A series representation of the nonlinear equation for axisymmetrical fluid membrane shape

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Whatever the fluid lipid vesicle is modeled as the spontaneous-curvature, bilayer-coupling, or the area-difference elasticity, and no matter whether a pulling axial force applied at the vesicle poles or not, a universal shape equation presents when the shape has both axisymmetry and up-down symmetry. This equation is a second order nonlinear ordinary differential equation about the sine \(\sin\psi(r)\) of the angle \(\psi(r)\) between the tangent of the contour and the radial axis \(r\). However, analytically there is not a generally applicable method to solve it, while numerically the angle \(\psi(0)\) can not be obtained unless by tricky extrapolation for \(r = 0\) is a singular point of the equation.

We report an infinite series representation of the equation, in which the known solutions are some special cases, and a new family of shapes related to the membrane microtubule formation, in which \(\sin\psi(0)\) takes values from 0 to \(\pi/2\), is given.

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Vesicles are closed surfaces of amphiphilic molecules dissolved in water, which form flexible bilayer membranes in order to minimize contact between the hydrocarbon chains of the lipid and water \[1\]. Recently, the vesicle shapes have attracted wide interest from different communities such as physics \[2\,3\,4\], mathematics \[5\,6\], chemistry \[7\,8\], and biology \[9\,10\,11\]. The naive model was given by Canham \[9\], in which only the surface bending elasticity is considered. An important progress was the introduction of the spontaneous curvature into the Canham’s theory \[12\], and it was made by Helfrich with analogue to the spontaneous splay in the liquid crystal molecular layer. Since the membrane consists in two monolayers, if assuming that two layers depart from each other at a fixed distance \[13\,14\], a so-called bilayer-coupling model was explored \[15\,16\]. However, the individual monolayers can in fact expand elastically under tensile stress, the so-called area-difference elasticity model \[13\] was introduced and investigated \[14\,15\,2\]. The latter three models are more realistic than the naive one, and have been intensively studied in recent years. A surprising common property of these three models is that they give exactly the same shapes \[14\,15\,2\], while differing from each other in accounting for the shape transitions, such as budding and vesiculation transition, transition from prolate to oblates etc. \[14\,15\]. Furthermore, pulling or pushing the vesicle axially making it up-down and axis symmetrical, as it used in the experimental investigation of the tether formation \[19\,17\], does not complicate the form of the mathematical equation for the general axisymmetrical vesicle in the spontaneous curvature model without force included. But the meanings of parameters need to re-specify. Except some numerical approach using the powerful software Surface Evolver \[20\], usual numerical as well as analytical method is employed to solve the shape equation representing axisymmetrical vesicle. However, in analytical side \[21\,22\], there is not a general applicable method to study the equation. In numerical side, \(r = 0\) (cf. the following Eq.\(1\)) is a singular point of the equation, so the shape around the point cannot be obtained unless by tricky extrapolation \[16\]. In this paper, we are going to reveal a novel property of the equation: the equation has an equivalent series representation, in which the two above problems do not present anymore. As a meaningful demonstration, a new family of shape related to the tether formation will be given.

Since the detailed or key steps of the derivation of the same equation from different models is available in many papers, e.g. \[17\,23\,24\], we can start our further discussion from the equation itself with clearly specifying the physics meaning of each quantity in it. This may of course makes this paper more concise. And the equation we start from reads: \[23\]

\begin{align}
\cos^2\psi \frac{d^2\psi}{dr^2} - \frac{\sin(2\psi)}{4} \left(\frac{d\psi}{dr}\right)^2 + \frac{\cos^2\psi}{r} \frac{d\psi}{dr} - \frac{\sin(2\psi)}{2r^2} \frac{\delta pr}{2kcos\psi} - \frac{\sin\psi}{2cos\psi} \left(\frac{sin\psi}{r} - c_0\right)^2 - \frac{\lambda sin\psi}{r cos\psi} = \frac{C}{rcos\psi}. \tag{1}
\end{align}

The quantities in this equation need some explanations. For an axisymmetrical shape, we can choose the symmetrical axis to be the \(z\)-axis. The contour of the shape can be plotted in \(rz\) plane, with \(r\) being the radial coordinate denoting the distance from the symmetric \(z\) axis. Then the tangent angle \(\psi(r)\) of the contour is measured clockwise from \(r\) axis. Using \(s\) to denote the arclength along
This is a second order nonlinear ordinary differential equation (ODE) not belonging to any well-studied mathematical type. For our purpose to attack it, let us recall the Taylor series expansion of a function. As well-known, for any analytical function $f(r)$ defining in a closed interval $r \in [r_1, r_2]$, global Taylor expansion of $f(r)$ around a point $r_0$ is

$$f(r) = \sum_{k=0}^{\infty} \frac{f^{(k)}(r_0)(r-r_0)^k}{k!} + R_n(r-r_0)$$

where $R_n(r-r_0) = (r-r_0)^{(n+1)}f^{(n+1)}(\xi)$ with $r_1 < \xi < r_2$. Both the above series are exact and equivalent to each other. The first finite series is easy to serve the digit purpose, while the second infinite one is useful to obtain a closed expression once the general form is determined. To note that every axisymmetrical shape must intersect the equatorial plane at right angle $\psi = \pi/2$. This means that there exists a point $r_0$, such that $f(r_0) = 1$. At this point $r_0$, the two terms containing the second derivative in Eq.~(1) cancel. We have then value of its first derivative $f'(r_0)$ of $f(r)$ at point $r_0$ as

$$f'(r_0) = \pm \sqrt{1 + 2Cr_0 - 2c_0r_0 + c_0^2r_0^2 + 2\lambda r_0^2 + \delta pr_0^2}.$$  

