Deformations of the geometry of lipid vesicles

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Abstract

Consider a closed lipid membrane (vesicle), modeled as a two-dimensional surface, described by a geometrical hamiltonian that depends on its extrinsic curvature. The vanishing of its first variation determines the equilibrium configurations for the system. In this paper, we examine the second variation of the hamiltonian about any given equilibrium, using an explicitly surface covariant geometrical approach. We identify the operator which determines the stability of equilibrium configurations.

1 Introduction

Many of the physical properties of a lipid membrane (or vesicle) are captured by a hamiltonian which describes the degrees of freedom of an idealized two-dimensional membrane surface. Typically, this hamiltonian is a sum of terms each of which either penalizes or constrains some geometrical characteristics of this surface. A term quadratic in the mean extrinsic curvature is a measure of the energy penalty associated with the bending of the membrane \([1, 2, 3]\). This term is supplemented by various constraints: the area as well as the enclosed volume are usually fixed. A constraint or (a term in the energy) linear in the mean extrinsic curvature describes an asymmetry between the lipid bilayers which constitute the membrane \([4]\).

(For a review see \([5, 6, 7, 8, 9]\).)

In equilibrium, this hamiltonian will be stationary with respect to arbitrary infinitesimal deformations in the surface. This infinitesimal deformation has both a tangential part and a normal part. The former corresponds to a reparametrization of the surface, and so can contribute only in boundary terms. The remaining normal infinitesimal deformation will completely describe the physical state of deformation of the membrane in its bulk. As a consequence, the equilibrium condition is a single equation, known somewhat prosaically as ‘the shape equation’ \([10]\). In the thirty or so years since the introduction of the model, a lot has been learnt about the solutions of this equation, both analytically and numerically (see, for example, \([11]\) and the references it contains).

In this paper, we will examine the second variation of the hamiltonian. From one point of view, the calculation of the second variation about an equilibrium configuration is necessary in order to assess its degree of stability; in addition, the fluctuations of the membrane due to its interaction with its environment, are encoded completely at lowest order in the second variation of the hamiltonian. This problem has, of
course, been addressed before and in both contexts. In the former, for example, perturbations about spherical or cylindrical configurations have been examined analytically \[11, 12, 13, 14\]. A decomposition of geometries with a convex hull into spherical harmonics has also proven very effective \[15\]. In the statistical mechanical context, while arbitrary background geometries have been considered, the focus has been on the part of the second variation contributing at one-loop to the renormalization of the parameters of the theory \[16, 17, 18, 19\]. In any case, there is a gap in perturbation theory which we would like to fill. We will write down the second variation of the hamiltonian about an arbitrary equilibrium configuration, approaching the problem from a manifestly geometrically covariant point of view. Two features of the approach we will adopt should be emphasized. At the level of the second variation, it is no longer justified to ignore tangential deformations of the membrane. This is because a finite tangential deformation unlike its infinitesimal counterpart is not a simple reparametrization of the surface. Indeed, it was by examining finite tangential deformations of a given surface of constant negative Gaussian curvature preserving the curvature that Backlund, Bianchi and others generated new surfaces \[20\]. We show, however, that when the background geometry is an equilibrium, tangential deformations contribute only boundary terms to the second variation of the Hamiltonian, and therefore for the consideration of bulk fluctuations about equilibrium, they can be neglected without incurring any error. A second simple but subtle technical point is the exploitation of the fact that the variation of the divergence of a vector density is equal to the divergence of the variation. Though this is not so essential computationally at the quadratic level we will work at, by facilitating the isolation of boundary terms, it does make higher order expansions in the fluctuations about a non-trivial background feasible in practice.

The paper is organized as follows. In section 2, we introduce our conventions for the geometrical description of a hypersurface embedded in \(R^{N+1}\). We extend our considerations to an \(N\)-dimensional hypersurface because of the little extra cost involved and because of potential applications in other geometrical problems in soft matter physics. In section 3, we examine how the geometry changes under an infinitesimal deformation of the hypersurface. This is used in section 3 to derive the first variation of a geometrical hamiltonian for lipid membranes, and to obtain its Euler-Lagrange derivative. In section 4 the the second variation is examined. In particular, we check that it vanishes at equilibrium when the deformation corresponds to a rigid normal translation. We end in section 6 with a few concluding remarks.

## 2 Geometry

We begin by describing briefly the geometry of a hypersurface embedded in Euclidean space \(R^{N+1}\). This allows us to introduce our conventions. We will emphasize the peculiarities associated with a surface embedded in \(R^3\). At the end of this section, we also address the issue of identifying the low order independent reparametrization invariants one can construct from the geometrical quantities that characterize the hypersurface.

Consider an orientable hypersurface \(\Sigma\) embedded in \(R^{N+1}\). This surface can be specified locally in parametric form by \(N + 1\) shape functions,

\[
\mathbf{x} = \mathbf{X}(\xi^a),
\]

where \(\mathbf{x} = x^\mu = (x^1, \cdots, x^{N+1})\) are coordinates for \(R^{N+1}\), \(\xi^a\) arbitrary coordinates on the surface \(\Sigma\) \((a, b, \cdots = 1, \cdots, N)\), and \(\mathbf{X} = (X^1, \cdots, X^{N+1})\) are the shape functions.

