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Periodic-cylinder vesicle with minimal energy*

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We give some details about the periodic cylindrical solution found by Zhang and Ou-Yang in [1996 *Phys. Rev.* E **53** 4206] for the general shape equation of vesicle. Three different kinds of periodic cylindrical surfaces and a special closed cylindrical surface are obtained. Using the elliptic functions contained in *mathematic*, we find that this periodic shape has the minimal total energy for one period when the period–amplitude ratio $\beta \simeq 1.477$, and point out that it is a discontinuous deformation between plane and this periodic shape. Our results also are suitable for DNA and multi-walled carbon nanotubes (MWNTs).

Keywords: vesicle, curvature, solution
PACC: 8720, 8725D, 8745

1. Introduction

Lipid bilayer membranes have abundant shapes in aqueous environment. The equilibrium shape of a vesicle is determined by the minimization of the Helfrich free energy:[1] $F_{\rm H} = \int\int [k_{\rm c}/2(2H+C_0)^2+\bar{k}\Lambda]{\rm d}A$. Where H, Λ and C_0 are the mean curvature, Gaussian curvature and spontaneous curvature, respectively, dA is the surface area element, and $k_{\rm c}$ and $\bar{k}$ are constants. For close shapes, we need the surface constraint and volume constraint:

$F_{\rm S} = \lambda \oint {\rm d}A$ and $F_{\rm V} = \Delta P \oint {\rm d}V$, respectively. Here ${\rm d}V$ is the volume element for the vesicle, λ and ΔP are constants. The total energy is $F = F_{\rm H}+F_{\rm S}+F_{\rm V}$. By studying the first variation of the total energy $\delta^{(1)}F = 0$, Ou-yang and Helfrich obtained the general shape equation of closed membranes[2,3]

$$k_{\rm c}(2H + C_0)(2H^2 - 2\Lambda - C_0H) - 2\lambda H + 2k_{\rm c}\nabla^2 H + \Delta P = 0, \quad (1)$$

where the ∇^2 is the Laplace–Beltrami operator. Equation (1) is a high order nonlinear partial differential equation. It is a hard task to solve it analytically. Only the general solution for cylindrical vesicles has been discussed[4,5] and other special solutions including the Clifford torus,[6] the discounts,[7] and the beyond-Delaunay surface[8] have been given. Since the numeric methods, such as finite element method using the surface Evolver,[9] were used to search solutions for this equation, many interesting shapes were obtained in Refs.[10]–[18]. Compared with those complicate shapes obtained by numeric methods, present known analytical solutions are only the tip of iceberg in the abundant solutions of Eq. (1). In addition, a generalized model with an arbitrary energy density function $\mathcal{F} = \mathcal{F}(H, \Lambda)$ was considered and the corresponding equilibrium equation was obtained.[19] Moreover, in Refs. [20]–[22], Tu and Ou-Yang obtained the basic equations for open vesicle with free edges using the exterior differential method. These basic equations are also complicated and we can suppose that they also have abundant solutions.

2. Periodic-cylinder vesicle with minimal energy

In cylindrical case, Eq. (1) is reduced to an elliptical equation which was fully discussed in Ref. [5]. Let a cylindrical surface along the y axis and $\tan\psi(x) = {\rm d}z/{\rm d}x$, here $\psi(x)$ is the angle between the x axis and the tangent to the curve at point x, the mean curvature and Gaussian curvature of this surface are

$$H = \frac{1}{2}\cos\psi\frac{{\rm d}\psi}{{\rm d}x} = \frac{1}{2}\frac{{\rm d}(\sin\psi)}{{\rm d}x}, \quad \Lambda = 0. \quad (2)$$

Besides the planar solution ${\rm d}\psi/{\rm d}x = 0$, the shape equation is reduced to

$$\frac{{\rm d}^2 g}{{\rm d}\psi^2} - 4\tan\psi\frac{{\rm d}g}{{\rm d}\psi} - (1 - 2\tan^2\psi)g = \frac{\sec^2\psi}{x_0^2}, \quad (3)$$

where $g = ({\rm d}\psi/{\rm d}x)^2$ and x_0 defined by $1/2x_0^2 = \lambda/k_{\rm c} + C_0^2/2$. Here we let $x_0 = \sqrt{k_{\rm c}/(k_{\rm c}C_0^2 + 2\lambda)}$. Furthermore, elastic theory is also used to analysis the

