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An integral case of the axisymmetric shape equation of open vesicles with free edges

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ABSTRACT

The equilibrium shapes of lipid vesicles are governed by the general shape equation which is derived from the minimization of the Helfrich free energy and can be reduced to the Willmore equation in a special case. The general shape equation is a high-order nonlinear partial differential equation and it is very difficult to find analytical solution even in axisymmetric case, which is reduced to a second-order ordinary differential equation. In the traditional axisymmetric shape equation, the turning radius is the variable. Here we study the shape equation by choosing the tangential angle as the variable. In this case, the Willmore equation is reduced to the Bernoulli differential equation and the general solution is obtained conveniently. We find that the curvature in this solution is discontinuous in some cases, which was not noticed previously. This solution can satisfy the boundary conditions for an open vesicle with free edges.

1. Introduction

Biological membranes are composed of two layers of phospholipid molecules. In aqueous environment, phospholipid bilayers can form closed vesicles [1–3] as well as open vesicles [4]. By comparing lipid bilayers with liquid crystals, Helfrich pointed out that membranes can be taken as two-dimensional (2D) surfaces and that their equilibrium shapes are determined by minimization of the following free energy [5]

$$E = \int\int [\frac{k_c}{2}(2H + C_0)^2 + k_g \Lambda] dA, \tag{1}$$

where H, Λ and C_0 are the mean curvature, Gaussian curvature and spontaneous curvature of the surface, respectively, dA is the surface area element, k_c and k_g are the bending moduli of the membrane. For closed vesicles, considering the surface area and volume constraints, the total free energy is

$$F = E + \lambda \int\int dA + p \oint dV, \tag{2}$$

where λ is the surface tension coefficient, p is the pressure difference between the outside and inside of the vesicle and dV is the volume element of the vesicle. By studying the first variation of $\delta^{(1)} F = 0$, Ou-yang and Helfrich obtained the following general shape equation of closed membranes [6,7]

$$k_c(2H + C_0)(2H^2 - 2\Lambda - C_0 H) - 2\lambda H + 2k_c \nabla^2 H + p = 0, \tag{3}$$

where ∇^2 is the Laplace–Beltrami operator in the 2D case. The above equation is a high-order nonlinear partial differential equation and it is very difficult to find analytical solutions even in the axisymmetric case, which can be reduced to a second-order ordinary differential equation. In the past two decades, several special analytical solutions have been found, such as the Clifford torus [8], discounts [9], the beyond-Delaunay surface [10] and the general solution for the cylindrical case [11,12]. All of these solutions are shown in Ref. [13]. Besides, numerical solutions in the axisymmetric case have been studied extensively and the phase diagram was obtained [14].

Moreover, the equilibrium shape equations for multi-component vesicles, open vesicles with free boundary as well as vesicle adhesion structures have been investigated and the corresponding shapes obtained [15–20]. In these models, Eq. (3) always needs to be satisfied (it needs $p = 0$ for open vesicles). Therefore, finding new analytical solutions for Eq. (3) is an attractive challenge [21].

Specially, if $\lambda = p = C_0 = 0$, Eq. (3) is reduced to the well-known Willmore equation which is used to describe the equilibrium configurations of thin shells [22]. Recently, some researchers found an analytical solution for the Willmore equation in the axisymmetric case [23,24]. It inspires us to find new solutions for the equilibrium shape equation (3). Traditionally, researchers defined the turning radius as the variable in the axisymmetric shape equation [25,26]. Here we study the shape equation by choosing the tangential angle as the variable. In this case, the Willmore equation is reduced to the Bernoulli

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differential equation and the general solution is obtained, which is nothing but the new solution in the recent works [23,24]. Meanwhile, we find that the curvature in this solution is discontinuous in some cases, which was not noticed by previous researchers. We also point out that this solution can satisfy the boundary conditions for open vesicle with free edges.

