

Warning: These notes have not been proofread and may contain typos and errors.

1 Math preliminaries

1.1 Parametrization: plane curve

reading: Giomi review in Soft Matter, 2013

Deserno notes https://www.cmu.edu/biolphys/deserno/pdf/diff_geom.pdf

1.2 Arclength parametrization:

A plane curve can be specified either by $\mathbf{r}(x(t), z(t))$ or the arclength $\mathbf{r}(s)$. The tangent and normal vectors are

$$\mathbf{t} = \frac{d\mathbf{r}}{ds}, \quad \mathbf{n} = \frac{1}{C} \frac{d\mathbf{t}}{ds}$$

hence the curvature and the bending energy

$$C = \left| \frac{d\mathbf{t}}{ds} \right|, \quad E = \frac{1}{2} \int_0^{L_c} ds \left| \frac{d\mathbf{t}}{ds} \right|^2$$

The length and the bending energy of the filament are

$$L_c = \int_0^{L_c} ds, \quad E = \frac{1}{2} \int_0^{L_c} ds C(s)^2$$

Exercise: show that the tangent vector is a unit vector, i.e. $|\mathbf{t}| = 1$.

Giomi's notation:

$$\mathbf{t} = \kappa \mathbf{n}, \quad \mathbf{n} = -\kappa \mathbf{t} \quad \kappa = \frac{d\psi}{ds}, \quad \psi \text{ is called turning angle.}$$

if κ is defined to be positive, then the normal vector is oriented toward the center of curvature.

1.3 Monge parametrization:

$\mathbf{r} = x\hat{\mathbf{x}} + h(x)\hat{\mathbf{z}}, z = h(x), t \equiv x$.

Exercise: show that

$$\mathbf{t} = \frac{1}{[1 + (h')^2]^{1/2}} (\hat{\mathbf{x}} + h'\hat{\mathbf{z}}), \quad \mathbf{n} = \frac{1}{[1 + (h')^2]^{1/2}} (-h'\hat{\mathbf{x}} + \hat{\mathbf{z}}), \quad C = \frac{h''}{[1 + (h')^2]^{3/2}}$$

(h' denotes dh/dx). Hint: Start from $\mathbf{n}C = \frac{d\mathbf{t}}{ds}$ and change variables

$$\frac{1}{[1 + (h')^2]^{1/2}} (-h'\hat{\mathbf{x}} + \hat{\mathbf{z}}) C = \frac{d\mathbf{t}}{dt} \frac{dt}{ds}$$

use that

$$\frac{dt}{ds} = \left(\left| \frac{d\mathbf{r}}{dt} \right| \right)^{-1} = \frac{1}{[1 + (h')^2]^{1/2}}$$

and finally solve for C .

Final note:

$$dx = ds (\mathbf{n} \cdot \hat{\mathbf{z}}) = ds (\mathbf{t} \cdot \hat{\mathbf{x}}) [1 + (h')^2]^{-1/2}$$

This can be generalized for surfaces in 3D:

$$z = h(x, y), \quad \mathbf{r}(x, y) = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + h(x, y)\hat{\mathbf{z}}$$

Then there are two tangential vectors

$$\frac{\partial \mathbf{r}}{\partial x} = \hat{\mathbf{x}} + \frac{\partial h}{\partial x} \hat{\mathbf{z}}, \quad \frac{\partial \mathbf{r}}{\partial y} = \hat{\mathbf{y}} + \frac{\partial h}{\partial y} \hat{\mathbf{z}}.$$

The normal vector which is the cross product of the tangential vectors.

The normal vector can be also obtained from the level set function $F = z - h(x, y)$. ∇F points in the direction of the normal,

$$F(\mathbf{r} + d\mathbf{r}) = F(\mathbf{r}) + d\mathbf{r} \cdot \nabla F$$

But $F(\mathbf{r} + d\mathbf{r}) = F(\mathbf{r})$ by definition, hence $d\mathbf{r} \cdot \nabla F = 0$

The relation between an area element in the xy plane (projected area) and the area element on the interface is the Jacobian

$$dA = dA_{xy} J(x, y), \quad J(x, y) = \left| \frac{\partial \mathbf{r}}{\partial x} \times \frac{\partial \mathbf{r}}{\partial y} \right| = \sqrt{1 + (\nabla h)^2} \quad (1)$$

1.4 Fourier transform

Fourier transform definition (note the convention about the 2π factor)

$$h(\mathbf{r}) = \frac{1}{(2\pi)^n} \int d\mathbf{q} e^{i\mathbf{q} \cdot \mathbf{r}} h(\mathbf{q}), \quad h(\mathbf{q}) = \int d\mathbf{r} e^{-i\mathbf{q} \cdot \mathbf{r}} h(\mathbf{r})$$

where n is the space dimensionality. Note that if $h(\mathbf{r})$ is real then $h^*(\mathbf{q}) = h(-\mathbf{q})$.

$$\int d\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} = (2\pi)^n \delta(\mathbf{q}) = L^n \delta_{\mathbf{q},0}$$

$\delta(\mathbf{q})$ is the Dirac delta function ($\mathbf{q}$ continuous) and $\delta_{\mathbf{q}+\mathbf{q}',0}$ is the Kronecker delta ($\mathbf{q}$ discrete)

The Dirac delta function is defined as

$$\delta(y) = 0, \quad \text{if } y \neq 0; \quad \int_{-\infty}^{\infty} \delta(y) dy = 1$$

(note that the Kronecker delta is the discrete version of the Dirac delta function.)

