Confining a fluid membrane vesicle of toroidal topology in an adhesive hard sphere

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Abstract. We discuss how the equilibrium shapes of a confined toroidal fluid membrane vesicle change when an adhesion between membrane and confining sphere is taken into account. The case without adhesion was studied in Ref. [1]. Different types of solution were found and assembled in a phase diagram as a function of area and reduced volume of the membrane. Depending on the degree of confinement the vesicle is either free, in contact along a circle (contact-circle solutions) or on a surface (contact-area solutions). All solutions without adhesion are up-down symmetric. When the container is adhesive, the phase diagram is altered and new kinds of solution without up-down symmetry are found. For increasing values of adhesion the region of contact-circle solutions shrinks until it vanishes completely from the phase diagram.

1. Introduction
Mitochondria are essential biological constituents which produce the chemical energy carriers of the cell. Their basic structure consists of two closed lipid membranes, one inside the other [2]. To model this system we consider a fluid membrane vesicle confined in a hard sphere. The case of a membrane of spherical topology has been studied by Kahraman et al. [3, 4]. These studies have shown that—under specific conditions—the topology of the membrane can change to a toroidal one. In nature, topology changes are frequent as well, particularly in mitochondria [5]. To shed some light on these processes, we consider confined fluid membranes of toroidal topology and their behaviour in equilibrium as a function of area, reduced volume and adhesion coefficient between the membrane and its confinement.

2. Model
Within the classical curvature model the simplest version of the bending energy of a fluid membrane is given by [6]

\[ E_b = \kappa \int dA 2H^2, \] (1)
where $\kappa$ is the bending rigidity, $H$ the mean curvature, and $dA$ the surface element. We fix the total area and volume of the membrane using the Lagrange multipliers $\sigma$, which corresponds to a surface tension, and $P$, which is the pressure difference between the inside and the outside of the vesicle.

If we suppose that the membrane is axisymmetric, we can use the angle arc-length parametrisation: the cross section of the membrane is given in terms of the tangent angle $\psi$ as a function of arc-length $s$. The whole surface can be obtained via a rotation about the azimuthal angle $\phi$. One portion of the membrane is in contact with the confining sphere. The scaled energy of the free part of the membrane writes

$$ E = \int ds \mathcal{L}, $$

where $\mathcal{L}$ is the scaled Lagrangian which equals

$$ \mathcal{L} = \rho \left( \dot{\psi} + \frac{\sin \psi}{\rho} \right)^2 + 2\sigma \rho + P \rho^2 \sin \psi + P_\rho (\dot{\rho} - \cos \psi) + P_z (\dot{z} - \sin \psi). $$

All variables are scaled with respect to the corresponding quantities of the spherical container. The conjugate momenta $P_i$ follow from

$$ P_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}. $$

The symbols $\rho$ and $z$ denote the radius and height of the membrane in cylindrical coordinates.

With the help of Hamilton's formalism the shape equations can be written as a system of coupled non-linear differential equations

$$ \dot{\psi} = \frac{P_\psi}{2\rho} - \frac{\sin \psi}{\rho}, $$

$$ \dot{P}_\psi = \left( \frac{P_\psi}{\rho} + P \rho^2 - P_z \right) \cos \psi + P_\rho \sin \psi, $$

$$ \dot{P}_\rho = \frac{P_\rho}{\rho} \left( \frac{P_\psi}{4\rho} - \frac{\sin \psi}{\rho} \right) + 2\sigma + 2P \rho \sin \psi, $$

$$ \dot{P}_z = 0, $$

to which the geometrical relations

$$ \dot{\rho} = \cos \psi, $$

$$ \dot{z} = \sin \psi $$

have to be added. This system can be solved with a standard shooting method using a forth-order Runge-Kutta algorithm. Equilibrium solutions in partial contact with the container (contact-area solutions) have to fulfill the boundary conditions at the contact lines between the free and the confined part of the membrane [7]

$$ \psi_0 = \psi_c, $$

$$ K_{\perp 0} = 1 + \sqrt{\frac{2\omega}{\kappa}}. $$

Eq. (10) states that the tangent to the membrane at the contact line, $\psi_0$, has to equal the container tangent $\psi_c$. Eq. (11) imposes a relation between the curvature $K_{\perp 0}$ of the membrane

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1 The details of the method can be found in appendix A of Ref. [1].

2 Similar conditions hold for the free and contact-circle solutions (see again Ref. [1]).
that is perpendicular to the contact line, the curvature of the confining sphere, and the adhesion coefficient $\omega$.

