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Biophysics Homework 4

9. Donut Vesicles

The microscopy pictures from [M. Mutz and D. Bensimon, Phys. Rev. A 43, 4525-4527 (1991)] show a toroidal vesicle from the side and top. The scale bar indicates ten microns. Since these curious objects evidently really exist, we take the liberty to look a bit into their properties in this problem.

In order to describe toroidal vesicles, we first need a convenient set of surface coordinates. One possibility is to characterize the torus by two radii, r_1 and $r_2 < r_1$. Any point within the torus can thus be parameterized by giving two angles, ϑ and φ, as well as a radius r from the center of the loop that passes through the center of the body of the torus. Restricting then to $r = r_2$ gets us onto the torus surface, so that (ϑ, φ) can be chosen as surface coordinates. These coordinates are curvilinear, so the area element is not just $d\vartheta d\varphi$ but rather $dA = r_2(r_1 - r_2 \cos\vartheta)d\vartheta d\varphi$. The two principal curvatures c_i point in ϑ- and φ-direction and are given by $c_\vartheta = \frac{1}{r_2}$ and $c_\varphi = \frac{-\cos\vartheta}{r_1 - r_2\cos\vartheta}$. Sadly, you need some differential geometry to actually prove this.

1. **What is the total surface area of the torus? If you have ever heard of Pappus' centroid theorem or Guldin's first rule, comment!**

$$\int_0^{2\pi}\int_0^{2\pi} dA = \int_0^{2\pi}\int_0^{2\pi} r_2(r_1 - r_2\cos\vartheta)d\vartheta d\varphi = 2\pi r_2\int_0^{2\pi}(r_1 - r_2\cos\vartheta)d\vartheta d\varphi = 4\pi^2 r_1 r_2$$

This can be predicted by Pappus' Centroid Theorem (another name for Guldin's first rule), which states that the surface area $S = 2\pi s\bar{x}$, where $\bar{x}$ is the distance from the axis of rotation to the centroid of the two-dimensional figure being rotated around the axis to generate the three-dimensional object and s is the surface area of the two-dimensional figure. In this case, a circle is rotated around an axis to produce a torus, $\bar{x} = r_1$ and $s = 2\pi r_2$.

2. **For vanishing spontaneous curvature c_0 and tension σ the curvature energy cannot depend on the absolute size of the vesicle – we know it's scale invariant. But it will depend on the aspect ratio $\xi = \frac{r_1}{r_2}$. Show that it is given by**

$$E_{curvature}(\xi) = \pi\kappa \int_0^{2\pi} d\vartheta \frac{(\xi - 2\cos\vartheta)^2}{\xi - \cos\vartheta} = \frac{2\pi^2\xi^2}{\sqrt{\xi^2 - 1}}\kappa$$ **, independent of $\bar{\kappa}$!**

Let me start with the Helfrich Hamiltonian:

$$e = \frac{1}{2}(c_\vartheta, c_\varphi)\begin{bmatrix} \kappa & \kappa + \bar{\kappa} \\ \kappa + \bar{\kappa} & \kappa \end{bmatrix}\begin{pmatrix} c_\vartheta \\ c_\varphi \end{pmatrix} = \frac{1}{2}\left[c_\vartheta^2 + c_\varphi^2\right]\kappa + (\kappa + \bar{\kappa})c_\vartheta c_\varphi .$$

Then, I seek:

$$E_{curvature} = \int_0^{2\pi}\int_0^{2\pi} e dA = \int_0^{2\pi}\int_0^{2\pi}\left[\frac{1}{2}\left[\frac{1}{r_2^2} + \frac{\cos^2\vartheta}{(r_1 - r_2\cos\vartheta)^2}\right]\kappa - (\kappa + \bar{\kappa})\frac{1}{r_2}\frac{\cos\vartheta}{r_1 - r_2\cos\vartheta}\right] r_2(r_1 - r_2\cos\vartheta)d\vartheta d\varphi$$

$$= \int_0^{2\pi}\int_0^{2\pi}\left[\frac{1}{2}\left[\frac{r_1 - r_2\cos\vartheta}{r_2} + \frac{r_2\cos^2\vartheta}{r_1 - r_2\cos\vartheta}\right]\kappa - (\kappa + \bar{\kappa})\cos\vartheta\right] d\vartheta d\varphi$$

$$= \pi\kappa \int_0^{2\pi}\left[\frac{r_1 - r_2\cos\vartheta}{r_2} + \frac{r_2\cos^2\vartheta}{r_1 - r_2\cos\vartheta}\right] d\vartheta$$

