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LETTER TO THE EDITOR

Conformal transformations of vesicle shapes

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Abstract. Conformal transformations are used to derive an exact geometrical relation for equilibrium vesicle shapes within the spontaneous curvature and bilayer coupling models. Stability criteria with respect to these transformations efficiently detect instabilities related to the breaking of reflection symmetry.

Vesicles are closed surfaces of lipid bilayers, which form already in simple binary systems of one lipid species plus water [1]. Studies by video microscopy reveal an amazing variety of shapes, between which transformations can be induced, e.g., by changing the temperature or the osmotic conditions [2-4].

Such experiments confirm the basic theoretical idea that the bending elasticity of the bilayer together with constraints on area A and enclosed volume V determine the vesicle shape [5]. If the vesicle is described as a two-dimensional surface embedded in three-dimensional space, the bending elastic energy can be expressed in terms of the curvature of this surface. Two models have been investigated in some detail. (i) In the *spontaneous curvature model* [5, 6], the bending energy is given by

$$F \equiv (\kappa/2) \oint dA (2H - C_0)^2 \quad (1)$$

where the H is the mean curvature and C_0 is the spontaneous curvature. The bending rigidity κ sets the energy scale. (ii) In the *bilayer coupling model* [7, 8], the area difference ΔA between the two monolayers is taken to be fixed, which leads to a constraint on the total mean curvature M ,

$$M \equiv \oint dA H \quad (2)$$

since $\Delta A \approx 2MD$, where D is the distance between the two monolayers. The bending energy G for this model is given by the scale-invariant part of (1),

$$G \equiv (\kappa/2) \oint dA (2H)^2. \quad (3)$$

The two models are related by a Legendre transformation. The phase diagram is determined by the 'ground state' shape S , whose energy E is given by $E \equiv \min_{|A, V, C_0} F$ or $E \equiv \min_{|A, V, M} G$, respectively.

So far, only axisymmetric stationary shapes have been obtained explicitly by solving the corresponding Euler-Lagrange equations (ELEs) for moderate values of the spontaneous curvature or the corresponding area difference. A systematic study of the (axisymmetric) phase diagram in this region, where the shapes of lowest energy are given by the four branches of oblate/discocyte, prolate/dumb-bell, stomatocyte and pear-shaped vesicles, has recently been performed for both models [9]. A comparison with experiment reached good agreement for the bilayer coupling model [4].

Open theoretical problems concern (i) a stability analysis for these shapes as outlined in [10], which has not been performed in general so far; (ii) an explicit determination of the non-axisymmetric shapes which are known to bridge a gap between the prolate and the oblate branch in the bilayer coupling model [9]. Perturbative calculations indicate that these shapes reduce in the spherical limit to ellipsoids with three different axes [11]. (iii) For large spontaneous curvature, the determination of the ground state has been investigated so far only for moderate values of the volume-to-area ratio [12]. For small volume-to-area ratio even the solution of the axisymmetric ELEs is difficult, since the shapes consist of different segments connected by narrow necks. Direct minimization procedures which require reasonable initial shapes may be more adequate there.

In this letter, we investigate the consequences of the following mathematical theorem, recently recalled by Duplantier *et al* [13]: *The bending energy (3) (or (1) for $C_0 = 0$) is conformally invariant* [14]. Thus, conformal mappings of three-dimensional space, which constitute the group of translations, rotations, dilations and *inversions in the sphere* (i.e. $\mathbf{R} \rightarrow \mathbf{R}' = \mathbf{R}/R^2$, if the inversion centre is at the origin), transform any vesicle shape into a new shape of the same bending energy G but, in general, different area, volume and area difference. Therefore, the constraints and the spontaneous curvature break this symmetry and continuous conformal deformations do not exist, in general [13].

We shall show below that, taking the constraints properly into account, one obtains nevertheless

(i) a surprising geometrical relation which any stationary shape, including, in particular, the ground state, must obey and

(ii) stability criteria with respect to conformal transformations, which are easy to check and remarkably effective in locating two already known instabilities. These criteria can, therefore, be expected to become a valuable tool for the stability analysis of non-axisymmetric shapes.