The Euclidean metric on \(R^{N+1}\) induces the metric \(g_{ab}\) on \(\Sigma\) defined by,

\[
g_{ab} := e_a \cdot e_b,
\]

where the \(N\) tangent vectors are defined by \(e_a(\xi^a) = \partial_a \mathbf{X} (\partial_a := \partial/\partial \xi^a)\). Latin indices are lowered and raised with \(g_{ab}\), and its inverse \(g^{ab}\), respectively. The metric \(g_{ab}\) determines the intrinsic geometry of the hypersurface \(\Sigma\). It defines the unique torsionless covariant derivative \(\nabla_a\) compatible with it, i.e. satisfying \(\nabla_a g_{bc} = 0\) and \((\nabla_a \nabla_b - \nabla_b \nabla_a) f(\xi^a) = 0\) for some surface function \(f(\xi^a)\). In terms of the Christoffel
symbol $\Gamma^c_{ab}$, acting on a hypersurface vector $V^a$, it reads
\[ \nabla_a V^b = \partial_a V^b + \Gamma^b_{ac} V^c, \quad (3) \]
where
\[ \Gamma^c_{ab} := g^{cd} e_d \cdot \partial_a e_b = \frac{1}{2} g^{cd} (\partial_a g_{bd} + \partial_b g_{ad} - \partial_d g_{ab}). \quad (4) \]
The intrinsic Riemann curvature $\mathcal{R}^a_{bcd}$ of $\nabla_a$ is defined by
\[ (\nabla_a \nabla_b - \nabla_b \nabla_a) V^c := \mathcal{R}^c_{dab} V^d. \quad (5) \]
In terms of the Christoffel symbol, the Riemann curvature tensor is given by
\[ \mathcal{R}^a_{bcd} = \partial_c \Gamma^a_{db} - \partial_d \Gamma^a_{cb} + \Gamma^a_{ce} \Gamma^e_{db} - \Gamma^a_{de} \Gamma^e_{cb}. \quad (6) \]
The Ricci tensor is defined by contraction, $\mathcal{R}_{ab} := \mathcal{R}^c_{acb}$; the scalar curvature $\mathcal{R}$ is defined by $\mathcal{R} := g^{ab} \mathcal{R}_{ab}$.

When the hypersurface $\Sigma$ is two-dimensional, $N = 2$, the Riemann curvature tensor is completely determined by the scalar curvature:
\[ \mathcal{R}^a_{abcd} = \frac{\mathcal{R}}{2} (g_{ac} g_{bd} - g_{ad} g_{bc}). \quad (7) \]
Note that, as a consequence, we then have that in two dimensions the Einstein tensor vanishes,
\[ \mathcal{G}_{ab} := \mathcal{R}_{ab} - \frac{1}{2} \mathcal{R} g_{ab} = 0. \quad (8) \]
The scalar curvature of a two-dimensional surface is related to the Gaussian curvature $G$ of the surface by $\mathcal{R} = 2G$.

The simplest geometrical quantity invariant under reparameterizations of the surface one can construct out of the intrinsic geometry of the hypersurface $\Sigma$ is its area,
\[ A := \int dA = \int d^N \xi \sqrt{g}, \quad (9) \]
where $g$ denotes the determinant of the metric $g_{ab}$. The next order invariant depending only on the intrinsic geometry of the surface is the average scalar curvature over the surface, $\int dA \mathcal{R}$. For a two-dimensional surface with no boundary, by the well-known Gauss-Bonnet theorem, this is not only a reparameterization invariant, it is also a topological invariant, with
\[ \int dA \mathcal{R} = 4\pi (1 - g), \quad (10) \]
where $g$ is the genus of the surface.

Let us turn now to the extrinsic geometry of $\Sigma$. The single normal vector $\mathbf{n}(\xi^a)$ to $\Sigma$ in $R^N$ can be defined in implicit form by,
\[ e_a \cdot \mathbf{n} = 0, \quad (11) \]
with the normalization,
\[ \mathbf{n} \cdot \mathbf{n} = 1. \quad (12) \]
Note that these equations determine $\mathbf{n}$ only up to a sign: the normal can be inward or outward. Since the surface is assumed to be orientable, we can pick one sign consistently, and we choose the normal to be outward. The unit normal vector field can also be given explicitly as
\[ n_\mu = \frac{1}{N! \sqrt{g}} \varepsilon_{\mu \rho_1 \cdots \rho_{N-1}} \varepsilon^{a_1 \cdots a_{N-1}} (e^\rho_{a_1}) \cdots (e^\rho_{N-1} a_{N-1}), \quad (13) \]
where $\varepsilon_{\mu_1 \ldots \mu_N}$ and $\varepsilon^{a_1 \ldots a_{N-1}}$ are the totally antisymmetric Levi-Civita symbols for $R^{N+1}$ and $\Sigma$, respectively ($\varepsilon_{1 \ldots N} = +1$). The factor of $\sqrt{g}$ is necessary in order to make $n$ a scalar under reparametrizations.

When $\Sigma$ is closed, as we are assuming in this paper, the total volume enclosed by the surface $\Sigma$ in $R^{N+1}$ is an invariant. The normal to $\Sigma$, as given by (13), allows us to provide an alternative definition of the volume occupied by the interior of $\Sigma$ as the surface integral

$$V = \frac{1}{N+1} \int dA \, n \cdot X.$$  \hfill (14)

The space vectors $\{n, e_a\}$ form a basis adapted to the hypersurface. Their gradients along the surface are themselves space vectors, and can be decomposed in turn with respect to this basis. These decompositions constitute the classical Gauss-Weingarten equations,

$$\partial_a e_b = \Gamma^c_{ab} e_c - K_{ab} n,$$  \hfill (15)

$$\partial_a n = K_{ab} g^{bc} e_c.$$  \hfill (16)

Here $\Gamma^c_{ab}$ is the Christoffel symbol defined in (4). The extrinsic curvature of $\Sigma$ is given by the symmetric rank two surface tensor,

$$K_{ab} = -n \cdot \partial_a e_b = K_{ba}.$$  \hfill (17)

(Note that many authors differ by a sign in this definition.) We define its trace with respect to the intrinsic metric,

$$K := g^{ab} K_{ab} =: 2H,$$  \hfill (18)

where $H$ represents the mean extrinsic curvature of the surface.

The intrinsic and the extrinsic geometries of $\Sigma$, determined respectively by $g_{ab}$ and by $K_{ab}$, cannot be specified independently. They are related by the well-known integrability conditions of Gauss-Codazzi, and Codazzi-Mainardi, given respectively by,

$$R_{abcd} - K_{ac} K_{bd} + K_{ad} K_{bc} = 0,$$  \hfill (19)

$$\nabla_a K_{bc} - \nabla_b K_{ac} = 0.$$  \hfill (20)

These equations follow as integrability conditions from taking a gradient along the surface of the Gauss-Weingarten equations (15), (16), and then the appropriate anti-symmetric part.

