Hamilton's equations for a fluid membrane

R Capovilla[1], J Guven[2] and E Rojas[3]

[1] Departamento de Física, Centro de Investigación y de Estudios Avanzados,
Apdo. Postal 14-740, 07000 México, DF, Mexico
[2] Instituto de Ciencias Nucleares, Universidad Nacional Autónoma de México,
Apdo. Postal 70-543, 04510 México, DF, Mexico
[3] Facultad de Física e Inteligencia Artificial, Universidad Veracruzana, 91000 Xalapa, Veracruz,
Mexico

Abstract
Consider a homogeneous fluid membrane described by the Helfrich–Canham
energy, quadratic in the mean curvature of the membrane surface. The
shape equation that determines equilibrium configurations is fourth order in
derivatives and cubic in the mean curvature. We introduce a Hamiltonian
formulation of this equation which dismantles it into a set of coupled first-
order equations. This involves interpreting the Helfrich–Canham energy as an
action; equilibrium surfaces are generated by the evolution of space curves.
Two features complicate the implementation of a Hamiltonian framework.
(i) The action involves second derivatives. This requires treating the velocity
as a phase-space variable and the introduction of its conjugate momentum.
The canonical Hamiltonian is constructed on this phase space. (ii) The action
possesses a local symmetry—reparametrization invariance. The two labels we
use to parametrize points on the surface are themselves physically irrelevant.
This symmetry implies primary constraints, one for each label, that need to be
implemented within the Hamiltonian. The two Lagrange multipliers associated
with these constraints are identified as the components of the acceleration
tangential to the surface. The conservation of the primary constraints implies
two secondary constraints, fixing the tangential components of the momentum
conjugate to the position. Hamilton's equations are derived and the appropriate
initial conditions on the phase-space variables are identified. Finally, it is
shown how the shape equation can be reconstructed from these equations.

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1. Introduction

A biological membrane consists, in a first approximation, of a bilayer of phospholipid
molecules in water [1, 2]. The thickness of the membrane is determined by the length of

the hydrocarbon tails $\sim$50 Å, whereas its overall size can reach 50 μm—it is thus sensible to describe it on mesoscopic scales as a two-dimensional surface. Remarkably, many of the physical properties of the membrane are completely described by the geometrical degrees of freedom associated with this surface. The language that is most appropriate to describe the membrane is differential geometry.

The phospholipid molecules move freely within the membrane so that the membrane behaves as a two-dimensional fluid. In a geometrical model, this feature is implemented by associating an energy, invariant under surface reparametrizations, with each possible shape of the membrane. One should think of reparametrization in its active sense, as the freedom of a point to move about on the surface, rather than as a change of coordinates.

In the early seventies, it was recognized that the leading term in the energy is proportional to the cost of bending the membrane—quadratic in the mean curvature [3–5]. This geometric invariant is known in the mathematical literature as the Willmore functional [6]. The geometry of a fluid membrane will generally also be subject to constraints: its area and (if closed) its volume are constant. Moreover, the bilayer structure is captured by the area difference between the layers, proportional to the integrated mean curvature. Its value is constrained in the minimal curvature model for fluid membranes [7]. This is the model we will focus our attention on. Other curvature models have superseded this simple model (see e.g. [8] for a review). In particular, it is worth mentioning the ADE model, with a non-local constraint involving the square of the area difference [9–11]. Our considerations can be extended to this and other geometrical models.

We are interested, in particular, in the equilibrium shapes of a closed fluid vesicle minimizing the Helfrich–Canham energy, defined below by equation (2), which describes the minimum curvature model. Typically, the addition of constraints, will increase the number of equilibrium solutions. The vanishing of the first variation of the energy is expressed in a single 'shape' equation [12–14]. It is a fourth-order nonlinear PDE. Beginning in the mid-seventies, with the work of Deuling and Helfrich on axisymmetric configurations [15], considerable effort and ingenuity has been dedicated to characterizing these shapes. For axisymmetric configurations, it is relatively straightforward to solve the shape equation: the symmetry reduces it to a third-order nonlinear ODE. Even in this simple case, however, solving this equation involves numerical approximations [8]. For more general configurations, analytical techniques have been as good as useless outside of the perturbation theory. Rather than attempt to solve the shape equation itself, one has relied on a combination of computational techniques, among them Monte-Carlo simulations and dynamical triangulations to minimize the energy (see e.g. [16, 17]).

In principle, how does one go about solving the shape equation when axisymmetry is relaxed? The method used to solve the axisymmetric shape equation numerically suggests a strategy. What one does is decompose the higher order shape equation into a set of coupled first-order equations. Initial conditions for these equations are specified, that will need to be tuned to obtain a geometry which closes smoothly. In practice, modulo the step involving tuning, what one does is formulate the problem in Hamiltonian terms. In this paper, we provide a novel formulation of the shape equation, in all its glory, as a Hamiltonian system. The basic idea is borrowed from the Hamiltonian formulation of general relativity, and more specifically, from the recent Hamiltonian formulation of the dynamics of relativistic extended objects [18]. Take any curve on the membrane surface. The surface is then generated by the evolution of the curve along some direction with appropriate initial data. The evolution is determined by a Hamiltonian that is derived from the Helfrich–Canham energy, reinterpreted as an action for the curve. To do this in one step is technically daunting. The reader may be interested in first working through the details in a simplified setting. The axisymmetric

case has been considered in [19], where the shape equation is formulated as a Hamiltonian system describing the motion of a particle, rather than a curve, in two dimensions. While the canonical structure itself is illustrated clearly in this restricted setting, it is too simple to capture the geometry.

The paper is organized as follows. In section 2, we introduce the geometry for the surface that describes the fluid vesicle, and the Helfrich–Canham energy. Next, we consider an arbitrary parametrized closed curve on the surface, and decompose the surface geometry along a tangential basis adapted to the curve: one vector is tangent to the curve, the other, not necessarily orthogonal to it, is parametrized by a second parameter t. The latter tangent vector acquires an interpretation as the velocity of the curve, parametrized by the time t. By implementing this decomposition of the surface geometry within the Helfrich–Canham energy, it can be written as an action describing the evolution of the curve. The corresponding Lagrangian depends not only on the position of the curve and its velocity, but also on its second derivative with respect to the parameter t: its acceleration. A second key feature is the presence of a local symmetry of the action, reparametrization invariance. Before looking at lipid vesicles, in section 3 we consider the simpler, but still non-trivial, case of a soap bubble. The energy is proportional to the area of the bubble with a constraint on the enclosed volume. The action does not involve second derivatives and we can address the problems associated with reparametrization invariance without the added complication of higher derivatives. In section 4 we return to fluid vesicles described by the Helfrich–Canham energy, and we identify the phase-space variables which are appropriate when the Lagrangian involves the acceleration; it becomes necessary to introduce canonical momenta not only conjugate to the position of the curve, but also to its velocity. We show how these momenta can be identified by examining the response of the energy to deformations of this curve. The momentum conjugate to position will be shown to be related directly to the conserved stress introduced by two of us in [14]. Not surprisingly, the stress plays a role in the Hamiltonian formulation; stresses get transmitted across closed curves [20]. In section 5, we construct the canonical Hamiltonian in terms of a Legendre transformation with respect to both position and velocity. This Hamiltonian will generate the evolution of the curve in terms of the phase-space variables. At a Hamiltonian level, the existence of a local symmetry, in our case reparametrization invariance, manifests itself in the appearance of constraints on the phase-space variables at fixed values of the evolution parameter. We find two primary constraints, that need to be added to the canonical Hamiltonian to generate evolution, as well as two secondary constraints. These four constraints are conserved in time. In particular, one of the secondary constraints is the vanishing of the canonical Hamiltonian—the hallmark of reparametrization invariance. The secondary constraints are the generators of reparametrizations. In section 6, we derive the Hamilton equations for this system. Appropriate initial conditions on the phase-space variables are discussed. Reparametrization invariance manifests itself in the appearance of two arbitrary functions in these equations. Ultimately the shape equation has been dismantled into its Hamiltonian building blocks: four constraints at fixed value of time and four first order, in time, evolution equations. In section 7, we show how the shape equation can be reconstructed using these blocks. We conclude in section 8 with some final remarks. Various technical details are collected in a set of appendices.

