Analytical solutions to Helfrich variation problem for shapes of lipid bilayer vesicles

Hiroyoshi Naito[1] and **Ou-Yang Zhong-can**[2]

[1]Department of Physics and Electronics, Osaka Prefecture University, Gakuen-cho, Sakai, Osaka 593, Japan

[2]Institute of Theoretical Physics, Academia Sinica, P.O.Box 2735 Beijing 100080, China

Surfaces of revolution with constant mean curvature, called Delaunay's surfaces, are catenoids, unduloids, nodoids, circular cylinders, and spheres. It is shown that all these surfaces are solutions of the Helfrich variation problem that is the determination of the equilibrium shapes of lipid bilayer vesicles.

1. Introduction

The minimal surfaces and surfaces with constant mean curvatures have extensively been studied since the study of soap bubbles by Plateau [1] and of the shape of air/liquid interfaces in a capillary tube by Young [2] and Laplace [3] in the middle of the nineteenth century. These surfaces also make their appearance in gas dynamics, stems of plants, and other biological systems (see Chapter V of the marvellous book by D'Arcy Thompson for an essay on the occurrence and properties of such surfaces in nature [4]). Even nowadays, there are still interesting problems in this field. For instance, many new problems of surfaces arise from the shapes of vesicles that are formed by lipid bilayers in aqueous solution and are simple models for biological membranes and cells. The theoretical approach for the determination of the equilibrium shapes is based on the elasticity of lipid bilayers proposed by Helfrich [5], and is called the Helfrich variation problem. In this approach, the shape free energy is give by

$$F = \frac{1}{2}k \oint (c_1 + c_2 - c_o)^2 dA + \bar{k} \oint c_1 c_2 dA + \Delta p \int dV + \lambda \oint dA, \tag{1}$$

where k is the bending rigidity, $\bar{k}$ Gaussian curvature modulus, c_1 and c_2 two principal curvatures, c_o the spontaneous curvature, dA surface area, dV volume elements, $\Delta p = (p_o - p_i)$ the osmotic pressure difference between outer (p_o) and inner media (p_i), and λ the tensile stress. Δp and λ are also regarded as the Lagrange multipliers to take account of the constraints of constant volume and area, depending on the situation.

The expression for the shape of the vesicle at mechanical equilibrium has been derived from the first variation of F with respect to normal to the vesicle surface by using general rules of differential geometry and imposing the closed surface condition [6]. The expression is called the general shape equation and is given by

$$\Delta p - 2\lambda H + k(2H + c_o)(2H^2 - 2K - c_o H) + 2k\nabla^2 H = 0, \tag{2}$$

where H $[= -(c_1 + c_2)/2]$ and K $(= c_1 c_2)$ are the mean and the Gaussian curvatures, respectively, and ∇^2 is the Laplace-Beltrami operator. Most studies in the Helfrich variation problem have been based on the numerical calculation of the shape equation for vesicles with special geometries such as axisymmetry so far [7, 8]. However, the general shapes surfaces have not been analytically examined yet except for a sphere, a cylinder, and a Clifford torus and its conformal transformations [6, 9].

In 1841 Delaunay [4, 10] has shown that the surfaces of revolution with constant mean curvature in Euclidean space are catenoids ($H = 0$), unduloids, nodoids, circular cylinders, and spheres. These surfaces are called Delaunay's surfaces. In this article, we show Delaunay's surfaces are solutions of the Helfrich variation problem [Eq. (2)].