The fundamental theorem for surfaces states that, given $g_{ab}$ and $K_{ab}$, these equations are not only necessary, but also sufficient for the existence of an embedding with these quantities as intrinsic metric and extrinsic curvature. Furthermore, the embedding is unique, up to rigid motions in the ambient space (see e.g. [21]).

Contraction of the Gauss-Codazzi-Mainardi equations with the contravariant intrinsic metric $g^{ab}$ results in

$$\mathcal{R}_{abcd} - K_{ac} K_{bd} + K_{ad} K_{bc} = 0,$$  \hfill (21)

$$\nabla_a K_{bc} - \nabla_b K_{ac} = 0.$$  \hfill (22)

For a two-dimensional surface, the contracted equations (21) and (22) possess the same content as the full Gauss-Codazzi-Mainardi equations, (19) and (20).

The lowest order geometrical invariant which involves the extrinsic geometry of the surface is the trace of the extrinsic curvature integrated over of the surface,

$$M := \int dA \, K.$$  \hfill (24)
This invariant, linear in \( n \), depends on the orientation of the surface. Note that \([K] = L^{-1}\), so that \([M] = L\). The next order reparameterization invariants are quadratic in the extrinsic curvature \((\approx L^0)\),

\[
\int dA K^2, \quad \int dA K^{ab} K_{ab},
\]

together with the Gaussian term, \(\int dA \mathcal{R}\). In general, these three invariants are not independent, as follows from the contracted Gauss equation, (22). Furthermore, in two dimensions, the Gaussian term is the Gauss-Bonnet topological invariant, see (10). For a two-dimensional surface, at this order there is then only one independent local scalar associated with the embedding, and it is customary to choose \(\int dA K^2\). The gradients of the extrinsic curvature \(\nabla_a K_{ab}\) which appear in the Codazzi-Mainardi equations do not feature. Differential bending can be ignored up to this order.

Let us now construct explicitly the geometrically independent terms of order \(L^{-2}\) and lower. In general, at order \(L^{-1}\), we have three independent scalars. Of the set, \(K^3, K K^{ab} K_{ab}, K^{ab} K_{be} K^e_a, K \mathcal{R}, \) and \(K_{ab} \mathcal{G}^{ab}\), the Gauss-Codazzi equations can be exploited to produce three that are independent

\[
\int dA K^3, \quad \int dA K \mathcal{R}, \quad \text{and} \quad \int dA K^{ab} \mathcal{G}_{ab}.
\]

The last of the three vanishes identically for two dimensional surfaces.

At order \(L^{-2}\) using the Gauss-Codazzi equation (13), it is easy to show that the independent scalars are \(\mathcal{R}^{abcd} \mathcal{R}_{abcd}, \mathcal{R}^{abc} \mathcal{R}_{abc}, \mathcal{R}^2, K^4, \mathcal{R} K^2, \) and \(\mathcal{G}_{ab} K^{ab}\). Of these, for a two-dimensional surface, only \(\mathcal{R}^2, K^4, \mathcal{R} K^2\) survive. Moreover, at this order gradients of the extrinsic geometry enter. We can reduce all terms quadratic in \(\nabla_a K_{bc}\) to the form \(\nabla_a K \nabla^a K + \text{terms that we have already considered}\). We exploit the uncontracted Codazzi-Mainardi integrability condition (20) to write

\[
\int dA (\nabla_a K_{bc})(\nabla^a K^{bc}) = \int dA (\nabla_a K_{bc})(\nabla^b K^{ac}) = - \int dA K_{bc} \nabla_a \nabla_b K^{ac},
\]

where we have integrated by parts. We now note that

\[
[\nabla_a, \nabla_b] K^{ac} = \mathcal{R}^{a dab} K^{dc} + \mathcal{R}^{c dab} K^{ad},
\]

so that

\[
\int dA (\nabla_a K_{bc})(\nabla^a K^{bc}) = - \int dA K^b_c (\nabla_b \nabla_a K^{ac} + \mathcal{R}_{db} K^{dc} + \mathcal{R}^{c dab} K^{ad}) = \int dA \left( K^{bc} \nabla_b \nabla_c K + \mathcal{R}_{db} K^{dc} K^b_c + \mathcal{R}_{c dab} K^{ad} K^{bc} \right),
\]

where we have used the contracted Codazzi-Mainardi equation (23) in the first term. We now integrate by parts again the first term, and use the Gauss-Codazzi-Mainardi equations to obtain

\[
\int dA (\nabla_a K_{bc})(\nabla^a K^{bc}) = \int dA (\nabla^a K)(\nabla_a K) + \mathcal{R}^{ab} \mathcal{R}_{ab} - K K^{ab} \mathcal{R}_{ab} + \frac{1}{2} \mathcal{R}_{abcd} \mathcal{R}^{abcd}.
\]

We conclude that for a two-dimensional surface, at this order there are four independent scalars,

\[
\int dA \left[ \mathcal{R}^2, \quad \int dA \mathcal{R} K^2, \quad \int dA K^4, \quad \text{and} \quad \int dA (\nabla^a K)(\nabla_a K) \right].
\]

These higher order terms appear in geometric models for the so called egg-carton membranes [22], and for tubular structures [23]. Note that if \(K\) is treated as a simple scalar field, \(\phi\), then the model described at this order is a \(\lambda \phi^4\) theory non-minimally coupled to the intrinsic curvature. The Euler-Lagrange equations of the two models are, of course, different.
3 Deformations

In this section, we consider infinitesimal deformations of a hypersurface $\Sigma$, and how the various geometrical quantities that characterize it change under deformation. A one-parameter deformation of the hypersurface is described by the functions $X(\xi^a, u)$. An infinitesimal change of the embedding functions

$$X \rightarrow X(\xi) + \delta X(\xi),$$

is characterized by the infinitesimal vector $\delta X(\xi) = \partial_\xi X(\xi^a, u)|_{u=0}\delta u$. This vector can be decomposed into its components normal and tangential to the hypersurface $\Sigma$:

$$\delta X = \delta_\perp X + \delta_\parallel X = \Phi n + \Phi^a e_a.$$  \hspace{1cm} (26)

The components $\Phi, \Phi^a$ have the dimensions of length. We will assume that they are much smaller than any characteristic length in the system, such as the curvature radii.