2. Helfrich–Canham energy

We model a fluid membrane as a two-dimensional surface Σ, defined locally by the embedding

$$\mathbf{x} = \mathbf{X}(\xi^a), \tag{1}$$

where $\mathbf{x} = x^i$ are local coordinate in space, ξ^a local coordinates on the surface Σ ($i, j, \ldots = 1, 2, 3; a, b, \ldots = 1, 2$) and $\mathbf{X} = X^i$ the embedding, or shape, functions. We denote by $\mathbf{e}_a = \partial \mathbf{X}/\partial \xi^a$ the two tangent vectors to the surface. The metric induced on Σ is given by their inner product, $g_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$, and its inverse is g^{ab}; indices are lowered and raised with g_{ab} and g^{ab}, respectively. The area of the surface Σ is $A = \int \mathrm{d}A = \int \mathrm{d}^2\xi \sqrt{g}$, with $g = \det g_{ab}$. The unit normal $\mathbf{n}$ to Σ is defined implicitly by $\mathbf{e}_a \cdot \mathbf{n} = 0$, $\mathbf{n}^2 = 1$. The extrinsic curvature tensor is $K_{ab} = -\mathbf{n} \cdot \partial_a \partial_b \mathbf{X}$, and the mean curvature is $K = g^{ab} K_{ab}$. In terms of the principal curvatures, $\{c_1, c_2\}$, we have $K = c_1 + c_2$. The intrinsic scalar curvature can be given in terms of the extrinsic curvature via the Gauss–Codazzi equation as $\mathcal{R} = K^2 - K^{ab} K_{ab}$; it is twice the Gaussian curvature, so that in terms of the principal curvatures $\mathcal{R} = 2c_1 c_2$.

The shape of a fluid membrane is obtained by minimizing the Helfrich–Canham energy, quadratic in the extrinsic curvature. In the bilayer coupling model, the membrane is subject to various global constraints: the enclosed volume, the area as well as the integrated mean curvature (the area difference between the layers) are fixed. One then searches for stationary points of the Helfrich–Canham energy $F[\mathbf{X}]$ defined by

$$F[\mathbf{X}] = \frac{\kappa}{2} \int \mathrm{d}A\,K^2 + \beta \int \mathrm{d}A\,K + \sigma A - \mathsf{P}V. \tag{2}$$

The constant κ is the bending rigidity; β, σ and P are Lagrange multipliers enforcing the constraints of constant integrated mean curvature, constant area and constant enclosed volume V, respectively. The constant σ is the bare surface tension, and P is the osmotic pressure. Of course, the inclusion of the volume term requires that the surface be closed. The volume can be written as a surface integral:

$$V = \frac{1}{3} \int \mathrm{d}A\,\mathbf{n} \cdot \mathbf{X}. \tag{3}$$

Despite appearances, this expression for V is translationally invariant. This is because $\int \mathrm{d}A\,\mathbf{n} \cdot \mathbf{a} = 0$ for any constant vector $\mathbf{a}$ on any closed surface. We have not included in the energy a term corresponding to the Gaussian bending, $F_G[\mathbf{X}] = \kappa_G \int \mathrm{d}A\mathcal{R}$, with κ_G being the Gaussian bending rigidity, since for a two-dimensional surface, by the Gauss-Bonnet theorem, it is a topological invariant, and so it does not contribute to the determination of equilibrium configurations.

The vanishing of the first variation of the energy (2), with respect to infinitesimal variations of the shape functions $\mathbf{X} \to \mathbf{X} + \delta\mathbf{X}$, gives the shape equation [12–14, 21]

$$\kappa \left[-\nabla^2 K - \frac{K}{2}(K^2 - 2\mathcal{R}) \right] + \beta\mathcal{R} + \sigma K - \mathsf{P} = 0, \tag{4}$$

where $\nabla^2 = g^{ab}\nabla_a\nabla_b$ denotes the surface Laplacian, and ∇_a the surface covariant derivative. This fourth-order nonlinear PDE determines the equilibrium configurations of fluid vesicles. Note that there is only one equilibrium condition. Naively varying $\mathbf{X}$, one would have expected three, since there are three independent deformations. However, reparametrization invariance tells us that two of the equations, corresponding to tangential deformations, must vanish identically [22]. The only physical deformations that enter in the determination of equilibrium are those normal to the surface.

Our basic proposal in this paper is to consider the surface Σ as the evolution of some closed curve $\mathcal{C}$. If the curve is parametrized by u, and its evolution by t, the surface generated by $\mathcal{C}$ will be given by $\mathbf{x} = \mathbf{X}(u, t)$. For any fixed t, the tangent vector to the curve is $\mathbf{X}' = \partial_u\mathbf{X} = \partial\mathbf{X}/\partial u$. The infinitesimal arclength along the curve is $\mathrm{d}s = h^{1/2}\mathrm{d}u$, where

$$h = \mathbf{X}' \cdot \mathbf{X}' \tag{5}$$

is the one-dimensional metric along $\mathcal{C}$; the unit tangent vector is $\mathbf{t} = h^{-1/2}\mathbf{X}'$. The curve $\mathcal{C}$ evolves along the surface vector field $\dot{\mathbf{X}} = \partial_t \mathbf{X} = \partial \mathbf{X}/\partial t$. This vector will not generally be orthogonal to $\mathcal{C}$. Let $\mathbf{l}$ denote the unit vector normal to the curve on the surface $\mathbf{l} \cdot \mathbf{X}' = 0$. We expand $\dot{\mathbf{X}}$ with respect to the vectors $\mathbf{l}$ and $\mathbf{X}'$:

$$\dot{\mathbf{X}} = N\mathbf{l} + N_\parallel \mathbf{X}'; \tag{6}$$

in analogy with the terminology used in general relativity, we will refer to the components $N, N_\parallel$ with respect to this basis as the lapse and shift functions, respectively. In terms of $\mathbf{X}'$ and $\dot{\mathbf{X}}$, they are given by

$$N^2 = \dot{\mathbf{X}}^2 - \frac{(\dot{\mathbf{X}} \cdot \mathbf{X}')^2}{h}, \qquad N_\parallel = \frac{(\dot{\mathbf{X}} \cdot \mathbf{X}')}{h}. \tag{7}$$

We now decompose the geometry of the surface Σ along the basis of tangent vectors adapted to the evolution of the curve, $\{\dot{\mathbf{X}}, \mathbf{X}'\}$. For the induced metric we have

$$g_{ab} = \begin{pmatrix} N^2 + hN_\parallel^2 & hN_\parallel \\ hN_\parallel & h \end{pmatrix}; \tag{8}$$

and for its inverse it follows that

$$g^{ab} = N^{-2} \begin{pmatrix} 1 & -N_\parallel \\ -N_\parallel & N^2h^{-1} + N_\parallel^2 \end{pmatrix}. \tag{9}$$

