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New solutions of the shape equation

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Abstract. The general shape equation describing the forms of vesicles is a highly nonlinear partial differential equation for which only a few explicit solutions are known. These solvable cases are briefly reviewed and a new analytical solution which represents the class of the constant mean curvature surfaces is described. Pearling states of the tubular fluid membranes can be explained as a continuous deformation preserving membrane mean curvature.

PACS. 87.16.Dg Membranes, bilayers, and vesicles – 68.15.+e Liquid thin films – 87.10.+e General theory and mathematical aspects – 02.40.Hw Classical differential geometry

1 Introduction

In water and at low concentrations some amphiphilic molecules like phospholipids assemble themselves and form flexible bilayers which can close in a single shell which nowadays is called a vesicle. Because these vesicles can be easily isolated and studied they are considered to be sufficiently realistic models of biomembranes and cells. On the other hand, since the thickness of the typical bilayer is in the nm range and the typical diameter of vesicles is in the μn range, one can regard the membrane bilayer as a two-dimensional surface in three-dimensional Euclidean space. Therefore, before starting to discuss vesicle morphology it is necessary to have a short summary of the classical differential geometry of surfaces. Then the Canham-Helfrich bending energy and the corresponding general shape equation into which enter such geometric quantities as the mean and Gaussian curvature, the area and the volume enclosed by the membrane will be introduced.

Finally, the list of the explicit solutions to the above mentioned equation will be briefly discussed and the new analytical formulae representing the axisymmetric constant mean curvature surfaces will be derived.

2 Differential geometry of surfaces

As the Canham-Helfrich approach is based on some notions of classical differential geometry we will sketch them below. Modern expositions of the subject can be found, *e.g.* in the books by Berger and Gostiaux [2] and Oprea [9]. The membrane is represented as a closed surface $\mathcal{S}$ in space and the position vector to a point on $\mathcal{S}$ is given in terms of two parameters u, v which label the material points

$$\mathbf{x} = \mathbf{x}[u, v] = (x(u, v), y(u, v), z(u, v))\,.$$

The surface itself is specified by its first and second fundamental forms

$$I = E\,\mathrm{d}u^2 + 2F\,\mathrm{d}u\mathrm{d}v + G\,\mathrm{d}v^2 \tag{1}$$

and

$$II = L\,\mathrm{d}u^2 + 2M\,\mathrm{d}u\mathrm{d}v + N\,\mathrm{d}v^2 \tag{2}$$

where the coefficients are given by

$$\begin{aligned} E = E[u,v] &= \mathbf{x}_u \cdot \mathbf{x}_u \quad & F = F[u,v] &= \mathbf{x}_u \cdot \mathbf{x}_v \\ G = G[u,v] &= \mathbf{x}_v \cdot \mathbf{x}_v \quad & L = L[u,v] &= \mathbf{n} \cdot \mathbf{x}_{uu} \\ M = M[u,v] &= \mathbf{n} \cdot \mathbf{x}_{uv} \quad & N = N[u,v] &= \mathbf{n} \cdot \mathbf{x}_{vv} \end{aligned} \tag{3}$$

where $\mathbf{n}$ is the unit vector normal to $\mathcal{S}$

$$\mathbf{n} = \mathbf{n}[u, v] = \frac{\mathbf{x}_u \times \mathbf{x}_v}{|\mathbf{x}_u \times \mathbf{x}_v|}\,\cdot \tag{4}$$