2. Shape Equation

We describe here the shape equation for axisymmetric vesicles that has been derived from Eq. (2) by Hu and Ou-Yang [11] and which is a third-order differential equation of $\psi(\rho)$,

$$\cos^3\psi\left(\frac{d^3\psi}{d\rho^3}\right) = 4\sin\psi\cos^2\psi\left(\frac{d^2\psi}{d\rho^2}\right)\left(\frac{d\psi}{d\rho}\right) - \cos\psi\left(\sin^2\psi - \frac{1}{2}\cos^2\psi\right)\left(\frac{d\psi}{d\rho}\right)^3$$

$$+ \frac{7\sin\psi\cos^2\psi}{2\rho}(\frac{d\psi}{d\rho})^2 - \frac{2\cos^3\psi}{\rho}(\frac{d^2\psi}{d\rho^2})$$
$$+ [\frac{c_o^2}{2} - \frac{2c_o\sin\psi}{\rho} + \frac{\lambda}{k} - \frac{\sin^2\psi - 2\cos^2\psi}{2\rho^2}]\cos\psi(\frac{d\psi}{d\rho})$$
$$+ [\frac{\Delta p}{k} + \frac{\lambda\sin\psi}{k\rho} + \frac{c_o^2\sin\psi}{2\rho} - \frac{\sin^3\psi + 2\sin\psi\cos^2\psi}{2\rho^3}], \tag{3}$$

where ρ is the distance from the symmetric axis (z axis) of rotation and $\psi(\rho)$ is the angle made by the surface tangent and the ρ axis. In this case, we have the following relations:

$$\frac{dz}{ds} = \sin\psi \tag{4}$$

and

$$\frac{d\rho}{ds} = \cos\psi, \tag{5}$$

where s is the arc-length of the vesicle with axisymmetry. The vesicle surface is hence represented by the vector $\vec{Y}(s,\phi)$ in Euclidean space as

$$\vec{Y}(s,\phi) = (\rho(s)\cos\phi, \rho(s)\sin\phi, z(s)), \tag{6}$$

where ϕ is the azimuth angle. Once $\psi(\rho)$ is solved from Eq. (3), we can obtain the contour $z(\rho)$ [$=z(s)$] by a simple integration,

$$z(\rho) - z(0) = \int_0^\rho \tan\psi(\rho')d\rho'. \tag{7}$$

3. Shape Equation Problem

Hu and Ou-Yang [11] have pointed out that three *different* shape equations for axisymmetric vesicles have been derived within the framework of the *same* Helfrich spontaneous curvature model [5]. We call this confused situation the shape equation problem. The three different shape equations for the axisymmetric vesicles have been reported by Deuling and Helfrich (DH) [7], Seifert, Berndl and Lipowsky (SBL) [8], and Hu and Ou-Yang (HO) [11] with different variational methods on the basis of the same Helfrich spontaneous curvature model. The three ways to obtain the shape equations are:
(i) Equation (1) is changed to an action form by using ρ as a parameter,

$$F_b + \lambda A + \Delta pV = 2\pi k\int_0^{\rho_c} L(\psi(\rho), \frac{d\psi}{d\rho}, \rho)d\rho, \tag{8}$$

where ρ_c is the equatorial radius of an axisymmetric vesicle, and L is the Lagrange function. After the parametrization of the vesicle shape, L is determined from Eq. (8). The DH shape equation [7] is then obtained from the Euler-Lagrange equation

$$\frac{\partial L}{\partial\psi} - \frac{d}{d\rho}\frac{\partial L}{\partial(d\psi/d\rho)} = 0. \tag{9}$$

(ii) The SBL shape equation [8] is derived in a way similar to (i) except for the parameter in the action form, which is the arclength of the contour s.
(iii) The HO shape equation, Eq. (3), [11] is obtained by simply substituting the mean and the Gaussian curvatures of an axisymmetric vesicle,

$$H = -\frac{1}{2}[\cos\psi\frac{d\psi}{d\rho} + \frac{\sin\psi}{\rho}], \tag{10}$$
$$K = \cos\psi\frac{\sin\psi}{\rho}\frac{d\psi}{d\rho}, \tag{11}$$

into the general shape equation [Eq. (2)].