We first determine how the basis $\{e_a, n\}$ changes under deformation. The key observation is that $\partial_e$ and $\partial_a$ commute, so that the change in the tangent vector satisfies

$$\delta e_a = (\nabla_a \Phi^b) e_b - K_{ab} \Phi^b n + \Phi K_{ab} g^{bc} e_c,$$  \hspace{1cm} (28)

where we have used the Gauss-Weingarten equations (15) and (16). We thus have for the deformations induced by $\delta X_\parallel$ and $\delta X_\perp$, respectively,

$$\delta_\parallel e_a = (\nabla_a \Phi^b) e_b - K_{ab} \Phi^b n,$$

$$\delta_\perp e_a = (\nabla_a \Phi) n + \Phi K_{ab} g^{bc} e_c.$$  \hspace{1cm} (29)

For the deformation of the induced metric, it follows that

$$\delta_\parallel g_{ab} = \nabla_a \Phi^b + \nabla_b \Phi_a,$$

$$\delta_\perp g_{ab} = 2K_{ab} \Phi.$$  \hspace{1cm} (30)

The tangential deformation is just the Lie derivative along the surface vector field $\Phi^a$. The normal deformation summarizes the geometrical content of the extrinsic curvature as one half of Lie derivative of the intrinsic metric along the normal vector field. Note that for the inverse metric one has that $\delta_\perp g^{ab} = -2K^{ab} \Phi$. It follows from these relations that the first order deformation of the infinitesimal area element is

$$\delta_\parallel dA = dA \nabla_a \Phi^a,$$

$$\delta_\perp dA = dA \ K \Phi.$$  \hspace{1cm} (31)

This last expression encodes the geometrical content of the trace of the extrinsic curvature as the relative change of area per unit normal deformation.

The variations of the normal vector,

$$\delta_\parallel n = K_{ab} \Phi^a g^{bc} e_c,$$

$$\delta_\perp n = -\nabla_a \Phi^a g^{ab} e_b,$$  \hspace{1cm} (32)

follow readily from the defining relations (11) and (12), together with (29).

For the remainder of this section we will focus on normal deformations of the hypersurface. The reason is that infinitesimal tangential deformations correspond to reparametrizations of the surface, and, as shown in the next section, they contribute only boundary terms to the variation of global quantities.

It is possible to evaluate the first order normal variation of the intrinsic scalar curvature $\mathcal{R}$ either intrinsically or extrinsically, the latter using the Gauss-Codazzi equation. Let us consider the former approach. Using the definition of the Riemann tensor given by (6), we have that the variation of the Riemann tensor is (see e.g. [24])

$$\delta \mathcal{R}^a_{bcd} = \nabla_c (\delta \Gamma^a_{db}) - \nabla_d (\delta \Gamma^a_{cb}),$$

6
which implies

\[ \delta R_{ab} = \nabla_c (\delta \Gamma^c_{ab}) - \nabla_b (\delta \Gamma^c_{ca}) . \]

For the scalar curvature we have then that its normal variation is

\[ \delta_\perp R = (\delta_\perp g^{ab}) R_{ab} + g^{ab} (\delta_\perp R_{ab}) \]

\[ = -2 R_{ab} K^{ab} \Phi + \nabla_c (g^{ab} \delta_\perp \Gamma^c_{ab}) - \nabla^a (\delta_\perp \Gamma^c_{ca}) . \]

Now, an arbitrary variation of the metric induces a variation

\[ \delta \Gamma^c_{ab} = \frac{1}{2} g^{cd} (\nabla_b \delta g_{ad} + \nabla_a \delta g_{bd} - \nabla_d \delta g_{ab}) \]

in the Christoffel symbols, so that using the Codazzi-Mainardi equations, we have that the normal variation of the Christoffel symbol is

\[ \delta_\perp \Gamma^c_{ab} = K_a^c \nabla_b \Phi + K_b^c \nabla_a \Phi - K_{ab} \nabla^c \Phi + (\nabla_a K_b^c) \Phi . \] (33)

As a consequence of the Codazzi-Mainardi equations, the (apparently unsymmetric) last term on the right hand side is, in fact, symmetric under the interchange of tangent indices. We determine then that the scalar curvature varies according to

\[ \delta_\perp R = -2 R_{ab} K^{ab} \Phi + 2 \nabla_a \left[ (K^{ab} - g^{ab} K) \nabla_b \Phi \right] . \] (34)

Note that for the densitized scalar curvature we have

\[ \delta_\perp \sqrt{g} R = \sqrt{g} (-2 g^{ab} K^{ab} \Phi + 2 \nabla_a \left[ (K^{ab} - g^{ab} K) \nabla_b \Phi \right] . \] (35)

It follows that the variation of the integrated scalar curvature is a pure divergence in two dimensions, as expected from the Gauss-Bonnet theorem [10].

Let us consider now the first order normal deformation of the extrinsic geometry. We have that

\[ \delta_\perp K_{ab} = -(\delta_\perp n) \cdot \partial_a e_b - n \cdot \partial_a (\delta_\perp e_b) \]

\[ = (\nabla_\perp \Phi) e^c \cdot \partial_a e_b - n \cdot \partial_a [(\nabla_b \Phi) n + \Phi K_b e^c] \]

\[ = \Gamma^c_{ab} \nabla_c \Phi - \partial_a \nabla_b \Phi + K_{ac} K^c_b \Phi \]

\[ = -\nabla_a \nabla_b \Phi + K_{ac} K^c_b \Phi . \] (36)

This is a remarkably simple expression. Using the contracted Gauss equation [21] we can cast this expression in the alternative form,

\[ \delta_\perp K_{ab} = -\nabla_a \nabla_b \Phi + (K K_{ab} - R_{ab}) \Phi . \] (37)

For the trace of the extrinsic curvature this gives (recall that \( \delta_\perp g^{ab} = -2 K^{ab} \Phi \)),

\[ \delta_\perp K = -\Delta \Phi + (R - K^2) \Phi , \] (38)

where \( \Delta := g^{ab} \nabla_a \nabla_b \) denotes the laplacian on \( \Sigma \), and we have used the contracted Gauss equation [22].