By definition the *normal curvature* $\mathbf{k_n}$ in the direction $(\mathrm{d}u : \mathrm{d}v)$ is

$$\mathbf{k_n} = \frac{II}{I} = \frac{L\,\mathrm{d}u^2 + 2M\,\mathrm{d}u\mathrm{d}v + N\,\mathrm{d}v^2}{E\,\mathrm{d}u^2 + 2F\,\mathrm{d}u\mathrm{d}v + G\,\mathrm{d}v^2}, \tag{5}$$

and the directions in which it attains extremal values (maximum and minimum) are called *principal directions*. If the coordinate curves coincide with the principal directions then

$$F = M \equiv 0 \tag{6}$$

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and the corresponding curvatures in these directions can be found by the formulae

$$\mathbf{k_1} = \frac{L}{E}, \qquad \mathbf{k_2} = \frac{N}{G} \cdot \tag{7}$$

It should be noted also that in this situation $\mathbf{k_1}$ and $\mathbf{k_2}$ are the principal curvatures along the meridians and parallels of latitude respectively. Classical differential geometry operates also with other important notions which are of immediate interest for us. These are the Gaussian curvature K and the mean curvature H

$$K = \mathbf{k_1} \cdot \mathbf{k_2}, \qquad H = \frac{\mathbf{k_1} + \mathbf{k_2}}{2}, \tag{8}$$

and the surface area element $\mathrm{d}A$

$$\mathrm{d}A = \sqrt{E\,G - F^2}\,\mathrm{d}u\mathrm{d}v = \sqrt{E\,G}\,\mathrm{d}u\mathrm{d}v. \tag{9}$$

3 Helfrich model and shape equation

According to the *fluid mosaic* model the biomembranes are considered as bilayers of amphiphilic lipids in which the lipid molecules can move freely on the membrane surfaces while other constituent molecules – proteins and enzymes are embedded in the lipid bilayers. Therefore no elastic energy is associated with the displacements within a given surface and only the energy coming from bending of the membrane should be taken into account. This is the essence of Canham's proposal [3] which states that the bending energy of membranes should be identified with the Willmore [14] functional built upon the curvatures of the embedded shape. This idea has been subsequently developed by Helfrich [5] who had introduced the so called *spontaneous curvature* $\mathrm{I\!h}$ that arises from the chemical asymmetry between interior and exterior of the membrane. So, within some topological class of surfaces, Helfrich's bending energy is modelled by the functional

$$F(\mathcal{S}) = \frac{k}{2}\int(\mathbf{k_1} + \mathbf{k_2} - \mathrm{I\!h})^2\,\mathrm{dA} + \lambda\int\mathrm{dA} + \delta\mathrm{p}\int\mathrm{dV} \tag{10}$$

in which k is bending rigidity, $\mathbf{k_1}$ and $\mathbf{k_2}$ are the principal curvatures, δp and λ are Lagrange multipliers due to the constraints of constant volume and area which denote respectively a tensile stress and osmotic pressure difference between outer and inner media. When spontaneous curvature is set to be equal to zero the Helfrich model reduces to the Canham model. The critical points of the Helfrich energy at which the above functional attains its minimum are assumed to correspond to the equilibrium shapes of phospholipid vesicles. Taking the variational derivative one gets the so called general shape equation of Ou-Yang and Helfrich [10] which reads

$$\Delta H + 2\left(H + \frac{\mathrm{I\!h}}{2}\right)\left(H^2 - K - \frac{\mathrm{I\!h}}{2}\right) - \sigma H + \frac{\rho}{2} = 0 \tag{11}$$

where $\Delta = 1/\sqrt{|g|}\partial_i(g^{ij}\sqrt{|g|}\partial_j)$ is the Laplace-Beltrami operator of $\mathcal{S}$, $|g| = EG - F^2$ is the determinant of the metric g, $g^{ij} = (g^{-1})_{ij}$, while $\sigma = \lambda/k$ and $\rho = \delta p/k$ denote the Lagrange multipliers, rescaled by k.

