Anchor ring-vesicle membranes

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A family of the exact and analytical solutions of the equilibrium shape equation of vesicle membranes is found. They are anchor rings with generating circles of radii in the ratio $1/\sqrt{2}$. It is shown that these ring vesicles are stable for some negative values of their spontaneous curvatures, such that experimental construction of such vesicles seems possible. A discussion shows that a positive Gauss-curvature elastic modulus favors the formation of these special vesicles.

Certain amphiphilic molecules, such as phospholipids, assemble in water to build bilayers which, at low concentration, close to form single shells called vesicles.[1] These structures are simple models for biological membranes and cells.[2,3] Other amphiphiles form surfactant films separating oil and water, thus giving rise to microemulsion.[4] The equilibrium shape of a vesicle is determined as that shape which minimizes the Helfrich curvature free energy,[5,6] namely, shape energy

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

Here dA and dV are the surface area and the volume elements, respectively, k_c is an elastic modulus, c_1 and c_2 are the two principal curvatures, and c_0, the spontaneous curvature, is a constant tending to bias the principal curvatures and serves to describe the effect of an asymmetry of the membrane or its environment.[7,8] The Lagrange multipliers Δp and λ take account of the constraints of constant volume and area, $\Delta p=p_0-p_i$ is the osmotic pressure difference between outer and inner media, and λ a tensile stress.

Applying standard techniques of the calculus of variations the author and Helfrich have derived from Eq. (1) the general equation of mechanical equilibrium of vesicle membranes[9,10]

$$\Delta p-2\lambda H+4k_c(H+\tfrac{1}{2}c_0)(H^2-K-\tfrac{1}{2}c_0H)+2k_c\nabla^2H=0\ , \quad (2)$$

where ∇^2, before H, denotes the Laplacian, H the mean curvature, and K Gauss curvature. So far, various solutions of Eq. (2) are calculated numerically by assuming azimuthal symmetry and topological spheres.[5,6,11,12] In these cases Eq. (2) reduces to an ordinary differential equation of the second order for the principal curvatures or fourth order for the contours. However, since the equation is highly nonlinear, finding exact and analytic solutions is quite a task. Up to now, besides the case of a sphere, no analytical solutions are known yet. It is interesting to ask the question: Do there exist closed surfaces of the vesicle which topologically are not spheres?

As a step towards solution of the problem, we report here on a theoretical finding of the vesicle surfaces of one genus, which are the special standard tori called anchor rings whose generating circles have radii in ratio $1/\sqrt{2}$. To show that these ring vesicles correspond to the stable infinitesimal extremum values of the shape energy shown in Eq. (1) and may be found in future experiment an investigation of the second variation of the shape energy of the shapes has been done. Applying the general formulation[10] we have shown that the ring vesicles are stable for some negative values of the spontaneous curvature by

$$c_0r_0<-(\pi\sqrt{2})^{1/2}(\tfrac{3}{2}+\sqrt{2}/4)\approx-3.9\ , \quad (3)$$

where $A=4\pi r_0^2$ is the area of the ring vesicles. The conditions of (3) are not very far from what are believed to be normal conditions for the red blood cells $(c_0r_0\approx-3)^2$, so that the torus vesicles may be constructed by biological membranes. In the following, we give an outline of our calculation.

With ring functions or toroidal functions,[13] the family of tori generated by the revolution around the z axis of the circles may be described in E^3 by

$$\mathbf{Y}=\left\{\frac{c\sinh\eta\cos\phi}{\cosh\eta-\cos\theta},\frac{c\sinh\eta\sin\phi}{\cosh\eta-\cos\theta},\frac{c\sin\theta}{\cosh\eta-\cos\theta}\right\}, \quad (4)$$

