Counterexample to some shape equations for axisymmetric vesicles

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Three different shape equations for axisymmetric vesicles have been derived from the same spontaneous-curvature model in literature. The validity of the equations has been examined by means of a rigorous analytical solution for axisymmetric vesicles. A counterexample is given to show the invalidity of two of the equations.

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Recently, Hu and Ou-Yang [1] have pointed out that three *different* shape equations for axisymmetric vesicles have been derived within the framework of the *same* Helfrich spontaneous-curvature model [2], in which the bending energy F_b is expressed as

$$F_b = \tfrac{1}{2}\, k \oint (c_1 + c_2 - c_0)^2 dA + \bar{K} \oint c_1 c_2 dA, \qquad (1)$$

where k, $\bar{K}$, c_1, c_2, and c_0 are the bending rigidity, Gaussian-curvature modulus, two principal curvatures, and the spontaneous curvature, respectively. The shape equation of the axisymmetric vesicles is determined by minimizing F_b for constant volume V and total area A. In practice, we can incorporate these constraints by Lagrange multipliers Δp and λ. The shape equation is obtained from

$$\delta(F_b + \lambda A + \Delta p V) = 0, \qquad (2)$$

where δ denotes the variant with respect to the shape of the vesicle. The three different shape equations for the axisymmetric vesicles have been reported by Deuling and Helfrich (DH) [3], Seifert, Berndl, and Lipowsky (SBL) [4], and Hu and Ou-Yang (HO) [1], and result from the different interpretations of the above variation. Hu and Ou-Yang [1] have carefully shown the reason why two of the equations (the DH and the SBL equations) are incorrect; these two equations were obtained from the erroneous calculus of variations by using a parameter (the radius or the arc length of the vesicles). They [1] have also given two examples, a Clifford torus [5] and a cylinder, to show the difference between the DH and the SBL equations, and the HO equation, which has been derived from the general shape equation [6],

$$\Delta p - 2\lambda H + k(2H + c_0)(2H^2 - 2K - c_0 H) + 2k\nabla^2 H = 0, \qquad (3)$$

where H and K are the mean and the Gaussian curvatures, respectively, and ∇^2 is the Laplace-Beltrami operator. The Lagrange multipliers Δp and λ take account of the constraints of constant area and volume of the vesicles, $\Delta p = p_o - p_i$ is the osmotic pressure difference between outer and inner media, and λ is the tensile stress. Since the two given examples in Ref. [1] are somewhat special in their topology, some researchers in this field, who use the DH or the SBL equations, may still think that the three shape equations predict the same shapes having smooth surfaces [7].

In this Brief Report we show a more general and significant example for the demonstration of the difference between the DH and the SBL equations, and the HO equation as well as of the invalidity of the two equations, because the two equations are widespread in literature [3,4]. For this purpose, we give an obvious and comprehensible counterexample to the DH and the SBL equations by using a rigorous analytical solution of the HO equation, which has been briefly reported to explain the human red-blood-cell (RBC) shape [8]. Prior to this counterexample, we briefly describe the three shape equations, the origin of the invalidity of the two equations, and the rigorous solution to the HO equation.

In the early stage of the theoretical investigation of an axisymmetric vesicle, efforts have been made to explain the shape of RBC's, which possess a well-known biconcave-discoid shape under normal physiological conditions. Since the axisymmetry reduces the complexity of the shape equations, only equilibrium shapes of axisymmetric vesicles have been extensively calculated with numerical methods so far [3,4]. In general, the shape equation derived from Eq. (1) is the nonlinear fourth-order ordinary differential equation. If we introduce the angle ψ made by the surface tangent and the plane perpendicular to the axisymmetric axis (z axis) as shown in Fig.1, the order of the equation can be further reduced. Once $\psi(\rho)$ is known, we can obtain the contour $z(\rho)$ by a simple integration

$$z(\rho) - z(0) = \int_0^{\rho} \tan\psi(\rho')d\rho', \qquad (4)$$

where ρ is the distance from the z axis.

We note that three different equations for axisymmetric vesicles have been derived from different variational

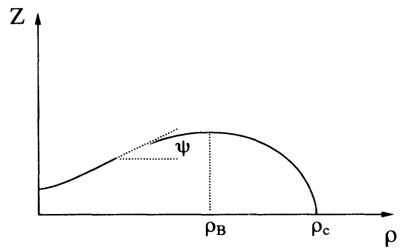

FIG. 1. Cross section of an axisymmetric vesicle described by Eq. (16) for $c_0 < 0$. Only one quadrant is shown. There is rotational symmetry around the z axis and reflection symmetry at the ρ axis.

methods on the basis of the same Helfrich spontaneous-curvature model [2]. The three ways to obtain the shape equations are as follows.