It is clear that (11) is a fourth order highly nonlinear partial differential equation and that finding any non-trivial solution of it is not an easy task. As always, symmetry is of some help. Assuming that our vesicles are axisymmetric the shape equation reduces to a third order nonlinear PDE and this can be further integrated so that the resulting equation simplifies to the following one which of a second order [15]

$$\cos^2\psi\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - \frac{\sin 2\psi}{4}\left(\frac{\mathrm{d}\psi}{\mathrm{d}x}\right)^2 + \frac{\cos^2\psi}{x}\frac{\mathrm{d}\psi}{\mathrm{d}x} - \frac{\sin 2\psi}{2x^2} - \frac{\rho x}{2\cos\psi} - \frac{\sin\psi}{2\cos\psi}\left(\frac{\sin\psi}{x} - \mathrm{I\!h}\right)^2 - \frac{\sigma\sin\psi}{\cos\psi} = \frac{C}{x\cos\psi} \cdot \tag{12}$$

Here, x is the distance of the surface point from the symmetry axis z, $\psi(x) = \psi$ is the angle of the surface tangent with the x axis and C is the integration constant.
In this parameterization the principal curvature along the meridians is $\cos\psi\frac{\mathrm{d}\psi}{\mathrm{d}x}$ and the one along the parallels is $\frac{\sin\psi}{x}$. The surface contour itself can be obtained by integration of the first order equation

$$\frac{\mathrm{d}z}{\mathrm{d}x} = \tan\psi(x) \tag{13}$$

which reflects the geometry of this plane curve.
Naito *et al.* [7] have shown that under some conditions on the constants a, C, σ and ρ, *i.e.* $a = \mathrm{I\!h}$, $\mathrm{C} = 2\mathrm{I\!h}$, $\sigma = \rho = 0$

$$\sin\psi = x(a\ln x + b) \tag{14}$$

represents a rigorous analytical solution of (12). To the previously known solutions of (11) – spheres and cylinders – the same authors [8] have added catenoids, nodoids and unduloids described by the general formula

$$\sin\psi = ax + \frac{d}{x} \cdot \tag{15}$$

Here the $a = 0$ case corresponds to the catenoid, when $ad < 0$ one gets nodoids and in the case $0 < ad < 1/4$, unduloids. While (15) describes constant mean curvature surfaces with $H = a$ as one can easily check by inserting the above expression into the general formula

$$H = \left(\cos\psi\frac{\mathrm{d}\psi}{\mathrm{d}x} + \frac{\sin\psi}{x}\right)/2 \tag{16}$$

the authors of [8] have noticed that

$$\sin\psi = ax + b + \frac{d}{x} \tag{17}$$

is still an exact solution of (12) but in this case $H \neq \mathrm{const}$. The complete list of the analytical solutions includes Willmore tori [11] and Dupin cyclides [12]. The book [13] and especially its chapter 4 contains many of the details regarding all kinds of solutions mentioned above.

4 Constant mean curvature surfaces

Extensive numerical computations had shown that (14) could be used to represent the curious biconcave shape of the red blood cell membrane, while *via* (15) one could generate the rotational constant mean curvature surfaces discovered a long time ago by Delaunay and bearing his name. The difficulty with both (14) and (15) is that the respective profile curve cannot be obtained in analytical form by integrating (13). Fortunately in the case of constant mean curvature surfaces there exist alternatives. The first one is that the contour representing these surfaces is given up to integration in the parametric form [4] (it is assumed that the symmetry axis is x)

$$\begin{aligned} x &= a\sin\varphi - a\tan\varphi\sqrt{1+\alpha-\sin^2\varphi} \\ &\quad + \int_0^{\varphi} \frac{a\alpha \mathrm{d}\varphi}{\cos^2\varphi\sqrt{1+\alpha-\sin^2\varphi}} \\ y &= -a\cos\varphi + a\sqrt{1+\alpha-\sin^2\varphi} \end{aligned} \tag{18}$$

where $a \neq 0$ and $\alpha > 0$ are two constants. The mean curvature H of these surfaces is $\frac{1}{2a}$. Delaunay [4] has isolated this class of surfaces guided by a nice geometrical argument - they are all just the traces of the foci of nondegenerate conics when they roll along a straight line in a plane (*roulettes* in French). In an Appendix to the same paper Sturm characterized Delaunay's surfaces variationally as those rotational surfaces having a minimal lateral area at a fixed volume. It turns out that these curves satisfy the equation (it is assumed again that the axis of rotation is x)