Hu and Ou-Yang have shown that these three equations are degenerate for a spherical vesicle, while

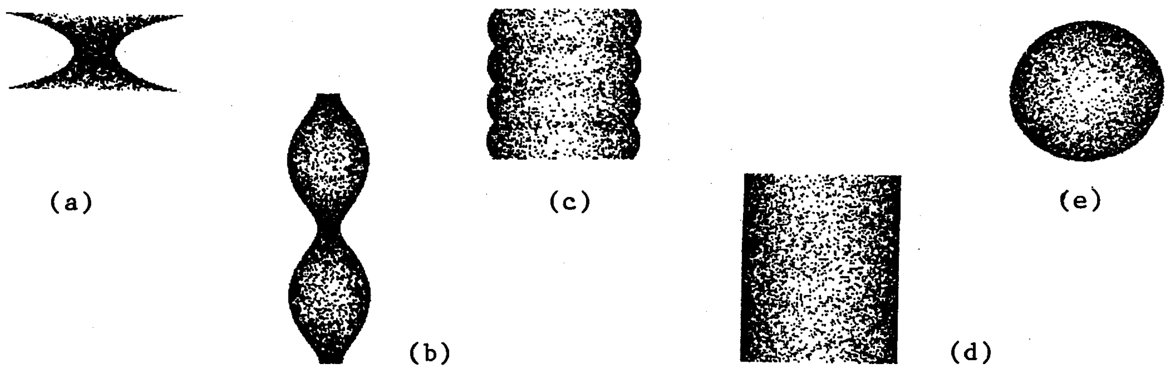

Figure 1: Delaunay's surfaces: (a) catenoid, (b) unduloid, (c) nodoid, (d) circular cylinder, and (e) sphere

the DH equation is not identical to the SBL and the HO equations in case of a cylindrical vesicle, and that a Clifford torus is a solution for all the equations, but the constraints on Δp, λ, and c_o are different [11].

The difference in the three shape equations is due to the different minimization procedure of the general action. In case of the HO approach, they first make minimization and then the specific parametrization of the shape. On the other hand, in the DH and the SBL approaches, they first make the parametrization of the shape and then minimization. This procedure leaves some free parameters which in general depend on the shape like ρ_c for example. These free parameters are not correctly variated in DH nor in SBL hamiltonians. Hu and Ou-Yang [11] have carefully shown the erroneous calculus of variations used in deriving the DH and the SBL equations. After the publication of the Hu and Ou-Yang paper, the shape equation problem was recognized and then several papers in which the shape equation problem was discussed have been published [12, 13, 14]. We believe that through the controversy on the shape equation problem the HO equation has been accepted as the correct shape equation for axisymmetric vesicles [12, 13, 14].

4. Analytical Solutions to the Shape Equation for Axisymmetric Vesicles: Delaunay's surfaces

We show here that Delaunay's surfaces are the solution to the Helfrich variation problem. In biological cells and vesicles, these surfaces can also be observed; the unduloidlike shapes have been found in myelin shapes of red blood cells and in lipid bilayers either treated by laser tweezer or by increasing osmotic pressure.

To do this, we first give the mathematical expression of Delaunay's surfaces [15], which is

$$\sin\psi(\rho) = a\rho + d\rho^{-1}, \tag{12}$$

where the two parameters, a and d determine the types of the surfaces: (i) the unduloids: $0 < ad < 1/4$ and (ii) the nodoids: $ad < 0$. The spheres and the circular cylinders are corresponding to the two limiting cases: when $d \to 0$ the unduloids become the spheres, and when $ad \to 1/4$ the unduloids degenerate to the cylinders. The catenoids are the only minimal surfaces of revolution when $a = 0$. These surfaces are shown in Fig. 1. By substituting Eq. (12) into Eq. (10), we have $H = -a$ and hence can show that the surfaces described by Eq. (12) are the surfaces of revolution with constant mean curvature.