We can replace summation with integration. Since

$$\int dq = \sum_q \Delta q = \frac{2\pi}{L} \sum_k \Delta k = \frac{2\pi}{L} \sum_k 1 \implies \int dq = \frac{2\pi}{L} \sum_q$$

(the increment of the integer is $\Delta k = 1$)

1.5 Fourier series

curve/planar membrane in 2D with projected length L

$$h(x) = \sum_{q=-\infty}^{\infty} h_q e^{iqx}, \quad q = \frac{2\pi}{L}k, \quad k = \pm 1, \dots, \infty \quad (2)$$

Note that $q = 0$ mode does not involve bending. $h = h_0 + \sum_{q>1} h_q e^{iqx}$ shows that h_0 is equivalent to translating the coordinate system along z .

closed curved/2D vesicle with projected shape circle with radius a (and contour length=perimeter $L = 2\pi a$). Shape can be parametrized in polar coordinates

$$r = a \left(1 + \sum_{k=0}^{\infty} u_k e^{ik\theta} \right) \quad \text{note that } qx = \frac{2\pi k}{L}s = k \frac{s}{a} = k\theta$$

The volume constrained fixes the $k = 0$ amplitude as a function of the other amplitudes

$$\begin{aligned} \pi a^2 &= \int_0^{2\pi} r dr d\theta = a^2 \frac{1}{2} \int_0^{2\pi} \left(1 + \sum_{k=0}^{\infty} u_k e^{ik\theta} \right)^2 d\theta \\ &= a^2 \left(\pi + \sum u_k \int e^{ik\theta} d\theta + \frac{1}{2} \sum_k \sum_{k'} u_k u_{k'} \int e^{i(k+k')\theta} d\theta \right) \\ u_0 &= -\frac{1}{2} \sum_{k>0} u_k u_{-k} \end{aligned}$$

Translation in x direction is given by velocity

$$\frac{dr}{dt} = U \cos \theta \implies \frac{du_1}{dt} = U$$

Thus the $n = 1$ modes are associated with translation of the center of mass. Reference: Finken et al, EPJE (2008)

2 Equilibrium

2.1 Simple fluid-fluid interface (only surface tension)

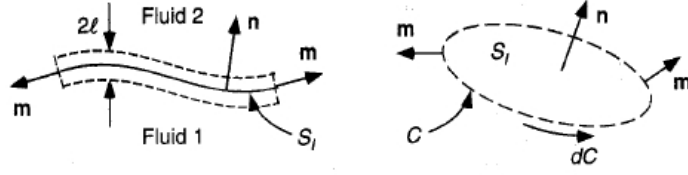


Figure 1: Figure from Dean "Analysis of Transport Phenomena"

Consider a surface area with normal $\mathbf{n}$. Conservation of momentum at the interface shows that inertia is negligible (due to its thinness, the interface mass is negligible). The mechanical equilibrium at the interface then reads

$$\int_S (\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n} dS = \int_C \mathbf{f}_s dC \quad (3)$$

$(\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n}$ is the jump in the bulk hydrodynamic stress. $\mathbf{f}_s$ are interfacial forces (surface tension, viscoelastic stresses, bending, etc...)

For an interface with surface tension $\mathbf{f}_s = \sigma \hat{\mathbf{m}}$, $\hat{\mathbf{m}} = \hat{\mathbf{t}} \times \mathbf{n}$

$$\int_C \mathbf{f}_s dC = \int_S [(\mathbf{n} \times \nabla) \times (\sigma \mathbf{n})] dS \quad (4)$$

$$(\mathbf{n} \times \nabla) \times (\sigma \mathbf{n}) = (\sigma \nabla \cdot \mathbf{n}) \mathbf{n} - \nabla_s \sigma, \quad \nabla_s = (\mathbf{I} - \mathbf{n} \mathbf{n}) \cdot \nabla$$

Proof:

$$\left[(\mathbf{n} \times \nabla)_j \times (\sigma \mathbf{n})_k \right]_i = \varepsilon_{ijk} (\mathbf{n} \times \nabla)_j (\sigma n_k) = \varepsilon_{ijk} \varepsilon_{jpq} n_p \frac{\partial}{\partial x_q} (\sigma n_k) = \varepsilon_{ijk} \varepsilon_{jpq} n_p n_k \frac{\partial \sigma}{\partial x_q} + \varepsilon_{ijk} \varepsilon_{jpq} n_p \sigma \frac{\partial n_k}{\partial x_q} =$$

using that $\varepsilon_{ijk} = \varepsilon_{jki}$ and

$$\varepsilon_{jki} \varepsilon_{jpq} = \delta_{kp} \delta_{iq} - \delta_{kq} \delta_{ip}$$

leads to

$$= n_k n_k \frac{\partial \sigma}{\partial x_i} + \sigma n_k \frac{\partial n_k}{\partial x_i} - n_i n_k \frac{\partial \sigma}{\partial x_k} - \sigma n_i \frac{\partial n_k}{\partial x_k} = [(\mathbf{I} - \mathbf{n} \mathbf{n}) \cdot \nabla \sigma + \sigma \mathbf{n} \cdot \nabla \mathbf{n} - \sigma \mathbf{n} \nabla \cdot \mathbf{n}]_i$$

note that $\mathbf{n} \cdot \nabla \mathbf{n} = 0$ because $\nabla (\mathbf{n} \cdot \mathbf{n}) = 0$