$$\mathrm{d}x = \frac{(y^2+c)\mathrm{d}y}{\sqrt{4a^2y^2-(y^2+c)^2}} \tag{19}$$

where c is some constant. Further on we will assume that this constant is strictly positive, *i.e.* $c = b^2$ (this case corresponds to the roulette of an ellipse with axes a and b, $a > b$). The expression in the radicand is real just when y varies in the interval (α, β), where

$$\alpha = a - \sqrt{a^2-b^2}, \qquad \beta = a + \sqrt{a^2-b^2}. \tag{20}$$

Introducing the eccentricity ε of the ellipse, *i.e.*

$$\varepsilon = \sqrt{1-\frac{b^2}{a^2}} \tag{21}$$

the interval endpoints can be rewritten in the form

$$\alpha = a(1-\varepsilon), \qquad \beta = a(1+\varepsilon). \tag{22}$$

This suggests the change of variable y as follows

$$y = a\sqrt{1+\varepsilon^2+2\varepsilon\sin u}, \qquad u \in [-\pi/2,\, \pi/2]. \tag{23}$$

Performing this change one gets

$$\mathrm{d}y \to \frac{a\varepsilon\cos u\mathrm{d}u}{\sqrt{1+\varepsilon^2+2\varepsilon\sin u}}, \qquad y^2+b^2 \to 2a^2(1+\varepsilon\sin u),$$

and

$$\sqrt{4a^2y^2-(y^2+b^2)^2} \quad\to\quad 2\varepsilon a^2\cos u.$$

As a result the integral in which we are interested becomes

$$x(u) = a\int_{-\pi/2}^{u} \frac{(1+\varepsilon\sin u)\mathrm{d}u}{\sqrt{1+\varepsilon^2+2\varepsilon\sin u}} \tag{24}$$

and can be split into the following types:

$$\int \frac{\mathrm{d}u}{\sqrt{p+q\sin u}} = -\frac{2}{\sqrt{p+q}}F(\phi,k)$$

and

$$\int \frac{\sin u\mathrm{d}u}{\sqrt{p+q\sin u}} = \frac{2p}{q\sqrt{p+q}}F(\phi,k) - \frac{2\sqrt{p+q}}{q}E(\phi,k).$$

Here $F(\phi\,,\,k)$ and $E(\phi\,,\,k)$ denote the first, respectively the second kind of incomplete elliptic integrals in which $\phi = \arcsin\sqrt{\frac{1-\sin u}{2}}$ and the so-called elliptic modulus k is given by $\sqrt{\frac{2q}{p+q}}$. In our case $p = 1+\varepsilon^2$, $q = 2\varepsilon$ so that

$$\phi = \frac{\pi}{4} - \frac{u}{2}, \qquad \text{and} \qquad k = \frac{2\sqrt{\varepsilon}}{1+\varepsilon}\cdot \tag{25}$$

Taken together the above considerations give us

$$\begin{aligned} x(u) &= a\,(1-\varepsilon)\,[F(\frac{2u-\pi}{4},k)+K(k)] \\ &\quad a\,(1+\varepsilon)\,[E(\frac{2u-\pi}{4},k)+E(k)] \end{aligned} \tag{26}$$

where $K(k) = K(\pi/2,k)$ and $E(k) = E(\pi/2,k)$ are the complete elliptic integrals of the first, respectively the second kind. The definition and properties of the elliptic functions and integrals can be found *e.g.* in Jahnke *et al.* [6]. Revolving the curve $(x(u),\,y(u))$ (with $x(u)$ and $y(u)$ given by (26) and (23)) around the x axis leads to a surface of revolution $\mathcal{S}$ with position vector

$$x[u,v] = (x(u),\, y(u)\cos v,\, y(u)\sin v). \tag{27}$$

The coefficients of its first and second fundamental forms are found to be (a computer algebra system like *Mathematica* or *Maple* could be of great help here):

$$\begin{aligned} &E = a^2, \qquad F = 0, \qquad G = a^2\,(1+\varepsilon^2+2\,\varepsilon\,\sin u) \\ &L = \frac{a\,\varepsilon\,(\varepsilon+\sin u)}{1+\varepsilon^2+2\,\varepsilon\,\sin u}, \quad M = 0, \quad N = a\,(1+\varepsilon\,\sin u) \end{aligned} \tag{28}$$

and therefore

$$H \equiv \frac{1}{2a} \tag{29}$$

as was claimed above.