The geometrical relation, derived below for any stationary shape, takes the form of a 'lever rule',

$$3(\partial E/\partial V)V(\mathbf{R}^A - \mathbf{R}^V) = 2\kappa C_0 M(\mathbf{R}^M - \mathbf{R}^A) \quad (4)$$

for the centres of volume (mass) \mathbf{R}^V , of area \mathbf{R}^A , and of mean curvature \mathbf{R}^M , defined as

$$\mathbf{R}^V \equiv \left(\int dV \mathbf{R} \right) V^{-1} \quad \mathbf{R}^A \equiv \left(\oint dA \mathbf{R} \right) A^{-1} \quad \mathbf{R}^M \equiv \left(\oint dA H \mathbf{R} \right) M^{-1} \quad (5)$$

respectively, where $\mathbf{R} = \mathbf{R}(s_1, s_2)$ parametrizes the vesicle shape as a function of the internal coordinates s_1 and s_2 . The relation (4) holds in both models, where $C_0 \equiv (\partial E/\partial M)/(2\kappa)$ in the bilayer coupling model. This derivative and $(\partial E/\partial V)$ are taken along the branch of stationary shapes under consideration. Note that $(\partial E/\partial V) = -P$,

where P denotes the Lagrange multiplier for the volume and is, thus, known from the numerical analysis.

This exact result implies, in particular, that the three centres R^V , R^A and R^M are collinear unless C_0 and $(\partial E/\partial V)$ both vanish†. For the axisymmetric shapes with a reflection plane, such as the prolate/dumb-bell and oblate/discocyte branches, as well as for non-axisymmetric shapes with three reflection planes, the lever rule holds by symmetry. However, for stomatocytes and pear-shaped vesicles, the lever rule is a non-trivial property. For example, at $C_0 = 0$, the centre of area and the centre of volume coincide for the stomatocytes.

For those parts of the phase diagrams where shapes with many necks dominate, shapes which are 'too' asymmetric can be excluded as trial ground states or initial shapes for direct minimization procedures whenever they violate collinearity, which is easy to check.

Both, the lever rule and the stability criteria can be derived by comparing the energy along a stationary branch of shapes with the energy of the shapes obtained therefrom by special conformal transformations (SCTs), as follows. An SCT is given by combining an inversion with a translation about the vector \mathbf{a} and a second inversion. This SCT maps \mathbf{R} to $\mathbf{R}' = (\mathbf{R}/R^2 + \mathbf{a})/(\mathbf{R}/R^2 + \mathbf{a})^2$. For small \mathbf{a} , the SCT becomes infinitesimal with $\mathbf{R}' = \mathbf{R} + R^2\mathbf{a} - 2(\mathbf{a} \cdot \mathbf{R})\mathbf{R} + (4(\mathbf{a} \cdot \mathbf{R})^2 - a^2R^2)\mathbf{R} - 2R^2(\mathbf{a} \cdot \mathbf{R})\mathbf{a} + O(a^3)$. (6)

The area element $dA \equiv (\det(\partial_i \mathbf{R} \cdot \partial_j \mathbf{R}))^{1/2}$, where $(i, j) \in (s_1, s_2)$, transforms under (6) as $dA' = dA(\mathbf{R}/R + \mathbf{a}\mathbf{R})^{-4}$. Expanding in \mathbf{a} and integrating over the surface, one obtains the transformed area,

$$A' = A[1 - 4\mathbf{a} \cdot \mathbf{R}^A - 2a^2(R^A)^2 + 12(\mathbf{a} \cdot \mathbf{R}^A)^2] - 2a^2 \oint dA(u^A)^2 + 12 \oint dA(\mathbf{a} \cdot \mathbf{u}^A)^2 + O(a^3) \tag{7}$$

with $\mathbf{u}^A \equiv \mathbf{R} - \mathbf{R}^A$. It is convenient to apply a spatial rescaling $\mathbf{R}'' \equiv \lambda \mathbf{R}'$, with $\lambda \equiv (A'/A)^{-1/2}$, in order to restore the original area, i.e. $A'' \equiv \lambda^2 A' = A$.

