·专论与综述·

The Morphology of Vesicles of Higher Topological genus*

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ABSTRACT: The equilibrium configuration of fluid - phase phospholipid vesicles in aqueous solutions are controlled by bending elasticity. We exploited a method for calculating explicitly the stability of arbitrary symmetric shapes. The morphology of lipid vesicles with topological genus g = 2, i.e. with two holes or two handles, is studied. We provided some stable shapes with results explicitly.

Key words: Vesicles; Genus 2; Morphology; Surface Evolver

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0 Introduction

Lipid is an amphipathic molecule which can be dissolved in an aqueous environment where they self - assemble and form two - dimensional bilayers or membranes[1,2]. In order to avoid the exposure of their hydrophobic tails of in water, the membranes formed by the lipid molecules tends to be closed surfaces or vesicles, which has been used in the pharmacology, cosmetology, drug carrier, environmental protecting, detergent development, oil exploiting, and so on. A rich variety of different shapes of vesicles had been observed under a special microscope in the experiments[3,6].

The assumption that vesicle shapes are determined by the bending elasticity of the membranes[7,8] allow the theoretical study of these shapes[9,14].

Vesicles can be classified by their topology. The topology of a vesicle is characterized by its topological genus g which counts the number of "handles" attached to a sphere to obtain a surface of given topology. Vesicles with the topology of a sphere, i.e. $g = 0$, are most common. However, vesicles with toroidal topology, i.e. $g = 1$[15,17], and vesicles with two, three and even more "handles" have been observed experimentally[18, 19].

In 1973, the SC (spontaneous curvature) model considering both asymmetry of the bilayer and the environments was proposed by Helfrich[20]. In this model, the shape energy is written as

$$F = \frac{1}{2} k_c \oint (C_1 + C_2 - C_0)^2 dA + \Delta p \int dV + \lambda \oint dA \qquad (1)$$

where k_c is an elastic modulus, c_1 and c_2 are two principle curvatures, c_0 is the spontaneous [1]curvature, $\Delta p$and λ are two Lagrange multipliers that take account of the constraints of constant volume and constant area. Physically, Δp can be understood as the osmotic pressure difference and λ can be understood as the tensile coefficient. The presence of the spontaneous curvature serves to describe the effect of asymmetry of the membrane and/or its environment.

By performing the variations of the above equation, the general equation was derived[21]

$$\Delta p - 2\lambda H + k_c(2H + C_0)(2H^2 - 2K - C_0 H) + 2K \nabla^2 H = 0 \qquad (2)$$

where the operator $\nabla^2 = (1/\sqrt{g})\partial_i(g^{ij}\sqrt{g}\partial_i)$ is the Laplace - Beltrami operator, g is the determinant of the metric g_{ij} associated with the first fundamental form, $g^{ij} = (g_{ij})^{-1}$, $H = (C_1 + C_2)$ is the local mean curvature, and $K = C_1 C_2$ is the Gaussian curvature. However, It is hard to resolve the equation analytically. Just the general solution for cylinder vesicles[22] has been discussed and the other special solutions including the Clifford torus, the discocyte, and the beyond - Delaunary surfaces have been studied.

In SC model, by using the scale invariance of the curvature energy function Eq. (1), the number of parameters can be reduced. The A is used to define a length scale $R_0 = \sqrt{A/4\pi}$, and the reduced volume $v = V/(4/3)\pi R_0^3$, and the reduced curvature $c_0 = C_0 R_0$. Then any solutions of Eq. (2) depend only on these two dimensionless quantities.

1 Tools and methods

In spite of the difficulty in finding the analytical solutions of Eq. (2), other complex vesicle shapes with genus 2 were found by the powerful software Surface Evolver [23].

The software is based on a discretization of the curvature energy, area, and volume on a triangulated surface. In this software, the resulting energy is minimized by a gradient descent procedure. The resulting shape is corresponding to a local energy minimum. Further more, it can calculate the Hessian matrix which is the second variations of the shape energy. All the shapes below are all calculated by Hessian matrix and have been evolved for a long time. So they are all stable shapes.

The energy in Surface Evolver is a combination of a few components. These components can be square mean curvature, surface tension, osmotic pressure difference, and gravitational energy, etc. In order to search the stable shapes based on spontaneous curvature mod-

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el, the energy function in the software takes the sum of square mean curvature, surface tension and osmotic pressure.

2 Results and discussion

We fix reduced volumebelow. And at the beginning, we just calculate under $c_0 = 0$. Two different shapes can be obtained by evolving different initial shapes [Fig.1].

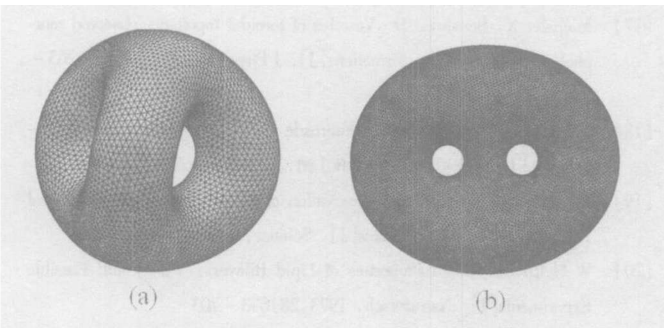

Fig. 1. Two different stable shapes which all minimize the curvature energy for F fixed reduced volume v = 056 and $c_0 = 0$. (a) The D_{3h} symmetric vesicle shape with energy $F \cong 50.526212$, $\Delta p = -23.97142$, $\lambda = 6.72141$, $m \cong 1.181851$. (b) The D_{2h} symmetric shape with energy $F \cong 48.809725$, $\Delta p = -21.717202$, $\lambda = 6.055103$, $m = 1.191350$.

