(\pm L'/2)$ is not predetermined, and the boundary conditions collected in Table 1 then show that we have to require the second derivative to vanish at the two ends:

$$0 \;=\; f''(\pm L'/2) \;=\; (-)\frac{c}{\lambda^2}\cos\frac{L'}{2\lambda}\,. \tag{45}$$

This equation is of course satisfied for $c = 0$, *i. e.* for the flat rod, but it is also satisfied when the argument of the cosine takes on the specific values

$$\frac{L'}{2\lambda} \;=\; \frac{\pi}{2} + n\pi \qquad n = 0, 1, 2, \ldots \tag{46}$$

It may be checked that the value $n = 0$ is the one we're looking for.[20] Hence we have

$$\lambda \;=\; \frac{L'}{\pi}\,. \tag{47}$$

Notice: Had we *not* changed the sign in front of our Lagrange parameter term in the constrained buckling functional (41) from $+$ to $-$, we would have obtained $\cosh$ and $\sinh$ as our solutions rather than $\cos$ and $\sin$. Instead of the condition (45) we then would have to find solutions of $(c/\lambda^2)\cosh(L'/(2\lambda)) = 0$, which at first sight only seems to work for $c = 0$, since $\cosh(x) \geq 1$ for all x. Right? No, wrong: $\cosh(x)$ can become zero, if its argument is *imaginary*! And since $\cosh(\mathrm{i}x) = \cos(x)$ this would then lead straight back to Eqn. (45), *i. e.*, of course the same physics. We should have been prepared for that, because λ contains the *square root* of our Lagrange multiplier Σ, and if for some reason Σ would "want" to be negative, this happens. Well, it happens here. And this "complex detour" is avoided by taking the minus sign out up front – something one either has to learn by going through the calculation once and stumble over this problem, or by thinking about it physically (as we'll do below).

Combining Eqn. (47) with the rod shape from Eqn. (44), we see that $f(0) = c$, which means that the remaining integration constant c is nothing but the *amplitude* by which the rod buckles out.

We finally need to impose the condition of constant rod length. This is easily done by working out the total length of the compression and requiring it to be ΔL:

$$\Delta L = \int_{-L'/2}^{L'/2}\mathrm{d}x\;\frac{1}{2}\big(f'(x)\big)^2 = \int_0^{L'/2}\mathrm{d}x\;\Big(\frac{c}{\lambda}\sin\frac{x}{\lambda}\Big)^2 = \Big(\frac{c}{\lambda}\Big)^2\underbrace{\int_0^{L'/2}\mathrm{d}x\;\sin^2\frac{\pi x}{L'}}_{=L'/4} \overset{(47)}{=} \frac{\pi^2 c^2}{4L'}\,, \tag{48}$$

from which we get the buckling amplitude

$$c \;=\; \pm\frac{2}{\pi}\sqrt{L'\Delta L}\,. \tag{49}$$

Of course, the *sign* of c is still unknown, because we can't tell energetically whether the rod buckles up or down (or, as a matter of fact, in *any* direction perpendicular to the line joining the ends). Let's just choose $c > 0$ for definiteness.

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[20] The other values correspond to shapes which are "multiply buckled", *i. e.*, they have more "waves" in it. Yet, $n = 1$ is not the next order buckle. Why? Because the next order one has an *antisymmetric* shape and would correspond to the solution $\sin(x/\lambda)$ which we had eliminated above for reasons that now don't apply.

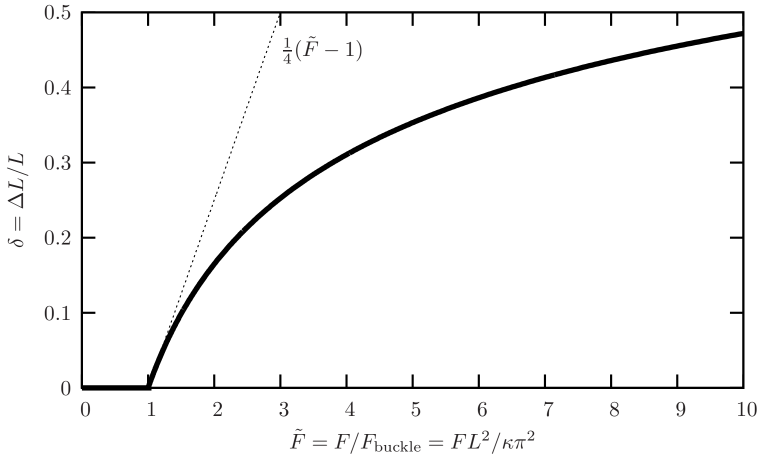

Figure 7: Stress-strain relation (53) for an elastic rod under compression.