Note that the component g^{uu} can also be written as $g^{uu} = \dot{\mathbf{X}}^2/h$. The determinant of the induced metric g_{ab} takes the simple form

$$g = N^2 h. \tag{10}$$

The vectors $\mathbf{t}, \mathbf{l}$, together with the normal to the surface $\mathbf{n}$ form a spatial basis adapted to the curve. We choose an orientation so that $\mathbf{n} = \mathbf{t} \times \mathbf{l}$. In terms of $\mathbf{X}'$ and $\dot{\mathbf{X}}$,

$$\mathbf{n} = \frac{1}{N\sqrt{h}}\mathbf{X}' \times \dot{\mathbf{X}}. \tag{11}$$

The decomposition of the extrinsic curvature along the basis $\{\dot{\mathbf{X}}, \mathbf{X}'\}$ is given by

$$K_{ab} = -\begin{pmatrix} \mathbf{n} \cdot \ddot{\mathbf{X}} & \mathbf{n} \cdot \dot{\mathbf{X}}' \\ \mathbf{n} \cdot \dot{\mathbf{X}}' & \mathbf{n} \cdot \mathbf{X}'' \end{pmatrix}, \tag{12}$$

which depends on the acceleration of the curve $\ddot{\mathbf{X}}$ projected along the normal to the surface. For the mean curvature it follows that

$$K = g^{ab}K_{ab} = \frac{1}{N^2}\left(-\mathbf{n} \cdot \ddot{\mathbf{X}} + J\right), \tag{13}$$

where we have isolated the part that does not depend on the acceleration in the quantity

$$J = 2N_\parallel(\mathbf{n} \cdot \dot{\mathbf{X}}') - h^{-1}(\dot{\mathbf{X}}^2)(\mathbf{n} \cdot \mathbf{X}''). \tag{14}$$

To make contact with the analysis in [19] for axisymmetric configurations, recall that an axisymmetric configuration can be described by cylindrical coordinates $\{R(t), Z(t), \phi\}$. The curve $\mathcal{C}$ is parametrized by the angle ϕ; the tangent vector is $\mathbf{X}' = \partial \mathbf{X}/\partial\phi$, and the one-dimensional metric is $h = R^2$. The velocity $\dot{\mathbf{X}}$ is along a meridian, with $N_\parallel = 0$, and $N = \sqrt{\dot{R}^2 + \dot{Z}^2}$. Moreover, in this case, $\mathbf{n} \cdot \dot{\mathbf{X}}' = 0, \mathbf{n} \cdot \mathbf{X}'' = -N^{-1}R\dot{Z}$, and $\mathbf{n} \cdot \ddot{\mathbf{X}} = N^{1/2}(\dot{Z}\ddot{R} - \dot{R}\ddot{Z})$; it follows that the quantity J takes the simple form $J = R^{-1}N\dot{Z}$, so that the mean curvature is $K = R^{-1}N^{-3/2}[R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + N^2\dot{Z}]$.

We now cast the energy $F[\mathbf{X}]$ given by (2) as an action describing the dynamics in time t of a curve parametrized by u, $\mathbf{X}(t, u)$:

$$F[\mathbf{X}] = \int \mathrm{d}t\, L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}], \tag{15}$$

where the Lagrangian functional is given by

$$L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}] = \oint du\, N\sqrt{h} \left[\frac{\kappa}{2N^4}(-\mathbf{n}\cdot\ddot{\mathbf{X}} + J)^2 + \frac{\beta}{N^2}(-\mathbf{n}\cdot\ddot{\mathbf{X}} + J) + \sigma - \frac{\mathsf{P}}{3}\mathbf{n}\cdot\mathbf{X} \right]. \tag{16}$$

Note the dependence of the Lagrangian on time derivatives of the field variables $\mathbf{X}$: it is *quadratic* in $\ddot{\mathbf{X}}$, the acceleration of the curve, and it is not possible to eliminate this dependence using integration by parts within the action. It depends on the velocity $\dot{\mathbf{X}}$ through its appearance in N, J and $\mathbf{n}$. In all but the last term, the position $\mathbf{X}$ appears only through its derivatives with respect to the parameter u along the curve, $\mathbf{X}'$ and $\mathbf{X}''$; note that there is an implicit dependence on $\mathbf{X}$ of N and $\mathbf{n}$.

The Hamiltonian formulation of the dynamical system defined by the action (15) is somewhat involved. As an aid to establishing our bearings, it will be useful to first understand the Hamiltonian formulation of a simpler system, without higher derivatives to contend with.

3. Soap bubble

In this section we will provide a Hamiltonian formulation of the equilibrium of a soap bubble, in which surface tension is pitted against the internal pressure. Here the energy is simply proportional to the area of the bubble, subject to a constraint fixing the enclosed volume. The energy involves no higher than the first derivatives of $\mathbf{X}$ with respect to the parameter t. This system illustrates, at the Hamiltonian level, the consequences of the presence of a local symmetry—reparametrization invariance—namely the presence of constraints on the phase-space variables. The reader should be warned, however, that the canonical structure is very different from that presented below for a lipid vesicle.

The energy is

$$F[\mathbf{X}] = \sigma A - \mathsf{P}V, \tag{17}$$

where σ is the surface tension, and P the pressure excess inside the bubble. The equilibrium condition obtained from the vanishing of the first variation of $F[\mathbf{X}]$ is given by the classical Laplace–Young equation, of second order in derivatives of the shape functions,

$$\sigma K - \mathsf{P} = 0. \tag{18}$$

Equilibrium configurations are surfaces of constant mean curvature.

We consider the energy (17) as an action, describing the motion in the parameter t of a curve parametrized by u, $\mathbf{X}(t, u)$. Decomposing the energy with respect to the coordinates $\{t, u\}$, we have

$$F[\mathbf{X}] = \int dt\, L[\mathbf{X}, \dot{\mathbf{X}}], \tag{19}$$

where the Lagrangian functional is

$$L[\mathbf{X}, \dot{\mathbf{X}}] = \oint du\, N\sqrt{h} \left(\sigma - \frac{\mathsf{P}}{3}\mathbf{n}\cdot\mathbf{X} \right). \tag{20}$$

We emphasize that this Lagrangian depends at most on the velocities via N and $\mathbf{n}$ related respectively to $\dot{\mathbf{X}}$ by (7) and (11). The factor of $\sqrt{h}$ appearing in (20) ensures invariance of L with respect to reparametrizations of the curve $\mathcal{C}$.

Our first step towards a Hamiltonian formulation of the problem is the derivation of the canonical momentum $\mathbf{p}$ conjugate to $\mathbf{X}$. A direct approach would be to define the canonical momentum $\mathbf{p}$ via the functional derivative $\mathbf{p} = \delta L/\delta\dot{\mathbf{X}}$. However, with an eye towards the higher order generalization for fluid vesicles, it is preferable to extract the canonical momentum

from the first variation of the action (19); we do this in some detail. Under an infinitesimal deformation of the embedding functions $\mathbf{X} \rightarrow \mathbf{X} + \delta\mathbf{X}$, the first variation of the action (19), can be written as

$$\delta F[\mathbf{X}] = \int dA\, \mathbf{E} \cdot \delta\mathbf{X} + \oint du\, \mathbf{p} \cdot \delta\mathbf{X}, \tag{21}$$

where $\mathbf{E}$ denotes the Euler–Lagrange derivative. This expression allows us to read the canonical momentum $\mathbf{p}$ from the second term. To carry out the first variation, we use the well-known variational expressions (see e.g. [22])

$$\delta A = \int dA\, \mathbf{e}^a \cdot \partial_a \delta\mathbf{X}, \tag{22}$$

$$\delta V = \frac{1}{3} \int dA\, \left[\mathbf{n} \cdot \delta\mathbf{X} + (\mathbf{n} \cdot \mathbf{X})\, \mathbf{e}^a \cdot \partial_a \delta\mathbf{X} - (\mathbf{e}^a \cdot \mathbf{X})\mathbf{n} \cdot \partial_a \delta\mathbf{X} \right]. \tag{23}$$

