Periodic cylindrical surface solution for fluid bilayer membranes

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The shape equation of cylindrical surfaces for lipid bilayer membranes expressed by the Gaussian maps of their cross sections is given. General cylindrical surface solution has been obtained for the case of $\Delta p=0$. This is the first case found that can be solved for the general shape equation. With this solution we show two kinds of periodic surface solutions to the general shape equation for fluid bilayer membranes.

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Amphiphilic molecules, such as phospholipids, asemble into bilayer membranes in water with the polor head groups in contact with water and the hydrocarbon chains facing inward. At low concentration, these bilayers tend to form vesicles [1], but at high enough concentration vesicles will transform into extended bilayers [2].

The equilibrium shapes of the membranes are determined by minimizing their shape energy [3]

$$F=\frac{1}{2}k_c \oint (c_1+c_2-c_0)^2 dA+\Delta p\int dV+\lambda \oint dA. \quad (1)$$

Here c_1 and c_2 are the two principal curvatures, c_0 is the spontaneous curvature, which serves to describe the intrinsic asymmetry in the lipid composition or different aqueous environments on the two sides of the bilayer, k_c is the bending rigidity, and dA and dV are the area and the volume element, respectively. The pressure difference $\Delta p=(p_o-p_i)$ between outer (p_o) and inner media (p_i) and the tensile stress λ serve as the Lagrange multipliers to take account of the constraints of constant volume and area.

The general shape equation has been derived via variational calculus [4]

$$\Delta p-2\lambda H+k(2H+c_0)(2H^2-2K-c_0H)+2k\nabla^2 H=0, \quad (2)$$

where H and K are the mean and the Gaussian curvatures, respectively, and ∇^2 is the Laplace-Beltrami operator. This equation is a high-order nonlinear partial differential equation. For a long time, the known analytic solutions to this equation have been restricted to spheres and circular cylinders. Except the well known case of $H=0$, which represents the shapes of soap films [5] and the case of $H=$ const, which represents the shapes of soap bubbles [6], it appears that no rigorous solution was known until the prediction of the Clifford torus solution by Ou Yang [7] and was experimentally verified by Mutz and Bensimon [8] later. Recently, two new axisymmetric solutions have been reported [9].

Circular cylinder is the only known cylinder solution to this equation. It has been shown under certain conditions, the circular cylinder may destabilize and tranform into other shapes [4]. Considering various cylindrical surfaces found in lipid bilayer membranes, it seems necessary to study this one-dimensional case more carefully.

The nonparametric form of a surface is

$$z=f(x,y).$$

If the equation does not involve one of the coordinates, say y, then the equation becomes

$$z=f(x). \quad (3)$$

Such a surface is called a cylinder and Eq. (3) defines the curve of its cross section. The curvature of the curve is given by

$$c_1=\frac{z_{xx}}{(1+z_x^2)^{3/2}}.$$

If we introduce $\tan\psi(x)=-z_x$, here $\psi(x)$ is the angle between the x axis and the tangent to the curve at point x, c_1 expressed by the Gauss map of the curve is

$$c_1=\cos\psi\frac{d\psi}{dx}.$$

The mean and the Gaussian curvature of this surface are represented by

$$H=-\frac{1}{2}\cos\psi\frac{d\psi}{dx}, \quad K=0. \quad (4)$$

$\nabla^2 H$ can now be written as

$$\nabla^2 H=-\frac{1}{2}\cos\psi\left[-\cos 2\psi\left(\frac{d\psi}{dx}\right)^3-2\sin 2\psi\frac{d^2\psi}{dx^2}\frac{d\psi}{dx}+\cos^2\psi\frac{d^3\psi}{dx^3}\right]. \quad (5)$$

Substituting Eq. (4) and Eq. (5) into the general shape equation (2), we obtain the shape equation of cylindrical surfaces

$$\cos^3\psi\left(\frac{d^3\psi}{dx^3}\right)-2\cos\psi\sin 2\psi\frac{d^2\psi}{dx^2}\frac{d\psi}{dx}-\left(\frac{1}{2}\cos^3\psi-\cos\psi\sin^2\psi\right)\left(\frac{d\psi}{dx}\right)^3-\left(\frac{\lambda}{k_c}+\frac{c_0^2}{2}\right)\cos\psi\frac{d\psi}{dx}-\frac{\Delta p}{k_c}=0. \quad (6)$$