Now that we know the shape, we can calculate the energy of the buckled rod:

$$E = \int_{-L'/2}^{L'/2} \mathrm{d}x \, \frac{1}{2}\kappa\big(f''(x)\big)^2 = \kappa \int_0^{L'/2} \mathrm{d}x \, \left(\frac{d}{\lambda^2}\cos\frac{x}{\lambda}\right)^2 = \frac{\kappa\pi^2\Delta L}{(L-\Delta L)^2} = \frac{\kappa\pi^2}{L}\,\frac{\delta}{(1-\delta)^2}\,, \tag{50}$$

where we introduced the scaled compressional strain $\delta = \Delta L/L$. This energy initially grows linearly with compression, but later it increases more strongly.

It is now time to think about the compression *force*. We have so far looked at the situation in an "ensemble" of constant *compression* (*i. e.*, *strain*) and would now like to change to an ensemble of constant *force* (*i. e.*, *stress*). As usual, this is accomplished by a Legendre transformation:

$$G(F) \;=\; \min_{\Delta L}\Big\{E(\Delta L) - F\,\Delta L\Big\} \;=\; \frac{\kappa\pi^2}{L}\min_{\delta}\Big\{\frac{\delta}{(1-\delta)^2} - \tilde{F}\delta\Big\}\,, \tag{51}$$

where we introduced the scaled force

$$\tilde{F} \;=\; \frac{FL^2}{\kappa\pi^2}\,. \tag{52}$$

Doing the minimization, we see that we have to solve the equation[21]

$$\frac{(1-\delta)^2 + 2\delta(1-\delta)}{(1-\delta)^4} - \tilde{F} \;=\; 0 \qquad \text{or} \qquad \tilde{F} \;=\; \frac{1+\delta}{(1-\delta)^3} \;=\; 1 + 4\delta + 9\delta^2 + 16\delta^3 + \cdots \tag{53}$$

This stress-strain relation is illustrated in Fig. 7. A positive compression $\delta > 0$ requires a (scaled) compression force $\tilde{F} \geq 1$. The initial stress-strain relation is *not* simply linear. One has to overcome a certain minimal force – the buckling force – before the rod will deflect:

$$F \;\geq\; F_{\text{buckle}} \;=\; \frac{\kappa\pi^2}{L^2}\,. \tag{54}$$

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[21] Of course, we might have guessed Eqn. (53) right away – it is nothing but a statement of the "obvious" fact that $F = \partial E/\partial\Delta x$. In some sense, the Legendre trafo shows, why this "obvious" fact indeed holds.

Eqn. (50) and its initial linear energy-compression relation shows rather vividly how strongly nonharmonic Euler buckling is. For a usual harmonic energy, *i. e.* $E \propto (\Delta x)^2$, the force would (linearly) go to zero as the compression goes to zero. Not so here: In the limit of vanishing compression a *finite* force remains, the buckling force, which – conversely – first needs to be overcome in order to compress the rod. Notice also that after F_{buckle} is exceeded the resulting deflection is quite finite. The rod does of course *not* catastrophically fail once the buckling limit is exceeded.

This scenario looks a bit like a second order "phase transition", even though a somewhat unusual one: If $\tilde{F}$ is the "driving variable" and δ the "order parameter", than $\partial\delta/\partial\tilde{F}$ does *not* diverge at the "critical" point but rather assumes the finite value $1/4$, while it has the value 0 below the transition.[22]

4.2.4 Nonlinear shape equation

Recall that the small gradient Hamiltonian (24) only was an approximation to the full expression (23). The full Hamiltonian can also be varied, giving rise to a shape equation. This variation is a bit more tedious to perform, but it can be done exactly.[23] However, the equation one now ends up with is a fourth order *nonlinear* partial differential equation [11, 17]. It is outrageously difficult to solve, and there exist *very* few exact solutions. However, many interesting problems involve membranes which are not essentially flat, such as for instance closed vesicles, and a lot of *numerical* research has thus been devoted (in the early 1990s) to understand specific solutions of the nonlinear shape equation. The reader will find a very good introduction to this (and much more in fact) in the review by Seifert [21].