Neither expression depends on the parametrization. For the first variation of the energy (19) it follows that, integrating by parts it can be cast in the form (21),

$$\delta F = \int dA\,(-\sigma \nabla_a \mathbf{e}^a - \mathsf{P}\mathbf{n}) \cdot \delta\mathbf{X} + \int dA \nabla_a \left\{ \sigma \mathbf{e}^a \cdot \delta\mathbf{X} - \frac{\mathsf{P}}{3}[(\mathbf{n} \cdot \mathbf{X})\mathbf{e}^a - (\mathbf{e}^a \cdot \mathbf{X})\mathbf{n}] \cdot \delta\mathbf{X} \right\}. \tag{24}$$

Now we use the Gauss–Weingarten equations for the surface Σ

$$\nabla_a \mathbf{e}_b = -K_{ab}\mathbf{n}, \tag{25}$$

$$\nabla_a \mathbf{n} = K_{ab} g^{bc} \mathbf{e}_c, \tag{26}$$

and Stokes' theorem as applied to a surface vector field V^a which states that, for a region of the surface enclosed by the curve $\mathcal{C}$,

$$\int dA \nabla_a V^a = \oint du\, \sqrt{h}\, l_a V^a, \tag{27}$$

where l^a is the normal to $\mathcal{C}$ on the surface Σ (note that $\mathbf{l} = l^a \mathbf{e}_a$). Therefore we obtain

$$\delta F = \int dA\,(\sigma K - \mathsf{P})\, \mathbf{n} \cdot \delta\mathbf{X} + \oint du\, \sqrt{h} \left\{ \sigma \mathbf{l} \cdot \delta\mathbf{X} - \frac{\mathsf{P}}{3}\,[(\mathbf{n} \cdot \mathbf{X})\mathbf{l} - (\mathbf{l} \cdot \mathbf{X})\mathbf{n}] \cdot \delta\mathbf{X} \right\}. \tag{28}$$

Comparison of (21) and (28) identifies the Euler–Lagrange derivative as $\mathbf{E} = E\mathbf{n}$, where E is given by the lhs of (18); the Euler–Lagrange derivative is normal to the surface. For the canonical momentum we read

$$\mathbf{p} = \sqrt{h} \left\{ \sigma \mathbf{l} - \frac{\mathsf{P}}{3}\,[(\mathbf{n} \cdot \mathbf{X})\mathbf{l} - (\mathbf{l} \cdot \mathbf{X})\mathbf{n}] \right\}$$

$$= \sigma \sqrt{h}\, \mathbf{l} - \frac{\mathsf{P}}{3}\mathbf{X} \times \mathbf{X}'. \tag{29}$$

The momentum transforms as a density under reparametrizations of the curve $\mathcal{C}$, as it should. It is normal to the curve. In this sense, it differs in an essential way from $\dot{\mathbf{X}}$ which is not necessarily normal. The contribution to $\mathbf{p}$ from area is proportional through σ to the densitized unit vector $\mathbf{l}$. The addition to $\mathbf{p}$ due to the volume constraint is independent of $\dot{\mathbf{X}}$, which introduces a component normal to the surface.

Note that neither N nor $N_\parallel$ are canonical variables for the soap bubble: they cannot be expressed as functionals of $\mathbf{X}$ and $\mathbf{p}$. They should not therefore appear within the canonical framework. For the same reason, the normal $\mathbf{n}$ (unlike the tangent vectors $\mathbf{t}$ and $\mathbf{l}$) is also not a

canonical variable, and has no place within this framework in this model. For fluid membranes, on the other hand, N, $N_\parallel$ as well as **n** will be identified as functions of the canonical variables.

We have now identified the phase-space variables appropriate for a Hamiltonian description of the equilibrium configurations of a soap bubble: the position of a given curve **X** and its conjugate momentum **p**, as given by (29). The canonical Hamiltonian is obtained via a Legendre transformation of the Lagrangian (20) with respect to $\dot{\mathbf{X}}$ as

$$H_0[\mathbf{p}, \mathbf{X}] = \oint \mathrm{d}u \, \mathbf{p} \cdot \dot{\mathbf{X}} - L[\mathbf{X}, \dot{\mathbf{X}}]. \tag{30}$$

It is immediate to see that it vanishes,

$$H_0[\mathbf{p}, \mathbf{X}] = 0. \tag{31}$$

Its vanishing is a direct consequence of the presence of reparametrization invariance. At first this might appear to indicate some inconsistency. However, a local symmetry such as reparametrization invariance also implies constraints. These constraints will generate the evolution. Let us examine these issues one at a time. Reparametrization invariance renders it impossible to invert for the velocity in terms of the momentum. To see this explicitly one considers the Hessian

$$H_{ij} = \frac{\delta^2 L}{\delta \dot{X}^i \delta \dot{X}^j} = \frac{\sigma \sqrt{h}}{N} n_i n_j. \tag{32}$$

H_{ij} is degenerate: its determinant vanishes. This is a feature of any Hamiltonian system with local symmetries. It means that at any value of the parameter t the phase-space variables are not all independent; there are constraints. We use the definition of the momentum (29) to identify the constraints as functions of the canonical variables: **p** is orthogonal to $\mathcal{C}$, and the function of the canonical variables $(\mathbf{p} + \mathsf{P}\mathbf{X} \times \mathbf{X}'/3)/\sigma \sqrt{h}$ is a unit vector. We thus find that, at each value of t, the phase-space variables must satisfy the primary constraints:

$$C_1 = \left(\mathbf{p} + \frac{\mathsf{P}}{3} \mathbf{X} \times \mathbf{X}' \right)^2 - \sigma^2 h = 0 \tag{33}$$

$$C_2 = \mathbf{p} \cdot \mathbf{X}' = 0. \tag{34}$$

The only freedom **p** possesses independent of **X** is a direction.

The constraints possess a geometrical role in phase space as generators of infinitesimal reparametrizations. In particular, whereas C_2 generates reparametrizations of the curve $\mathcal{C}$ itself, C_1 generates motions off the curve $\mathcal{C}$ onto the surface. This can be shown by considering the Poisson bracket of the constraints with the phase-space variables, where, for two arbitrary functions of the phase-space variables f and g, the Poisson bracket is

$$\{f, g\} = \oint \mathrm{d}u \left[\frac{\delta f}{\delta \mathbf{X}} \cdot \frac{\delta g}{\delta \mathbf{p}} - (f \leftrightarrow g) \right]. \tag{35}$$

It should be mentioned that analogous constraints with $\mathsf{P} = 0$ occur in the Hamiltonian formulation of a relativistic bosonic string (see e.g. [18]).

The Hamiltonian that generates the motion of the curve $\mathcal{C}$ is proportional to the constraints themselves,

$$H = \oint \mathrm{d}u (\lambda_1 C_1 + \lambda_2 C_2), \tag{36}$$

where $\lambda_1 = \lambda_1(u, t)$ and $\lambda_2 = \lambda_2(u, t)$ are two arbitrary Lagrange multiplier functions that enforce the constraints. The time derivative of a phase-space function f is given by its Poisson bracket with this Hamiltonian,

$$\dot{f} = \{f, H\}. \tag{37}$$

In particular, it is important to note that the time derivative of the constraints (33) and (34) does not generate any new constraints.