Thus

$$(\mathbf{T}_2 - \mathbf{T}_1) \cdot \mathbf{n} = (\sigma \nabla \cdot \mathbf{n}) \mathbf{n} - \nabla_s \sigma \quad (5)$$

At equilibrium, tension is uniform and the hydrodynamic stress $\mathbf{T} = -p\mathbf{I}$. The mechanical equilibrium condition reduces to

$$p_1 - p_2 = \sigma H, \quad H = \nabla \cdot \mathbf{n}$$

Minimal surfaces: $H=0$

2.2 Shape of vesicles (closed membranes)

References:

for vesicles in 2D

Seifert Phys. Rev. A (1991) 43:6803–6814

Veerapaneni et al, International Journal of Non-Linear Mechanics (2009) 44:257–262

Giomi Soft Matter (2013) 9:8121

for vesicles in 3D (axisymmetric)

Seifert et al. Phys. Rev. A (1991) 44:1182–1202

for criticism of Seifert's equations see Blyth and Pozrikidis, European Journal of Mechanics A Solids (2004) 23:877–892

Reboucas et al. Soft Matter (2024) 20:2258-2271 <https://arxiv.org/abs/2311.14193>

big review on vesicles Seifert "Advances in physics" (1997)

In 3D, a vesicle is a closed inextensible surface with area A enclosing volume V . In 2D, it is a closed contour with perimeter L enclosing area A_{2D} . The reduced volume compares the volume of the vesicle to the volume of an equivalent sphere with the same surface area.

$$v = \frac{V}{\frac{4\pi}{3} \left(\frac{A}{4\pi}\right)^{3/2}} \quad \text{in 3D}$$

$$v = \frac{A_{2D}}{\pi \left(\frac{L}{2\pi}\right)^{3/2}} \quad \text{in 2D}$$

2.2.1 Euler-Lagrange equations

Bending energy

$$E = \int \left(\frac{\kappa}{2} H^2 + \kappa_G K \right) dA - \Delta p V + \sigma A \quad (6)$$

where $\Delta p = p_{(2)} - p_{(1)}$ is the pressure difference between inside and outside the vesicle (a Lagrange multiplier enforcing bulk-incompressibility), σ is the tension (a Lagrange multiplier enforcing area-incompressibility). $K = c_1 c_2$ is the Gaussian curvature and $H = c_1 + c_2$ (c_1, c_2 being the principal curvatures; $H = \nabla \cdot \mathbf{n}$, where $\mathbf{n}$ is the outward pointing normal vector to the surface). If there are no topological changes $\int \kappa_G K dA = \text{const}$.

Variation of the energy Eq. [6] yields

$$\Delta p = \sigma H - \kappa \left(\frac{1}{2} H^3 - 2HK - \nabla_s^2 H \right) \quad (7)$$

∇_s^2 is the Laplace-Beltrami operator. For a given reduced volume v , σ and Δp , there are many solutions of Eq. [7]. The equilibrium shape is the lowest energy shape.

Derivation: idea EL equation is a PDE whose solution is the function u for which a given functional E is stationary. [recall example with finding the minimum distance between two points]

$$E(u) = \int F(t, u, u') dt$$

$$\frac{\partial F}{\partial u} - \frac{d}{ds} \frac{\partial F}{\partial u'} = 0$$

Exercise: For a surface with no bending (only tension σ) derive the Laplace law using EL (Laplace law describes shapes of soap films). For simplicity use Monge parametrization $z = h(x)$ The energy is

$$E = \sigma \int \sqrt{1 + \dot{h}^2} dx + p \int h dx \implies F(x, h, \dot{h}) = \sigma \sqrt{1 + \dot{h}^2} + ph$$

(p denotes pressure difference across the interface)

$$\frac{\partial F}{\partial h} - \frac{d}{dx} \frac{\partial F}{\partial \dot{h}} = p + \sigma \frac{d}{dx} \left(\frac{\dot{h}}{(1 + \dot{h}^2)^{1/2}} \right) = p + \sigma H = 0$$

Note: equilibrium surfaces governed by surface tension have constant curvature, e.g., sphere, catenoid, unduloid

2.2.2 Variational approach

Deserno Fluid lipid membranes: From differential geometry to curvature stresses, Chemistry and Physics of Lipids (2015) 185:11-45

2.2.3 Derivation from mechanical equilibrium

The membrane stresses (for per unit length in 2D) are

$$\mathbf{f} = \frac{d}{ds} (\tau \mathbf{t} - q \mathbf{n}) = \left(H\tau - \frac{dq}{ds} \right) \mathbf{n} + \left(\frac{d\tau}{ds} + Hq \right) \mathbf{t} \quad (8)$$

H is curvature, τ is tension, $q = dm/ds$ is transverse shear (this relation comes from torque balance), m is the bending moment. Use a constitutive law

$$m = \kappa H$$

Hence,

$$\mathbf{f} = \frac{d}{ds} (\tau \mathbf{t} - q \mathbf{n}) = \left(H\tau - \kappa \frac{d^2 H}{ds^2} \right) \mathbf{n} + \left(\frac{d\tau}{ds} + \kappa H \frac{dH}{ds} \right) \mathbf{t} \quad (9)$$

At equilibrium, there is only the normal pressure force acting on the membrane from the bulk. Mechanical equilibrium requires

$$f_n = p, \quad f_t = 0$$

$$f_t = 0 \quad \text{integrate} \implies \tau = \sigma - \frac{\kappa}{2} H^2$$

σ is a constant of integration.

