Lecture notes
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Soft matter in and out of equilibrium

Geometric frustration and handedness

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This series of three lecture will deal with two basic notions that are encountered in many different soft matter systems; geometric frustration and handedness. The first two lectures will focus on geometric frustration. We will introduce different kinds of geometric frustration, and discuss different possible strategies of resolving the resulting frustration, emphasizing differences between local and global strategies. The third lecture will introduce a quantitative path to handed phenomena. We will discuss the history of chirality as defined by Lord Kelvin, and the difficulties that arise when using it as a source for a quantitative treatment of handedness. We will then present the orientation dependent generalization of this notion, and its implications. Both notions, that of geometric frustration and that of handedness, are of exceptional use in may soft matter systems where the constituents of a structure are ofter big enough to possess a non-trivial internal structure.

1 Geometric frustration: Examples and Riemannian formulation

When a multicellular tissue grows or a ductile material irreversibly deforms, the different cells and different regions in the material may experience different conditions and thus deform differently. However, the restriction that the tissue remains connected and continuous, forces the different cells or parts of the material to fit next to one another. As the deformation profile was not necessarily programed to make the different parts snugly fit next to one another, this will result in frustration; the inability to simultaneously satisfy all intrinsic tendencies in the material (in the present case, matching all the rest-lengths).

This frustration is not always unwanted. It can be exploited to produce elaborate shapes from very simple inputs, as well as to strengthen the material against failure (for example in tempered gorilla glass covering our smart phones).

The resolution of geometric frustration may be local (resolving the frustration uniformly), or resolve the frustration globally, incorporating into the solution quantities of the object as a whole, such as total volume and aspect ratio.

In what follows we shall explore natural and man-made examples of geometric frustration, and understand how to treat such phenomena quantitatively. This will naturally require some use of differential geometry. I will introduce the notions needed for our discussion, but will do so not in the most general framework. The less restricted form of these derivations can be found in elementary differential geometry books (e.g. *Lectures on classical differential geometry* by Struik, and *Differential geometry* by Pogorelov. A more mathematically advanced account may be found in *An introduction to differential geometry with applications to elasticity* by Ciarlet). I also want to draw the participants' attention to the 2002 summer school lecture notes by Randy Kamien *"The geometry of soft materials: A primer"* which also saw light as a review article in Rev. Mod. Phys.

1.1 Examples of geometrically frustrated systems

1.1.1 Flattening the sphere

One of the most familiar notion of geometric incompatibility is that of flattening the sphere. For hundreds of years cartographers have been faced with the challenge of accurately describing the spherical surface of the earth on flat pieces of paper. We know that any such "flattening" will necessarily distort distances and shapes. There are two types of questions concerning such maps, the first is to find the most accurate way of mapping a region in space, and the second concerns the most accurate description of the whole globe. We will discuss both of these notions (termed local and global notions) of incompatibility, and will address the question of minimal distortion quantitatively.

1.1.2 Doubly curved bilayer: The Bauhinia seed-pod geometry

Next let us consider the following geometry: Two thin elastic sheets of thickness t are uniaxially stretched by a factor $1+\alpha$ with respect to each other along perpendicular directions and are then glued to one another. Along each direction we can estimate the difference in length between the center of the layers when curved to a radius R:

$$\frac{l_{out}}{l_{in}} = \frac{R+t/2}{R-t/2} = \frac{1+\alpha/2}{1-\alpha/2} \Rightarrow \kappa = R^{-1} = \frac{\alpha}{t}.$$

The curvature along the two directions is equal in magnitude but points along opposite directions (and thus associated with opposite signs). We note that we can keep R constant and take α to be arbitrarily small provided also diminish the thickness t accordingly. In this limit, we do not change the two dimensional geometry of each of the layers (which both start planar, and thus with zero Gaussian curvature, $K = 0$). However, the desired geometry is associated with a non-vanishing Gaussian curvature $K = \kappa_1\kappa_2 = -R^{-2}$. Gauss' theorema egregium which relates the metric properties of a surface to its allowed conformation in space through the Gaussian curvature thus precludes the ability to simultaneously conform to the 2D geometry and the prescribed curvatures.