(i) Equation (2) is changed to an action form by using ρ as a parameter,

$$F_b + \lambda A + \Delta p V = 2\pi k \int_0^{\rho_c} L\left(\psi(\rho), \frac{d\psi}{d\rho}, \rho\right) d\rho\,, \quad (5)$$

where ρ_c is the equatorial radius of an axisymmetric vesicle and L is the Lagrange function. After the parametrization of the vesicle shape, L is determined from Eq. (5). The minimal solutions to the axisymmetric vesicles are given by the DH shape equation [3], which is obtained from the Euler-Lagrange equation

$$\frac{\partial L}{\partial \psi} - \frac{d}{d\rho}\frac{\partial L}{\partial(d\psi/d\rho)} = 0. \quad (6)$$

(ii) The SBL shape equation [4] is derived in a way similar to (i) except for the parameter in the action form, which is the arc length of the contour s.

(iii) The HO shape equation [1] is obtained by simply substituting the mean and the Gaussian curvatures of an axisymmetric vesicle into the general shape equation [Eq. (3)], which describes the shape of the vesicle at mechanical equilibrium, and which has been derived from the first variation of $F_b + \lambda A + \Delta p V$ by using general rules of differential geometry and imposing the closed condition of the surface of the vesicle only [6].

The DH [3], the SBL [4], and the HO [1] shape equations of $\psi(\rho)$ are

$$\cos^2\psi\left(\frac{d^2\psi}{d\rho^2}\right) = \frac{\sin\psi\cos\psi}{2}\left(\frac{d\psi}{d\rho}\right)^2 - \frac{\cos^2\psi}{\rho}\left(\frac{d\psi}{d\rho}\right) + \frac{\sin 2\psi}{2\rho^2} + \frac{\Delta p\rho}{2k\cos\psi} + \frac{\lambda\sin\psi}{k\cos\psi} + \frac{\sin\psi}{2\cos\psi}\left(\frac{\sin\psi}{\rho} - c_0\right)^2, \quad (7)$$

$$\begin{aligned}\cos^3\psi\left(\frac{d^3\psi}{d\rho^3}\right) = {} & \left(3\sin\psi\cos^2\psi + \frac{\cos^2\psi}{\sin\psi}\right)\left(\frac{d^2\psi}{d\rho^2}\right)\left(\frac{d\psi}{d\rho}\right) - \cos\psi\sin^2\psi\left(\frac{d\psi}{d\rho}\right)^3 \\ & + \frac{(2+5\sin^2\psi)\cos^2\psi}{2\rho\sin\psi}\left(\frac{d\psi}{d\rho}\right)^2 - \frac{2\cos^3\psi}{\rho}\left(\frac{d^2\psi}{d\rho^2}\right) - \left[\frac{c_0\sin\psi}{\rho} + \frac{\sin^2\psi}{\rho^2} + \frac{\Delta p\rho}{2k\sin\psi}\right]\cos\psi\left(\frac{d\psi}{d\rho}\right) \\ & + \left[\frac{\Delta p}{k} + \frac{\lambda\sin\psi}{k\rho} + \frac{c_0^2\sin\psi}{2\rho} - \frac{\sin\psi(1+\cos^2\psi)}{2\rho^3}\right],\end{aligned} \quad (8)$$

and

$$\begin{aligned}\cos^3\psi\left(\frac{d^3\psi}{d\rho^3}\right) = {} & 4\sin\psi\cos^2\psi\left(\frac{d^2\psi}{d\rho^2}\right)\left(\frac{d\psi}{d\rho}\right) - \cos\psi\left(\sin^2\psi - \frac{1}{2}\cos^2\psi\right)\left(\frac{d\psi}{d\rho}\right)^3 \\ & + \frac{7\sin\psi\cos^2\psi}{2\rho}\left(\frac{d\psi}{d\rho}\right)^2 - \frac{2\cos^3\psi}{\rho}\left(\frac{d^2\psi}{d\rho^2}\right) + \left[\frac{c_0^2}{2} - \frac{2c_0\sin\psi}{\rho} + \frac{\lambda}{k} - \frac{\sin^2\psi - 2\cos^2\psi}{2\rho^2}\right]\cos\psi\left(\frac{d\psi}{d\rho}\right) \\ & + \left[\frac{\Delta p}{k} + \frac{\lambda\sin\psi}{k\rho} + \frac{c_0^2\sin\psi}{2\rho} - \frac{\sin^3\psi + 2\sin\psi\cos^2\psi}{2\rho^3}\right],\end{aligned} \quad (9)$$

respectively. We change the parameter s to ρ in Eq. (8) for the sake of comparison. Hu and Ou-Yang have shown that these three equations are degenerate for a spherical vesicle, while the DH equation is not identical to the SBL and the HO equations in case of a cylindrical vesicle, and that a Clifford torus is a solution for all the equations, but the constraints on Δp, λ, and c_0 are different [1].

Obviously, these three equations are different from each other in general. The difference is due to the different minimization procedure of the general action [Eq. (2)]. In case of the HO approach, they have utilized the general shape equation in Eq. (3). This equation describes the equilibrium shape of a vesicle. The HO equation can be obtained by only substituting the mean and the Gaussian curvatures of an axisymmetric vesicle. In this procedure, they first make minimization and then the specific parametrization of the shape. On the other hand, in the DH and the SBL approaches, they first make the parametrization of the shape and then minimization. This procedure leaves some free parameters which, in general, depend on a shape such as ρ_c for example. These free parameters are not correctly variated in DH nor in SBL Hamiltonians.