As a check of the consistency of the expressions we have derived, one can verify that they imply the vanishing of the first order variation of the contracted Gauss equation, \( i.e. \delta_\perp (R - K^2 + K^{ab} K_{ab}) = 0 \).

In the calculations of higher order variations, an essential ingredient is the commutator of the deformation operator and the covariant derivative on \( \Sigma \). This commutator allows one to express deformations of the covariant derivative of any geometrical quantity of interest in terms of the covariant derivative of the variation of such quantity. For instance, when acting on an arbitrary second rank tensor \( A_{ab} \) in \( \Sigma \), it is given by

\[ [\delta_\perp, \nabla_a] A^c_b = -(\delta_\perp \Gamma^d_{ab}) A^c_d + (\delta_\perp \Gamma^c_{ad}) A^d_b , \] (39)
where $\delta_\perp \Gamma^c_{ab}$ is defined in (33). Also for this case, it is a useful check of the validity of these expressions, to verify that the first order variation of the Codazzi-Mainardi equation (20), which involves such commutator, vanishes identically.

A useful expression is the commutator of the deformation derivative with the Laplacian, acting on an arbitrary function $f$,

$$[\delta_\perp, \Delta]f = -2K^{ab}\Phi \nabla_a \nabla_b f - 2K^{ab}\nabla_a f \nabla_b \Phi + K \nabla^a f \nabla_a \Phi - (\nabla_a K)(\nabla^a f)\Phi .$$  \hspace{1cm} (40)

### 4 First variation

In this section, we apply the formalism for deformations we have developed to the systematic determination of the Euler-Lagrange derivatives of the geometrical invariants which appear in the hamiltonian for the strict bilayer couple model

$$F[X] = \alpha \int dA K^2 + \beta M + \mu A + PV. \hspace{1cm} (41)$$

The first term is the bending energy, with $\alpha$ the bending rigidity, the constants $\mu, P, \beta$ are lagrange multipliers that enforce the constraints of constant area, constant volume and constant area difference, respectively. For the sake of simplicity, we have not included the non-local bending rigidity term, necessary in a realistic description of lipid vesicles [25, 26].

We first comment on tangential deformations. For the surface area element we have that under a tangential deformation it transforms according to (31). In addition, any surface scalar satisfies $\delta_\parallel f(X) = \Phi^a \partial_a f(X)$. Thus, any reparameterization invariant functional of the form

$$F[X] = \int dA f(X), \hspace{1cm} (42)$$
deforms tangentially as

$$\delta_\parallel F[X] = \int dA \nabla_a [\Phi^a f(X)]. \hspace{1cm} (43)$$

Using Stokes theorem this becomes

$$\delta_\parallel F[X] = \int ds \eta^a \Phi^a f(X), \hspace{1cm} (44)$$

where the integral ranges over the boundary of $\Sigma$ and $\eta^a$ denotes the unit normal to the boundary into $\Sigma$. If this boundary is empty, the integral vanishes identically. It is worthwhile emphasizing that in the case of a surface with a boundary, this integral in general will be non-vanishing, and it is no longer correct to neglect the tangential variations of the surface. In fact, in the variational principle, the vanishing of such terms will determine the boundary conditions to be imposed on the shape functions (see e.g. [27]).

If the surface has no boundary, the tangential part of the variation can always be associated with a reparametrization. Since we are interested, to begin with, in quantities that are invariant under surface reparametrizations, we disregard this contribution and focus on normal deformations of the geometry of $\Sigma$. We write

$$\delta_\perp F[X] = \int dA \left\{ \mathcal{E}[f] \Phi + \nabla_a V^a_{(1)} f \right\}. \hspace{1cm} (45)$$

The divergence comes about when we integrate by parts to remove all derivatives from the normal deformation $\Phi$. The subscript in the vector appearing in the second term refers to the order of the variation.

We begin with the first order normal variation of $A$ and $V$. For the normal variation of the total area it follows immediately from (31) that

$$\delta_\perp A = \int dA K \Phi. \hspace{1cm} (46)$$
The difference in area between two surfaces separated by an infinitesimal constant normal distance \( \Phi \) is proportional to the integrated mean curvature. The area of the surface is extremal for arbitrary normal deformations, \( \delta \perp A = 0 \), when \( K = 0 \) at each point on the surface.

One way to determine the normal deformation of the volume enclosed by the surface is to exploit the definition given in (14). We have

\[
\delta \perp V = \frac{1}{N+1} \int d\Sigma \left[ (\delta \perp \sqrt{g}) \mathbf{n} \cdot \mathbf{X} + \sqrt{g} (\delta \perp \mathbf{n}) \cdot \mathbf{X} + \sqrt{g} \mathbf{n} \cdot \delta \perp \mathbf{X} \right]
\]

Integrating by parts the second term and dropping a total divergence gives

\[
\delta \perp V = \frac{1}{N+1} \int d\Sigma \left[ \Phi \mathbf{n} \cdot \mathbf{X} - (\nabla_a \Phi) g^{ab} e_b \cdot \mathbf{X} + \Phi \right]
\]

(47)

Integrating by parts the second term and dropping a total divergence gives

\[
\delta \perp V = \frac{1}{N+1} \int d\Sigma \left[ \Phi \mathbf{n} \cdot \mathbf{X} + \Phi \right] + \Phi \]

(48)

where we have used the Gauss-Weingarten equations (15) to obtain the second term of the second line. This final expression should come as no surprise. The infinitesimal change in volume is simply proportional to the area of the surface times the normal displacement.