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shape of DNA chain and MWNTs. In planar case, total energy of DNA[23] and MWNT[24] can be written as $F = (k_c/2)\int (K - C_0)^2 \mathrm{d}s + \lambda \int \mathrm{d}s$ (K is the curvature of the central line of DNA and MWNT and ds is the element of arc length), which induces the same shape equation as Eq. (3). Zhang and Ou-Yang found a solution for Eq. (3) with the form[4]

$$\sin\psi = \frac{1}{4\alpha}\left(\frac{x}{x_0} + C_1\right)^2 - \alpha, \tag{4}$$

here α and C_1 are constants and we choose $C_1 = 0$ because it is corresponding to a remove along x axis. Choosing the reduced value $X = x/x_0$, expression (4) can be written as

$$\sin\psi = \frac{1}{4\alpha}X^2 - \alpha. \tag{5}$$

The cross section of this cylinder can be obtained by

$$Z(X) - Z(X_1) = \int_{X_1}^{X} \tan\psi \mathrm{d}X, \tag{6}$$

where $Z = z/x_0$. By choosing different α, we find that this solution can have four kinds of different shapes as shown in Fig. 1. Here we only discuss the case $\alpha > 0$, because we will obtain the similar results when $\alpha < 0$. Valid shapes are only in the range $0 < \alpha < 0.462$. When $\alpha \geq 0.462$, the shape will be self-intersected.

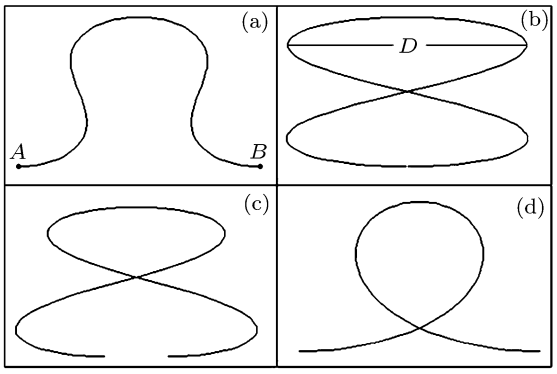


Fig. 1. Four kinds of different shapes obtained by choosing different α in expression (5). (a) A period of a kind of periodic cylinder when $0 < \alpha < 0.462$; (b) A special closed cylinder when $\alpha = 0.652$, the width–height ratio $D/(2X_\mathrm{m}) \simeq 0.328$; (c) A period for a new kind of self-intersected periodic cylinder when $0.652 < \alpha < 1$; (d) A period for a kind of self-intersected periodic cylinder when $\alpha > 1$.

In Fig. 2, we give a new kind of periodic shape using Fig. 1(c). Specifically, when $\alpha \simeq 0.652$, the points A and B in Fig. 1(a) will be superposed and we get a closed cylinder with the width–height ratio $D/(2X_\mathrm{m}) \simeq 0.328$ in Fig. 1(b). Simultaneously we need

$$-X_\mathrm{m} \leq X \leq X_\mathrm{m} \text{ for } 0 < \alpha < 1, \tag{7}$$

$$-X_\mathrm{m} \leq X \leq X_\mathrm{n} \text{ or } X_\mathrm{n} \leq X \leq X_\mathrm{m} \text{ for } \alpha > 1, \tag{8}$$

where $X_\mathrm{m} = 2\sqrt{\alpha(\alpha+1)}$ and $X_\mathrm{n} = 2\sqrt{\alpha(\alpha-1)}$.

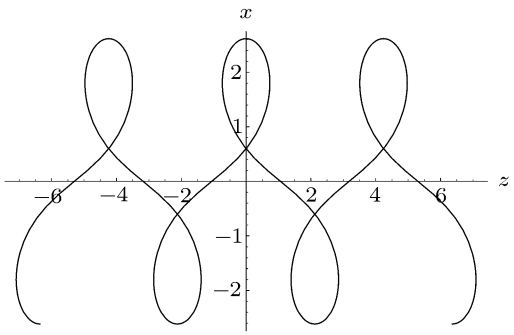


Fig. 2. A kind of periodic shape (three periods) by choosing $\alpha = 0.9$ in expression (5). This shape and the shape in Fig. 2 of Ref. [4] are close to the experimental shapes in Fig. 1 of Ref. [25].