Thus, the shape equation for a vesicle in 2D is then

$$H\sigma - \kappa \left(\frac{d^2 H}{ds^2} + \frac{1}{2} H^3 \right) = p \quad (10)$$

Since $H = d\psi/ds$ Eq. [10] is a third order ODE for $\psi(s)$. Integrating Eq. [10] yields $\psi(s)$, and another integration gives the shape of the curve

$$\mathbf{r}(s) = \mathbf{r}(0) + \int_0^s ds [\cos \psi \hat{\mathbf{x}} + \sin \psi \hat{\mathbf{z}}], \quad \frac{dz}{ds} = \sin \psi, \quad \frac{dx}{ds} = \cos \psi$$

Side note: For a closed, inextensible surface in 2D, a membrane stress of the form

$$\mathbf{f}_o = \frac{d}{ds} \left(g(s) \frac{d\mathbf{r}}{ds} \right)$$

where $g(s)$ is an arbitrary function, does zero work. So it can be added to the membrane force Eq. [10] at equilibrium. Prove this, i.e. show that

$$\int \mathbf{f}_o \cdot d\mathbf{r} = 0 \text{ over a closed contour}$$

So the tangential force component (coming from bending, $-Hq$) in Eq. [9] can be eliminated by adding

$$-\kappa \frac{d}{ds} \left(H^2 \frac{d\mathbf{r}}{ds} \right)$$

2.3 Fluctuating filament/1D membrane

Energy spectrum of the fluctuations: see for detailed derivation Deserno notes on "Fluid membranes", p. 26 (it is for a surface but here we just treat the wavevector q as scalar). The total bending energy is

$$E_b = \int_0^{L_c} ds C^2 = \frac{k_f}{2} \int_0^L dx \left[1 + \left(\frac{dh}{dx} \right)^2 \right]^{1/2} \left(\frac{\frac{d^2h}{dx^2}}{\left[1 + \left(\frac{dh}{dx} \right)^2 \right]^{3/2}} \right)^2 \approx \frac{k_f}{2} \int_0^L dx \left(\frac{d^2h}{dx^2} \right)^2$$

$$E_b = \frac{k_f}{2} \int_0^L dx \sum_q \sum_{q'} (q^2 q'^2) h_q h_{q'} e^{i(q+q')x}$$

use that

$$\int_0^L dx e^{i(q+q')x} = L \delta_{q+q',0}$$

$$E_b = \frac{k_f}{2} L \sum_q q^4 h_q h_{-q} \quad \text{:independent oscillators}$$

each degree of freedom has $k_B T/2$ energy (equipartition theorem). Hence for each mode

$$\frac{k_B T}{2} = \frac{k_f}{2} L \langle h_q h_{-q} \rangle$$

$$\langle h_q h_{q'} \rangle = \frac{1}{L} \frac{k_B T}{k_f q^4} \delta_{q+q',0} \quad (11)$$

$\delta_{q+q',0}$ is the Kronecker delta function.

Apparent length L : Polymers/membranes "store" length in the thermal contour/shape undulations. So, the apparent length L is smaller than the actual length L_c .

$$L_c = \int_0^{L_c} ds = \int_0^L dx \left(1 + \frac{1}{2} \left(\frac{dh}{dx} \right)^2 \right) = L + \frac{1}{2} \int_0^L dx \left(\frac{dh}{dx} \right)^2 \quad (12)$$

$$\frac{L_c - L}{L} = \frac{1}{2} \sum_q q^2 \langle |h_q^2| \rangle = \frac{1}{24} \frac{L}{\xi_p} \sim \frac{L}{\xi_p}$$

For semiflexible filaments, the persistence length is $\xi_p = k_f/k_B T$. Note that the correction to the length is quadratic in the small parameter, $ds = dx + O(\varepsilon^2)$, i.e., $L_c = L(1 + O(\varepsilon^2))$. Averaging over all possible conformations taken by the fluctuating filament gives the average end-to-end distance (apparent length)

$$L = L_c - \frac{1}{2} \int_0^L dx \left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle$$

From Eq. [29] and Eq. [38] we have

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = c \frac{k_B T}{\xi_p}, \quad \text{where } c = O(1) \text{ constant}$$

Hence

$$L = L_c - \frac{1}{2} \int_0^L dx \left(c \frac{k_B T}{\xi_p} \right) = L_c - L \left(c \frac{k_B T}{\xi_p} \right)$$

and

$$\frac{L_c - L}{L} \approx \frac{L_c - L}{L_c} \approx \frac{k_B T}{\xi_p}$$

Force-extension curve: References: Marko and Siggia "Stretching DNA", Macromolecules, 1995, v.28:8759-8770

Evans and Rawicz, "Entropy-driven tension and bending elasticity in condensed-fluid membranes", PRL 64:2094 (1990)

Polymers/membranes "store" length in the thermal contour/shape undulations. So, the apparent length L is smaller than the actual length L_c . The polymer/filament is inextensible, i.e. the total length L_c is fixed. However, the apparent length L increases if we pull on one end of the polymer. The end-to-end distance L increases at the expense of decreasing amplitude of the contour fluctuations.

Here we will calculate $L(f)$.

