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Stress and geometry of lipid vesicles

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Abstract

We consider lipid fluid vesicles described by the Helfrich Hamiltonian. We develop a geometrically covariant approach to derive the appropriate equilibrium conditions for these objects. This also allows us to derive general expressions for the stresses and torques acting within the vesicle. The appropriate generalization to models for inhomogeneous lipid vesicles is briefly described.

In water, lipid molecules assemble spontaneously into vesicles which are described remarkably well at mesoscopic scales by a purely geometrical Hamiltonian. On such scales there is a difference of several orders of magnitude between the thickness and the size of the vesicle. This makes it sensible to describe it as an idealized two-dimensional surface. Moreover, the vesicle acts like a two-dimensional fluid as there is no cost in energy associated with tangential displacements of the lipid constituents. Geometrically, tangential displacements can be identified with a reparametrization of the surface. Therefore, the appropriate effective Hamiltonian must be an invariant under reparametrizations. The Hamiltonian describing the penalty associated with the bending of the vesicle is quadratic in the mean extrinsic curvature [1–3]. In addition, there are global constraints on the vesicle shape. The total area is fixed and, on time scales relevant to experiment, the enclosed volume is also. In a first approximation, the particular architecture of the lipid bilayer that forms the vesicle, and in particular the asymmetry between the layers, is described by a constraint on the total mean extrinsic curvature of the surface, which captures the constancy of the area difference between the two layers. For the sake of simplicity we will restrict our attention to a minimal geometric model for fluid vesicles which is known as the strict bilayer couple model, or Helfrich Hamiltonian [2, 4]. A more realistic geometric model, the area-difference model, takes into account more precisely the bilayer architecture [5, 6]. In any case, the two are related by a Legendre transformation, so that our considerations extend to the latter model as well (for a review see [7]).

The model is defined by the Hamiltonian

$$F[\mathbf{X}] = \alpha F_b + \overline{\alpha} F_{\mathrm{G}} + \beta M + \mu A. \tag{1}$$

The variables are the shape functions $\mathbf{X}$ that describe the surface. The first term is proportional to the bending energy quadratic in the mean extrinsic curvature K, $F_b := \int \mathrm{d}A\, K^2$, where the constant α is the bending rigidity. The second term is proportional to the Gaussian bending energy $F_{\mathrm{G}} := \int \mathrm{d}A\, \mathcal{R}$, with $\overline{\alpha}$ the Gaussian bending rigidity, and $\mathcal{R}$ the intrinsic scalar curvature, or twice the Gaussian curvature of the surface. If the surface has no boundary, by the Gauss–Bonnet theorem, the Gaussian bending energy is a topological invariant $F_{\mathrm{G}} = 8\pi(1-g)$, where g is the genus of the surface. As such it does not contribute to the determination of the equilibrium configurations of the membrane. A denotes the area. $M = \int \mathrm{d}A\, K$ is the total mean extrinsic curvature. μ, β are the Lagrange multipliers that enforce the constraints of constant area and total mean extrinsic curvature (constant area difference) respectively. In order to account for the constant volume constraint, we subtract from the Hamiltonian (1) the term PV, where P is a Lagrange multiplier and V the enclosed volume.

For the determination of the equilibrium shapes of the vesicle, one needs to extremize the Hamiltonian (1). One approach is to consider a Monge parameterization of the surface in terms of a height function, which is appropriate when considering small deformations from a specified reference surface. An alternative simplification is to specialize to axisymmetric configurations, with an emphasis on the principal curvatures of the surface. However, although certainly convenient in specific applications, the use of special parametrizations leads to unnecessary complications when considering the purely geometrical problem of the variation of the Hamiltonian (1) under an infinitesimal deformation of the surface. A treatment that is explicitly covariant with respect to surface parametrization is preferable [8–11]. The price one pays is the introduction of a little mathematical formalism. But, as we hope to illustrate below, this price is well worth paying.