2. Axisymmetrical shape equation and a special solution

For an axisymmetric surface, let the generating line be around the z-axis and ρ be the turning radius,

$$x = \rho\cos\phi, y = \rho\sin\phi, z = \int \tan\psi(\rho)d\rho, \tag{4}$$

where ϕ is the azimuthal angle and ψ is the tangent angle of the profile curve. The surface can be expressed as

$$\mathbf{r} = \{\rho\cos\phi, \rho\sin\phi, z\}. \tag{5}$$

Defining $()' = \frac{d()}{d\rho}$, we have

$$2H = \frac{\sin\psi}{\rho} + (\sin\psi)', \quad \Lambda = \frac{\sin\psi}{\rho}(\sin\psi)', \tag{6}$$

$$\nabla^2 = \frac{\cos\psi}{\rho}\left[\frac{\partial}{\partial\rho}(\rho\cos\psi\frac{\partial}{\partial\rho}) + \frac{\partial}{\partial\phi}(\frac{\sec\psi}{\rho}\frac{\partial}{\partial\phi})\right]. \tag{7}$$

Hu et al. obtained the general shape equation, which is a third-order ordinary differential equation [25]. Zheng et al. provided the first integral of the shape equation as follow [26].

$$2H'\cos\psi + (2H - C_0)\psi'\sin\psi - \tilde{\lambda}\tan\psi + \frac{\eta - \tilde{p}\rho^2}{2\rho\cos\psi} - \frac{\tan\psi}{2}(2H - C_0)^2 = 0, \tag{8}$$

where η is a constant of integration, $\tilde{\lambda} = \lambda/k_c$ and $\tilde{p} = p/k_c$. The above is a second-order ordinary differential equation with the variable ρ. Although it is very difficult to solve generally, several analytic solutions have been found [13].

Now, let us consider another way to express this equation by using the tangential angle ψ as the variable. Defining $\dot{\rho} = \frac{d\rho}{d\psi}$, we have $()' = \frac{d()}{d\rho} = \frac{d()}{d\psi}\frac{d\psi}{d\rho} = \frac{1}{\dot{\rho}}\frac{d()}{d\psi}$ and

$$2H = \frac{\sin\psi}{\rho} + \frac{\cos\psi}{\dot{\rho}}, \quad \Lambda = \frac{\sin\psi\cos\psi}{\dot{\rho}\rho}, \tag{9}$$

$$\nabla^2 = \frac{\cos\psi}{\rho}\left[\frac{1}{\dot{\rho}}\frac{\partial}{\partial\psi}(\frac{\rho}{\dot{\rho}}\cos\psi\frac{\partial}{\partial\psi}) + \frac{\partial}{\partial\phi}(\frac{\sec\psi}{\rho}\frac{\partial}{\partial\phi})\right]. \tag{10}$$

The shape equation is changed to

$$\frac{2\dot{H}}{\dot{\rho}}\cos\psi + \frac{1}{\dot{\rho}}(2H - C_0)\sin\psi - \tilde{\lambda}\tan\psi + \frac{\eta - \tilde{p}\rho^2}{2\rho\cos\psi} - \frac{\tan\psi}{2}(2H - C_0)^2 = 0. \tag{11}$$

A trial solution can be defined as $\rho = \exp[f(\psi)]$. Substituting it into above equation we attain

$$\left[2\tilde{p}e^{3f}\sec\psi - 2e^{2f}(C_0^2 + 2\tilde{\lambda})\tan\psi + 2e^{f}(\eta\sec\psi + 2C_0\sin\psi\tan\psi) - (3 + \cos 2\psi)\tan\psi\right]\dot{f}^3 - 4\cos^2\psi\ddot{f} - \sin 2\psi\dot{f} = 0. \tag{12}$$

If $\tilde{p} = \tilde{\lambda} = C_0 = \eta = 0$, the above equation should be the axisymmetric Willmore equation. It is reduced to the following Bernoulli differential equation

$$(3 + \cos 2\psi)\tan\psi\dot{f}^3 + 4\cos^2\psi\ddot{f} + \sin 2\psi\dot{f} = 0. \tag{13}$$

This equation has following general solution

$$\dot{f}^{-2} = -2e^{2\int P(\psi)d\psi}\left[\int Q(\psi)e^{-2\int P(\psi)d\psi}d\psi - \frac{I}{2}\right] = \tan^2\psi + I\sec\psi, \tag{14}$$

where $P(\psi) = \frac{1}{2}\tan\psi$, $Q(\psi) = -\frac{(3+\cos 2\psi)\sin\psi}{4\cos^3\psi}$ and I is a constant of integration. Then we obtain

$$\rho = \rho_0\exp\left(\pm\int\frac{d\psi}{\sqrt{\tan^2\psi + I\sec\psi}}\right), \tag{15}$$

where ρ_0 is a constant of integration. This solution was obtained by using the Noether theorem in a recent work [24]. Considering $\tan\psi = \frac{dz}{d\rho}$, we obtain

$$\frac{dz}{d\psi} = \frac{dz}{d\rho}\frac{d\rho}{d\psi} = \frac{\pm\rho}{\sqrt{\tan^2\psi + I\sec\psi}}\tan\psi. \tag{16}$$

