

XIth International Conference Geometry, Integrability and Quantization June 5-10, Varna, Bulgaria

Explicit parametrization of a class of equilibrium shapes of fluid membranes under pressure

Vassil Vassilev, Peter Djondjorov Institute of Mechanics – Bulgarian Academy of Sciences

and

Ivaïlo Mladenov Institute of Biophysics – Bulgarian Academy of Sciences

Fluid lipid bilayer membranes

• In aqueous solution, amphiphilic molecules (e.g., phospholipids) may form bilayers, the hydrophilic heads of these molecules being located in both outer sides of the bilayer, which are in contact with the liquid, while their hydrophobic tails remain at the interior.



• A bilayer may form a closed membrane - vesicle. Vesicles constitute a well-defined and sufficiently simple model system for studying basic physical properties of the more complex cell biomembranes.



Membrane Shapes

• The equilibrium shapes of a fluid lipid vesicle are determined by the extremals of the curvature (shape) energy (*Helfrich*, 1973):

$$F_{c} = \frac{k_{c}}{2} \int_{S} (2H + c_{0})^{2} dA + k_{G} \int_{S} K dA$$

under the constraints of fixed enclosed volume and membrane area.

• Using Lagrangian multipliers, this yields the functional

$$F = \frac{k_c}{2} \int_{S} (2H + c_0)^2 dA + k_G \int_{S} K dA + \lambda \int_{S} dA + P \int_{S} dV$$

- k_c, k_G bending and Gaussian rigidities of the membrane λ – tensile stress (chemical potential) of the membrane c_0 – spontaneous curvature of the bilayer P – pressure difference H, K – mean and Gaussian curvatures of the middle surface S
- dA, dV area and volume elements

Membrane Shape Equation

• The corresponding Euler-Lagrange equation (Ou-Yang and Helfrich Phys. Rev. A 39 1989)

 $2k_{c}\Delta H + k_{c}(2H + c_{0})(2H^{2} - c_{0}H - 2K) - 2\lambda H + P = 0$

is often referred to as the membrane shape equation. Here Δ is the Laplace-Beltrami operator on the surface S.

• The membrane shape equation describes the equilibrium shapes of lipid vesicles in terms of the mean *H* and Gaussian *K* curvatures of the membrane middle surface *S* and the physical parameters:

- k_c bending rigidity of the membrane
- λ tensile stress (chemical potential) of the membrane
- $\mathcal{C}_0~$ spontaneous curvature of the bilayer
- P pressure difference between the outer and inner media

Analytic solutions of the membrane shape equation

For more than three decades, the study of the equilibrium shapes of the vesicles has attracted much attention nevertheless only a few analytic solutions to the MS equation have been reported. These are the solutions determining:

- spheres and circular cylinders (Ou-Yang & Helfrich Phys. Rev. A 39 1989)
- Clifford torus and toroidal shapes (Ou-Yang Phys. Rev. A 41 1990, Phys. Rev. E 47 1993, Hu & Ou-Yang Phys. Rev. E 47 1993)
- several types of configurations with constant squared mean curvature density and Willmore surfaces (Konopelchenko Phys. Lett. B 414 1997, Vassilev & Mladenov GIQ 5 2004)
- circular biconcave discoids (Naito et al. Phys. Rev. E: 48 1993, 54 1996)
- cylindrical surfaces (Vassilev & Djondjorov & Mladenov J. Phys A.: Math. Theoret. 41 2008)

• Delaunay surfaces, nodoidlike and unduloidlike shapes (Naito et al. Phys. Rev. Lett. 74 1995, Mladenov Eur. Phys. J. B 29 2002, Mladenov et al. AIP CP1076 2008)