Exercise: show that the action of the external tensile force f results in additional energy

$$E_t \approx \frac{f}{2} \int_0^L dx \left(\frac{dh}{dx} \right)^2$$

Hence, the total energy of the filament is then

$$E = E_t + E_b \approx \int_0^L dx \left[\frac{k_f}{2} \left(\frac{d^2 h}{dx^2} \right)^2 + \frac{f}{2} \left(\frac{dh}{dx} \right)^2 \right]$$

Exercise: show that

$$\langle h_q h_{q'} \rangle = \frac{1}{L} \frac{k_B T}{k_f q^4 + f q^2} \delta_{q+q', 0} \quad (13)$$

and use

$$L = L_c - \frac{1}{2} \int_0^L dx \left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle$$

to evaluate $L/L_c(f)$. Note: there is a factor of 2 in Marko because the polymer fluctuations are in 3D, undulation in both transverse directions, z and y. We consider for simplicity curve in a plane, 2D.

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{1}{L} k_B T \sum_q \frac{1}{k_f q^2 + f} = \frac{k_B T}{L} \frac{L}{(2\pi)} \int_{-\infty}^{+\infty} \frac{dq}{k_f q^2 + \tau} = \frac{k_B T}{2\pi k_f} \pi \sqrt{\frac{k_f}{f}} = \frac{1}{2\xi_p} \sqrt{\frac{k_f}{f}} \quad (14)$$

$$L = L_c - \frac{1}{2} \int_0^L dx \left(\frac{1}{2\xi_p} \sqrt{\frac{k_f}{f}} \right) = L_c - L \frac{1}{4\xi_p} \sqrt{\frac{k_f}{f}} \quad (15)$$

To leading order, $L \approx L_c$ in the second term, hence

$$\frac{L}{L_c} = 1 - \frac{1}{4} \sqrt{\frac{k_B T}{\xi_p f}} \quad (16)$$

At large forces, L approaches L_c with $f^{-1/2}$ behavior, in contrast to the FJC model in which $L_c - L \sim 1/f$ for large forces.

another way (Marko): Stretching energy is $E_t = -fL = f(L_c - \int dx (dh/dx)^2)$ The filament extension is

$$\begin{aligned} \frac{L}{L_c} &= \mathbf{t} \cdot \hat{\mathbf{x}} = 1 - \frac{1}{2} \langle (dh/dx)^2 \rangle \\ \frac{E}{k_B T} &= \int ds \left(\frac{\xi_p}{2} \left(\frac{d\mathbf{t}}{ds} \right)^2 - F \mathbf{t} \cdot \hat{\mathbf{x}} \right) \\ (\mathbf{n} \cdot \hat{\mathbf{x}}) &\equiv t_x = \sqrt{1 - t_z^2}, \quad ds = dx \sqrt{1 - t_z^2} \end{aligned}$$

to leading order

$$\begin{aligned} L &= \int_0^{L_c} ds (\mathbf{n} \cdot \hat{\mathbf{x}}) = \int_0^{L_c} ds - \frac{1}{2} \int_0^{L_c} dx t_z^2 \\ \langle (t_z)^2 \rangle &= \left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{1}{L} k_B T \sum_q \frac{1}{k_f q^2 + f} = \frac{k_B T}{L} \frac{L}{(2\pi)} \int_{-\infty}^{+\infty} \frac{dq}{k_f q^2 + \tau} = \frac{k_B T}{2\pi k_f} \pi \sqrt{\frac{k_f}{f}} = \frac{1}{2\xi_p} \sqrt{\frac{k_f}{f}} \end{aligned} \quad (17)$$

$$\mathbf{t} = \left(1, \frac{dh}{dx} \right)$$

The projected length

$$\begin{aligned} dx &= ds (\mathbf{n} \cdot \hat{\mathbf{x}}), \quad L = \int_0^{L_c} ds (\mathbf{n} \cdot \hat{\mathbf{x}}) \\ (\mathbf{n} \cdot \hat{\mathbf{x}}) &\equiv t_x = \sqrt{1 - t_z^2}, \quad ds = dx \sqrt{1 - t_z^2} \end{aligned}$$

to leading order

$$\begin{aligned} L &= \int_0^{L_c} ds (\mathbf{n} \cdot \hat{\mathbf{x}}) = \int_0^{L_c} ds - \frac{1}{2} \int_0^{L_c} dx t_z^2 \\ \langle (t_z)^2 \rangle &= \left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{1}{L} k_B T \sum_q \frac{1}{k_f q^2 + f} = \frac{k_B T}{L} \frac{L}{(2\pi)} \int_{-\infty}^{+\infty} \frac{dq}{k_f q^2 + \tau} = \frac{k_B T}{2\pi k_f} \pi \sqrt{\frac{k_f}{f}} = \frac{1}{2\xi_p} \sqrt{\frac{k_f}{f}} \end{aligned} \quad (18)$$

2.4 Fluctuating membrane

Power spectrum of the curvature fluctuations: Expand the membrane profile $h(x, y)$ in Fourier modes

$$h(x, y) = \sum_{\mathbf{q}} h_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{r}}, \quad \mathbf{q} = \frac{2\pi}{L} (n_x \hat{\mathbf{x}} + n_y \hat{\mathbf{y}}), \quad n_x, n_y = \pm 1, \pm 2, \dots \infty \quad (19)$$

see for detailed derivation Deserno notes on "Fluid membranes", p. 26.

$$E = L^2 \sum_{\mathbf{q}} h_{\mathbf{q}} h_{-\mathbf{q}} \frac{\kappa}{2} q^4$$