We now examine the integrated powers of the mean extrinsic curvature. The deformation of the density \( \sqrt{g}K \), using (31), (38), is

\[
\delta \perp \sqrt{g} K = -\Delta \Phi + R \Phi .
\]

(49)

We thus find for the total mean curvature, up to a total divergence,

\[
\delta \perp M = \int d\Sigma \Phi .
\]

(50)

It is interesting that this expression depends only on the intrinsic geometry of the surface. If the scalar curvature vanishes, so also does \( \delta \perp M \). This is to be expected in a two-dimensional surface where \( R = 0 \) implies that it is flat. It is, however, a non-trivial statement for higher dimensions.

For the variation of the integrated second power of the extrinsic curvature we have

\[
\delta \perp \int d\Sigma K^2 = \int d\Sigma K \left[ -2\Delta \Phi + (2R - K^2) \Phi \right] ;
\]

(51)

We now integrate by parts twice to obtain, again up to a total divergence,

\[
\delta \perp \int d\Sigma K^2 = \int d\Sigma \left[ -2\Delta K + (2R - K^2) K \right] \Phi .
\]

(52)

We are now in the position to derive the Euler-Lagrange derivative for the model defined by the Helfrich hamiltonian (41). Using the expressions (46), (48), (51), (52), in (45), we find [10]

\[
\mathcal{E} = -2\alpha \Delta K + (2\alpha K + \beta) R - \alpha K^3 + \lambda K + P .
\]

(53)

At equilibrium, \( \mathcal{E} = 0 \), it is known as the shape equation. Note that it involves four derivatives of the shape functions. It determines the equilibrium configurations of lipid membranes described by the hamiltonian (41). Recently it was shown how to cast the shape equation in the form of a conservation law [28].
5 Second variation

In this section, we derive the second variation of the hamiltonian \([11]\). Before we proceed, we note that because the shape functions \(X\) are the variables to be varied, we have that \(\delta_{\perp} \Phi \neq 0\), to second order, and similarly for the remaining three possibilities, \(\delta_{\perp} \Phi^a\), \(\delta_{\parallel} \Phi\) and \(\delta_{\parallel} \Phi^a\). In fact, using \([29], [32]\), we have

\[
\delta_{\perp} \Phi = -\Phi^a \nabla_a \Phi, \quad \delta_{\parallel} \Phi = K_{ab} \Phi^a \Phi^b,
\]

together with

\[
\delta_{\perp} \Phi^a = \Phi \nabla_a \Phi + K_{ab} \Phi^b, \quad \delta_{\parallel} \Phi^a = \Phi^b \nabla_a \Phi^b - K_{ab} \Phi^b \Phi.
\]

This appears to suggest that the computation of the second variation is a formidable task and that the decomposition of deformations into tangential and normal parts will not be so useful. As we will show, the formal apparatus we have developed simplifies the calculation enormously and all of the troublesome tangential terms are collected in a divergence when the Euler-Lagrange equations are satisfied: no actual error is incurred in setting \(\delta_{\perp} \Phi = 0\) and neglecting \(\Phi^a\) in the sequel.

Let \(F = \sqrt{\mathbf{g}} f\), where \(f\) is a scalar, introduced in \([12]\). At first order, we have

\[
\delta F = \int d^N \xi \left[ \delta_\parallel \Phi + \delta_{\perp} \Phi \right] = \int d^n \xi \left[ \sqrt{\mathbf{g}} \mathcal{E} \Phi + \nabla_a (\mathcal{V}_{(1)}[\mathcal{F}] + \mathcal{F} \Phi^a) \right],
\]

where \(\mathcal{V}_{(1)}[\mathcal{F}] = \sqrt{\mathbf{g}} \mathcal{V}^{(1)}[\mathcal{F}]\) is the densitized vector defined by Eq.\([12]\). Now the divergence of a vector density is independent of the surface affine connection \(\Gamma^c_{ab}\), and thus variation of the divergence of a vector density \(\mathcal{V}^a\) is equal to the divergence of the variation,

\[
\delta (\nabla_a \mathcal{V}^a) = \nabla_a (\delta \mathcal{V}^a).
\]

We thus have at second order,

\[
\delta^2 F = \int d^N \xi \delta \left[ \sqrt{\mathbf{g}} \mathcal{E} \Phi \right],
\]

modulo another divergence. Thus, whereas for the second variation of \(F\) we cannot legitimately discard the divergence, we can for \(F\). Furthermore, we have

\[
\delta \left[ \sqrt{\mathbf{g}} \mathcal{E} \Phi \right] = \delta_{\perp} \left( \sqrt{\mathbf{g}} \mathcal{E} \Phi \right) + \nabla_a (\sqrt{\mathbf{g}} \mathcal{E} \Phi^a) \Phi + \sqrt{\mathcal{E}} \delta \Phi.
\]

Thus, modulo the Euler-Lagrange equation, \(\delta \left[ \sqrt{\mathbf{g}} \mathcal{E} \Phi \right] = \delta_{\perp} \left( \sqrt{\mathbf{g}} \mathcal{E} \Phi \right)\). But \(\delta_{\perp} \left( \sqrt{\mathbf{g}} \mathcal{E} \right)\) can always be expressed as \(\mathcal{L} \Phi\), for some local differential operator \(\mathcal{L}\), and therefore the second order variation of the hamiltonian can itself be written in the form

\[
\delta^2 F[X] = \int dA \; \Phi \; \mathcal{L} \Phi.
\]

It must be remembered, however, that this is not true for the individual terms contributing to \(F\), for which \(\mathcal{E} \neq 0\). When the second variation of these terms is written down it, it should be understand that the expression refers to the second normal variation; off diagonal terms \(\sim \Phi \Phi_n\) as well as purely tangential terms \(\sim \Phi_a \Phi_b\) have been suppressed.

A second order variation can also be seen as a different deformation \(X^\mu \rightarrow X^\mu (\xi) + \Phi^\mu \mathbf{n}\) applied to the first order variations, and then letting \(\Phi^\prime = \Phi\). From a computational point of view, this is clearly equivalent to a repeated application of the normal deformation operator \(\delta_{\perp}\).