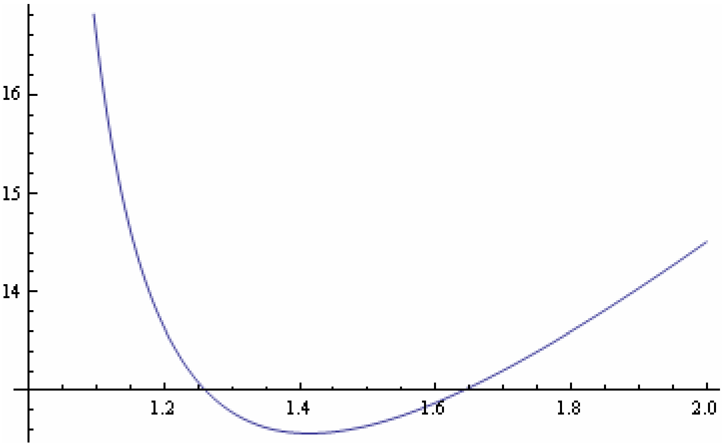
$$= \pi\kappa \int_0^{2\pi}\left[\xi - \cos\vartheta + \frac{\cos^2\vartheta}{\xi - \cos\vartheta}\right] d\vartheta$$

$$= \pi\kappa \int_0^{2\pi}\left[\frac{\xi^2 - 2\xi\cos\vartheta + 2\cos^2\vartheta}{\xi - \cos\vartheta}\right] d\vartheta$$

Integrating this in Mathematica gives the correct result in spite of the slight difference between this and the expected integral (their difference integrates to zero):

$$E_{curvature}(\xi) = \pi\kappa \int_0^{2\pi}\left[\frac{\xi^2 - 2\xi\cos\vartheta + 2\cos^2\vartheta}{\xi - \cos\vartheta}\right] d\vartheta = \frac{2\pi^2\xi^2}{\sqrt{\xi^2 - 1}}\kappa$$

3. **Sketch $E_{curvature}(\xi)$. You'll see that the energy is minimized by one particular value of the aspect ratio, $\xi_{\min}$. What is it, and what is $E_{curvature}^{\min} \equiv E_{curvature}(\xi_{\min})$? Are the experimental pictures compatible with your finding?**



$E_{curvature}(\xi)$ as a function of ξ.

The minimum should occur at $\partial_\xi\left[\frac{2\pi^2\xi^2}{\sqrt{\xi^2-1}}\right]\kappa = 0$, or $\frac{2\pi\xi\left(\xi^2-2\right)}{\left(\xi^2-1\right)^{\frac{3}{2}}} = 0$. Thus, this minimum occurs where $\xi_{\min} = \sqrt{2}$ and $E_{curvature}^{\min} = 4\pi^2\kappa$.

In this case, then, I would expect the hole's diameter to be $\frac{\sqrt{2}-1}{\sqrt{2}+1} \approx 17\%$ of the total diameter of the torus. Measuring from the picture, the hole appears to be 2.5 microns in diameter and the torus to be 15 microns in diameter, so that the hole's diameter is indeed about 16.6% of the total diameter of the torus, corroborating my findings.

4. **Is it conceivable that for some given values of the bending moduli κ and $\bar{\kappa}$ an optimal toroidal vesicle has a lower energy than a spherical one? What does your answer tell you about the experimental pictures shown above?**

The curvature of a sphere is $c = \frac{1}{R}$. Locally, then, using the Helfrich Hamiltonian,

$$e_{sphere} = \frac{1}{2}\left(c_{sphere}, c_{sphere}\right)\begin{bmatrix} \kappa & \kappa + \bar{\kappa} \\ \kappa + \bar{\kappa} & \kappa \end{bmatrix}\begin{pmatrix} c_{sphere} \\ c_{sphere} \end{pmatrix} = \left(2\kappa + \bar{\kappa}\right)c_{sphere}^2$$

Integrating this over the entire surface, however, I pick up a factor of $4\pi R^2$ so that $E_{curvature,sphere} = 4\pi\left(2\kappa + \bar{\kappa}\right)$. Thus, I see that $E_{curvature--sphere} = 4\pi\left(2\kappa + \bar{\kappa}\right) > E_{curvature--torus}^{\min} = 4\pi^2\kappa$ when $\bar{\kappa} > (\pi - 2)\kappa$.