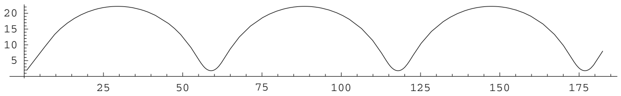

Fig. 1. The profile curve of the unduloid with parameters $a = 12$ and $\varepsilon = 0.85$.

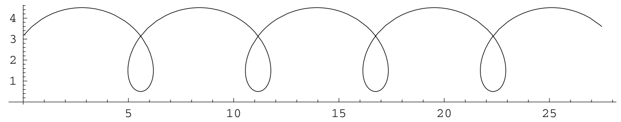

Fig. 2. The profile curve of the nodoid with parameters $a = 5$ and $\varepsilon = 1.25$.

In addition, it is clear that (27) is a solution of the general shape equation (11) provided

$$a = -\mathbb{h}^{-1} \qquad \text{and} \qquad \rho = -\sigma\mathbb{h}. \tag{30}$$

A few extra remarks are in order here. The first one is about the values which ε can take. Up to now it was implicitly assumed that they belong to the interval (0, 1) but it is easy to see that (27) produces a constant mean curvature (possibly not embedded but immersed) surface for any $\varepsilon \in \mathbb{R}^+$. More precisely:

- for $\varepsilon = 0$ the elliptic modulus k is zero as well and one gets a circular cylinder.
- for $\varepsilon \in (0, 1)$ the profile curve is wavy (see Fig. 1.) and the revolved surface is called an unduloid.
- when $\varepsilon = 1$ the resulting surface is a sequence of spheres centered on the x axis.
- if $\varepsilon > 1$ one gets the so called *nodary* curve (see Fig. 2) and respectively a self-intersecting nodoid surface which describes *e.g.* cell deformation under compression and will be discussed in more details elsewhere.

The second remark is about the recent hypothesis raised by Ou-Yang *et al.* [13] that the extension (17) of the constant mean curvature solution (15) could be appropriate for the description of the pearling cylinder observed by Bar-Zip and Moses [1]. Looking at Figures 3 and 4 in their paper one can understand how the cylinder can be deformed in a continuous way to the "pearling state" shown in the Figure 3 below. Without any doubt this transition corresponds to the continuous change of the parameter ε from 0 to the values that are close to, but strictly less than 1.

A remarkable fact is that this smooth transformation preserves the mean curvature!

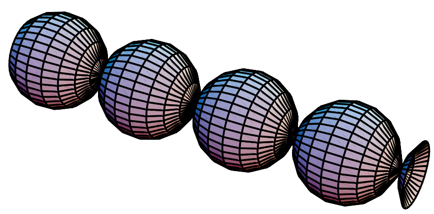

Fig. 3. Pearls obtained *via* (27) with $a = 5$ and $\varepsilon = 0.99$.

Quite interesting also is the possibility of introducing an additional non-zero deformation parameter μ, namely

$$\tilde{\mathbf{x}}[u, v] = (x(\mu u),\, y(\mu u)\cos v,\, y(\mu u)\sin v)/\mu. \tag{31}$$

It is easily checked that in this case the mean curvature is

$$H = \frac{\mu}{2a} \tag{32}$$

and that (31) is a solution of the general shape equation when

$$\mu = -a\mathbb{h} \qquad \text{and} \qquad \rho = -\sigma\mathbb{h}. \tag{33}$$

In some sense the presence of this second parameter is not by chance because otherwise we will not have constant mean curvature membranes of different geometry and size as these are controlled just by a and μ.

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