where ϕ varies from 0 to 2π, θ from $-\pi$ to π, and c and η are parameters specifying the different rings. In detail, as shown in Fig. 1, A and B are points on a straight line through the origin O, $AB=2c$, perpendicular to the z axis, and making an angle ϕ with the x axis, we take as coordinates of a point P in the plane ϕ=const, $\eta=\ln(AP/BP)$, and θ is the angle APB. The surfaces for η=const will be the family of tori generated by the revolution around the z axis of the circles of the family of coaxial circles of which A and B are the limiting points. Equation (2) is an invariant under similarity transformations of scale. It is only necessary to consider the case of $c=1$. With the same notation used in Ref. 9, a straightforward calculation yields

$$H=\frac{1}{2}\left\{\sinh\eta+\frac{\cosh\eta\cos\theta-1}{\sinh\eta}\right\},$$
$$K=\cosh\eta\cos\theta-1\ , \quad (5)$$
$$\nabla^2H=-\tfrac{1}{2}\cos\theta(\cosh\eta-\cos\theta)^2\coth\eta\ .$$

Substitution of Eq. (5) into Eq. (2) gives

$$\Delta p-2k_c c_0(\cosh\eta\cos\theta-1)-(k_c c_0^2+2\lambda)\tfrac{1}{2}\left[\sin\eta+\frac{\cosh\eta\cos\theta-1}{\sinh\eta}\right]$$
$$+\tfrac{1}{2}k_c(\cosh\eta-\cos\theta)^2\left[\frac{\cosh^2\eta(\sinh^2\eta-1)}{\sinh^3\eta}+\left[\frac{\cosh^3\eta}{\sinh^3\eta}-2\frac{\cosh\eta}{\sinh\eta}\right]\cos\theta\right]=0\ . \quad (6)$$

Observing the coefficients of $\cos^m\theta$ for different m ($m=0,1,2,3$), one finds that Eq. (6) is satisfied only when

$$\sinh\eta=1,\ \text{i.e.,}\ \cosh\eta=\sqrt{2}\ , \quad (7)$$

and

$$\Delta p=-2k_c c_0,\quad \lambda=-2k_c(c_0+\tfrac{1}{4}c_0^2)\ . \quad (8)$$

Equations (4) and (7) imply that Eq. (2) is satisfied by the standard torus if and only if its generating circles have radii in the ratio of $1/\sqrt{2}$. For example, with $\phi=\pi/2$, one has $(y-\sqrt{2})^2+z^2=1$, i.e., generating circle on the yz plane.

The shape equation, Eq. (2), comes from the first variation[10] of the shape energy and Eqs. (7) and (8) are the necessary conditions for the shape energy to attain a stationary value. To show that they correspond to the infimum value of the energy it is necessary to consider the second variation of shape energy. The second variation of the shape energy for such an arbitrary shape is given in Ref. 10. Now, let us consider the distorted rings

$$\mathbf{Y}'=\mathbf{Y}+\mathbf{n}\psi\ , \quad (9)$$

where $\mathbf{n}$ is the normal of the ring surface described by Eqs. (4) and (7), and

$$\psi=\sum_m[a_m(\theta)\sin m\phi+b_m(\theta)\cos m\phi]\ . \quad (10)$$

From Eqs. (4), (5), (7), (8), (10), and Eq. (39) of Ref. 10, after a lengthy calculation,[14] we have the second variations of the shape energy as follows:

$$\delta F=\pi\int_{-\pi}^{\pi}d\theta\sum_m\Big\{(a_{m,\theta\theta}^2+b_{m,\theta\theta}^2)(\sqrt{2}-\cos\theta)^2+(a_{m,\theta}^2+b_{m,\theta}^2)[m^2(\sqrt{2}-\cos\theta)^2+\sqrt{2}(1+c_0)\cos\theta-\tfrac{1}{2}\cos^2\theta-2-2c_0]$$
$$+(a_m^2+b_m^2)\Big[m^2\Big[\frac{m^2}{2}(\sqrt{2}-\cos\theta)^2+3\sqrt{2}\cos\theta-\tfrac{1}{2}\cos^2\theta\Big]$$
$$+(\sqrt{2}-\cos\theta)^{-2}[4\cos^4\theta+\sqrt{2}(c_0-9)\cos^3\theta+(12-4c_0)\cos^2\theta$$
$$-\sqrt{2}(2+c_0)\cos\theta+2c_0]\Big]\Big\}\ , \quad (11)$$