The axisymmetry of these solutions can be broken using conformal transformations as in Ref. [8]. These transformations conserve the curvature energy but change the area and the volume of the membrane. Since the membrane is confined in a hard sphere, the transformed solution must fulfill the boundary conditions (10) and (11). In Ref. [1] we have shown that—for the case without adhesion—this restriction reduces the possible transformations to a subgroup defined by the constant parameter $\vec{\Lambda}$

$$\vec{r}' = \frac{\vec{r}}{(\vec{r}^2 + \vec{\Lambda})^2} \left(1 - \Lambda^2\right) + \vec{\Lambda},$$

(12)

where $\vec{r}'$ is the transformed shape of the original surface $\vec{r}$. To break axisymmetry $\vec{\Lambda}$ has to have a component perpendicular to the symmetry axis. $\vec{\Lambda} = 0$ yields the identity transformation. When $\Lambda = |\vec{\Lambda}|$ tends to 1, the surface becomes a sphere with a hole of infinitesimal diameter at the edge.

The total force on these transformed shapes due to the confining sphere does not necessarily vanish. With the help of finite element simulations we were, however, able to confirm that the shapes approximate the non-axisymmetric solutions remarkably well [1].

3. Results

The complete phase diagram for the case without adhesion can be found in Ref. [1]. Figure 1 shows, for example, shapes that a toroidal vesicle of fixed reduced volume adopts for increasing area. When the area of the membrane equals the container area ($a = 1$), the vesicle is sickle-shaped and does not touch the confinement. In this phase without contact, we exactly retrieve the behaviour of a free toroidal vesicle [8]. When we increase the area, the membrane touches the sphere along a circular contact line (contact-circle solutions). The confinement induces a discontinuity in the derivative of the curvature perpendicular to the contact line which is proportional to the radial contact force. An increase in area will increase this force whereas the curvature at the contact line decreases until it reaches the container curvature. Above this limit the contact line extends to a zone of contact ($a > 1.23$ for $v_r = 0.6$). Subsequently, the vesicle breaks axisymmetry (see the profile with $a = 1.26$ in figure 1 for an example). For very large values of the area shapes with self-contact appear.

To determine the axisymmetric equilibrium shapes of confined adhesive membrane vesicles one has to solve the same shape equations as in the case without adhesion. The only difference

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3 The simulation program also allowed us to distinguish between energy minima and maxima.

4 A similar transition from free to contact-circle to contact-area solutions is found at smaller areas for circular tori.
Figure 2. Equilibrium profiles of a membrane with adhesion ($\omega = 1$) for fixed reduced volume $v_r = 0.6$ and increasing area. Colors indicate the density of the bending energy.

Lies in one of the boundary conditions, Eq. (11), which implies that the curvature at the contact line is discontinuous due to the adhesion. With adhesion one finds regions of solutions that are not up-down symmetric with respect to the midplane. For example, for the reduced volume $v_r = 0.6$ and small area $a$, the transition from free shapes to confined ones can either be accomplished via symmetric circular tori (similar to the case with no adhesion, see the first two profiles of figure 1), or via shapes that are less symmetric (see figure 2). This is due to Eq. (11): when the adhesion coefficient $w$ is large, the curvature of the membrane at the contact line has to be large. The sickle-shaped profiles have a greater perpendicular curvature far from the midplane. With adhesion they will attach to the confining sphere along a circular contact line which does not lie in the midplane (see the profile with $a = 0.75$ in figure 2). When we increase the area, the contact zone increases because of the negative adhesion energy (see the profiles with $a = 0.9$ and $a = 1.2$ in figure 2) until the symmetry with respect to the midplane is recovered.

A closer look at the transition from contact-circle to contact-area solutions reveals that an increasing adhesion induces a shift of this transition towards smaller areas (see curves $C_1^\omega$ in figure 3 for the circular tori). Fixing the reduced volume to $v_r = 0.6$ again, one finds contact-area solutions for $a > 0.85$ when $\omega = 0$. For $\omega = 2$ the transition point shifts to $a = 0.73$. When the adhesion is large one does not find any contact-circle solutions but a discontinuous transition from free to contact-area solutions ($\omega > 6.6$ for $v_r = 0.6$).

4. Conclusion
In this work we have studied toroidal vesicles in an adhesive spherical container using the classical curvature model. We only had a first glance at the rich solution space by focusing on shapes with axisymmetry. A more detailed study would not only have to include non-axisymmetric shapes but also consider questions of stability. Finite element simulations—similar to those made for the case without adhesion—could help to accomplish this task.

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Figure 3. Partial phase diagram showing the axisymmetric extrema together with the conformal transformations of the free vesicles for the case without adhesion (adapted from figure 4 of Ref. [1]). Regions of circular tori are colored in orange-red, regions of sickle-shaped tori are in green. Non-axisymmetric regions are hatched. The shades represent the different degrees of confinement: light shading corresponds to free solutions, medium shading corresponds to contact-circle solutions, and dark shades to contact-area solutions. The curve $C_0^1$ separates the regions of contact-circle and contact-area solutions when there is no adhesion between membrane and container. The dashed curves $C_0^{1'}$ indicate how this boundary shifts to the left when adhesion is switched on. All other line styles correspond to those of Ref. [1].