As an example, let us consider the case of a circular cylinder,

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$$\sin\psi = \frac{x}{\rho_0},$$

where ρ_0 is the radius of the circular cylinder. Equation (6) now gives

$$\Delta p \rho_0^3 + \lambda \rho_0^2 + \frac{k}{2}(c_0^2 \rho_0^2 - 1) = 0, \tag{7}$$

which is just the relation derived in [4]. Equation (6) is a nonlinear ordinary differential equation of the third order, however, for the case of $\Delta p = 0$, it can be linearized. For this purpose, we introduce $d\psi/dx = \pm\sqrt{g(\psi)}$, then the equation becomes

$$\sqrt{g}\left[\frac{d^2 g}{d\psi^2} - 4\tan\psi\frac{dg}{d\psi} - (1 - 2\tan^2\psi)g - \frac{1}{x_0^2}\sec^2\psi\right] = 0, \tag{8}$$

where for convenience, we have introduced the parameter x_0 defined by

$$\left(\frac{\lambda}{k_c} + \frac{c_0^2}{2}\right) = \frac{1}{2x_0^2}. \tag{9}$$

We note that $\sqrt{g} = \pm d\psi/dx = 0$ is just the trivial case of a plane. If $d\psi/dx \neq 0$, we have

$$\frac{d^2 g}{d\psi^2} - 4\tan\psi\frac{dg}{d\psi} - (1 - 2\tan^2\psi)g = \frac{1}{x_0^2}\sec^2\psi. \tag{10}$$

Two linearly independent solutions to the homogeneous equation corresponding to Eq. (10) are found to be $\sin\psi/\cos^2\psi$ and $1/\cos\psi$. Recall that the circular cylinder is a particular solution to Eq. (10), the general solution to Eq. (10) is therefore

$$g = \frac{1}{x_0^2\cos^2\psi} + C_1\frac{\sin\psi}{\cos^2\psi} + C_2\frac{1}{\cos\psi}, \tag{11}$$

where C_1 and C_2 are arbitrary constants. Let $C_1 = k_1/x_0^2$, $C_2 = k_2/x_0^2$; the general solution of Eq. (6) in the case of $\Delta p = 0$ can be written as

$$\psi = \text{const}$$

or

$$\pm\int\frac{\cos\psi\, d\psi}{\sqrt{1 + k_1\sin\psi + k_2\cos\psi}} = \frac{x}{x_0} + C. \tag{12}$$

In general, the integral in Eq. (12) is reducible to elliptic integrals. Equation (12) defines various interesting cross sections, which will be discussed elsewhere. We point out here that only for particular parameters Eq. (12) represents closed shapes (for example, the circular cylinder corresponds to the case of $k_1 = k_2 = 0$); the general shapes of the solution in the case of $\Delta p = 0$ are not closed and the case of $k_2 = 0$ represents two important and interesting kinds of periodic shapes. With substitution of $\alpha = 1/k_1, k_2 = 0$, Eq. (12) gives

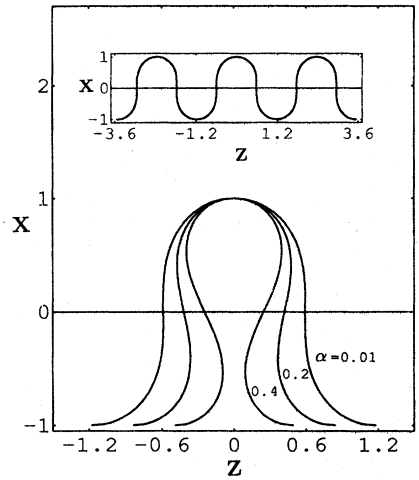

FIG. 1. One period of the cross sections of the undulation cylindrical surfaces for different values of α. The inset shows three periods of this undulation shape for $\alpha = 0.01$. Note that the vertical axis is the X axis.

$$\sin\psi = \frac{1}{4\alpha}\left(\frac{x}{x_0} + C\right)^2 - \alpha. \tag{13}$$