As shown in Fig.1, two shapes are of different symmetric properties. But the biggest differences lie in the energy and reduced integral of mean curvature. Obviously, in the energy and reduced integral of mean curvature, the former is higher than the latter when calculating other reduced volunes within willmore surfaces($V < 0.66$)[Fig 2], the two kinds of shapes exist stably. One D_{2h} symmetric shape has been observed experimentally.[25] In SC model, such a shape can be easily found.

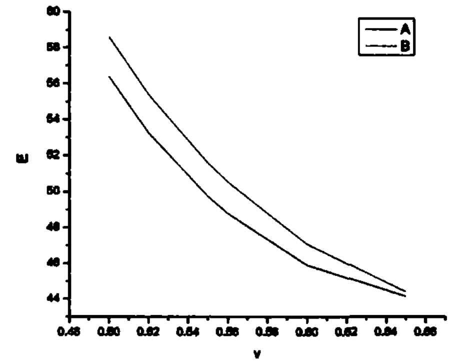

Fig.2 Phase diagram for v - E. A(the bold one) and B have the same symmetry with Fig.1(a),(b), respectively.

图 2 对应的相图。A(粗线),B线分别对应着图1中a,b所具有的对称性。

Drawn from Fig.2, one can find the energy of the one with D_{3h} symmetry is always higher than the one with D_{2h} symmetry under the same reduced volume when keeping $c_0 = 0$ outside of willmore surface region.

More shapes have been found while we change c0 under [Fig.3].

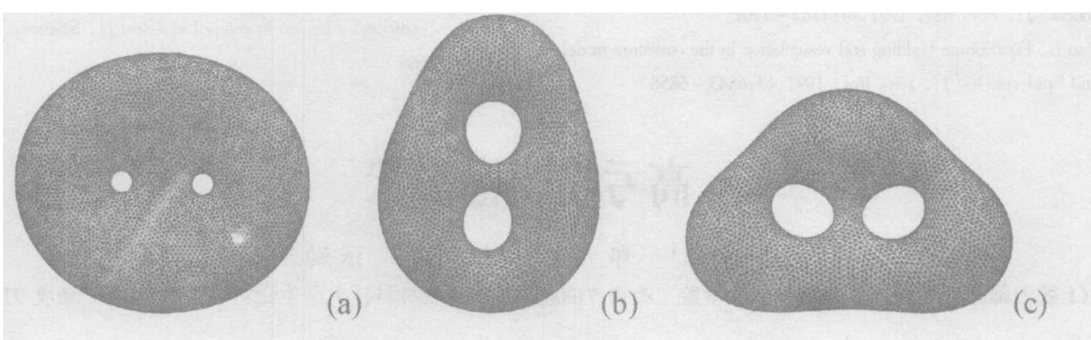

Fig.3 Three different shapes with genus 2 under v = 052. (a) The shape with $c_0 \cong 0.000000$, $m \cong 1.143488$, $F \cong 53.076624$, $\Delta p = -26.862336$, $\lambda = 7.054473$; (b) The shape with $c_0 = 1.900000$, $m \cong 1.385660$, $F \cong 12.506893$, $\Delta p = -7.364980$, $\lambda = 1.105188$; (c) the shape with $c_0 = 2.000000$, $m \cong 1.417304$, $F \cong 11.484585$, $\Delta p = -6.570478$, $\lambda = 0.897029$.

图 3 下对应的亏格为2囊泡的不同形状。(a) $c_0 \cong 0.000000$, $m \cong 1.143488$, $F \cong 53.076624$, $\Delta p = -26.862336$, $\lambda = 7.054473$;的膜泡。(b) The shape with $c_0 = 1.900000$, $m \cong 1.385660$, $F \cong 12.506893$, $\Delta p = -7.364980$, $\lambda = 1.105188$ 的膜泡。(c) the shape with $c_0 = 2.000000$, $m \cong 1.417304$, $F \cong 11.484585$, $\Delta p = -6.570478$, $\lambda = 0.897029$ 的膜泡。

From Fig.3, one can easily find that two phase transformations occur when c_0 grows. And the energy decreases with integral mean curvature. So it is interesting to find out whether they are continuous phase transformations or not, which is within our capability.

3 Conclusion

By building some initial configuration, we can easily find some interesting shapes. We believe that some of other more complex shapes can be found by this way. Furthermore each eigenvector of the Hessian matrix stands for a king of transformation in the configuration space. A stable shape scan is used in the phase diagram, its nontrivial eigenvalues are noted down. If one of them crosses 0 or reaches a lower value, an bifurcation point or an unstable point occurs, so we can obtain a more perfect phase diagram in SC model.

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高亏格膜泡形状*

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摘要:溶液中流体相磷脂膜泡的平衡形状是由其弯曲弹性能决定的。我们用 Surface Evolver 软件找到了一个具体的模拟稳定膜泡形状的方法,对亏格为2的膜泡进行了研究。我们提供了具体的计算结果。

关键词:膜泡;亏格2;形状;Surface Evolver

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