We have already shown that the HO shape equation has a rigorous analytical solution,

$$\psi = \arcsin[\rho(a\ln\rho + b)], \quad (10)$$

where a and b are constants determined by the shape equation and a vesicle size, respectively [8]. First, second, and third differentiation of ψ with respect to ρ are

$$\frac{d\psi}{d\rho} = \frac{1}{\cos\psi}\left(\frac{\sin\psi}{\rho} + a\right), \tag{11}$$

$$\frac{d^2\psi}{d\rho^2} = \frac{\sin\psi}{\cos^3\psi}\left(\frac{\sin\psi}{\rho} + a\right)^2 + \frac{a}{\rho\cos\psi}, \tag{12}$$

and

$$\frac{d^3\psi}{d\rho^3} = \left(\frac{3\sin^2\psi}{\cos^5\psi} + \frac{1}{\cos^3\psi}\right)\left(\frac{\sin\psi}{\rho} + a\right)^3 + \frac{3a\sin\psi}{\rho\cos^3\psi}\left(\frac{\sin\psi}{\rho} + a\right) - \frac{a}{\rho^2\cos\psi}, \tag{13}$$

respectively. With these three expressions, we can easily show that Eq. (10) is a rigorous solution for the HO shape equation under the condition

$$\begin{aligned} a &= c_0, \\ \Delta p &= \lambda = 0, \end{aligned} \tag{14}$$

as reported in Ref. [8]. We introduce a new parameter

$$\rho_B = \exp[-b/a]. \tag{15}$$

This modifies Eq. (10) to

$$\psi = \arcsin[a\rho\ln(\rho/\rho_B)]. \tag{16}$$

For $c_o < 0$, the solution represents a circular biconcave discoid, the shape of the RBC, as illustrated in Fig. 1 [8]. A more detailed analysis [9] gives the expression for the outward normal vector on the vesicle surface defined by Eq. (16), which is

$$\mathbf{n} = (-\sin\psi(\rho)\cos\phi, -\sin\psi(\rho)\sin\phi, \cos\psi(\rho)), \tag{17}$$

where ϕ is the rotational angle ($0 \leq \phi \leq 2\pi$). It is obvious from the property of Eq. (16) that the normal vector, Eq. (17), is analytically and uniquely defined everywhere on the vesicle surface. In the geometry, such a surface is called a smooth surface. Therefore, this solution can be utilized for examining whether the three shape equations give the same shapes having smooth surfaces [7], and thereby for giving a good counterexample to the DH and the SBL equations. It is easy to show whether the DH and the SBL equations have the same solution as the HO equation. Substituting Eqs. (11)–(13) and (16) into Eqs. (7) and (8), we can rewrite Eqs. (7) and (8) as

$$\frac{\Delta p}{2k}\,\rho - \frac{2a}{\rho} + a^2(a - c_0)\rho[\ln(\rho/\rho_B)]^2 + a\left(\frac{\lambda}{k} + \frac{1}{2}\,c_0^2 - \frac{1}{2}\,a^2\right)\rho\ln(\rho/\rho_B) = 0 \tag{18}$$

and

$$\frac{\Delta p}{2k} + \frac{2a}{\rho^2} + a^2(a - c_0)[\ln(\rho/\rho_B)]^2 + a\left(\frac{\lambda}{k} + \frac{1}{2}\,(a - c_0)^2\right)\ln(\rho/\rho_B) + \left(\frac{2a}{\rho^2} - \frac{\Delta p}{2k}\right)[\ln(\rho/\rho_B)]^{-1} = 0, \tag{19}$$

respectively. These two equations are satisfied when

$$\begin{aligned} a &= c_0 = 0, \\ \Delta p &= \lambda = 0. \end{aligned} \tag{20}$$

It can be seen from the comparison of Eq. (14) and Eq. (20) that the rigorous solution, Eq. (10), can simultaneously satisfy the three shape equations only for $c_0 = 0$. Equation (10) is nothing but a perfect sphere when $c_0 = 0$; let $a = c_0 = 0$ and $b = 1/R_0$, then Eq. (10) becomes $\rho = R_0\sin\psi$, which represents a sphere with radius R_o. The present result confirms the previous prediction by Hu and Ou-Yang [1] that the three shape equations are degenerate for a spherical vesicle. Hence, we expect that the DH and the SBL shape equations can give approximate solutions to the HO equation only for a spherical vesicle with infinitesimal deformation. This has been verified in Ref. [6]; the numerical results for nearly spherical vesicles having ℓth-polygon symmetry (where ℓ=3, 5, and 7) calculated by Deuling and Helfrich [3] are in excellent agreement with the analytical results obtained from Eq. (3). However, for vesicles whose shapes are far from spheres, the DH and the SBL shape equations are not useful: a smooth surface, which describes the famous RBC shape, for instance, is a rigorous solution for the HO shape equation but not for the DH and the SBL equations. This is the most important conclusion drawn from the present counterexample. We therefore consider that the attempts to show the three shape equations predicting the same shapes are futile.

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