where the subscript θ of $a_{m,\theta}$, $b_{m,\theta}$, $a_{m,\theta\theta}$, and $b_{m,\theta\theta}$ means derivatives with respect to θ, e.g., $a_{m,\theta}=(d/d\theta)a_m(\theta)$, $a_{m,\theta\theta}=(d^2/d\theta^2)a_m(\theta)$. The stability analysis requires δF to be positive definite for any $\psi\neq 0$. From Eq. (11) we see that the necessary condition for the coefficients of $a_{m,\theta}^2$ and $b_{m,\theta}^2$ in Eq. (11) to be positive is

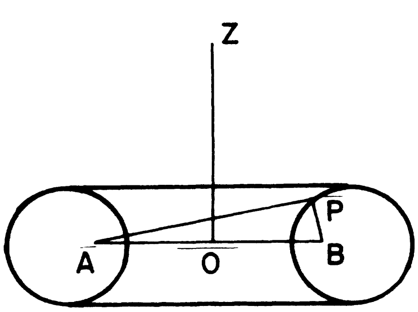

FIG. 1. The family of tori generated by the revolution around the z axis of coaxial circles of which A and B are the limited points.

$$c_0<-(\tfrac{3}{2}+\sqrt{2}/4)\ , \quad (12)$$

which also ensures the positivity for the coefficients of $a_m^2+b_m^2$ in Eq. (11). Moreover, considering that the special torus has the area

$$A\equiv 4\pi r_0^2=4\pi^2\sqrt{2}\ , \quad (13)$$

the result of (3) follows immediately.

Similarly, with Eq. (13) the conditions of Eq. (8) may change into the following general forms:

$$\Delta p=-2\pi\sqrt{2}\left[\frac{k_c}{r_0^3}\right]c_0 r_0\ ,$$
$$\lambda=-2\left[\frac{k_c}{r_0^2}\right][(2\sqrt{\pi})^{1/2}c_0 r_0+\tfrac{1}{4}c_0^2 r_0^2]\ . \quad (14)$$

These last two conditions indicate that both the pressure difference Δp and tensile stress λ are fixed by the $c_0 r_0$ and the sizes of the ring vesicles, while one of them can be freely chosen in the case of spheres.[9] Obviously, the situations which satisfy simultaneously conditions (3) and (14) are quite rare. In a sense, that is why so far ring vesicles have not been observed. For this fact an additional reason may relate to the sign of Gauss-curvature elastic modulus $\bar{k}$. In its complete form the shape energy of Eq. (1) still needs to be supplemented by another elastic energy[5,6]

$$F_G=\tfrac{1}{2}\bar{k}\oint c_1c_2\,dA\ . \tag{15}$$

According to the Gauss-Bonnet theorem in differential geometry, this term gives a contribution to the total energy only by a constant $2\pi\bar{k}(1-g)$, where g is the genus of the vesicle and is, obviously, independent of the shape equation of (2). For a vesicle of topological spheres, $F_G=2\pi\bar{k}$, but in the case of the ring vesicles it is zero. Hence if $\bar{k}<0$ the construction of the latter needs an extra curvature energy. For example, let us consider a special case in which the sphere and the anchor ring can coexist. From the conditions of Eq. (14) and the sphere equation [which comes from Eq. (2)]

$$\Delta p r_0^3+2\lambda r_0^2-k_c c_0 r_0(2-c_0r_0)=0\ , \tag{16}$$

one can show that two types of vesicles may coexist only when $c_0=0$. With this and Eqs. (1), (5), (14), and (15) one finds the total shape energies of the sphere and the ring vesicle are, respectively,

$$F_S=8\pi k_c+2\pi\bar{k}\ , \tag{17}$$

and

$$F_R=4\pi^2k_c\ . \tag{18}$$

If one assumes the membranes of both vesicles are the same, the case is advantageous to the ring vesicle only when $F_R<F_S$, that is,

$$\bar{k}>2(\pi-2)k_c\ . \tag{19}$$

In other words, a positive k favors the formation of a ring vesicle. This is an intrinsic limit for building these special vesicle membranes. However, as we mentioned at the beginning, the construction of them with biological membranes under the normal physiological conditions remains possible and will be an interesting subject for the experiments.