We consider an infinitesimal deformation of the shape functions $\mathbf{X}(\xi^a)$ that describe the surface ($\xi^a = \{\xi^1, \xi^2\}$ are arbitrary coordinates on the surface) of the form $\mathbf{X}(\xi^a) \to \mathbf{X}(\xi^a) + \epsilon \mathbf{W}(\xi^a)$, with $\mathbf{W}$ an arbitrary vector field, and the constant ϵ an infinitesimal parameter. This shape deformation induces, at first order, a variation of the Hamiltonian of the form

$$F_{(1)}[\mathbf{X}, \mathbf{W}] = \epsilon \int \mathrm{d}A\, [\mathbf{E} \cdot \mathbf{W} + \nabla_a \mathcal{Q}^a]. \tag{2}$$

Here $\mathbf{E} = E\mathbf{n}$ denotes the Euler–Lagrange derivative, with $\mathbf{n}$ the (outward) normal to the surface. The fact that the Euler–Lagrange derivative is purely normal follows from the reparametrization invariance of the Hamiltonian; tangential deformations contribute only boundary terms. The quantity $\mathcal{Q}^a$ appearing in the total divergence in the second term is the Noether charge, which can be used to derive the stresses and torques acting on the surface associated with the Hamiltonian (1) [8].

Let us focus first on the variation of the area. One finds that under an infinitesimal deformation of the shape functions,

$$A_{(1)} = \epsilon \int \mathrm{d}A\, (\mathbf{e}_a \cdot \mathbf{W}^a),$$

where $\mathbf{e}_a = \partial \mathbf{X}/\partial \xi^a$ are the two tangent vectors to the surface. To cast this expression in the form (2), we integrate by parts, and obtain

$$A_{(1)} = \epsilon \int \mathrm{d}A\, [K\mathbf{n} \cdot \mathbf{W} + \nabla_a (\mathbf{e}^a \cdot \mathbf{W})], \tag{3}$$

where ∇_a denotes the covariant derivative on the surface. Latin indices are lowered and raised with the induced metric $g_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$ and its inverse, respectively. As expected, the Euler–Lagrange derivative of the area is purely normal, and given by the mean extrinsic curvature, $E = K$. Minimal surfaces (extremizing the area) have vanishing mean extrinsic curvature, $K = 0$.

For the curvature terms in (1) note that (see e.g. [10]),

$$K_{(1)} = -\epsilon[(\mathbf{n} \cdot \nabla_a \mathbf{W}^a) + 2K^{ab}(\mathbf{e}_a \cdot \mathbf{W}_b)], \tag{4}$$

where $K_{ab} = -\mathbf{n} \cdot \nabla_a \mathbf{e}_b = K_{ba}$ denotes the extrinsic curvature tensor of the surface, together with

$$\mathcal{R}_{(1)} = 2\epsilon[(K^{ab} - Kg^{ab})(\mathbf{n} \cdot \nabla_a \mathbf{W}_b) - \mathcal{R}(\mathbf{e}^a \cdot \mathbf{W}_a)]. \tag{5}$$

With the help of these expressions, it is straightforward to obtain the variation of the Hamiltonian in the form (2). After various integrations by parts we identify the Euler–Lagrange derivative as

$$E = \alpha[-2\nabla^2 K + K^3 - 2K_{ab}K^{ab}] + \mu K + \beta\mathcal{R}, \tag{6}$$

where $\nabla^2 = g^{ab}\nabla_a\nabla_b$ is the Laplacian on the surface. At this point, we take into account the constraint on the enclosed volume, which we write as a surface integral with $V = (1/3)\int \mathrm{d}A\, \mathbf{n} \cdot \mathbf{X}$, so that its first variation is $V_{(1)} = \epsilon \int \mathrm{d}A\, \mathbf{n} \cdot \mathbf{W}$. Therefore we obtain the equilibrium condition

$$E = P, \tag{7}$$

where the left-hand side is given by (6). This is known as the shape equation [12, 13]. It is a fourth-order non-linear PDE. A great deal of effort has been dedicated to its study (see e.g. [7]). As expected, the Gaussian bending energy does not contribute to the shape equation.