1.1.3 Bend-Splay coupling in 2D nematic liquid crystals

A two dimensional nematic liquid crystal is characterized by a unit vector field $\hat{\mathbf{n}}$ named the director which is indicative of a local preferred orientation of the constituents in the liquid. The constituents in a nematic liquid crystal, named *nematogens*, have a broken symmetry and are typically elongated rod-like structures. In its ground state a nematic liquid crystal attempts to align the nematogens, leading to a uniform and constant director field. However, this configuration may be distorted by imperfections, boundary conditions, and other external forces. The energetic cost of such deformations is given by the Frank free energy:

$$F = \tfrac{1}{2}K_s(\nabla \cdot \hat{\mathbf{n}})^2 + \tfrac{1}{2}K_b\left((\hat{\mathbf{n}} \cdot \nabla)\hat{\mathbf{n}}\right)^2.$$

The first term is called the splay term, and the second is called the bending term. We could define $s = |\nabla \cdot \hat{\mathbf{n}}|$ and $b = |(\hat{\mathbf{n}} \cdot \nabla)\hat{\mathbf{n}}|$ to obtain the energy in compact form:

$$F = \tfrac{1}{2}K_s s^2 + \tfrac{1}{2}K_b b^2.$$

A third term (called the saddle splay) can be written as the divergence of a function, and for simplicity was omitted above. In three dimensions the above terms naturally extend to their three dimensional forms and an additional term, named twist (or helicity) appears, $\frac{1}{2}K_T(\hat{\mathbf{n}} \cdot \nabla \times \hat{\mathbf{n}})^2$.

For an unconstrained liquid crystal it is easy to see that the Frank energy in 2D yields a trivial minimizer where $s = 0$ and $b = 0$. However if we now consider a nematogen of a slightly more structured form, say having a slight longitudinal bend, things may look different. Such a liquid crystal will possess a non-vanishing preferred spontaneous bend. Its Frank energy, given by

$$F = \tfrac{1}{2}K_s s^2 + \tfrac{1}{2}K_b(b - b_0)^2,$$

favors a zero splay configuration with a constant bend of value b_0, and one may naïvely expect that we should only consider small perturbations about this ground state. However, as we next show, there exists no ground state with vanishing splay and a constant bending.

Setting $\hat{\mathbf{n}} = (\cos(\theta), \sin(\theta))$, the vanishing splay requirement amounts to $\theta_y = \tan(\theta)\theta_x$. This gives for the bending the expression

$$b = \theta_x/\cos(\theta) = \theta_y/\sin(\theta).$$

This can be immediately shown to be incompatible with the no splay condition as

$$\theta_{xy} = -b\sin(\theta)\theta_y = -b^2\sin^2(\theta) \neq b^2\cos^2(\theta) = b\cos(\theta)\theta_x = \theta_{yx}.$$

The uniformly bent ground state is therefore frustrated and the ground state will inevitably contain some splay or display non-uniform bending.

1.1.4 2D axially symmetric exponential growth

Last let us consider a circular ring of N cells that produces a new layer of ΛN cells, where $\Lambda > 1$ every generation. Had Λ been equal to unity this would have resulted in a cylindrical tube. The restriction that $\Lambda > 1$ requires the perimeter of the next generation to be longer. This growth of the perimeter occurs at an increasing rate. The most a circular perimeter can grow between layer of height Δh is $\rho(s+\Delta h)-\rho(s) = 2\pi\Delta h$, which occurs when the growth is planar. Beyond this point no axially symmetric solution can continue to increase the perimeter at an accelerating rate. This is known as the finite horizon of the pseudosphere. Beyond this point, growth must lead to a strong symmetry breaking of the configuration.

1.2 Formulation of the problem via Riemanian geometry

We now come to make these notions of frustration quantitative within the framework of Riemannian geometry. The main tool in Riemannian geometry is the Riemannian metric, g. This is the tool with which infinitesimal distances are defined. The metric is given with respect to a set of coordinates x^α:

$$ds^2 = g_{ij} dx^i dx^j,$$

where above, and hereon-after we assume the Einstein summation convention where repeated indices in a product are summed over. On a smooth Riemannian manifold every point locally looks like Euclidean space. A general Riemannian space differs from Euclidean space in that the former does not require to support the parallel postulate which holds in Euclidean space (that to every straight line and every point not on the line there exists a single straight line that passes through the point and never intersects the line). This gives Riemannian manifolds all their exotic behavior. In particular it allows for something called non-holonomy or non-trivial parallel transport. For pedagogical reasons, in what follows next we will consider the notion of connection, covariant derivative, and parallel transport for surfaces embedded in 3D. Each of these notions can, of course, be defined in arbitrary dimensions and without the need to resort to an embedding.