Likewise, one obtains for the transformation of the volume element, $dV' = dV(\mathbf{R}/R + \mathbf{a}\mathbf{R})^{-6}$, which leads after integration and rescaling to

$$V'' \equiv \lambda^3 V' = \lambda^3 \int dV' = V(1 + 6\mathbf{a} \cdot (\mathbf{R}^A - \mathbf{R}^V) + \mathbf{a}\mathcal{B}^V\mathbf{a}) + O(a^3). \tag{8}$$

Here, the matrix \mathcal{B}^V has elements $\mathcal{B}_{\alpha\beta}^V$ with

$$\mathcal{B}_{\alpha\beta}^V \equiv 3 \left\{ \delta_{\alpha\beta} \left[(R^A)^2 - (R^V)^2 + (1/A) \oint dA(u^A)^2 - (1/V) \int dV(u^V)^2 \right] + 8R_\alpha^V R_\beta^V + 4R_\alpha^A R_\beta^A - 12R_\alpha^A R_\beta^V - (6/A) \oint dA u_\alpha^A u_\beta^A + (8/V) \int dV u_\alpha^V u_\beta^V \right\} \tag{9}$$

with $\mathbf{u}^V \equiv \mathbf{R} - \mathbf{R}^V$. For axisymmetric shapes with a reflection plane, $\mathbf{R}^A = \mathbf{R}^V$, and these expressions reduce to the simple integrals,

$$\mathcal{B}_{zz}^V = (12\pi/A) \int_0^{s^*} ds(r^3 - 5rz^2) + (4\pi/V) \int_0^{s^*} ds(7rz^3 - 3r^3z) \cos \psi \tag{10}$$

† This interesting case can occur for vesicles of toroidal topology [15].

and

$$\mathcal{B}_{xx}^V = \mathcal{B}_{yy}^V = (12\pi/A) \int_0^{s^*} ds (rz^2 - 2r^3) + (4\pi/V) \int_0^{s^*} ds (9r^3z - rz^3) \cos \psi \quad (11)$$

while the non-diagonal elements vanish. Here, $z(s)$ and $r(s)$ denote the distance of the contour from the mirror plane and axis of symmetry, respectively. The arc length s is measured from the north pole at $s=0$ to the mirror plane at $s=s^*$ while $\psi(s)$ is the tilt angle, i.e. $dr/ds = \cos \psi$.

The transformation of the total mean curvature M is also required. With the definition $H \equiv -(1/2)g^{ij}(\partial_i \partial_j \mathbf{R}) \cdot \mathbf{n}$, where $g^{ij} = (g_{ij})^{-1}$ and $\mathbf{n} \equiv (\partial_i \mathbf{R} \times \partial_j \mathbf{R}) / |\partial_i \mathbf{R} \times \partial_j \mathbf{R}|$ is the unit normal vector, one obtains with (6)

$$H' = H + 2\mathbf{a} \cdot (\mathbf{H}\mathbf{R} - \mathbf{n}) + a^2 R^2 H - 2a^2 (\mathbf{R} \cdot \mathbf{n}). \quad (12)$$

This leads after integration and rescaling to the transformed total mean curvature,

$$M'' \equiv \lambda M' = \lambda \oint dA' H' = M[1 + 2\mathbf{a} \cdot (\mathbf{R}^A - \mathbf{R}^M) + \mathbf{a} \mathcal{B}^M \mathbf{a}] + O(a^3). \quad (13)$$

Here, the matrix elements of \mathcal{B}^M are given by

$$\begin{aligned} \mathcal{B}_{\alpha\beta}^M &\equiv \delta_{\alpha\beta} [(R^A)^2 - (R^M)^2 - 6V/M] + 4(R_\alpha^M R_\beta^M - R_\alpha^M R_\beta^A) \\ &+ (1/M) \oint dA [8u_\alpha^M n_\beta + 4Hu_\alpha^M u_\beta^M - \delta_{\alpha\beta} H(u^M)^2] \\ &+ (1/A) \oint dA [\delta_{\alpha\beta} (u^A)^2 - 6u_\alpha^A u_\beta^A] \end{aligned} \quad (14)$$

with $\mathbf{u}^M \equiv \mathbf{R} - \mathbf{R}^M$. For axisymmetric shapes with a reflection plane, these expressions reduce again to simple integrals over the contour.