(8)

Since $f(r) \leq f(r_0) = 1$, we have $f'(r_0) = \lim_{r \rightarrow r_0^-} f(r) - 1/(r - r_0) \geq 0$ if and only if $r_0$ is the maximum radius of vesicle. Since we treat $f(r)$ a single valued function of $r$ and $r_0$ is really the maximum radius of vesicle, only the positive $f'(r_0)$ is relevant. To note that the physically interesting vesicles are either free or axially forced, and there is no force or torque acting on the waist. It implies that the high rank derivatives of $f(r)$ at $r_0$ as $f^{(k)}(r_0), k = 2, 3...$ exist, and they can be obtained by the following method. Taking derivative with respect to variable $r$ in both side, Eq.~(1) becomes a third order differential equation. Putting $r = r_0$ and substituting the value $f(r_0) (= 1)$ and $f'(r_0)$ (given by Eq.~(8)) into the third order equation, the third order terms cancel, and we can obtain the value of its second derivative $f''(r_0)$. Similarly, taking derivative with respect to variable $r$ in both side of the third order derivative equation, we can obtain $f^{(3)}(r_0)$, and so forth, all its higher rank derivatives $f^{(k)}(r_0), k = 4, 5...$ can be determined. It is a remarkable result: the nonlinear ODE~(1) can be transformed into an infinite series with the recurrence relation between coefficients uniquely determined by the equation itself~[25]. In the mathematical point of view, all its solutions with physical significance are obtained.

In this paper, we only treat the simplest aspect of the solution without considering the congruence of the segments of shapes. Since the parameterization of the axisymmetrical surface is $\psi(r)$ rather than $\psi(s)$, from Eq.(1) $f(r)$ is a single value function of $r$ in interval
ψ(r) ∈ [0, π/2]. We can therefore expand f(r) in Taylor series directly. Conversely, once all Taylor coefficients \( f^{(k)}(r_0)/k! \), \( (k = 1, 2, 3, \ldots) \), are known, the function \( f(r) \) is determined from the relation (6). In principle, we can give such a series for each shape. As checks of our method, we like to give two examples. 1) Cylinder with arbitrary radius \( r = r_0 \). It is the case \( f(r_0) \equiv 1 \) provided all parameters \( k, \delta p, \lambda, c_0, C \) satisfying \( \delta p r_0^2 + 2C r_0^2 + k(c_0 r_0 - 1)^2 = 0 \) and \( C = 0 \). It is the result discussed previously [29,23]. 2) The Delaunay surfaces \( f(r) = ar + b/r \) \( (a, b \) are two constants). These constant mean curvature surfaces appear when \( \lambda = \delta p = C = 0 \). Now we have simply \( f^{(1)}(r_0) = \pm(c_0 - 1/r_0) \) at position \( r_0 \) satisfying \( f(r_0) = 1 \). We study the case with positive sign. We can easily find \( f^{(k)}(r_0) = (-1)^{(k+1)}k!(c_0 r_0 - 2)/(2r_0^k) \), \( (k = 2, 3, 4, \ldots) \). Then the solution can be exactly written as \( f(r) = ar + b/r \) with \( a = c_0/2, b = (r_0 - c_0 r_0^2)/2 \). It is the result discussed also previously [22]. One can verify this method using another analytical or numerical solution as exercises, and can easily find that they are some special cases of the infinite series with special relation between the parameters.

Now we wish to give new family of shapes. These shapes can be inferred from the works of three research groups in studying the meaning of the integral constant \( C \). First by Zheng and Liu [23], they noted that the constant \( C \) roughly meant that the constant pressure difference \( \delta p \) in Helfrich shape equation [23] was replaced by \( \delta p + 2kC/r^2 \). Since that the all Helfrich shapes with axisymmetry are smooth at the poles \( r = 0 \) [24,14], the constant \( C \) means a stress singularity at two poles. This singularity may lead to two horns at both poles. Secondly, Jülicher and Seifert claimed that the nonvanishing \( C \) connected to shapes with torus topology [30]. Thirdly, Podgornik, Svetina, and Žekš in [31] and Božič, Svetina, and Žekš in [17] showed that a point axial force can lead to such a constant \( C \). We have known that such a force can lead to microtubule formation of vesicle [17,14], and in real experiment a finite force is enough to produce such structure. However, the expected shapes with two horns at both poles as exerting finite force have not been obtained theoretically.