Let us consider a surface in Euclidean three dimensional space,

$$\mathbf{r}(\mathbf{x}) = \big(r^1(x^1,x^2), r^2(x^1,x^2), r^3(x^1,x^2)\big).$$

The metric is obtained by examining infinitesimal displacements along the surface (dx^1, dx^2):

$$ds^2 = d\mathbf{r}\cdot d\mathbf{r} = \frac{d\mathbf{r}}{dx^\alpha}\cdot\frac{d\mathbf{r}}{dx^\beta} dx^\alpha dx^\beta = g_{\alpha\beta} dx^\alpha dx^\beta.$$

The inverse metric is also a useful tool in geometry

$$g^{\alpha\beta} = (g_{\alpha\beta})^{-1}, \quad \text{i.e.} \quad g_{\alpha\beta}g^{\beta\gamma} = g^{\gamma\beta}g_{\beta\alpha} = \delta^{\gamma}_{\alpha}.$$

A vector on the surface in our specific embedded context should be thought of as the possible velocity vector of a particle moving on the surface. It is a vector in $\mathbb{R}^3$ that is locally tangent to the surface. Such a vector can be defined through its contravariant (marked by upper indices) components, or through its covariant (marked by lower indices) components:

$$\mathbf{v} = v^{\alpha}\partial_{\alpha}\mathbf{r} = v_{\beta}g^{\alpha\beta}\partial_{\alpha}\mathbf{r} = v_{\beta}\partial^{\beta}\mathbf{r}$$

where $\partial_{\alpha}\mathbf{r} = \partial\mathbf{r}/\partial x^{\alpha}$ and $\partial^{\alpha}\mathbf{r} = g^{\alpha\beta}\partial_{\beta}\mathbf{r}$. We now are able to differentiate the components of a vector. We recall that the component of the vector at different points are defined with respect to different basis vectors. It thus will surprise us that a correction term should be introduced to compensate for this effect.

$$\partial_{\alpha}\mathbf{v} = \partial_{\alpha}v^{\beta}\partial_{\beta}\mathbf{r} + v^{\beta}\partial_{\alpha}\partial_{\beta}\mathbf{r} = (\partial_{\alpha}v^{\beta} + \Gamma^{\beta}_{\alpha\gamma}v^{\gamma})\partial_{\beta}\mathbf{r} = (\nabla_{\alpha}v^{\beta})\partial_{\beta}\mathbf{r},$$

where we have defined the Christoffel symbol: $\partial_{\alpha}\partial_{\beta}\mathbf{r} = \Gamma^{\gamma}_{\alpha\beta}\partial_{\gamma}\mathbf{r}$. This compensated differentiation is called the covariant derivative. Similarly one can show that for the covariant components the covariant derivative reads

$$\nabla_{\alpha}v_{\beta} = \partial_{\alpha}v_{\beta} - \Gamma^{\gamma}_{\alpha\beta}v_{\gamma}. \tag{1}$$

One can also easily show that the Chrisftoffel symbol can be calculated directly from the metric:

$$\Gamma^{\gamma}_{\alpha\beta} = \tfrac{1}{2}g^{\gamma\delta}(\partial_{\alpha}g_{\beta\delta} + \partial_{\beta}g_{\alpha\delta} - \partial_{\delta}g_{\alpha\beta}). \tag{2}$$

The Christoffel symbol is the central tool in defining the **connection** on the manifold, that is in determining how to compare vector in different locations, or alternatively in determining how to parallel translate vectors. The notion of parallel translation of a vector along a path is trivial in Euclidean space, "one only needs to keep the direction of the vector constant". This is because the connection in this case is trivial and directions can be defined globally. This is the case of general Riemannian geometry in which directions are cannot be defined globally. One can formulate the notion of parallel transport locally: Two parallel vectors in Euclidean space form with a given straight line a constant angle. Similarly, to infinitesimally translate a vector v_{α} along a path γ we simply construct at every point a geodesic curve that is locally tangent to the curve γ, and keep a constant angle between the vector and the geodesic. Unlike the case in Euclidean space, parallel translating a vector around a closed loop in a general Riemannian manifold results in a rotation which is proportional to the area enclosed by the loop. The local manifestation of this non-holonomy is the non-commutativity of second derivatives

$$\nabla_{\alpha}\nabla_{\beta}v_{\gamma} - \nabla_{\beta}\nabla_{\alpha}v_{\gamma} = R^{\delta}_{\gamma\alpha\beta}v_{\delta},$$

where the Riemannian curvature tensor appearing above reads

$$R^{\delta}_{\gamma\alpha\beta} = \partial_\alpha \Gamma^{\delta}_{\beta\gamma} - \partial_\beta \Gamma^{\delta}_{\alpha\gamma} + \Gamma^{\nu}_{\beta\gamma}\Gamma^{\delta}_{\alpha\nu} - \Gamma^{\nu}_{\beta\gamma}\Gamma^{\delta}_{\beta\nu}. \tag{3}$$