Stability criteria for local equilibrium shapes can now be derived using the relations (8) and (13). First, consider the spontaneous curvature model and choose a stationary shape S with energy E , volume V and total mean curvature M . Apply an SCT parametrized by \mathbf{a} and, subsequently, a spatial rescaling to this shape. The transformed shape S'' has an energy

$$F(\mathbf{a}) = E - 2\kappa C_0 (M''(\mathbf{a}) - M) \quad (15)$$

and a volume $V''(\mathbf{a})$, as given by (8). The energy of this conformally transformed shape has to be compared with the energy $E(V''(\mathbf{a}))$ of the neighbouring stationary shape with volume $V''(\mathbf{a})$. This energy can be expanded as

$$\begin{aligned} E(V''(\mathbf{a})) &= E + (\partial E / \partial V) \left[\sum_\alpha a_\alpha (\partial V'' / \partial a_\alpha) + (1/2) \sum_{\alpha\beta} a_\alpha a_\beta (\partial^2 V'' / \partial a_\alpha \partial a_\beta) \right] \\ &+ (1/2) (\partial^2 E / \partial V^2) \left[\sum_\alpha a_\alpha (\partial V'' / \partial a_\alpha) \right]^2 + O(a^3). \end{aligned} \quad (16)$$

In order for S to be locally stable with respect to SCTs,

$$E(V''(\mathbf{a})) \leq F(\mathbf{a}) \quad (17)$$

must hold for small \mathbf{a} . This condition leads to $O(\mathbf{a})$ and using (8), (13), (15) and (16) to the lever rule (4), since the linear terms in (17) must coincide.

For the derivation of this lever rule it is sufficient to assume that S is a stationary shape, since only the linear terms in \mathbf{a} enter so far. Note that a relation of the type $(\partial E/\partial V)(\partial V/\partial \varepsilon)|_{\varepsilon=0} = -2\kappa C_0(\partial M/\partial \varepsilon)|_{\varepsilon=0}$ can be derived for *any* area preserving transformation parametrized by a small parameter ε . The significance of the SCT lies in the fact that $(\partial M/\partial \mathbf{a})$ and $(\partial V/\partial \mathbf{a})$ can be expressed by the quantities \mathbf{R}^A , \mathbf{R}^V and \mathbf{R}^M , which have a nice geometrical interpretation.

The stability criterion is obtained from the second-order terms in (17). Inserting (13) into (15) and (8) into (16) leads for (17) at $O(\mathbf{a})^2$ to the relation,

$$-[(\partial E/\partial V)V\mathcal{B}^V + 18(\partial^2 E/\partial V^2)V^2\mathcal{P}^V + 2\kappa C_0 M\mathcal{B}^M] \geq 0 \quad (18)$$

where \mathcal{P}^V is the projector onto $\mathbf{R}^V - \mathbf{R}^A$, i.e. $\mathcal{P}_{\alpha\beta}^V \equiv (R_\alpha^V - R_\alpha^A)(R_\beta^V - R_\beta^A)$. The \geq sign means positive when applied to $\mathbf{a} \neq 0$.

The stability criterion for the bilayer coupling model can be derived quite similarly. In this case, the shape $S''(\mathbf{a})$ obtained from a stationary shape S by a SCT and rescaling has the same energy, $G(\mathbf{a}) = E$, since G as given by (3) is conformally invariant. This energy has to be compared with the energy $E(V''(\mathbf{a}), M''(\mathbf{a}))$ of the neighbouring stationary shape with the corresponding volume $V''(\mathbf{a})$ and mean curvature $M''(\mathbf{a})$. The stability criterion for S now reads $E(V''(\mathbf{a}), M''(\mathbf{a})) \leq E$ for small \mathbf{a} . Expanding as in (16) and taking the dependence on $M''(\mathbf{a})$ into account, one obtains, again, from the first-order term in \mathbf{a} the lever rule (4). The second-order terms yield

$$-[(\partial E/\partial V)V\mathcal{B}^V + 18(\partial^2 E/\partial V^2)V^2\mathcal{P}^V + 2\kappa C_0 M\mathcal{B}^M + 16\kappa(\partial C_0/\partial M)M^2\mathcal{P}^M] \geq 0 \quad (19)$$

where \mathcal{P}^M is the projector onto $\mathbf{R}^M - \mathbf{R}^A$, i.e. $\mathcal{P}_{\alpha\beta}^M \equiv (R_\alpha^M - R_\alpha^A)(R_\beta^M - R_\beta^A)$. In general, the stability criteria differ in the two ensembles; but, they become identical for axisymmetric shapes with a reflection plane, since $\mathcal{P}^V = \mathcal{P}^M = 0$ in this case.