4.3 Membrane fluctuations

The fact that the small-gradient version of the Helfrich Hamiltonian, Eqn. (24), is quadratic, implies that the shape equation (28) is linear. But it also means that we can rather easily treat additional *thermal fluctuations*, because the partition function of quadratic Hamiltonians can be easily worked out. In fact, we don't even have to do this, the equipartition theorem will suffice for what we want to look at now.

We start by Fourier-expanding the membrane shape $h(\boldsymbol{r})$. For this we assume that the membrane spans a quadratic frame of size $L \times L$, and for convenience we assume periodic boundary conditions. The shape can then be expanded in a Fourier series according to

$$h(\boldsymbol{r}) \;=\; \sum_{\boldsymbol{q}} h_{\boldsymbol{q}}\, \mathrm{e}^{\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}} \qquad , \qquad \boldsymbol{q} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \end{pmatrix} \qquad , \qquad n_x, n_y \in \mathbb{Z}\;. \tag{55}$$

Since the membrane surface $h(\boldsymbol{r})$ is a real function, the complex Fourier modes must satisfy the

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[22] If you want, the critical exponent β takes on the unusual value $\beta = 0$.

[23] A particularly clever method, which relies on fixing the tedious geometrical constraints by Lagrange multiplier functions, has recently been proposed by Guven [11].

condition $h_{-\boldsymbol{q}} = h^*_{\boldsymbol{q}}$. Using this, we find immediately

$$\begin{aligned}
\boldsymbol{\nabla} h &= \sum_{\boldsymbol{q}} h_{\boldsymbol{q}} \, \mathrm{i}\boldsymbol{q} \, \mathrm{e}^{\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}} \, , && \text{(56a)} \\
\big(\boldsymbol{\nabla} h\big)^2 &= \sum_{\boldsymbol{q},\boldsymbol{q}'} h_{\boldsymbol{q}} h_{\boldsymbol{q}'} \, (-\boldsymbol{q}\cdot\boldsymbol{q}') \, \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{q}')\cdot\boldsymbol{r}} \, , && \text{(56b)} \\
\boldsymbol{\nabla}^2 h &= \sum_{\boldsymbol{q}} h_{\boldsymbol{q}} \, (-q^2) \, \mathrm{e}^{\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}} \, , && \text{(56c)} \\
\big(\boldsymbol{\nabla}^2 h\big)^2 &= \sum_{\boldsymbol{q},\boldsymbol{q}'} h_{\boldsymbol{q}} h_{\boldsymbol{q}'} \, (q^2 q'^2) \, \mathrm{e}^{\mathrm{i}(\boldsymbol{q}+\boldsymbol{q}')\cdot\boldsymbol{r}} \, . && \text{(56d)}
\end{aligned}$$

If we now make use of the Fourier representation of the Kronecker-δ

$$\int_{L\times L} \mathrm{d}^2 r \; \mathrm{e}^{-\mathrm{i}\,\boldsymbol{q}\cdot\boldsymbol{r}} \;=\; L^2 \, \mathrm{e}^{\mathrm{i}qL/2} \, \frac{\sin\frac{qL}{2}}{\frac{qL}{2}} \;=\; L^2 \, \delta_{\boldsymbol{q},\boldsymbol{0}} \, , \tag{57}$$

we find upon inserting Eqns. (56) back into the small gradient energy (24)

$$\begin{aligned}
E_{\text{bend}} &= \int_{L\times L} \mathrm{d}^2 r \sum_{\boldsymbol{q},\boldsymbol{q}'} h_{\boldsymbol{q}} h_{\boldsymbol{q}'} \, \mathrm{e}^{i(\boldsymbol{q}+\boldsymbol{q}')\cdot\boldsymbol{r}} \left\{ \frac{1}{2}\kappa(q^2 q'^2) + \frac{1}{2}\Sigma(-\boldsymbol{q}\cdot\boldsymbol{q}') \right\} \\
&= \sum_{\boldsymbol{q},\boldsymbol{q}'} h_{\boldsymbol{q}} h_{\boldsymbol{q}'} \, L^2 \, \delta_{\boldsymbol{q}+\boldsymbol{q}',\boldsymbol{0}} \left\{ \frac{1}{2}\kappa(q^2 q'^2) + \frac{1}{2}\Sigma(-\boldsymbol{q}\cdot\boldsymbol{q}') \right\} \\
&= L^2 \sum_{\boldsymbol{q}} h_{\boldsymbol{q}} h_{-\boldsymbol{q}} \left\{ \frac{1}{2}\kappa q^4 + \frac{1}{2}\Sigma q^2 \right\} \;=\; \underline{\underline{L^2 \sum_{\boldsymbol{q}} |h_{\boldsymbol{q}}|^2 \left\{ \frac{1}{2}\kappa q^4 + \frac{1}{2}\Sigma q^2 \right\}}} \, .
\end{aligned} \tag{58}$$