Hamilton's equations are given by (see the appendices for useful formulae)

$$\dot{\mathbf{X}} = \frac{\delta H}{\delta \mathbf{p}} = 2\lambda_1 \left(\mathbf{p} + \frac{\mathsf{P}}{3}\mathbf{X} \times \mathbf{X}' \right) + \lambda_2 \mathbf{X}', \tag{38}$$

$$\dot{\mathbf{p}} = -\frac{\delta H}{\delta \mathbf{X}} = -\frac{2\mathsf{P}}{3}\lambda_1 \mathbf{X}' \times \left(\mathbf{p} + \frac{\mathsf{P}}{3}\mathbf{X} \times \mathbf{X}' \right) - \frac{2\mathsf{P}}{3}\left[\lambda_1 \mathbf{X} \times \left(\mathbf{p} + \frac{\mathsf{P}}{3}\mathbf{X} \times \mathbf{X}' \right) \right]'$$
$$- (2\sigma^2 \lambda_1 \mathbf{X}' + \lambda_2 \mathbf{p})'. \tag{39}$$

These two couple first-order equations reproduce the equilibrium condition $\mathbf{E} = E\mathbf{n} = 0$, where E is given by the lhs of the Laplace–Young equation (18), that follows from extremization of the energy. The first equation identifies both the momentum $\mathbf{p}$ and the Lagrange multipliers λ_1, λ_2. Using the constraints, one finds that the Lagrange multipliers are proportional to the lapse and shift functions appearing in (6):

$$\lambda_1 = \frac{N}{2\sigma\sqrt{h}}, \qquad \lambda_2 = N_{\parallel}. \tag{40}$$

These expressions for the Lagrange multipliers indicate that, given the curve $\mathcal{C}$, the surface we generate depends only on the normal $\mathbf{l}$: the specific linear combination of $\mathbf{l}$ and $\mathbf{t}$ entering the velocity $\dot{\mathbf{X}}$ is gauge—it is not determined by the Hamilton equations. For the soap bubble, reparametrization invariance manifests itself in a freedom within the velocity $\dot{\mathbf{X}}$ (for a fluid membrane this will become a freedom within the acceleration $\ddot{\mathbf{X}}$). The definition (29) of the momentum is reproduced when we substitute (40) for the Lagrange multipliers back into (38). Using this information in the second of Hamilton's equations (39), one finds the following relationship:

$$-\sqrt{g}E\mathbf{n} = \dot{\mathbf{p}} + \frac{\delta H}{\delta \mathbf{X}}, \tag{41}$$

where E is given by the left-hand side of (18). To check this, one can use the geometrical expressions given in appendix A.

Hamilton's equations (38), (39), together with the constraints (33), (34), provide an alternative formulation of the single Euler–Lagrange equilibrium equation (18). Once we have confirmed that this set of equations is equivalent to (18), we can forget about the latter.

The basic strategy to construct an equilibrium configuration is to choose a closed curve in space defined by its position $\mathbf{X}(u, 0)$. We choose a momentum $\mathbf{p}(u, 0)$ consistent with the constraints (33) and (34). This corresponds to a direction. Now we let $\mathbf{X}, \mathbf{p}$ evolve according to the Hamilton's equations (38) and (39) for any λ_1 and λ_2 of our choosing. An equilibrium configuration $\mathbf{X}(u, t)$ will be generated.

In practice, when we discretize these equations, we will find that the canonical variables will stray off the constrained surface in phase space; the formalism itself suggests a strategy to nudge them back. One simply introduces explicit damping terms proportional to the numerical value of the constraints on the rhs of Hamilton's equations. It is also possible to tune λ_1 and λ_2 so as pace the evolution most appropriately.

Unless we have been extremely lucky, we will find that the initial data we have prescribed generate a surface that does not close smoothly. This is not surprising: after all, the unique non-self-intersecting geometry is a sphere of radius $R_0 = 2\sigma/\mathsf{P}$. One needs to tune the initial conditions to produce this sphere.

4. Phase space for the fluid membrane

We now turn to the Hamiltonian formulation of the evolution of a curve described by the action (15). We first identify the phase-space variables. Because the Lagrangian (16) depends on the acceleration $\ddot{\mathbf{X}}$, in addition to the position of the curve $\mathbf{X}$ and its conjugate momentum $\mathbf{p}$, the phase space will need to be enlarged to include the velocity $\dot{\mathbf{X}}$ and its conjugate momentum $\mathbf{P}$. (A pedagogical introduction to the Hamiltonian formulation of higher order systems is given in the appendix of [19].) The momenta are defined by the functional derivatives

$$\mathbf{P} = \frac{\delta L}{\delta \ddot{\mathbf{X}}}, \tag{42}$$

$$\mathbf{p} = \frac{\delta L}{\delta \dot{\mathbf{X}}} - \partial_t \left(\frac{\delta L}{\delta \ddot{\mathbf{X}}} \right). \tag{43}$$

Using the expression (13) for the mean curvature K, one immediately obtains for the momentum $\mathbf{P}$ conjugate to $\dot{\mathbf{X}}$,

$$\mathbf{P} = -\frac{\sqrt{h}}{N}(\kappa K + \beta)\mathbf{n}. \tag{44}$$

$\mathbf{P}$ is normal to the surface, and transforms as a density under a reparametrization of the curve. The part due to bending is proportional to the mean curvature. We anticipate that this expression will be the content of one of Hamilton's equations for this system (see (79)). Note that $\mathbf{P}$ depends on $\mathbf{X}$, $\dot{\mathbf{X}}$ and $\ddot{\mathbf{X}}$.

The functional derivatives involved in the determination of the momentum $\mathbf{p}$ are somewhat less simple. A more convenient approach, generalizing that used in the previous section for the soap bubble, see (21), focuses on the first variation of the energy. For a system that depends on the acceleration, (21) generalizes to

$$\delta F[\mathbf{X}] = \int \mathrm{d}A\, \mathbf{E} \cdot \delta \mathbf{X} + \oint \mathrm{d}u\, (\mathbf{p} \cdot \delta \mathbf{X} + \mathbf{P} \cdot \delta \dot{\mathbf{X}}), \tag{45}$$

where $\mathbf{E}$ is the Euler–Lagrange derivative. Therefore, just as we did for a soap bubble, it is possible to read the momenta from this expression. To carry out the variation, we use variational results described e.g. in [22], such as (22), (23), together with

$$\delta K = -\mathbf{n} \cdot \nabla^2 \delta \mathbf{X} + 2K^{ab}\mathbf{e}_a \cdot \partial_b \delta \mathbf{X}. \tag{46}$$

The Euler–Lagrange derivative is normal, $\mathbf{E} = E\mathbf{n}$, where E is given by the lhs of the shape equation (4). Let us focus our attention on the second term of (45). Integrating by parts and using Stokes' theorem (27), one finds that

$$\oint \mathrm{d}u\, (\mathbf{p} \cdot \delta \mathbf{X} + \mathbf{P} \cdot \delta \dot{\mathbf{X}}) = \oint \mathrm{d}u\, \sqrt{h}\, l_a \left\{ \kappa \left[(\nabla^a K)\mathbf{n} + \left(\frac{1}{2}K^2 g^{ab} - KK^{ab} \right) \mathbf{e}_b \right] \right.$$
$$\left. + \beta(Kg^{ab} - K^{ab})\mathbf{e}_b + \sigma \mathbf{e}^a - \frac{\mathsf{P}}{3}[(\mathbf{n} \cdot \mathbf{X})\mathbf{e}^a - (\mathbf{e}^a \cdot \mathbf{X})\mathbf{n}] \right\} \cdot \delta \mathbf{X}$$
$$- \oint \mathrm{d}u\, \sqrt{h}\, l^a(\kappa K + \beta)\mathbf{n} \cdot \nabla_a \delta \mathbf{X}. \tag{47}$$