These stability criteria determine whether a shape is locally stable with respect to SCTs, which are, of course, only a subset of all deformations. Therefore, the validity of (18) or (19) as in general a necessary but not sufficient condition for local stability. The violation of (18) or (19) indicates that a shape is unstable; however, the breakdown of these criteria will not locate the precise value of the instabilities, since the conformal deformation (6) will not be an eigenvector of the second variation of the curvature energy.

As an illustrative example, consider the oblate/discocyte shapes. From the analysis of the ELEs, one knows that this branch becomes unstable with respect to a mode which breaks the reflection symmetry but preserves the axisymmetry for $v < v^{\text{ELE}}(c_0)$ [9]. Here, $v \equiv V/[4\pi(A/4\pi)^{3/2}/3] \leq 1$ is the reduced volume and $c_0 \equiv C_0(A/4\pi)^{1/2}$ is the scaled spontaneous curvature. An SCT with \mathbf{a} parallel to the axis of symmetry applied to the oblate/discocyte branch preserves also the axisymmetry. The stability criterion (18) is found numerically to be violated for $v < v^{\text{SCT}}(c_0)$, which thus determines the instability of this branch with respect to the SCT. The surprising fact is that the 'true' instability as given by v^{ELE} and the conformal instability as given by v^{SCT} are very close together. In fact, $v^{\text{ELE}} - v^{\text{SCT}} < 10^{-2}$, for the range $-2 < c_0 < 1$. The same bound holds for the instability of the prolate/dumb-bell branch with respect to the pear-shaped vesicles for $c_0 < 4$. These results indicate that the mode which breaks the reflection symmetry is nearly given by the conformal transformation (6). Since it is far easier to check the stability criteria (18) for axisymmetric shapes with a reflection plane than it is to search for shapes lacking this symmetry without knowing where they are,

these findings may have a practical significance for the determination of reflection-symmetry-breaking instabilities in the low volume-to-area range for large spontaneous curvature.

It might appear even more interesting to choose \mathbf{a} perpendicular to the axis of symmetry, which leads to non-axisymmetric shapes. Numerical testing of the stability criteria in this case shows that both the prolate/dumb-bell and the oblate/discocyte branch are stable with respect to these SCTs. On the other hand, it is known that in the spherical limit the prolate (the oblate) branch is unstable for $c_0 < -1.2$ ($c_0 > -1.2$) [11]. The instability drives the prolate (oblate) shape into the oblate (prolate) shape through ellipsoids with three different axis. The unstable mode, thus, preserves *three* reflection planes. The SCT with \mathbf{a} perpendicular to the axis of symmetry, applied to an oblate or prolate, however, preserves only *two* reflection planes and is antisymmetric with respect to a plane perpendicular to \mathbf{a} . Therefore, this SCT is *orthogonal* on the unstable mode, and the instability cannot show up in a violation of (18).

The SCT, thus, will only (if ever) be efficient in detecting a new instability, if the unstable mode has the same symmetry as the SCT. Promising candidates are the non-axisymmetric ellipsoids with *three reflection planes mentioned above*, which bridge the gap in the phase diagram of the bilayer coupling model. If these shapes become unstable, e.g. with decreasing volume, it will be generically through a mode which breaks one reflection plane. Such a mode would have the same symmetry as an SCT applied to these shapes with \mathbf{a} perpendicular to one of the reflection planes. One might, then, expect that the stability criteria developed here give a reasonable value for this instability. So far, this consideration is speculative, since its verification would first require the explicit calculation of these non-axisymmetric shapes, which is far from trivial.

In summary, we have exploited a conformal symmetry in order to derive an exact geometrical property of the ground state and to discuss necessary stability criteria for local minima.

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