However, this result conflicts with the requirement that $\bar{\kappa} < 0$ since $\kappa > 0$. Then, clearly, this object is not in thermal equilibrium with its surroundings and as such has a finite lifetime.

10. **Linearized Shape Equation for the Helfrich Hamiltonian**

Let us study membranes which deviate only weakly from the flat xy-plane, so that we can describe them by the height function $z = h(x,y)$. With a little bit of differential geometry one may show that to lowest order the curvature in this parameterization is given by the Laplacian Δh and the excess area is given by the squared gradient $\frac{1}{2}(\nabla h)^2$. The total energy is therefore

$$E[h(x,y)] = \frac{1}{2}\int dxdy\left\{\kappa(\Delta h(x,y))^2 + \sigma(\nabla h(x,y))^2\right\}$$

We would like to know which differential equation $h(x,y)$ must satisfy in order to minimize this energy.

1. **Let us perform a little variation, $h(x,y) \rightarrow h(x,y) + \delta h(x,y)$. Show that up to linear order in the small variation the change is given by**

   $$\delta E[h(x,y)] = \int dxdy\{\kappa(\Delta h)(\Delta\delta h) + \sigma(\nabla h)\cdot(\nabla\delta h)\}.$$

$$E[h(x,y)+\delta h(x,y)] = \frac{1}{2}\int dxdy\left\{\kappa(\Delta[h(x,y)+\delta h(x,y)])^2 + \sigma(\nabla[h(x,y)+\delta h(x,y)])^2\right\}$$

$$= \frac{1}{2}\int dxdy\left\{\kappa(\Delta h + \Delta\delta h)^2 + \sigma(\nabla h + \nabla\delta h)^2\right\}$$

Expanding the squares and dropping terms quadratic in the variation, I have:

$$E[h(x,y)+\delta h(x,y)] = \frac{1}{2}\int dxdy\left\{\kappa\left((\Delta h)^2 + 2(\Delta h)(\Delta\delta h)\right) + \sigma\left((\nabla h)^2 + 2(\nabla\delta h)\cdot(\nabla h)\right)\right\}$$

However, subtracting the original expression for energy from the above I have:

$$\delta E[h(x,y)] = E[h(x,y)+\delta h(x,y)] - E[h(x,y)] = \int dxdy\{\kappa(\Delta h)(\Delta\delta h) + \sigma(\nabla\delta h)\cdot(\nabla h)\}$$

QED.

2. **The two terms $\Delta\delta h$ and $\nabla\delta h$ contain derivatives of the variation rather than just the variation itself. This is not nice. Remove these derivatives by partial integration (you may ignore boundary terms). You'll then have an integral of the form $\delta E[h(x,y)] = \int dxdy \mathrm{E}(h)\delta h$, where $\mathrm{E}(h)$ is the so-called Euler-Lagrange derivative. Since in equilibrium $\delta E = 0$, and**

since $\delta h(x,y)$ was completely arbitrary, it follows that $\mathrm{E}(h)$ must vanish. This is the shape equation. What is it?

I will start by converting this to tensor notation since it will help me stay organized.

$$\delta E[h(x,y)] = \int dxdy\{\kappa(\Delta h)(\Delta \delta h) + \sigma(\nabla \delta h)\cdot(\nabla h)\}$$
$$= \kappa \sum_{i,j,k,l} \int dxdy\left[\partial_i \partial_j \delta^{ij} h\right]\left[\partial_k \partial_l \delta^{kl} \delta h\right] + \sigma \sum_{i,j} \int dxdy\left[\partial_i \delta h\right]\left[\partial_j h\right]\delta^{ij}$$

Now it is clear that I must simply move my derivatives over and re-interpret the results. I will ignore all of the boundary terms.

$$\delta E[h(x,y)] = \kappa \sum_{i,j,k,l} \int dxdy\left[\partial_i \partial_j \partial_k \partial_l \delta^{kl} \delta^{ij} h\right]\delta h - \sigma \sum_{i,j} \int dxdy\left[\partial_i \partial_j \delta^{ij} h\right]\delta h$$
$$= \kappa \int dxdy\left[\Delta^2 h\right]\delta h - \sigma \int dxdy[\Delta h]\delta h$$

Now since in equilibrium $\delta E = 0$ and $\delta h(x,y)$ is completely arbitrary, then the Euler-Lagrange derivative is:

$$\mathrm{E}(h) = \kappa\left(\Delta^2 h\right) - \sigma(\Delta h) = 0$$

This is also known as the “shape equation”.