For a membrane under tension σ , the energy cost for the undulations away from the flat state is

$$E = \frac{\kappa}{2} \int dA H^2 + \sigma \left(\int dA - \iint dxdy \right) \approx \int_0^L dx \int_0^L dy \left(\frac{\kappa}{2} (\nabla^2 h)^2 + \sigma (\nabla h)^2 \right)$$

Exercise: Show that

$$\langle |h_{\mathbf{q}}|^2 \rangle = \frac{1}{L^2} \frac{k_B T}{\kappa q^4 + \sigma q^2} \quad (20)$$

Apparent (also called projected) area A_p Reading: Boal, Chapter 8

$$A_p = L^2 = \int_0^L \int_0^L dxdy, \quad \text{for a square patch}$$

The contour (true area)

$$A = \iint dxdy \sqrt{1 + (\nabla h)^2} \approx \iint dxdy \left(1 + \frac{1}{2} (\nabla h)^2 \right)$$

The projected area $A_p = \iint dxdy$ is reduced below the contour area A by thermal fluctuations. The reduction of in-plane area with respect to the contour area is

$$\begin{aligned} A_{red} = A - L^2 &= \frac{1}{2} \iint dxdy \langle (\nabla h)^2 \rangle = \frac{1}{2} L^2 \sum_{\mathbf{q}} q^2 \langle |h_{\mathbf{q}}|^2 \rangle = \frac{1}{2} L^2 \frac{L^2}{(2\pi)^2} \int d\mathbf{q} q^2 \langle |h_{\mathbf{q}}|^2 \rangle \\ &= \frac{1}{2} L^2 \frac{L^2}{(2\pi)^2} \int_{q_{min}}^{q_{max}} (2\pi q dq) q^2 \frac{k_B T}{L^2 (\kappa q^4 + \sigma q^2)} \end{aligned}$$

Exercise: Derive that the area reduction at given tension is

$$\frac{A - L^2}{L^2} \approx \frac{A - L^2}{A} = \frac{k_B T}{8\pi\kappa} \ln \left(\frac{\sigma/\kappa + q_{max}^2}{\sigma/\kappa + q_{min}^2} \right)$$

$q_{min} = \pi/L$ and $q_{max} = \pi/d$, where d is the thickness of the membrane.

Evans and Rawicz (1990) evaluate the area change with respect to the tensionless reference state, which has the largest area reduction ($\sigma = 0$). Then, applying a tension τ increases the projected area by an amount α . Find α

$$\alpha = \frac{A_{red}(0) - A_{red}(\tau)}{A} = ?$$

2.5 Persistence length ζ_p

Length over which the filament is nearly straight /membrane is nearly flat (note that inearly flat means there is high degree of correlation between the normal vectors). At lengthscales $\gg \zeta_p$, the filament is "random coil" / the membrane is crumpled.

This so called persistence length can be estimated as the projected ("apparent") length L at which the Monge approximation breaks down (the bending become significant), i.e.

$$\langle |\nabla h|_{\xi_p=L} \rangle \sim 1$$

where

$$\langle \dots \rangle$$

denotes average over all possible conformations taken by the membrane while fluctuating at a given temperature.

2D: filament: Note that

$$|\nabla h| = \sqrt{\nabla h \cdot \nabla h} = \sqrt{\left(\frac{dh}{dx}\right) \left(\frac{dh}{dx}\right)}$$

So we can evaluate the persistence length from

$$\left(\frac{dh}{dx}\right) \left(\frac{dh}{dx}\right) \sim 1$$

Expand the (fluctuating) filament contour $h(x)$ in Fourier modes

$$h(x) = \sum_{q=-\infty}^{\infty} h_q e^{iqx}, \quad q = \frac{2\pi}{L}n, \quad n = \pm 1, \pm 2, \dots \infty \quad (21)$$

Note: mode 0 involves no bending therefore is excluded.

The modes amplitudes h_q fluctuate about average zero value $\langle h_q \rangle = 0$, but nonzero $\langle |h_q|^2 \rangle$ (to be determined).

$$\frac{dh}{dx} = \sum_q (iq) h_q e^{iqx} \quad (22)$$

$$\left(\frac{dh}{dx}\right)^2 = \sum_q \sum_{q'} (-qq') h_q h_{q'} e^{i(q+q')x} \quad (23)$$

Taking average

$$\left\langle \left(\frac{dh}{dx}\right)^2 \right\rangle = \sum_q \sum_{q'} (-qq') \langle h_q h_{q'} \rangle e^{i(q+q')x} \quad (24)$$

The shape modes are independent, i.e., uncorrelated

$$\langle h_q h_{q'} \rangle = \langle |h_q|^2 \rangle \delta_{q+q',0} \quad (25)$$

where $\delta_{q+q',0}$ is the Kronecker delta ($\delta_{a,b} = 1$ if $a = b$, and $\delta_{a,b} = 0$ otherwise) Hence in the sum Eq. [24] only the terms with $q' = -q$ survive

$$\left\langle \left(\frac{dh}{dx}\right)^2 \right\rangle = \sum_q q^2 \langle h_q h_{-q} \rangle \quad (26)$$

Next lecture we will see that (for a tensionless filament)

$$\langle |h_q|^2 \rangle = \frac{1}{L} \frac{k_B T}{k_f q^4} \quad (27)$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{1}{L} \frac{k_B T}{k_f} \sum_q \frac{1}{q^2} = \frac{1}{L} \frac{k_B T}{k_f} \frac{L^2}{(2\pi)^2} 2 \sum_{n=1}^{\infty} \frac{1}{n^2} \quad (28)$$

The sum (Basel problem)

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{1}{L} \frac{k_B T}{k_f} \frac{L^2}{(2\pi)^2} 2 \frac{\pi^2}{6} = \frac{k_B T}{k_f} \frac{L}{12} \quad (29)$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle \sim 1, \quad \text{when } L \sim \frac{k_f}{k_B T} \equiv \xi_p \quad (30)$$

(ignore the $O(1)$ numerical factor of 12, which anyways is incorrect because we assumed that the largest wavenumber is ∞ while in reality there is truncation due to the finite thickness of the filament, $q_{max} = 2\pi/d$, where d is the thickness of the filament, and $q_{min} = 2\pi/L$).