This tells us several things:

1. Whether a particular undulation mode costs predominantly bending energy or tension energy is a question of the wave vector. For wave vectors smaller than $q_{\text{crossover}} := \sqrt{\Sigma/\kappa}$, *i. e.* on large length scales, tension is the dominant energy contributing to Eqn. (58). Conversely, for wave vectors bigger than $q_{\text{crossover}}$, *i. e.* on small length scales, bending dominates.
2. In Fourier space the membrane energy is diagonal, *i. e.*, the different wave vectors decouple:

$$\langle h_{\boldsymbol{q}} h_{\boldsymbol{q}'} \rangle \;=\; \langle |h_{\boldsymbol{q}}|^2 \rangle \, \delta_{\boldsymbol{q},-\boldsymbol{q}'} \, . \tag{59}$$

3. These modes are *harmonic*, *i. e.*, we can simply use the equipartition theorem to get

$$L^2 \, \langle |h_{\boldsymbol{q}}|^2 \rangle \left\{ \frac{1}{2}\kappa q^4 + \frac{1}{2}\Sigma q^2 \right\} \;=\; \frac{1}{2} k_{\mathrm{B}} T \, . \tag{60}$$

Equation (60) immediately gives us the important result

$$\underline{\underline{\langle |h_{\boldsymbol{q}}|^2 \rangle \;=\; \frac{k_{\mathrm{B}} T}{L^2 \big[\kappa q^4 + \Sigma q^2\big]}}} \, . \tag{61}$$

Eqn. (61) is the *fluctuation spectrum* or *static structure factor* of a membrane. It tells us the mean-square-amplitude of membrane modes. Since they are thermally excited, they are also proportional to temperature: More fluctuations give bigger amplitudes. Importantly, the fluctuation spectrum depends on the elastic constant κ and on the applied tension Σ. Measuring the fluctuation spectrum and fitting to Eqn. (61) is thus a viable method to extract the bending modulus in an experiment. The method is called *flicker spectroscopy* [2, 9, 20].

What kind of average undulation amplitude do we have to expect for the entire membrane, and not just for a single mode? Evidently, the full membrane amplitude is the sum over all individual modes, and we can easily calculate

$$\begin{aligned} \langle h^2 \rangle &= \sum_{\boldsymbol{q}} \langle |h_{\boldsymbol{q}}|^2 \rangle = \sum_{\boldsymbol{q}} \frac{k_{\rm B}T}{L^2(\kappa q^4 + \Sigma q^2)} \approx \left(\frac{L}{2\pi}\right)^2 \int_{q_{\min}}^{q_{\max}} {\rm d}q \; 2\pi q \, \frac{k_{\rm B}T}{L^2(\kappa q^4 + \Sigma q^2)} \\ &= \frac{k_{\rm B}T}{4\pi\Sigma} \ln \frac{q_{\max}^2(q_{\min}^2\kappa + \Sigma)}{q_{\min}^2(q_{\max}^2\kappa + \Sigma)} \xrightarrow{\Sigma\to 0} \frac{k_{\rm B}T}{4\pi\kappa} \frac{q_{\max}^2 - q_{\min}^2}{(q_{\max}q_{\min})^2} \approx \frac{k_{\rm B}T}{16\pi^3\kappa} L^2 \ , \end{aligned} \tag{62}$$

where we in the first line replaced the sum by an integral, in which we introduced a large wavelength cutoff $q_{\min} = 2\pi/L$ and a small wavelength cutoff $q_{\max} = 2\pi/a$, where a is comparable to bilayer thickness. In the last step we neglected $q_{\min}^2$ against $q_{\max}^2$ in the numerator.

The final approximate relation gives rise to a nice rule of thumb: Since a very typical value for the bending stiffness is $\kappa = 20\, k_{\rm B}T$, inserting it we readily find

$$\Delta h \ \equiv \ \langle h^2 \rangle^{1/2} \ \simeq \ \frac{L}{100} \qquad\qquad (\Sigma = 0, \, \kappa \approx 20\, k_{\rm B}T) \ , \tag{63}$$

i. e., the root mean square amplitude of the membrane fluctuations under vanishing tension are typically about 1% of the lateral extension of the membrane. Notice the scale invariance inherent in such a statement. Of course, if the membrane is under tension, this value is reduced.

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