Making use of $\frac{dz}{d\rho} = \frac{1}{\dot{\rho}}\frac{dz}{d\psi}$ and $\frac{d^2z}{d\rho^2} = \frac{1}{\dot{\rho}^2}\frac{d^2z}{d\psi^2} - \frac{\ddot{\rho}}{\dot{\rho}^3}\frac{dz}{d\psi}$, the above equation is changed to the following Willmore equation [23]

$$\frac{d^2z}{d\rho^2} = \pm\frac{1}{\rho}\left[(\frac{dz}{d\rho})^2 + 1\right]\sqrt{(\frac{dz}{d\rho})^2 + I\sqrt{(\frac{dz}{d\rho})^2 + 1}}. \tag{17}$$

By solving this equation, one can get Willmore surfaces. Several example shapes were shown in Refs. [23,24]. However, we will see that the curvature on these shapes is discontinuous in certain cases.

3. Discontinuity of curvature on axisymmetric Willmore surfaces

In Eq. (17), the "±" indicates that the solution has two parts. Defining

$$Y = \frac{1}{\rho}\left[(z')^2 + 1\right]\sqrt{(z')^2 + I\sqrt{(z')^2 + 1}}, \tag{18}$$

for part I, we have $z = z_1(\rho)$ and $z_1'' = Y$ and for part II, we have $z = z_2(\rho)$ and $z_2'' = -Y$. Because $Y \geq 0$, we have $z_1'' \geq 0$ and $z_2'' \leq 0$. This result determines the concave and convex configurations of $z_1(\rho)$ and $z_2(\rho)$. An example is shown in Fig. 1, where part I is concave and part II is convex. Refs. [23,24] shows several shapes with concave and convex parts in a solution. According to our analysis, each shape is possibly the combination of the $z_1(\rho)$ and $z_2(\rho)$ parts. If so, the continuity of this solution on the combination point needs to be discussed. Making use of Eqs. (9) and (18), the mean curvature H and H' are

$$H_1 = \frac{z'\left[(z')^2 + 1\right] + Y\rho}{2\rho\left[(z')^2 + 1\right]^{3/2}}, H_2 = \frac{z'\left[(z')^2 + 1\right] - Y\rho}{2\rho\left[(z')^2 + 1\right]^{3/2}}, \tag{19}$$

$$H_1' = H_2' = -\frac{Iz'}{4\rho^2}. \tag{20}$$

where the subscripts 1 and 2 correspond to part I and part II, respectively. Supposing that the combination point satisfies $\rho = \rho_a$, the shape equation (8) requires that $z(\rho)$, $H(\rho)$, $H'(\rho)$ and $\psi'(\rho) = z''/(1 + (z')^2)$ are continuous at $\rho = \rho_a$.

If $z_1'(\rho_a) = z_2'(\rho_a)$, we can see that H' is continuous, while we cannot ensure that H is continuous. Let $H_1 = H_2$, we have

$$(z')^2 + I\sqrt{(z')^2 + 1} = 0. \tag{21}$$

If $I > 0$, there is no real solution for z'. Therefore we cannot find a point to combine the concave and convex parts in a solution in this case. So, the corresponding shapes in Refs. [23,24] have discontinuous mean curvature (the Gaussian curvature also is discontinuous). But if $I < 0$, it seems possible to find the suitable joint point. Then let $z'(\rho_1)$ and $z'(\rho_2)$ be two real solutions of Eq. (21); we have

$$z'(\rho_1) = -z'(\rho_2) = \frac{1}{\sqrt{2}}\sqrt{I^2 - I\sqrt{4 + I^2}}. \tag{22}$$

It is not difficult to find that H, H' and ψ' are continuous at $\rho = \rho_i$ ($i = 1,2$). Therefore, if the connect point between the concave and convex parts is at $\rho = \rho_i$, the combined shape is a solution for Eq. (8) without curvature singularity. However, by solving Eq. (17) with condition (22), we find there is nothing but the straight line solution, which gives the conical surface in 3D case. But it is not an exact solution for Eq. (8). Fig. 2 shows several example shapes with $I = -1$, $z(1) = 0$ and different

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