Now, we turn to discuss the total energy of this solution. For simplicity, we only consider the case $0 < \alpha < 1$. Then, the total energy (actually the energy density along y axis) for a period is

$$\begin{aligned}\mathcal{F}_1(\alpha) &= x_0 \int_{X_\mathrm{m}}^{-X_\mathrm{m}} \frac{k_\mathrm{c}(2H + C_0)^2 + 2\lambda}{\cos\psi}\mathrm{d}X \\ &= 4\sqrt{k_\mathrm{c}^2 C_0^2 + 2\lambda k_\mathrm{c}}\,\Gamma(\alpha),\end{aligned} \tag{9}$$

here we define

$$\theta = \mathrm{i}\,\mathrm{arcsinh}\sqrt{\frac{1+\alpha}{1-\alpha}}, \quad k = \frac{\alpha - 1}{\alpha + 1}, \tag{10}$$

the function $\Gamma(\alpha)$ is

$$\begin{aligned}\Gamma(\alpha) = \frac{\mathrm{i}}{\sqrt{\alpha(\alpha+1)}}\Big\{&(\alpha+1)\times E[\theta, k] \\ &- (2\alpha+1)\times F[\theta, k]\Big\},\end{aligned} \tag{11}$$

where $F[x, y]$ and $E[x, y]$ are the elliptic integral of the first kind and the seconde kind, respectively. We find that $\Gamma(\alpha)$ has the minimum $\Gamma_\mathrm{min} \simeq 2.235$ at $\alpha \simeq 0.256$ (see Fig. 3). Thus, the minimal total energy for one period is

$$\mathcal{F}_\mathrm{min} = 8.94\sqrt{k_\mathrm{c}^2 C_0^2 + 2\lambda k_\mathrm{c}}. \tag{12}$$

Since it is difficult to discuss the stability of this infinite periodic solution, we only can think that the stable shapes satisfy $\alpha \simeq 0.256$.

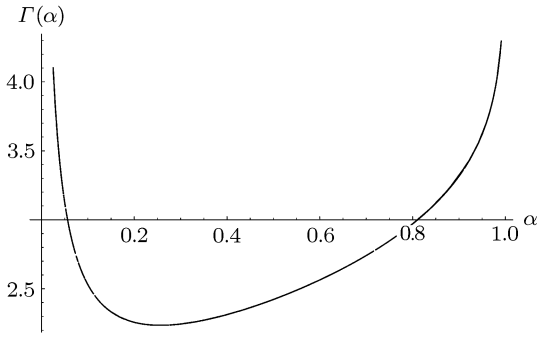


Fig. 3. The curve of $\Gamma(\alpha)$. It has the minimum $\Gamma_{\min} \simeq 2.235$ at $\alpha \simeq 0.256$. When $\alpha \to 0$ and $\alpha \to 1$, we have $\Gamma \to \infty$.

The reduced period T is

$$T(\alpha) = 2\int_{-X_{\rm m}}^{X_{\rm m}} \tan\psi {\rm d}X = \frac{8\,{\rm i}\,\alpha}{\sqrt{\alpha(\alpha+1)}}\{(\alpha+1)\times E[\theta,k] - F[\theta,k]\}. \tag{13}$$

We show $T(\alpha)$ in Fig. 4 and find that $T(\alpha)$ has the maximum $T_{\max} \simeq 1.672$ at $\alpha \simeq 0.256$. Here we should note that the real period which can be measured in experiment is $T' = x_0 T$ and we have $T'_{\max} \simeq 1.672 x_0$. Further, it is interesting to know why $\mathcal{F}_1(\alpha)$ and $T(\alpha)$ have the minimum and maximum when $\alpha \simeq 0.256$, respectively. However, because the elliptic function is everywhere continuous but everywhere non-derivable, it is difficult to discuss this coincidence.

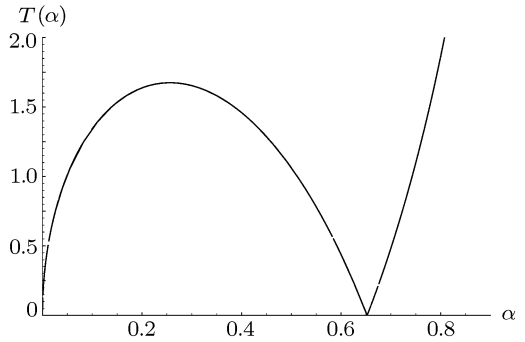


Fig. 4. The curve of reduced period $T(\alpha)$. It has the maximum (for not self-intersected shapes) $T_{\max} \simeq 1.672$ at $\alpha \simeq 0.256$. When $\alpha \to 0$, we have $T \to 0$.