The terms in parenthesis spanning the first two lines contribute to the momentum $\mathbf{p}$. The third line needs some massaging to bring it into the form (45); we use the definition of the velocity (6), to decompose $l^a \nabla_a \delta \mathbf{X} = N^{-1}(\delta \dot{\mathbf{X}} - N_{\parallel} \delta \mathbf{X}')$. The third line of (47) thus contributes to

both $\mathbf{P}$ and $\mathbf{p}$:

$$-\oint \mathrm{d}u\,\sqrt{h}(\kappa K\mathbf{n} + \beta\mathbf{n})l^a\nabla_a\delta\mathbf{X} = \oint \mathrm{d}u\,\mathbf{p}\cdot\left(\delta\dot{\mathbf{X}} + N_\parallel(\delta\mathbf{X})'\right)$$

$$= \oint \mathrm{d}u[\mathbf{P}\cdot\delta\dot{\mathbf{X}} - (N_\parallel\mathbf{P})'\cdot\delta\mathbf{X}]. \tag{48}$$

Definition (44) of the momentum $\mathbf{P}$ is recovered, and we identify the momentum $\mathbf{p}$ conjugate to $\mathbf{X}$ as

$$\mathbf{p} = \sqrt{h}l_a\left\{\kappa\left[\left(\frac{1}{2}K^2g^{ab} - KK^{ab}\right)\mathbf{e}_b + (\nabla^a K)\mathbf{n}\right] + \beta(Kg^{ab} - K^{ab})\mathbf{e}_b\right\}$$

$$+ \sigma\sqrt{h}\mathbf{l} - \frac{\mathsf{P}}{3}\mathbf{X}\times\mathbf{X}' + (N_\parallel\mathbf{P})'. \tag{49}$$

The momentum $\mathbf{p}$ also transforms as a density under reparametrization of the curve. Note that it depends on $\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}$ and $\mathbf{X}$ with three dots. For $\kappa = \beta = 0$ the momentum for a soap bubble (29) is recovered. We also anticipate that one of Hamilton's equations will reproduce this expression (see (80)). Geometrically, the momentum $\mathbf{p}$ given by (49) is very simple; $\mathbf{p}$ is also related in a very direct way to the conserved stress for fluid membranes derived by two of us in [14]. To illustrate the relationship, it is convenient to set P to vanish. The conserved stress for the energy (2) is

$$\mathbf{f}^a = \kappa\left[\left(KK^{ab} - \frac{1}{2}K^2g^{ab}\right)\mathbf{e}_b - (\nabla^a K)\mathbf{n}\right] + \beta(K^{ab} - Kg^{ab})\mathbf{e}_b - \sigma\mathbf{e}^a. \tag{50}$$

Its divergence gives the shape equation as a conservation law:

$$\nabla_a\mathbf{f}^a = E\mathbf{n} = 0, \tag{51}$$

where E is given by the lhs of (4). We exploit the completeness of the surface tangent vectors $g^{ab} = l^al^b + t^at^b$, where $l_a = \mathbf{l}\cdot\mathbf{e}_a$, and $t_a = \mathbf{t}\cdot\mathbf{e}_a$ to decompose the stress as

$$\mathbf{f}^a = \mathbf{f}\,l^a + \mathbf{g}\,t^a. \tag{52}$$

The canonical momentum $\mathbf{p}$ is given by (minus) the projection of the stress along the normal to the curve l^a, up to a total divergence:

$$\mathbf{p} = -\sqrt{h}\,\mathbf{f} + (N_\parallel\mathbf{P})'. \tag{53}$$

Note that integrated over the closed curve:

$$\oint \mathrm{d}u\,\mathbf{p} = -\oint \mathrm{d}u\,\sqrt{h}l_a\mathbf{f}^a. \tag{54}$$

The integrated momentum is the total force acting on the region enclosed by the curve; if there are no external forces acting and $\mathsf{P} = 0$, this integral will vanish.

One of Hamilton's equations will be an equation for $\dot{\mathbf{p}}$ (see (81)). Modulo the remaining canonical equations, this equation should reproduce the conservation law. Using the decomposition of the stress tensor (52) in (51), we find

$$N\sqrt{h}\nabla_a\mathbf{f}^a = \partial_t(\sqrt{h}\mathbf{f}) + (N\mathbf{g} - N_\parallel\sqrt{h}\,\mathbf{f})', \tag{55}$$

where we also make use of the identities (A.11), (A.12) given in appendix A. If we now use (53), we find that the (densitized) shape equation can be cast as a continuity equation,

$$\sqrt{g}E\mathbf{n} = \sqrt{g}\nabla_a\mathbf{f}^a = -\dot{\mathbf{p}} + \mathbf{m}' = 0, \tag{56}$$

with a current $\mathbf{m}$ given by

$$\mathbf{m} = \partial_t(N_\parallel\mathbf{P}) + N\mathbf{g} + N_\parallel\mathbf{p} - N_\parallel(N_\parallel\mathbf{P})'. \tag{57}$$

If now we restore a non-vanishing pressure P, the continuity equation (56) acquires a source term, see (81).

5. Hamiltonian and constraints

The canonical Hamiltonian is given by a Legendre transformation of the Lagrangian $L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}]$, as given by (16), with respect to both the velocity $\dot{\mathbf{X}}$ and the acceleration $\ddot{\mathbf{X}}$,

$$H_0[\mathbf{X}, \mathbf{p}; \dot{\mathbf{X}}, \mathbf{P}] = \oint \mathrm{d}u \left(\mathbf{P} \cdot \ddot{\mathbf{X}} + \mathbf{p} \cdot \dot{\mathbf{X}} \right) - L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}], \tag{58}$$

where the definition of the momentum $\mathbf{P}$ is used to express the acceleration $\ddot{\mathbf{X}}$ in terms of the phase-space variables. It should be emphasized that the term $\mathbf{p} \cdot \dot{\mathbf{X}}$ is left alone; the only place $\mathbf{p}$ appears in H_0 is in the first term. The only tricky bit is the elimination of $\ddot{\mathbf{X}}$. To do this, first note that from the definition of $\mathbf{P}$ (44), and the decomposition of the mean curvature (13), we have

$$\mathbf{P} \cdot \ddot{\mathbf{X}} = \frac{\kappa \sqrt{h}}{N^3} (\mathbf{n} \cdot \ddot{\mathbf{X}})^2 - \frac{\sqrt{h}}{N^3} (\kappa J + \beta N^2)(\mathbf{n} \cdot \ddot{\mathbf{X}}); \tag{59}$$

the quantity J, defined in (14), does not depend on the acceleration. Setting

$$L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}] = \oint \mathrm{d}u \, \mathcal{L}(\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}), \tag{60}$$

we find that

$$\mathbf{P} \cdot \ddot{\mathbf{X}} - \mathcal{L}(\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}) = \sqrt{h} N \left[\frac{\kappa}{2N^4} (\mathbf{n} \cdot \ddot{\mathbf{X}})^2 - \frac{\kappa}{2N^4} J^2 - \frac{\beta}{N^2} J - \sigma + \frac{\mathsf{P}}{3} \mathbf{n} \cdot \mathbf{X} \right]; \tag{61}$$

the acceleration has been isolated in a single term. We can express this term with respect to the phase-space variables by inverting the definition for $(\mathbf{n} \cdot \ddot{\mathbf{X}})^2$:

$$\mathbf{P} = \frac{\sqrt{h}}{N^3} [\kappa (\mathbf{n} \cdot \ddot{\mathbf{X}}) - (\kappa J + \beta N^2)] \mathbf{n} \tag{62}$$

implies

$$(\mathbf{n} \cdot \ddot{\mathbf{X}})^2 = \frac{N^6}{\kappa^2 h} \left[\mathbf{P} + \frac{\sqrt{h}}{N} \left(\frac{\kappa}{N^2} J + \beta \right) \mathbf{n} \right]^2. \tag{63}$$