It is easily shown that Eq. (12) is an analytical solution to Eq. (3) by substituting Eq. (12) and its first, second and third differentiations of ψ with respect to ρ into Eq. (3) under the conditions,

$$\Delta p/\lambda = -c_o \tag{13}$$

and

$$a = \frac{c_o}{2}. \tag{14}$$

Ou-Yang and Helfrich [6] have derived the relations for a sphere with radius r_o $(= 1/a)$

$$\Delta p r_o^3 + 2\lambda r_o^2 - k c_o r_o (2 - c_o r_o) = 0,$$

and for a circular cylinder with radius ρ_o $(= 1/2a)$

$$\Delta p \rho_o^3 + \lambda \rho_o^2 + \frac{k}{2}(c_o^2 \rho_o^2 - 1) = 0.$$

It is important to note that Eqs. (13) and (14) satisfy these relations.

5. Conclusions

We have shown that surfaces of revolution with constant mean curvature (catenoids, unduloids, nodoids, circular cylinders, and spheres), called Delaunay's surfaces, are solutions of the Helfrich variation problem for the equilibrium shapes of lipid bilayer vesicles. The present analytical results for Delaunay's surfaces are valuable for the investigation of the shapes of vesicles such as the unduloidlike shape in red blood cells and in vesicles.

References

[1] J. Plateau *Statique expérimentale et théorique des liquides soumis aux seules forces moléculaires* (Gauthier-Villars, Paris, 1873).

[2] T. Young, Philos. Transact. Roy. Soc. London **95**, 65 (1805).

[3] P. S. Laplace, *Traité de mécanique céleste*, Supplément au livre X, 1805 and 1806, resp. In Oeuvres compl. Vol. 4 (Gauthier-Villars, Paris, 1839).

[4] D'Arcy Thompson, *On Growth and Form* (Cambridge, 1917).

[5] W. Helfrich, Z. Naturforsch. **28C**, 693 (1973).

[6] Ou-Yang Zhong-can and W. Helfrich, Phys. Rev. Lett. **59**, 2486 (1987); Phys. Rev. A **39**, 5280 (1989).

[7] H. Deuling and W. Helfrich, J. Phys. (Paris) **37**, 1335 (1976), J. Jenkins, J. Math. Biophys. **4**, 149 (1977), M. Peterson, J. Appl. Phys. **57**, 1739 (1985), S. Svetina and B. Zeks, Eur. Biophys. J. **17**, 101 (1989), L. Miao, B. Fourcade, M. Rao, M. Wortis and R. Zia, Phys. Rev. A **43**, 6843 (1991). L. Miao, B. Fourcade, M. Wortis and H. Döbereiner, Phys. Rev. E **49**, 5389 (1994).

[8] U. Seifert, Phys. Rev. Lett. **66**, 2404 (1991), U. Seifert, K. Berndl, and R. Lipowsky, Phys. Rev. A **44**, 1182 (1991), J. Berndl, J. Käs, R. Lipowsky, E. Sackmann, and U. Seifert, Europhys. Lett. **13**, 659 (1990),

[9] Ou-Yang Zhong-can, Phys. Rev. A **41**, 4517 (1990); Phys. Rev. E **47**, 747 (1993), Xie Yu-zhang and Ou-Yang Zhong-can, Acta Physica Sinica **2**, 881 (1993).

[10] C. Delaunay, J. Math. Pures et Appl. Ser 1(6), 309 (1841); J. Eells, Math. Intelligen. **9**, 53 (1987).

[11] Hu Jian-guo and Ou-Yang Zhong-can, Phys. Rev. E **47**, 461 (1993).

[12] W. M. Zheng and J. Liu, Phys. Rev. E **48**, 2856 (1993).

[13] F. Jülicher and U. Seifert, Phys. Rev. E **49**, 4728 (1994).

[14] H. Naito, M. Okuda, and Ou-Yang Zhong-can, Phys. Rev. E **48**, 2304 (1993).

[15] H. Naito, M. Okuda, and Ou-Yang Zhong-can, Phys. Rev. Lett. **74**, 4345 (1995).