We now note that the central formulas above (**??**), (**??**) and (**??**) rely only on knowledge of the metric and do not require the specific embedding we used to understand the intuition behind these notion. Given a Riemannian metric we can paralle transport vector, define curvature, and use covariant differentiation as we wish.

In order to discuss physical properties of a manifold we will need to parameterize it. Naturally, many of the calculated quantities will depend on the specific parametrization. In particular, the components of the metric tensor and and of the christtoffel symbols will differ between different parametrizations. However, we will see that all relevant scalar quantities will be parametrization independent. If we contract a contravariant vector field v^α with a covariant vector field u_α the resulting scalar field $v^\alpha u_\alpha = \phi$ will be independent of the parametrization used (despite the fact that the component of both vector fields will depend on the parametrization). This will also bring us to conclude that when formulated properly, if a vectorial equation holds with respect to one parametrization, it will hold true for every parametrization despite the fact that the components of the vectors will strongly depend on the parametrization. Higher indexed quantities, such as the metric, are called tensors and should be thought of as an external product of vectors. We note in passing that the Christoffel symbol is not a tensor in this sense (and thus is not allowed into covariant equations), however the difference of two Christoffel symbols with respect to two different metrics is a tensor.

1.3 Existence and uniqueness of an embedding for flat metrics

Let us now consider a three dimensional flat manifold, again given by the mapping $\mathbf{r}(\mathbf{x})$. One could think of this structure as endowing space with curvilinear coordinates. Recalling that the Christoffel symbol reads

$$\partial_i \partial_j \mathbf{r} = \Gamma^k_{ij} \partial_k \mathbf{r}, \tag{4}$$

As we know that parallel transport is trivial in Euclidean space, we expect the Riemann curvature tensor to vanish. We can ask if that is a sufficient condition on the metric to produce such a flat manifold. The way to answer such a question is constructive. We try to reconstruct the manifold from knowledge of the metric alone. One could think of the definition of the Christoffel symbol above as a first order PDE for $\mathbf{V}_\alpha = \partial_\alpha \mathbf{r}$. Such a set of PDE's allows a solution only if $\partial_\alpha \partial_\beta \mathbf{V} = \partial_\beta \partial_\alpha \mathbf{V}$. Thus given a metric g_{ij}, and corresponding Christoffel symbols Γ^i_{jk} we can reconstruct from these a three dimensional structure in Eculidean space provided that

$$0 = \partial_j \partial_k \partial_i \mathbf{r} - \partial_k \partial_j \partial_i \mathbf{r} = (\partial_j \Gamma^m_{ik} - \partial_k \Gamma^m_{ij} + \Gamma^l_{ik}\Gamma^m_{lj} - \Gamma^l_{ij}\Gamma^m_{lk})\partial_m \mathbf{r} = R^m_{ijk}\partial_m \mathbf{r}.$$

Which again implies vanishing of all coordinates of the Riemann curvature tensor. Thus a Riemannianly flat (vanishing curvature) 3D manifold can be has a unique realization in 3D Euclidean space (up to rigid motions).

1.4 Generation of incompatibility in non-uniform isotropic expansion

We now come to exemplify how difficult it is to construct a flat metric through a specific example. Consider a strain-free body, parameterized by Cartesian coordinates, i.e. $g = I$. Allow every point in the body to expand isotropically but non-homogeneously by a factor $\lambda(x)$, thus giving rise to a reference metric $\bar{g} = \lambda^2 I$. Such expansion may result for example from thermal expansion, or in growth induced by turgor pressure in plants' cells. We now ask a simple question: what isotropic growth profiles will result in a compatible reference metric, i.e. will be realizable by an Euclidean metric, g, and will therefore not induce residual stress?