For the second order variation of the enclosed volume no work is needed, since, using \([31]\), it is simply related to the first variation of the area with

\[
\delta^2 V = \delta \int dA \; \Phi = \int dA \; K \; \Phi^2.
\]
In order to derive the second variation of the area, various strategies are possible. On one hand one can simply calculate the second variation of the metric. Using (37) one obtains,

\[
\delta_2^\perp g_{ab} = 2(\delta_\perp K_{ab}) \Phi = -2\Phi [\nabla_a \nabla_b \Phi - K_a^c K_{cb}] \Phi ,
\]

(62)

so for the area element this gives

\[
\delta_2^\perp \sqrt{g} = \sqrt{g}(-\Phi \Delta \Phi + \mathcal{R} \Phi^2) ,
\]

(63)

and the second variation of the area is given by the well-known expression (see e.g. [29])

\[
\delta^2 A = \int dA \Phi \{-\Delta + \mathcal{R}\} \Phi .
\]

(64)

There is an alternative route to the second variation of the area, which becomes increasingly useful as one considers higher variations. The idea is to exploit the natural hierarchy in the variations illustrated by the relations

\[
\delta_\perp \sqrt{g} = \sqrt{g} K \Phi \delta_2^\perp \sqrt{g} = \delta_\perp (\sqrt{g} K) \Phi .
\]

Using (49), this gives directly (63). The usefulness of this approach is apparent: the \(n\)th variation of the surface volume element can be expressed in terms of the \((n-1)\)th variation of the densitized mean extrinsic curvature.

We now exploit this observation to derive the second variation of the densitized mean extrinsic curvature. We rewrite (50) as

\[
\delta_\perp (\sqrt{g} K) = \sqrt{g} \mathcal{R} \Phi + \nabla_a V^{a(1)}[K] ,
\]

(65)

where we have defined the vector density \(V^{a(1)}[K] := -\sqrt{g} \nabla_a \Phi\). Using the fact that the variation of the divergence of a vector density is equal to the divergence of the variation, we have

\[
\delta_\perp^2 (\sqrt{g} K) = \delta_\perp \{-\sqrt{g} \mathcal{R} \Phi + \nabla_a V^{a(1)}[K]\} \]

\[
= \Phi \delta_\perp (\sqrt{g} K) + \nabla_a V^{a(2)}[K] \]

\[
= 2\sqrt{g} \Phi \left[ (K^{ab} - \mathcal{R} g^{ab}) \nabla_a \nabla_b \Phi - \mathcal{G}_{ab} K^{ab} \Phi \right] + \nabla_a V^{a(2)}[K] ,
\]

(66)

where we have used (53), and defined the vector density

\[
V^{a(2)}[K] = \delta_\perp V^{a(1)}[K] = \sqrt{g} \Phi (2K^{ab} - g^{ab}) \nabla_b \Phi .
\]

We have therefore for the second variation of \(M\),

\[
\delta^2 M = \int dA \{2\Phi [((K^{ab} - \mathcal{R} g^{ab}) \nabla_a \nabla_b - \mathcal{G}_{ab} K^{ab}) \Phi]\} .
\]

(68)

Note that if the surface is flat then the second order variation, like the first, vanishes. Thus, in a gaussian approximation about a flat background geometry, this term is absent.

Our final task in this section is to compute the second variation of the densitized squared mean extrinsic curvature. Unfortunately, this quantity does not fit naturally in the hierarchy of variations we have been exploiting. One approach is to calculate the second variation of \(K\) directly. From (38), using (34), (40), we have that

\[
\delta_\perp^2 K = 4K^{ab} \Phi \nabla_a \nabla_b \Phi + (2K^{ab} - K g^{ab}) \nabla_a \Phi \nabla_b \Phi + 2K (K^2 - \mathcal{R}) \Phi^2 - 2\mathcal{R}_{ab} K^{ab} \Phi^2 .
\]

(69)

We prefer to capitalize on the relative simplicity of the expressions for the variation of the densitized mean curvature and use the identity

\[
\delta_\perp^2 (\sqrt{g} K^2) = 2K \delta_\perp^2 (\sqrt{g} K) + 2[\delta_\perp (\sqrt{g} K)]^2 g^{-1/2} - 5K^2 \Phi \delta_\perp (\sqrt{g} K) + 2\sqrt{g} K^4 \Phi^2 .
\]