The first variation of the Hamiltonian, in addition to yielding the shape equation, allows us to determine the stresses and the torques acting locally on the surface. This was done in [8] using Noether's theorem with an emphasis on the role of the normal component of the deformation. (For an earlier treatment that exploits an analogy with plate theory in the special case of axisymmetric configurations, see [14].) The identification of the stresses and torques acting on the surface is important in a number of experimental applications which involve micro-manipulation techniques (see, e.g., [15–17]).

Here we offer an alternative, more direct route to the determination of stresses and torques. The first step is to collect the total divergences that appear in the Noether charge, obtaining

$$\begin{aligned}\mathcal{Q}^a = \alpha[&(K^2 g^{ab} - 2KK^{ab})(\mathbf{e}_b \cdot \mathbf{W}) + 2(\nabla^a K)(\mathbf{n} \cdot \mathbf{W}) - 2K(\mathbf{n} \cdot \mathbf{W}^a)] \\ &+ \overline{\alpha} 2(K^{ab} - Kg^{ab})(\mathbf{n} \cdot \mathbf{W}_b) \\ &+ \beta[(Kg^{ab} - K^{ab})(\mathbf{e}_b \cdot \mathbf{W}) - \mathbf{n} \cdot \mathbf{W}^a] + \mu(\mathbf{e}^a \cdot \mathbf{W}).\end{aligned} \tag{8}$$

The second step is to consider a (simply connected) piece of the membrane, which we denote by Σ_0, bounded by a curve C, and to specialize the variation of the Hamiltonian (2) to this arbitrary region of the membrane,

$$F_{(1)} = \epsilon \int_{\Sigma_0} \mathrm{d}A\, [E\mathbf{n} \cdot \mathbf{W} + \nabla_a \mathcal{Q}^a]. \tag{9}$$

Now, we consider an infinitesimal translation $\epsilon\mathbf{W} = \mathbf{a}$, with $\mathbf{a}$ constant. As the Hamiltonian is invariant under translations, the left-hand side of (9) vanishes, and with the stress tensor $\mathbf{f}^a$ defined by

$$\mathcal{Q}^a = -\mathbf{a} \cdot \mathbf{f}^a, \tag{10}$$

it follows that we can write the shape equation as a conservation law

$$E\mathbf{n} = \nabla_a \mathbf{f}^a = P\mathbf{n}, \tag{11}$$

where the stresses associated with the Hamiltonian (1) are given by

$$\mathbf{f}^a = -\alpha[(K^2 g^{ab} - 2KK^{ab})\mathbf{e}_b + 2(\nabla^a K)\mathbf{n}] - \beta(Kg^{ab} - K^{ab})\mathbf{e}_b - \mu\mathbf{e}^a. \tag{12}$$

We emphasize that it is far from obvious from the shape equation itself (7) that it can be written as a conservation law.

There are three conservation laws, and only one shape equation. As mentioned above, this is a consequence of the reparametrization invariance of the Hamiltonian. This statement can be made explicit using the decomposition of the stress tensor into tangential and normal parts as follows:

$$\mathbf{f}^a = f^{ab}\mathbf{e}_b + f^a\mathbf{n}. \tag{13}$$

The surface covariant derivative then gives

$$\nabla_a f^a - K_{ab} f^{ab} = E = P, \tag{14}$$

$$\nabla_a f^{ab} + K^b{}_a f^a = 0. \tag{15}$$

The first equation is the shape equation expressed in terms of the projections f^a and f^{ab}. The second equation expresses the content of reparametrization invariance as a consistency check: the normal stress and the tangential stress must balance exactly in this way. Note that this identity is potentially useful in numerical simulations, where reparametrization invariance is necessarily lost, and one is interested in quantifying the degree of violation.