To answer this question we write down the components of the Riemannian curvature tensor of the metric $\bar{g}$ in terms of the expansion factor λ and its derivatives. Taking independent linear combination of the covariant components of the Riemannian curvature tensor yields the following compatibility conditions:

$$\begin{aligned} 2(\partial_1\lambda)^2 - \lambda\partial_1\partial_1\lambda - \triangle\lambda &= 0, & 2\partial_1\lambda\partial_2\lambda - \lambda\partial_1\partial_2\lambda &= 0, \\ 2(\partial_2\lambda)^2 - \lambda\partial_2\partial_2\lambda - \triangle\lambda &= 0, & 2\partial_1\lambda\partial_3\lambda - \lambda\partial_1\partial_3\lambda &= 0, \\ 2(\partial_3\lambda)^2 - \lambda\partial_3\partial_3\lambda - \triangle\lambda &= 0, & 2\partial_2\lambda\partial_3\lambda - \lambda\partial_2\partial_3\lambda &= 0, \end{aligned}$$

where $\triangle = \nabla \cdot \nabla = \partial_1^2 + \partial_2^2 + \partial_3^2$ is the standard Laplacian operator. It takes straightforward algebra and integration to find that the only non-constant solution of the above equations is

$$\lambda = \frac{C^2}{|\mathbf{x} - \mathbf{x_0}|^2},$$

for some constants C and $\mathbf{x_0}$. Every other isotropic expansion profile of an initially Euclidean 3D body will give rise to a non-Euclidean metric and inevitably result in a residually stressed body. This result, may be surprising when considering growth profiles. However it is a consequence of a well-known geometric result whereby all conformal mappings in $\mathbb{R}^3$ are inversions of a sphere. It implies that any growth that does not result in residual stress requires delicate global control, or some mechanical feedback.

1.5 Differential geometry of surfaces in three dimension

When coming to describe surfaces we will need to resort to slightly more complicated structures; namely the first and second fundamental forms. For surfaces embedded in three dimensions we distinguish between intrinsic properties (essentially the metric and quantities that can be derived from it) and extrinsic properties that can be changed without altering the metric, such as the principal curvature in a specific location. The latter properties will be said to depend on the specific embedding.

Given a surface $\mathbf{r}(x^1, x^2)$ and a surface normal $\hat{\mathbf{N}}$ we construct the first and second fundamental forms via

$$a_{\alpha\beta} = \partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r}, \qquad b_{\alpha\beta} = \partial_\alpha \partial_\beta \mathbf{r} \cdot \hat{\mathbf{N}}.$$

The second fundamental form measures curvature per unit of coordinate length. This is related to true length through the metric. A third tensor called the shape operator $c^\alpha_\beta = g^{\alpha\gamma} b_{\gamma\beta}$ gives curvatures in real units, independent of the parametrization. Two scalar quantities can be calculated from it; Its determinant is the Gaussian curvature $K = det(c) = \kappa_1\kappa_2$, and its trace is the mean curvature, $H = \frac{1}{2}(\kappa_1 + \kappa_2)$. Gauss' theorema egregium identifies the Gaussian curvature with the Riemannian curvature which can be calculated from the metric alone. This theorem naturally restricts the allowable pairs of fundamental forms. For example, the Eulidean metric $g = I$ cannot support a uniformly curved configuration $b = \kappa I$, or as we discussed in the examples a saddle like negative Gaussian curvature.

In addition to Gauss' equation there are two more differential restrictions on the fundamental forms These can be written compactly as

$$\nabla_\alpha b_{\beta\gamma} = \nabla_\beta b_{\alpha\gamma}.$$

The compatibility conditions for surfaces are called the Gauss-Peterson-Mainardi-Codazzi (GPMC) equations. Similarly to the case of Riemannian curvature satisfaction of these equations is a necessary and sufficient condition for the existence of a unique surface with a given first and second fundamental forms. An exceptionally elegant derivation of these equations starts with a surface and extends it along its normal vector:

$$\mathbf{r}(x^1, x^2, x^3) = \boldsymbol{\rho}(x^1, x^2) + x^3 \hat{\mathbf{N}}(x^1, x^2)$$

The resulting metric g^{3D} can be expressed in terms of the 2D metric and curvature tensors, a and b:

$$g^{3D} = \begin{pmatrix} a - 2x^3 b & & 0 \\ & & 0 \\ 0 & 0 & 1 \end{pmatrix} + \mathcal{O}((x^3)^2)$$

Calculating the Riemannian curvature tensor of g^{3D} reproduces the GPMC equations.

1.6 Homework assignment (optional)

Derive the compatibility condition for splay-free bending in a 2D liquid crystal.