ASIDE: doing the calculation using integrals.

$$\left(\frac{dh}{dx} \right)^2 = \sum_{q, q'} (-qq') h_q h_{q'} e^{i(q+q')x} = \frac{L^2}{(2\pi)^2} \int dq \int dq' (-qq') h_q h_{q'} e^{i(q+q')x} \quad (31)$$

Taking average

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{L^2}{(2\pi)^2} \int dq \int dq' (-qq') \langle h_q h_{q'} \rangle e^{i(q+q')x} \quad (32)$$

The shape modes are independent, i.e., uncorrelated

$$\langle h_q h_{q'} \rangle = \langle |h_q|^2 \rangle \delta_{q+q', 0} = \langle |h_q|^2 \rangle \delta(q+q') \frac{2\pi}{L} \quad (33)$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{L}{(2\pi)} \int dq \langle |h_q|^2 \rangle \int dq' (-qq') \delta(q+q') e^{i(q+q')x} \quad (34)$$

use the property of the delta function that

$$\int dy \delta(y) f(y) = f(0)$$

Hence

$$\begin{aligned} \int dq' (-qq') \delta(q+q') e^{i(q+q')x} &= q^2 \\ \left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle &= \frac{L}{2\pi} \int dq \langle |h_q|^2 \rangle q^2 \end{aligned} \quad (35)$$

We know (for a tensionless filament)

$$\langle |h_q|^2 \rangle = \frac{1}{L} \frac{k_B T}{k_f q^4} \quad (36)$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{L}{2\pi} \int dq q^2 \frac{1}{L} \frac{k_B T}{k_f q^4} = \frac{k_B T}{k_f 2\pi} \int dq \frac{1}{q^2} \quad (37)$$

Let us discuss the limits of the integral. The sum is from $-\infty$ to $+\infty$ (in reality this is q_{max} corresponding to molecular scales (the rod has finite thickness)), excluding $q = 0$. $1/q^2$ is even hence

$$\int_{-\infty}^{+\infty} = 2 \int_{q_{min}}^{\infty}$$

The lowest mode (corresponding $n = 1$) is not zero but it is set by the size of the system $q_{min} = 2\pi/L$. Hence the integral does not start at 0.

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle = \frac{k_B T}{k_f \pi} \int_{q_{min}}^{\infty} dq \frac{1}{q^2} = \frac{k_B T}{k_f \pi} \left(\frac{1}{q_{min}} \right) = \frac{k_B T}{k_f} \frac{L}{2\pi^2} \quad (38)$$

$$\left\langle \left(\frac{dh}{dx} \right)^2 \right\rangle \sim 1, \quad \text{when} \quad L \sim \frac{k_f}{k_B T} \equiv \xi_p \quad (39)$$

(ignore the $O(1)$ numerical factor of $2\pi^2$).

Exercise: Go over the calculations, check for accuracy. Any idea why there is a difference between Eq. [38] and Eq. [29]?

3D: membranes: Note that $\mathbf{r} \cdot \mathbf{q} = q_x x + q_y y$

$$\nabla h = \sum_{\mathbf{q}} h_{\mathbf{q}} (i q_x e^{i\mathbf{r} \cdot \mathbf{q}} + i q_y e^{i\mathbf{r} \cdot \mathbf{q}}) = \sum_{\mathbf{q}} h_{\mathbf{q}} (i\mathbf{q}) e^{i\mathbf{r} \cdot \mathbf{q}}$$

$$(\nabla h)^2 = \sum_{\mathbf{q}, \mathbf{q}'} h_{\mathbf{q}} h'_{\mathbf{q}'} (-\mathbf{q} \cdot \mathbf{q}') \exp(i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{r})$$

going from sums to integrals

$$(\nabla h)^2 = \left(\frac{L^2}{(2\pi)^2} \right)^2 \int d\mathbf{q} \int d\mathbf{q}' \exp(i(\mathbf{q} + \mathbf{q}') \cdot \mathbf{r}) (-\mathbf{q} \cdot \mathbf{q}') h_{\mathbf{q}} h'_{\mathbf{q}'}$$

$$\int d\mathbf{q}' e^{i\mathbf{r} \cdot (\mathbf{q} + \mathbf{q}')} = \delta(\mathbf{q} - \mathbf{q}') = \delta_{\mathbf{q} + \mathbf{q}', 0} \frac{L^2}{(2\pi)^2}$$

$$\langle (\nabla h)^2 \rangle = \frac{L^2}{(2\pi)^2} \iint d\mathbf{q} q^2 \langle |h_{\mathbf{q}}|^2 \rangle = \frac{L^2}{(2\pi)^2} \iint 2\pi q dq \frac{k_B T}{L^2 \kappa q^2} = \frac{k_B T}{2\pi} \ln \left(\frac{q_{max}}{q_{min}} \right)$$

$q_{min} \sim 1/L$, and the microscopic cut-off is $q_{max} \sim 1/d$, $d \sim$ thickness of the membrane
 $\langle (\nabla h)^2 \rangle \sim 1$ when

$$L \sim \zeta_p \equiv d \exp \left(\frac{2\pi \kappa}{k_B T} \right)$$

Compare to filaments!!!!!!