Axially symmetric equilibrium shapes of fluid membranes

For an axisymmetric fluid membrane the MS equation takes the form

$$\cos^{3}\varphi\left(\frac{d^{3}\varphi}{dx^{3}}\right) = 4\sin\varphi\cos^{2}\varphi\left(\frac{d^{2}\varphi}{dx^{2}}\right)\left(\frac{d\varphi}{dx}\right) - \cos\varphi\left(\sin^{2}\varphi - \frac{1}{2}\cos^{2}\varphi\right)\left(\frac{d\varphi}{dx}\right)^{3}$$
$$+ \frac{7\sin\varphi\cos^{2}\varphi}{2x}\left(\frac{d\varphi}{dx}\right)^{2} - \frac{2\cos^{3}\varphi}{x}\left(\frac{d^{2}\varphi}{dx^{2}}\right)$$
$$+ \left[\frac{c_{0}^{2}}{2} - \frac{2c_{0}\sin\varphi}{x} + \frac{\lambda}{k_{c}} - \frac{\sin^{2}\varphi - 2\cos^{2}\varphi}{2x^{2}}\right]\cos\varphi\left(\frac{d\varphi}{dx}\right)$$
$$+ \frac{P}{k_{c}} + \frac{\lambda\sin\varphi}{k_{c}x} + \frac{c_{0}^{2}\sin\varphi}{2x} - \frac{\sin^{3}\varphi + 2\sin\varphi\cos^{2}\varphi}{2x^{3}}$$

in terms of the slope angle φ regarded as a function of the distance x of a point on the profile curve of the surface from the axsis of symmetry z. Then

$$z\left(x\right) = \int \tan\varphi\left(x\right) dx$$

A class of exact solutions of the axisymmetric MS equation

Naito, Okuda and Ou-Yang (Phys. Rev. Lett. 74 1995) have found that the axisymmetric MS equation with nonzero pressure and spontaneous curvature, i.e., $P \neq 0$ and $c_0 \neq 0$, has the following class of exact solutions

$$\sin \varphi = \varepsilon + \frac{1}{c_0 x} + \frac{1}{4} c_0 \left(\varepsilon^2 + 2\right) x, \qquad \varepsilon \in \mathbb{R}$$

the pressure P and the tensile stress λ being given as follows

$$\frac{P}{k_c} = -\frac{1}{8} \left(\varepsilon^2 + 2\right)^2 c_0^3, \quad \frac{\lambda}{k_c} = \frac{1}{4} c_0^2 \left(2\varepsilon^2 + 3\right).$$

Our aim is to find an explicit parametrization of the profile curves of the corresponding axisymmetric surfaces by representing the integral in the r.h.s. of expression $z(x) = \int \tan \varphi(x) dx$ in terms of elliptic integrals and functions.

For the considered class of solutions we have

$$z = \pm \int \frac{\varepsilon + \frac{1}{c_0 x} + \frac{1}{4} c_0 \left(\varepsilon^2 + 2\right) x}{\sqrt{1 - \left(\varepsilon + \frac{1}{c_0 x} + \frac{1}{4} c_0 \left(\varepsilon^2 + 2\right) x\right)^2}} dx$$

which can be rewritten in the form

$$z(x) = \pm \int \frac{x^2 + \frac{4\varepsilon}{c_0(\varepsilon^2 + 2)}x + \frac{4}{(\varepsilon^2 + 2)c_0^2}}{\sqrt{-(x - \alpha)(x - \beta)(x - \gamma)(x - \delta)}} dx$$

where α , β , γ and δ are the roots of the polynomial

$$\mathcal{P} = \left(x^2 + \frac{4(\varepsilon+1)}{c_0(\varepsilon^2+2)}x + \frac{4}{(\varepsilon^2+2)c_0^2}\right)\left(x^2 + \frac{4(\varepsilon-1)}{(\varepsilon^2+2)c_0}x + \frac{4}{(\varepsilon^2+2)c_0^2}\right)$$

Evidently, at least two of the forgoing roots have to be real, otherwise z(x) can not be a real-valued function. For that reason, it turned out that either $\varepsilon < -1/2$ or $\varepsilon > 1/2$. In what follows, the second case will be considered.