Substituting this expression into (61), we identify the canonical Hamiltonian as

$$H_0[\mathbf{X}, \mathbf{p}; \dot{\mathbf{X}}, \mathbf{P}] = \oint \mathrm{d}u \left[\mathbf{p} \cdot \dot{\mathbf{X}} + \frac{N^3}{2\kappa \sqrt{h}} \mathbf{P}^2 + \left(J + N^2 \frac{\beta}{\kappa} \right) \mathbf{P} \cdot \mathbf{n} \right.$$
$$\left. + \frac{N \sqrt{h} \beta^2}{2\kappa} - \sigma N \sqrt{h} + \frac{\mathsf{P}}{3} N \sqrt{h} (\mathbf{n} \cdot \mathbf{X}) \right]. \tag{64}$$

Unlike its soap bubble counterpart, this Hamiltonian does not vanish at the level of its definition, although it turns out that it does vanish anyway, see below. It is quadratic in the higher momentum $\mathbf{P}$; it is linear in $\mathbf{p}$—indeed, $\mathbf{p}$ only appears in the first term. The dependence on $\dot{\mathbf{X}}$ is rather more complicated: linearly in the first term through $\mathbf{p} \cdot \dot{\mathbf{X}}$, and nonlinearly everywhere else through its appearance in N, $\mathbf{n}$ and J. The dependence on $\mathbf{X}$ is similarly complicated; it appears always through its spatial derivatives with respect to the parameter u along the curve $\mathcal{C}$ with the exception of the last term proportional to the pressure P in which $\mathbf{X}$ appears directly. While this dependence does not break translation invariance, it signals that $\dot{\mathbf{p}}$ will not be a divergence.

The reparametrization invariance of the energy manifests itself, at a Hamiltonian level, in the presence of constraints: the phase-space variables are not all independent at a fixed value of the parameter t. Primary constraints appear because it is impossible to invert for the higher momentum $\mathbf{P}$ in terms of the acceleration $\ddot{\mathbf{X}}$, just as, in section 4, it was impossible to invert

for the momentum $\mathbf{p}$ in terms of the velocity $\dot{\mathbf{X}}$. Note, however, that this did not hinder the completion of the Legendre transformation. The primary constraints are identified by the null eigenvectors of the Hessian of the Lagrangian with respect to the higher derivatives

$$\mathcal{H}_{ij} = \frac{\delta^2 L[\mathbf{X}, \dot{\mathbf{X}}, \ddot{\mathbf{X}}]}{\delta \ddot{X}^i \delta \ddot{X}^j} = -\kappa \frac{\sqrt{h}}{N^3} n_i n_j. \tag{65}$$

There are two null eigenvectors, $\dot{\mathbf{X}}$ and $\mathbf{X}'$; we therefore identify the two primary constraints

$$C_1 = \mathbf{P} \cdot \dot{\mathbf{X}} = 0, \tag{66}$$

$$C_2 = \mathbf{P} \cdot \mathbf{X}' = 0. \tag{67}$$

Their geometrical content is simple: the momentum $\mathbf{P}$ is normal to the surface.

The Hamiltonian function that generates the motion is given by adding the primary constraints to the canonical Hamiltonian (64), giving the total Hamiltonian

$$H[\mathbf{X}, \mathbf{p}; \dot{\mathbf{X}}, \mathbf{P}] = H_0[\mathbf{X}, \mathbf{p}; \dot{\mathbf{X}}, \mathbf{P}] + \oint \mathrm{d}u \, (\lambda_1 C_1 + \lambda_2 C_2) , \tag{68}$$

where $\lambda_1 = \lambda_1(u, t), \lambda_2 = \lambda_2(u, t)$ are arbitrary Lagrange multipliers that enforce the constraints.

The Poisson bracket appropriate for this higher derivative system is, for any two functions on the phase space f, g,

$$\{f, g\} = \oint \mathrm{d}u \left[\frac{\delta f}{\delta \dot{\mathbf{X}}} \cdot \frac{\delta g}{\delta \mathbf{P}} + \frac{\delta f}{\delta \mathbf{X}} \cdot \frac{\delta g}{\delta \mathbf{p}} - (f \leftrightarrow g) \right]. \tag{69}$$

The time derivative of any function on phase space f is then given by its Poisson bracket with the total Hamiltonian (68)

$$\dot{f} = \{f, H\}. \tag{70}$$

We have identified the primary constraints on the phase-space variables. For consistency, these constraints must be conserved in time. This requires us to introduce new *secondary* constraints. First, note that the primary constraints are in involution under the Poisson bracket, i.e. $\{C_1, C_2\} = C_2$. The conservation in time of the primary constraints (66) and (67) implies the existence of the secondary constraints, with $H_0 = \oint \mathrm{d}u \, \mathcal{H}_0$,

$$S_1 = \mathcal{H}_0 = 0, \tag{71}$$

$$S_2 = \mathbf{p} \cdot \mathbf{X}' + \mathbf{P} \cdot \dot{\mathbf{X}}' = 0. \tag{72}$$

A detailed proof that these constraints follow from the conservation in time of the primary constraints is provided in appendix B. As we will show below, a far simpler derivation follows directly from reparametrization invariance.

Among the secondary constraints is the vanishing of the canonical Hamiltonian, the hallmark of reparametrization invariance. Together, the two secondary constraints completely fix the two tangential components of the momentum $\mathbf{p}$, $\mathbf{p} \cdot \dot{\mathbf{X}}$ and $\mathbf{p} \cdot \mathbf{X}'$. There are no other, tertiary constraints—the four constraints we have identified are in involution under the Poisson brackets.

The secondary constraints are the generators of reparametrizations. In particular, S_2 generates reparametrizations tangential to the curve $\mathcal{C}$, as follows from the fact that if we denote by $\mathbf{Z}$ any of the phase-space variables,

$$\delta \mathbf{Z} = \{\mathbf{Z}, S_2\} = \mathbf{Z}'. \tag{73}$$

On the other hand, $S_1 = -\mathcal{H}_0$ generates reparametrizations off the curve $\mathcal{C}$, as it will become clear in the next section, where we consider the evolution it determines. The details of the model will enter through $\mathcal{H}_0$.

Conversely, one can show that reparametrization invariance implies all four constraints: the primary constraints (66) and (67) as well as the secondary constraints (71), (72). To see this, let us re-examine the expression (45) for the first variation of the energy. Consider first a temporal reparametrization $\delta \mathbf{X} = \omega(u, t)\dot{\mathbf{X}}$, where the parameter ω is some function of the parameters u and t. In equilibrium, we have for the right-hand side of (45)

$$\oint du\,(\mathbf{p} \cdot \delta \mathbf{X} + \mathbf{P} \cdot \delta \dot{\mathbf{X}}) = \oint du\,\omega(\mathbf{p} \cdot \dot{\mathbf{X}} + \mathbf{P} \cdot \ddot{\mathbf{X}}) + \oint du\,\dot{\omega}\mathbf{P} \cdot \dot{\mathbf{X}}, \qquad (74)$$

On the other hand, for the left-hand side of (45), we have

$$\delta F[\mathbf{X}] = \oint du\,\omega L. \qquad (75)$$

We conclude that

$$\oint du\,\omega \mathcal{H}_0 + \dot{\omega} C_1 = 0. \qquad (76)$$

Because ω and $\dot{\omega}$ are completely arbitrary, we conclude that the invariance of F under a redefinition of time implies the constraints (66) and (71). In exactly the same way, reparametrization invariance tangential to the curve implies the constraints (67) and (72). The structure of the constraints depends only on the number of derivatives; it is independent of the details of the model.