For our purpose, we treat a case in which the quantity in the square of Eq. (8) to form the square of a quantity with nonzero \( C \). For our purpose, we choose the simplest parameters as \( C = c_0, \delta p = 0, \lambda = -c^2/2, \) and the positive sign of \( f'(r_0) \). The first seven derivatives \( f^{(k)}(r_0) \), \( (k = 0, 1, 2, \ldots 6) \) are

\[
\begin{align*}
&\left\{1, \frac{1}{r_0}, \frac{2C}{r_0}, -\frac{4C}{r_0^2}, 2\left(35C + 4C^2 r_0\right), \frac{5r_0^3}{35}, -2C \left(1155 + 268C r_0 + 12C^2 r_0^2\right), \frac{35r_0^6}{8C \left(5040 + 1689C r_0 + 99C^2 r_0^2 + 32C^3 r_0^3\right)} \right\}.
\end{align*}
\]

Since the conformal invariance of the shape [14,26,17], the magnitude of \( C \) does not matter. We can therefore choose \( C = 1 \). Then the Taylor series Eq. (6) cannot give real and positive root of \( r_0 \) for equation \( f(0) = 0 \). It means that in this case the equation is not self-consistent. In contrast, it can give a unique and positive root for equation \( f(0) = 0 \) a positive constant. To note that \( \arcsin f(0) \) is the angle between the tangent of the contour at pole and the \( r \) axis. For a sequence of numbers of \( f(0) \) as

\[N = \{0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.972, 1\}, \]

we have form the equation \( f(0) = N \) a corresponding sequence of unique and (semi-)positive roots for \( r_0 \) as

\[
\begin{align*}
&\{0, 0.0095195, 0.0189412, 0.0282679, 0.0375022, 0.0466463, 0.0557024, 0.0646727, 0.0735589, 0.0823627, 0.0886836, 0.0910858\}. \tag{10}
\end{align*}
\]

Do not care the magnitude of these values. The energy of the vesicle depends on the shape due to the conformal invariance. For clearly specifying each shape, a conformal invariant, the so called relative volume \( v = V/(4\pi R^3/3) \) with \( R = \sqrt{A/4\pi} \) is usually used [4], where \( V \) and \( A \) are the volume and area of the vesicle respectively. The one-to-one corresponding relative volumes are:

\[
v = \{1, 0.999971, 0.999879, 0.999725, 0.999505, 0.999213, 0.998844, 0.998386, 0.997819, 0.997107, 0.996449, 0.996136\}. \tag{12}
\]

In FIG. 1, the two limit shapes, sphere (thick solid line) and the prolate with the sharpest horn (thin line), are plotted. Other shapes with the horns of angles \( \psi(0) \) satisfying \( 0 < \psi(0) < \pi/2 \) will occupy the domain between these two.

For studying the relation between the “external force” \( C \) and the relative volume, we define a dimensionless external force as \( C(z_0 - r_0) \) with \( z_0 \) being half of the length of the prolate, and rescale the relative volume as \( v' = 4.725(1 - v) \). We can find that both the dimensionless external force and the rescaled relative volume have nearly the same relationship to the zenith angle, as shown in FIG. 2. Results plotted in FIG.1 and FIG.2 clearly show that the zenith angle becomes sharper as the external force becomes larger, or equivalent, the less.
the relative volume, the sharper the horn.

FIG. 1. The two limit shapes: sphere (thick solid line) and the prolate with right angle horns on two poles (thin solid line). They have relative volumes 1 and 0.996 respectively. Only a quarter of the contour is plotted.

FIG. 2. The correlation between the axial force $C$ and the relative volume $v$. We plot the dimensionless force $C(z_0 - r_0)$ (solid line) with the $z_0$ being half of the length of the prolate and the rescaled relative volume $v' = 4.725(1 - v)$ (solid dots). The larger axial external force and the smaller relative volume, the sharper angle of the corn.

In summary, we have found that the second order nonlinear different equation for axisymmetrical fluid vesicle shapes with up-down symmetry has an equivalent Taylor series representation, in which the recurrence relation of Taylor coefficients are uniquely and completely determined be the equation. Using this representation, we can not only reproduce the known solutions, but also new ones. The new solutions discussed in this article give the shapes with horns at two poles. These horns can never form simultaneously if no axially external force exerted. So, our study directly answers a question whether the constant $C$ is related to the presence of the axially external force. This result is compatible with that obtained previously [31,17,30]. The obtained shapes are related to the formation of the membrane microtubule on the axially strained vesicles, and finite force is enough to lead to such structure. Results also show that the shapes with less relative volume is easier to form such microtubule.

Finally, we give two comments. First, even the Taylor series method is useful in obtaining and analyzing the solution to the equation, one should be careful to check the convergence of the series. In fact, we explore many cases with different parameter set of $\delta p, \lambda, c_0, C$, the convergence is sometime uncertain. Secondly, the presence of the constant $C$ may not be the sufficient condition to relate the axial force [17,26,19], especially in the torus topology situation [30].

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