An important characteristic parameter for this periodic shape is the period–amplitude ratio, it is

$$\beta(\alpha) = \frac{T(\alpha)}{X_{\rm m}} = \frac{4\,{\rm i}}{\alpha+1}\Big\{(\alpha+1)\times E[\theta,k] - F[\theta,k]\Big\}. \tag{14}$$

We find that $\beta(\alpha)$ has the maximum (for not self-intersected shapes) $\beta_{\max} \simeq 2.4$ when $\alpha \to 0$ (see Fig. 5), which is in accord with the value in Ref.[4]. Specially, when $\alpha = 0.256$, we get $\beta = 1.477$. Through measuring the shapes in Ref.[26], we obtain $\beta \approx 2$ for Fig. 9, $\beta \approx 3.3$ for Fig. 11(a), and $\beta \approx 2.7$ for Figs. 11(b) and 11(c). It indicates that not all these shapes can be explained by this solution. Moreover, in Ref.[26] the authors found that planar surface can gradually change into periodic cylinder. But in this solution, it seems that the planar surface cannot change into periodic cylinder continuously, because planar surface means $\beta \to \infty$ which is out of the range $\beta < 2.4$. Considering planar surface is always stable scampered with any periodic surface,[27] we think that there is an energy barrier between this two kinds of surfaces. Supposing that a plane with $\tilde{C}_0$ and $\tilde{\lambda}$ changes into a periodic cylinder with C_0 and λ, then the energy change between this deformation can be obtained by the following way.

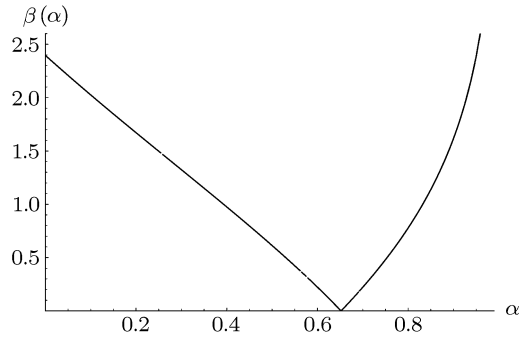


Fig. 5. The curve of period–amplitude ratio $\beta(\alpha)$. It has the maximum (for not self-intersected shapes) $\beta_{\max} \simeq 2.4$ when $\alpha \to 0$, and $\beta(0.256) \simeq 1.477$.

For this periodic cylinder, the length for one period of the cross section line is

$$L_1(\alpha) = 2x_0\int_{-X_{\rm m}}^{X_{\rm m}} \frac{1}{\cos\psi}{\rm d}X = -\,{\rm i}\,8x_0\sqrt{\frac{\alpha}{\alpha+1}}\times F[\theta,k]. \tag{15}$$

Consider the energy density for planar surface solution is $\mathcal{F}_{\rm p} = k_{\rm c}\tilde{C}_0^2/2 + \tilde{\lambda}$, the energy change for a period is

$$\Delta\mathcal{F}_{\rm p} = \mathcal{F}_1(\alpha) - \mathcal{F}_{\rm p}L_1(\alpha) = \mathcal{F}_1(\alpha) - \left(\frac{k_{\rm c}}{2}\tilde{C}_0^2 + \tilde{\lambda}\right)L_1(\alpha). \tag{16}$$

Let $\tilde{C}_0 = C_0$ and $\tilde{\lambda} = \lambda$, there is

$$\Delta\mathcal{F}_{\rm p} = 4\sqrt{k_{\rm c}^2C_0^2 + 2\lambda k_{\rm c}}\,\Omega(\alpha),$$

with

$$\Omega(\alpha) = \Gamma(\alpha) + {\rm i}\sqrt{\frac{\alpha}{\alpha+1}}\times F[\theta,k]. \tag{17}$$

We show $\Omega(\alpha)$ in Fig. 6 and find that $\Omega(\alpha)$ has a minimum $\Omega_{\min} \simeq 1.325$ at $\alpha \simeq 0.652$, which is corresponding to the closed shape in Fig. 1(b). Simply

let the barrier be equal to the energy difference, then the minima barrier is between the plane and the self-intersected 8-shape in Fig. 1(b). Clearly, in phase space, if we want that a plane drops to a periodic cylinder, we need $\Delta\mathcal{F}_{\rm p} < 0$ in Eq. (16). It cannot be satisfied if $\tilde{C}_0 = C_0$ and $\tilde{\lambda} = \lambda$, because $\Omega(\alpha) > 0$. Thus, in this downward transition process, λ (or C_0) will change.