Exercise: Estimate the persistence length for a membrane with typical bending rigidity $\kappa = 10k_B T$

3 A bit more on vesicle shapes

The equilibrium shapes of a vesicle (in absence of flow) satisfy the generalized Laplace's equation, which for the Helfrich model is

$$p^{(2)} - p^{(1)} = -2\sigma_0 H + \kappa (4H^3 - 4HK + 2\nabla_s^2 H) , \quad (40)$$

where σ_0 is the membrane tension. Eq. [40] is a nonlinear equation for the surface profile and yields a plethora of solutions as a function the vesicle deflation. As an example, the equilibrium shapes predicted by Eq. [40] for vesicles with an intermediate aspect ratio e (defined as the ratio of the long and short axes) possess both axial and top-down mirror symmetry: prolate-dumbbell for $v > 0.652$ ($e < 4$), and oblate-discocyte (the shape of the red blood cell) for $0.591 < v \leq 0.651$ ($3.44 < e < 3.95$).

Nondimensionalize Eq. [40] using R_0 and κ . Solve the shape equation to find different vesicle shapes for given reduced volume v , Δp and $\bar{\sigma}$.

$$4H^3 - 4HK + 2\nabla_s^2 H - 2\Sigma H = \Delta p , \quad (41)$$

$$\Sigma = \sigma_0 R_0^2 / \kappa , \quad P = (p^{(2)} - p^{(1)}) R_0^3 / \kappa$$

3.1 2D shapes

In 2D a vesicle is a closed curve. The curvature of a curve κ is defined by $\frac{d^2 \mathbf{r}}{ds^2} = \kappa \mathbf{n}$ and the bending energy is

$$\frac{1}{2} \int_0^1 \kappa^2 ds$$

Note that the reduced volume is

$$v = \frac{A}{\pi R_0^2} \quad R_0 = \frac{L}{2\pi}$$

3.1.1 approach 1

Follow Veerapaneni et al “Analytical and numerical solutions for shapes of quiescent two-dimensional vesicles” International Journal of Non-Linear Mechanics 44 (2009) 257–262

Using arc length parametrization Eq. Eq. [41] becomes

$$\frac{d^2 \kappa}{ds^2} + \frac{1}{2} \kappa^3 - 2\Sigma \kappa + P = 0 \quad (42)$$

(check $\kappa = -H/2$?)

Need to solve this equation using

$$\kappa(0) = c_0 , \quad \frac{d\kappa}{ds} = 0 \quad (43)$$

3.1.2 approach 2

Derive and solve equation for the profile $Z(s)$

3.2 Axisymmetric shapes

Seifert et al “SHAPE TRANSFORMATIONS OF VESICLES - PHASE-DIAGRAM FOR SPONTANEOUS-CURVATURE AND BILAYER-COUPPLING MODELS”, PRA (1991) vol. 44 (2) pp. 1182-1202

We will use shape parametrization shown in Figure 1.

$$\dot{X} = \cos \psi \quad \dot{Z} = -\sin \psi \quad (44)$$

dot denotes derivative wrt arc length s . The two principal curvatures are

$$C_1 = \dot{\psi} \quad C_2 = \frac{\sin \psi}{X} \quad (45)$$

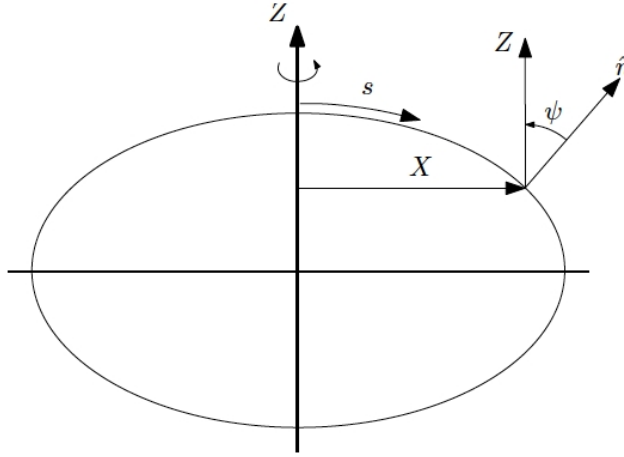


Figure 2: Coordinate system for axisymmetric shape

Show that Eq. [41] transforms to

$$\begin{aligned} \frac{d^3\psi}{ds^3} = & -\frac{1}{2} \left(\frac{d\psi}{ds} \right)^3 + \frac{3 \sin \psi}{2X} \left(\frac{d\psi}{ds} \right)^2 + \frac{3 \cos(2\psi) + 1}{4X^2} \frac{d\psi}{ds} + \Delta p \\ & + \Sigma \left(\frac{d\psi}{ds} + \frac{\sin \psi}{X} \right) - \frac{2 \cos \psi}{X} \frac{d^2\psi}{ds^2} - \frac{(3 + \cos(2\psi)) \sin \psi}{4X^3} \end{aligned} \quad (46)$$

How to solve this equation? What are the boundary conditions ?

See newer paper by Reboucas et al. Soft Matter (2024)