Here α and C are dimensionless constants and with the proper choice of the origin of the x axis we can take $C = 0$. For $0 < \alpha < 1$, Eq. (13) describes undulation surfaces and the amplitude of the surface is $X_A = 2\sqrt{(\alpha+1)\alpha}x_0$. By introducing a new variable $X = x/x_A$, Eq. (13) now can be written in the following form:

$$\sin\psi = (\alpha + 1)X^2 - \alpha \quad (-1 \leq X \leq 1). \tag{14}$$

The contour of the cross section can be obtained by calculating the following integral:

$$Z(X) - Z(X') = -\int_{X'}^{X}\tan\psi\, dX, \tag{15}$$

where $Z = z/x_A$, so both the x and z axes are scaled by x_A. In Fig. 1 we display one period of the contour of the cross sections for different values of α. We can see that the shapes and periods of the cross sections change with α. The period (actually period-amplitude ratio) of the cross section reaches its maximum value as $\alpha \to 0$ and the shape equation approaches

$$\sin\psi = X^2. \tag{16}$$

The maximum period T is

$$T = 2\int_{-1}^{1}\frac{t^2}{\sqrt{1 - t^4}}dt \approx 2.4. \tag{17}$$

We note that the shape shown in the inset of Fig. 1 was observed by Harbich and Helfrich [10] in the experiment of the swelling of egg lecithin in excess water. But they did not give an explanation of the appearance of this wavy kind of

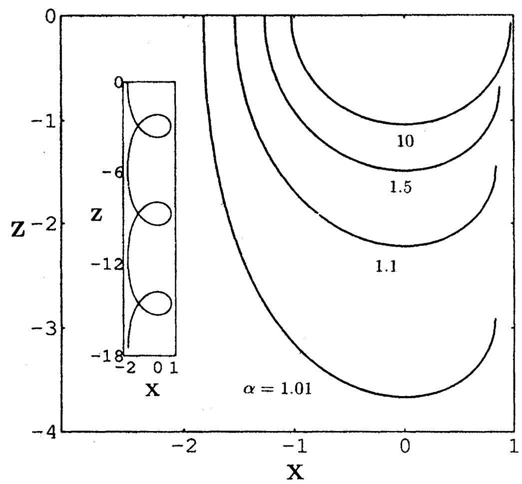

FIG. 2. Half period of the cross sections of the nodoidlike cylindrical surfaces for different α. The inset shows three periods of this kind of surface for $\alpha = 1.01$. Note that the vertical axis is the Z axis.

surface. We now realize that such a kind of surface is just a solution to the general shape equation.

For $\alpha > 1$, Eq. (13) represents another kind of period surface shown in the inset of Fig. 2. Choose $C = 2\alpha$, Eq. (13) can be rewritten in the following form:

$$\sin\psi = \frac{1}{4\alpha}(X + 2\alpha)^2 - \alpha, \tag{18}$$

where $X = x/x_0$, and $2\sqrt{(\alpha-1)\alpha} - 2\alpha < X < 2\sqrt{(\alpha+1)\alpha} - 2\alpha$. In Fig. 2 we show the half period of this kind of surface for different α. We find when $\alpha \to \infty$ this kind of surface degenerates to a circular cylinder with radius of $X = 1$ because

$$\sin\psi = \lim_{\alpha \to \infty} \alpha \left(\frac{X}{2\alpha} + 1 \right)^2 - \alpha = X, \tag{19}$$

where $-1 \leqslant X \leqslant 1$ for $2\sqrt{(\alpha-1)\alpha} - 2\alpha$ and $2\sqrt{(\alpha+1)\alpha} - 2\alpha$ tend to -1 and 1, respectively.

We know that ordered bicontinuous structures can be expressed by triply periodic minimal surfaces in the case of $\Delta p = 0$ for it is easy to check that minimal surfaces are solutions to the general shape equation (2) in the case of $\Delta p = 0$. Triply periodic minimal surfaces were discovered last century by Schwarz [11] and many new examples were given more recently by Schoen [12]. Just as Schwarz's primitive and diamond minimal surfaces can be obtained by fusion of droplets on a primitive or diamond lattice [13], Figs. 1 and 2 actually display two ways for tubes to transform into one-dimensional extended structures. We hope the shape shown in the inset of Fig. 2 may be demonstrated by experiment soon.

In conclusion, we have derived the general cylindrical surface solution in the case of $\Delta p = 0$. With it we have shown two kinds of periodic solutions to the general shape equation. The surfaces degenerate to circular cylinders in certain limiting cases. One interesting point is that the cross sections of our surfaces are quite similar to the contour of the unduloidlike and nodoidlike solutions for axisymmetric membranes [9]. At last we point out here that we have also studied the case of $\Delta P \neq 0$, which is more complicated and in general is not integrable in terms of elementary functions, algebraic or classical transcendental [14].

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