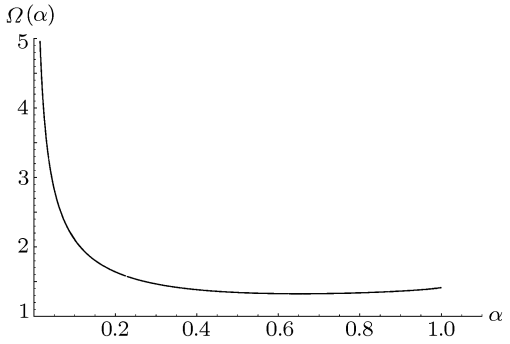


Fig. 6. The curve of $\Omega(\alpha)$. It has the minimum $\Omega_{\rm min} \simeq 1.325$ when $\alpha \simeq 0.652$. When $\alpha \to 0$ we have $\Omega \to \infty$ and when $\alpha \to 1$ we get $\Omega \simeq \sqrt{2}$. In addition, we have $\Omega(0.256) \simeq 1.526$, $\Omega(0.462) \simeq 1.356$.

When $\alpha > 1$ we find that $\mathcal{F}_1(\alpha)$ is monotone decreasing following the increase of α and $\mathcal{F}_1 = 4\pi k_{\rm c} C_0$ when $\alpha \to \infty$. Another way, when $\Delta P = 0$, a circular cylinder solution with radii R needs $C_0 R = 1$.[28] Its total energy is $\mathcal{F} = \oint \frac{k_{\rm c}}{2}(1/R + C_0){\rm d}s = 4\pi k_{\rm c} C_0$ which is in accordance with the above result (note that $\alpha \to \infty$ is corresponding to a circular cylinder[4]).

Remarkably, although the shape in Fig. 1(b) is self-intersected for 2D surface, it is useful to describe the DNA and MWNT shapes, because that any perturbations on the binormal direction will probably lead it to be not self-intersected. A ring solution: $x = R\sin\psi$ for Eq. (3) induces

$$\tilde{\lambda}R^2 + \frac{1}{2}k_{\rm c}(\tilde{C}_0^2 R^2 - 1) = 0. \tag{18}$$

If a DNA ring changes into the shape in Fig. 1(b) and $\tilde{C}_0$ and $\tilde{\lambda}$ change to C_0 and λ, respectively, we have

$$2\pi R = L_1(0.652). \tag{19}$$

Equations (18) and (19) yield the relationship

$$2.846 \times (\tilde{C}_0^2 + 2\tilde{\lambda}/k_{\rm c}) = C_0^2 + 2\lambda/k_{\rm c}. \tag{20}$$

If $\tilde{C}_0 = C_0 = 0$, expression (20) indicates that the tension λ will increase in this deformation.

3. Discussion and conclusion

In conclusion, we have studied the particulars about the periodic cylinder in Ref.[4] for the closed shape equation of vesicle. Several characteristics for this periodic shape are obtained, which give us some interesting details about this solution. For instance, when the period–amplitude ratio $\beta \simeq 1.477$, this periodic shape has a minimal total energy for one period. We hope the shape with period–amplitude ratio $\beta \simeq 1.477$ can be found in experiment. As for the other periodic surface: beyond-Delaunay surface,[8] because there is not an analytic integral function of its total energy, we do not know whether there is a similar result.

Finally, we point out an interesting revelation. We know that if the energy density of a one-dimensional structure, such as DNA[23] and MWNTs,[24] can be written as

$$\mathcal{F} = \frac{1}{2}k_{\rm c}(K - C_0)^2, \tag{21}$$

the corresponding shape equation in planar case is

$$2\ddot{K} + K^3 - (C_0^2 + 2\lambda/k_{\rm c})K = 0, \tag{22}$$

where $\dot{K} = {\rm d}K/{\rm d}s$. This equation is equal to Eq. (3) (except the straight line solution $K = 0$). The shapes of DNA and MWNT in planar case satisfy this equation. Thus, the solutions of Eq. (3) have broad meaning. Ou-Yang *et al.* proved that the energy density of MWNTs can be written as $\mathcal{F} = \alpha K^2$,[24] but this model seems not suitable for single-walled carbon nanotubes (SWNTs), because the constant α will be zero for SWNTs. However, we note that the shape in Fig. 2 of Ref. [4] and the new shape in Fig. 2 of this paper seems to be in good agreement with the experimental SWNT shapes in Fig.1 of Ref. [25]. Thus, we suppose that the energy density of SWNTs satisfies expression (21) under suitable approximation. We will try to prove this supposition in our future work.

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