For $\varepsilon > 1/2$ we have

$$\alpha = -\frac{2\left(\varepsilon + 1 - \sqrt{2\varepsilon - 1}\right)}{c_0\left(\varepsilon^2 + 2\right)}, \quad \beta = -\frac{2\left(\varepsilon + 1 + \sqrt{2\varepsilon - 1}\right)}{c_0\left(\varepsilon^2 + 2\right)}$$
$$\gamma = -\frac{2\left(\varepsilon - 1 + i\sqrt{2\varepsilon + 1}\right)}{c_0\left(\varepsilon^2 + 2\right)}, \quad \delta = -\frac{2\left(\varepsilon - 1 - i\sqrt{2\varepsilon + 1}\right)}{c_0\left(\varepsilon^2 + 2\right)}$$

The integral in the r.h.s. of the expression for z(x) turned out to be quite complicated and that is why we decided to introduce a new variable t such that

$$\frac{dt}{dx} = \frac{1}{\sqrt{-(x-\alpha)(x-\beta)(x-\gamma)(x-\delta)}}$$

Here, $0 < \alpha \leq x \leq \beta$ for $c_0 < 0$ and $\beta \leq x \leq \alpha < 0$ for $c_0 > 0$. Thus

$$t = \int \frac{dx}{\sqrt{-(x-\alpha)(x-\beta)(x-\gamma)(x-\delta)}}$$

Then

$$x(t) = \frac{2}{c_0\sqrt{\varepsilon^2 + 2}} \left(1 - \frac{2h}{h + \operatorname{cn}(ut, k)}\right)$$

where

$$h = \sqrt{\frac{1 + \varepsilon + \sqrt{2 + \varepsilon^2}}{1 + \varepsilon - \sqrt{2 + \varepsilon^2}}}, \quad u = \frac{4}{c_0 \left(2 + \varepsilon^2\right)^{3/4}}, \quad k = \sqrt{\frac{1}{2} - \frac{3}{4\sqrt{2 + \varepsilon^2}}}.$$

and

$$z(t) = \pm \int x^{2}(t) dt \pm \frac{4\varepsilon}{c_{0}(\varepsilon^{2}+2)} \int x(t) dt \pm \frac{4t}{(\varepsilon^{2}+2)c_{0}^{2}}$$
$$0 \le t \le \frac{T}{2}, \quad T = \frac{4}{u} \mathbf{K}(k)$$

Finally

$$x(t) = \frac{2}{c_0\sqrt{\varepsilon^2 + 2}} \left(1 - \frac{2h}{h + \operatorname{cn}(ut, k)}\right)$$

$$\begin{split} z\left(t\right) &= \frac{8h^2}{c_0^2\left(2+\varepsilon^2\right)\left(h^2-1\right)\left[1+\left(h^2-1\right)k^2\right]} \left(\frac{\mathrm{sn}(ut,k)\mathrm{dn}(ut,k)}{\mathrm{cn}(ut,k)+h} - \mathrm{F}\left(ut,k\right)\right) \\ &+ \frac{8h}{c_0^2\left(2+\varepsilon^2\right)} \left(1+\frac{\varepsilon}{\sqrt{2+\varepsilon^2}} + \frac{h^3\left[1+2\left(h^2-1\right)k^2\right]}{\left(h^2-1\right)^2\left[1+\left(h^2-1\right)k^2\right]}\right) \Pi\left(ut,k\right) \\ &+ \frac{4ut}{c_0^2\left(2+\varepsilon^2\right)} \left(\frac{2h^2}{h^2-1} - \frac{\varepsilon+\sqrt{2+\varepsilon^2}}{\sqrt{2+\varepsilon^2}}\right) \end{split}$$

 $\varepsilon = 3, c_0 = -1, P = 15.125k_c, \lambda = 110.25k_c$