(70)
A short calculation gives
\[
\delta^2 \left( \sqrt{g} K^2 \right) = \sqrt{g} [2(\Delta \Phi)^2 + 4\Phi K K^{ab} \nabla_a \nabla_b \Phi + (K^2 - 4R) \Phi \Delta \Phi + (2R^2 + 2K^4 - 5R K^2 - 4G_{ab} K^{ab} K^2) + 2K \nabla_a V_a^{(2)}[K],
\]
where $V_a^{(2)}[K]$ is defined by (71). We isolate a total divergence in the final term using
\[
2K \nabla_a V_a^{(2)}[K] = -2(\nabla_a K) V_a^{(2)}[K] + \nabla_a V_a^{(2)}[K^2],
\]
where we define
\[
V_a^{(2)}[K^2] = 2\sqrt{g} [\Delta \Phi \nabla^a \Phi - \Phi \nabla^a \Delta \Phi + \Phi (2K^{ab} - Kg^{ab}) \nabla_b \Phi],
\]
to obtain
\[
\delta^2 \int dA K^2 = \int dA \Phi [2\Delta^2 + 4K K^{ab} \nabla_a \nabla_b + (K^2 - 4R) \Delta + 2R^2
\]
\[- 2(\nabla_a K)(2K^{ab} - g^{ab} K) \nabla_b + 2K^4 - 5R K^2 - 4G_{ab} K^{ab} K] \Phi,
\]
We can simplify this expression using
\[
-2 \int dA \Phi(\nabla_a K)(2K^{ab} - g^{ab} K) \nabla_b \Phi = \int dA[2K^{ab} \nabla_a \nabla_b K - K \Delta K + (\nabla^a K)(\nabla_a K)] \Phi^2,
\]
to arrive at the final expression
\[
\delta^2 \int dA K^2 = \int dA \Phi [2\Delta^2 + 4K K^{ab} \nabla_a \nabla_b + (K^2 - 4R) \Delta + 2K^{ab} \nabla_a \nabla_b K
\]
\[- K \Delta K + (\nabla^a K)(\nabla_a K) + 2R^2 + 2K^4 - 5R K^2 - 4G_{ab} K^{ab} K] \Phi.
\]
Therefore, for the second order variation of the Helfrich hamiltonian (41), as expressed in (60), we can write the local differential operator $L$ as
\[
L = 2\alpha \Delta^2 + 2\lambda \Delta + 2A^{ab} \nabla_a \nabla_b + 2B,
\]
where
\[
2A = \alpha(K^2 - 4R) - 2\beta K - \lambda,
\]
\[
2A^{ab} = 4\alpha K K^{ab} + 2\beta K^{ab},
\]
\[
2B = \alpha(2R^2 + 2K^4 - 5R K^2 - 4G_{ab} K^{ab} K + 2K^{ab} \nabla_a \nabla_b K
\]
\[- K \Delta K + (\nabla^a K)(\nabla_a K)] - 2\beta G_{ab} K^{ab} + \lambda R + PK.
\]
We note that $A^{ab}$ is symmetric. Furthermore, the operator $L$ is always self-adjoint, by which we mean that
\[
\int dA \Phi_1 L \Phi_2 = \int dA \Phi_2 L \Phi_1.
\]
Thus, the eigenvalues of $L$ are assured to be real valued. To see this, consider the terms that could potentially spoil self-adjointness originating in the contributions proportional to $\alpha$ with two derivatives of $\Phi$. Let $\tilde{A}^{ab} = A^{ab} + g^{ab} A$. Now,
\[
\Phi \tilde{A}^{ab} \nabla_a \nabla_b \Phi = \Phi \nabla_a (\tilde{A}^{ab} \nabla_b \Phi) - \Phi \nabla_a \tilde{A}^{ab} \nabla_b \Phi
\]
\[= \Phi \nabla_a (\tilde{A}^{ab} \nabla_b \Phi) + \frac{1}{2} \nabla_a \nabla_b \tilde{A}^{ab} \Phi^2,
\]
modulo a total divergence which we discard. In this form the operator \( \tilde{A}^{ab} \nabla_a \nabla_b \) is manifestly self-adjoint: we have

\[
\Phi_1 \nabla_a (\tilde{A}^{ab} \nabla_b \Phi_2) = \Phi_2 \nabla_b (\tilde{A}^{ab} \nabla_a \Phi_1)
\]

modulo two total divergences. We can write

\[
\mathcal{L} = 2\alpha \Delta^2 + 2\nabla_a \tilde{A}^{ab} \nabla_b + 2B_1,
\]

where

\[
2B_1 = \alpha[2R^2 + 2K^4 - 5R K^2 - 4G_{ab} K^{ab} K + 2\Delta(K^2 - R)] - 2\beta G_{ab} K^{ab} + \lambda R + PK.
\]

We note that the expression Eq.(76) agrees with the one obtained in [16, 17], in the terms containing derivatives of \( \Phi \). These previous studies were focused on the effect of short wavelength fluctuations, where only these terms contribute. We also note that the expression we have obtained disagrees with the one obtained previously in [12]. Agreement is restored in the special case of spherical and cylindrical configurations.

It is clear that a rigid translation of the surface should not alter the second variation, at equilibrium. This provides a non-trivial check of our expression (77). As it is not entirely obvious, we will outline the details. Throughout, we will use extensively the Gauss-Weingarten equations (15), (16), and the contracted Gauss-Codazzi-Mainardi equations (21), (22), (23). Consider a constant normal deformation \( \delta X = a \), such that \( a \cdot e_a = 0 \). We have for the derivatives of \( \Phi \) that appear in (77),

\[
\nabla_a \nabla_b \Phi = -K_{ac} K^c_b (n \cdot a),
\]

\[
\Delta^2 \Phi = \left[-2K^{ab} \nabla_a \nabla_b \Phi - (\nabla_a K)(\nabla^a K) - \Delta(K_{ab} K^{ab}) + (K_{ab} K^{ab})^2 \right](n \cdot a).
\]

If we now insert these expressions in the second variation, we find

\[
\delta^2 F = \int dA \left\{ \alpha \left[ -2K^{ab} \nabla_a \nabla_b \Phi - (\nabla_a K)(\nabla^a K) - \Delta(K_{ab} K^{ab}) - K\Delta K + 2RK^2 - K^4 \right] + \beta RK + \lambda K^2 + PK \right\} (n \cdot a)^2.
\]

We now integrate by parts the terms that involve derivatives of the extrinsic curvature. The desired simplifications follow from the crucial identity, for any surface vector \( V^a \),

\[
\int dA \left( \nabla_a V^a \right)(n \cdot a)^2 = 0,
\]

up to boundary terms. This is a consequence of \( \nabla_a (n \cdot a) = K_{ab} (e_a \cdot a) = 0 \), by hypothesis. Using this identity, we easily arrive at

\[
\delta^2 F = \int dA K E (n \cdot a)^2,
\]

where \( E \) is the Euler-lagrange derivative defined by (53). Therefore at equilibrium the second variation vanishes for rigid translations.

Note that a similar check has been used for the second variation of particular configurations, as, for example, spheres in [11, 10]. However, not all of the terms appearing in the second variation can be checked considering only symmetric configurations, since many terms simply vanish identically in these limits.

6 Concluding remarks

In this paper we have presented a covariant geometric approach for examining the variation of geometric models of lipid membranes. For concreteness, we have restricted our attention to the first and second variation of the rigid bilayer couple hamiltonian (41). We note that it is straightforward to specialize the
second variation in the form (77) to axisymmetric configurations. Moreover, our approach can be extended
straightforwardly to other geometric models. However, computational difficulties are to be expected if
the membrane has a free edge and it is no longer legitimate to throw away boundary terms. When
considering higher order variations, a different difficulty arises. It is no longer justified to neglect tangential
deformations. We will address this issue in a future publication.

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