On the theoretical side, the existence of the ring vesicles and spherical ones, whose genus is equal to one and zero, respectively, raises a mathematical question whether there exist vesicle solutions of other genus. The general equation (2) can be extended to give a positive answer to this question. It is not difficult to see that if $c_0=\Delta p=0$ there exist the vesicle surfaces whose mean curvature at every point on the surfaces is equal to zero, namely, the minimal surfaces. Following Lawson's[15] theorem: there exist closed minimal surfaces of arbitrary genus, we then have immediately the above answer. However, for $H\neq 0$ the question remains open. The shape equation of (2) is new. A special case of Eq. (2) is the Plateau problem of soap films ($H=0$ and $H=-c_0/2=$const), which is known for its richness, complexity, and beauty. The investigation of this equation in connection with biological cells, artificial vesicle membranes, and microemulsions will probably develop into a new broad field in mathematical physics.

Finally we would like to clarify an important case: In Ref. 10 it was shown that straight cylinders are in a large parameter range stable solutions. One then thinks that closing such a cylinder to a large torus with small radius ratio should lead to stable solutions. Does this cast doubt on the claim that the radius ratio $1/\sqrt{2}$ is singled out? In fact, such a limiting torus is included in our above calculations. If we return to normal unit of scale, then Eqs. (5) and (6) change into the following:

$$\begin{aligned}H&=\frac{1}{2c}\left[\sinh\eta+\frac{\cosh\eta\cos\theta-1}{\sinh\eta}\right],\\ K&=c^{-2}(\cosh\eta\cos\theta-1)\ ,\\ \nabla^2H&=-\tfrac{1}{2}c^{-2}\cos\theta(\cosh\eta-\cos\theta)^2\coth\eta\ ,\end{aligned} \tag{20}$$

and

$$\Delta p-2k_cc^{-2}c_0(\cosh\eta\cos\theta-1)-(k_cc_0^2+2\lambda)\frac{1}{2c}\left[\sin\eta+\frac{\cosh\eta\cos\theta-1}{\sinh\eta}\right] +\tfrac{1}{2}k_cc^{-3}(\cosh\eta-\cos\theta)^2\left[\frac{\cosh^2\eta(\sinh^2\eta-1)}{\sinh^3\eta}+\left[\frac{\cosh^3\eta}{\sinh^3\eta}-2\frac{\cosh\eta}{\sinh\eta}\right]\cos\theta\right]=0\ . \tag{21}$$

From the last equation, especially from the coefficient of $\cos^3\theta$, one again finds that under limited scale, i.e., c is definite, the radius ratio $1/\sqrt{2}$ is singled out. However, if we let $\eta\to\infty$, $c\to-\infty$ (the negative sign is to adjust the unit normal vector of the torus surface in agreement with that in Ref. 10), and $c/\sinh\eta$, $c/\cosh\eta\to-\rho_0$. We then have, from the mentioned equations,

$$H=-\frac{1}{2\rho_0},\quad K=0,\quad \nabla^2H=0\ , \tag{22}$$

and

$$\Delta p\rho_0^3+\lambda\rho_0^2+\tfrac{1}{2}k_c(c_0^2\rho_0^2-1)=0\ . \tag{23}$$

Obviously, Eqs. (22) and (23) are the same as Eqs. (64) and (58) of Ref. 10, respectively. These just serve to describe an equilibrium cylinder with radius ρ_0 as shown in Ref. 10. In other words, the limiting torus is nothing but a true straight cylinder.

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