The physical meaning of the stress tensor $\mathbf{f}^a$ is perhaps best illustrated by considering the total force per unit length acting on the curve C. Concretely, C may be the shape of an edge of the membrane [18], or the line boundary between the two phases of a two-component vesicle [19]. If we consider a basis $\{\mathbf{t}, \mathbf{l}\}$ on the surface adapted to the curve C that bounds Σ_0, with $\mathbf{t}$ tangent to C, and $\mathbf{l} = l^a\mathbf{e}_a$ the (outward) normal to C on the surface, we obtain the force per unit length acting on C, $l_a\mathbf{f}^a = \mathbf{f}$, as

$$\mathbf{f} = [K_{\parallel\perp}(2\alpha K + \beta)]\mathbf{t} + [\alpha K(K_\perp - K_\parallel) - \beta K_\parallel - \mu]\mathbf{l} - 2\alpha(\nabla_a K)\mathbf{n}, \tag{16}$$

where we denote the projections of the extrinsic curvature onto the surface as $K_\parallel = K_{ab}t^a t^b$, $K_\perp = K_{ab}l^a l^b$ and $K_{\perp\parallel} = K_{ab}t^a l^b$. Note that $K = K_\perp + K_\parallel$ and $\mathcal{R} = 2(K_\parallel K_\perp - K_{\perp\parallel}^2)$.

Similarly, as we showed for translations, for an infinitesimal rotation of the form $\epsilon\mathbf{W} = \mathbf{b} \times \mathbf{X}$, we can obtain the torques acting on the surface associated with the Hamiltonian (1). We define the total angular momentum $\mathbf{m}^a$

$$\mathcal{Q}^a = -\mathbf{b} \cdot \mathbf{m}^a, \tag{17}$$

where the torque $\mathbf{m}^a$ can be split in its 'orbital' and 'differential' parts as

$$\mathbf{m}^a = \mathbf{X} \times \mathbf{f}^a + \mathbf{s}^a. \tag{18}$$

From the Noether charge (8) we obtain directly

$$\mathbf{s}^a = [(2\alpha K + \beta)g^{ab} + 2\overline{\alpha}(Kg^{ab} - K^{ab})]\mathbf{e}_b \times \mathbf{n}. \tag{19}$$

Note that it is tangential to the surface.

The differential torque and the stress tensor are related by the relation

$$\nabla_a \mathbf{s}^a = \mathbf{f}^a \times \mathbf{e}_a. \tag{20}$$

We emphasize that this expression is valid also when not in equilibrium.

So far, we have focused on the case of a homogenous lipid vesicle. Inhomogeneities within the vesicle can be described in an effective way by introducing fields on the surface [20]. The

simplest possibility is to consider a scalar field $\phi(\xi^a)$, that may represent a local variation in density. For our purposes here, it is sufficient to add to the geometrical Hamiltonian (1) the Hamiltonian describing an inhomogeneity,

$$F_\phi[\mathbf{X}, \phi] = \int \mathrm{d}A \left[\frac{\lambda}{2}(\nabla\phi)^2 + V(\phi) + \beta_\phi K\phi\right], \tag{21}$$

where λ, β_ϕ are coupling constants, and the last term represents an interaction between the membrane mean curvature and the field ϕ. Variation with respect to ϕ gives

$$\lambda\nabla^2\phi - \frac{\partial V}{\partial\phi} = \beta_\phi K. \tag{22}$$

The shape equation (7) is modified by the addition of source terms,

$$E - \lambda K^{ab}\left[\nabla_a\phi\nabla_b\phi - \tfrac{1}{2}g_{ab}(\nabla\phi)^2\right] - V + \beta_\phi(\phi\mathcal{R} - \nabla^2\phi) = P, \tag{23}$$

where the Euler–Lagrange derivative E is given by (6).

The stress tensor is modified by the addition of

$$\mathbf{f}^a_\phi = \left[\lambda\nabla^a\phi\nabla^b\phi - \frac{\lambda}{2}g^{ab}(\nabla\phi)^2 - g^{ab}V + \beta_\phi\phi(K^{ab} - Kg^{ab})\right]\mathbf{e}_b - \beta_\phi(\nabla^a\phi)\mathbf{n}. \tag{24}$$

We emphasize that the analogues for this case of the expressions (14) and (15) still hold. In contrast to the purely geometrical situation, the latter (tangential) conservation laws now also encode the conservation of the scalar field stress tensor.

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