This analysis also clarifies the role of the primary constraints. In the transformation for the velocity induced by $\delta \mathbf{X} = \omega \dot{\mathbf{X}}$, $\delta \dot{\mathbf{X}} = \omega \ddot{\mathbf{X}} + \dot{\omega} \dot{\mathbf{X}}$, the second term is a scaling of $\dot{\mathbf{X}}$. The constraint C_1 is the generator of this scale transformation. An equal and opposite scaling of $\mathbf{P}$ is required to preserve its Poisson bracket with $\dot{\mathbf{X}}$.

A result of reparametrization invariance is that the phase-space variables provide a redundant description of our system. The four constraints do, however, permit us to identify the independent degrees of freedom: these are position of the curve $\mathbf{X}$ and its velocity $\dot{\mathbf{X}}$ as well as the normal components of $\mathbf{P}$ and $\mathbf{p}$ (or, equivalently, $\ddot{\mathbf{X}}$ and $\mathbf{X}^{(3)}$ (with three dots)). Whereas both $\mathbf{X}$ and $\dot{\mathbf{X}}$ can be freely specified, the primary constraints kill the tangential components of $\mathbf{P}$ and the secondary constraints fix the tangential components of $\mathbf{p}$ in terms of the remaining canonical variables.

6. Hamilton's equations

In this section, we present the complete set of Hamilton's equations that follow from the Hamiltonian (68). We find it convenient to consider the equations in this order:

$$\partial_t \mathbf{X} = \frac{\delta H}{\delta \mathbf{p}}; \qquad \partial_t \dot{\mathbf{X}} = \frac{\delta H}{\delta \mathbf{P}}; \qquad \partial_t \mathbf{P} = -\frac{\delta H}{\delta \ddot{\mathbf{X}}}; \qquad \partial_t \mathbf{p} = -\frac{\delta H}{\delta \mathbf{X}}. \qquad (77)$$

There is one equation for each phase-space variable; the equations are first order in time.

(1) The first equation is

$$\partial_t \mathbf{X} = \delta H / \delta \mathbf{p} = \dot{\mathbf{X}}. \qquad (78)$$

Note that the only dependence on $\mathbf{p}$ in the Hamiltonian is through the linear term $\mathbf{p} \cdot \dot{\mathbf{X}}$ appearing in the canonical Hamiltonian H_0 (64). Although it may appear to be a mere identity, its content is the identification of the canonical variable $\dot{\mathbf{X}}$ with the time derivative of $\mathbf{X}$.

(2) The second of Hamilton's equation $\partial_t \dot{\mathbf{X}} = \delta H/\delta \mathbf{P}$ is (see appendix B):

$$\partial_t \dot{\mathbf{X}} = \ddot{\mathbf{X}} = \frac{N^3}{\kappa \sqrt{h}} \mathbf{P} + \left(J + N^2 \frac{\beta}{\kappa} \right) \mathbf{n} + \lambda_1 \dot{\mathbf{X}} + \lambda_2 \mathbf{X}'. \tag{79}$$

Note that the rhs does not depend on the momentum $\mathbf{p}$ conjugate to $\mathbf{X}$. The content of this equation is to identify the momentum $\mathbf{P}$ in terms of $\ddot{\mathbf{X}}$, $\dot{\mathbf{X}}$ and $\mathbf{X}$, reproducing the expression (44). This equation also identifies the form of the Lagrange multipliers λ_1 and λ_2. As we show in the next section, they are proportional to the tangential components of the acceleration $\ddot{\mathbf{X}}$.

(3) For the third of Hamilton's equation $\partial_t \mathbf{P} = -\delta H/\delta \dot{\mathbf{X}}$, we obtain (see appendix C):

$$\partial_t \mathbf{P} = -\mathbf{p} + 2h^{-1}(\mathbf{p} \cdot \mathbf{X}')\mathbf{X}' + 2(N_\| \mathbf{P})' + \{h^{-1}N^{-1}[2N_\| h(\mathbf{l} \cdot \dot{\mathbf{X}}') - \dot{\mathbf{X}}^2(\mathbf{l} \cdot \mathbf{X}'')] - \lambda_1\}\mathbf{P}$$

$$+ 2h^{-1}(\mathbf{P} \cdot \mathbf{X}'')\dot{\mathbf{X}} - \left[\frac{3N^2}{2\kappa \sqrt{h}} \mathbf{P}^2 + \frac{2N\beta}{\kappa}(\mathbf{P} \cdot \mathbf{n}) + \frac{\beta^2 \sqrt{h}}{2\kappa} - \sigma \sqrt{h} \right] \mathbf{l} - \frac{\mathsf{P}}{3} \mathbf{X} \times \mathbf{X}'. \tag{80}$$

This equation identifies the momentum $\mathbf{p}$ in terms of $\mathbf{X}$, $\dot{\mathbf{X}}$, $\mathbf{P}$ and $\dot{\mathbf{P}}$. It is independent of λ_2. This presentation of $\mathbf{p}$ is very different from the form written in (49) where it is cast as a functional of $\mathbf{X}$, $\dot{\mathbf{X}}$, $\ddot{\mathbf{X}}$ and $\mathbf{X}$ with three dots. A little work is required to establish that indeed the two are the same $\mathbf{p}$. We will return to this issue in the next section.

At this point, it is worth emphasizing that the secondary constraints identified in the previous section, (71) and (72), specify the tangential part of $\mathbf{p}$ in terms of the remaining phase-space variables, and initial data will need to be chosen accordingly.

(4) Finally, the fourth Hamilton equation $\partial_t \mathbf{p} = -\delta H/\delta \mathbf{X}$ is

$$\partial_t \mathbf{p} = \dot{\mathbf{p}} = -\mathbf{m}' - \frac{\mathsf{P}}{3} N \sqrt{h} \mathbf{n}, \tag{81}$$

where the current $\mathbf{m}$ is given by

$$\mathbf{m} = \left[\frac{3N^2}{2\kappa \sqrt{h}} N_\| \mathbf{P}^2 + \frac{2\beta}{\kappa} N N_\| (\mathbf{P} \cdot \mathbf{n}) - 2Nh^{-1}(\mathbf{P} \cdot \dot{\mathbf{X}}') + \sqrt{h} N_\| \left(\frac{\beta^2}{2\kappa} - \sigma \right) \right] \mathbf{l}$$

$$+ \left[h^{-3/2} \frac{N^3}{2\kappa} \mathbf{P}^2 - h^{-2} \dot{\mathbf{X}}^2 (\mathbf{P} \cdot \mathbf{X}'') + 2h^{-1} N_\| (\mathbf{P} \cdot \dot{\mathbf{X}}') - h^{-1/2} N \left(\frac{\beta^2}{2\kappa} - \sigma \right) \right] \mathbf{X}'$$

$$+ \frac{1}{N\sqrt{h}} [h^{-1} \dot{\mathbf{X}}^2 (\mathbf{n} \times \dot{\mathbf{X}} \cdot \mathbf{X}'') - 2N_\| (\mathbf{n} \times \dot{\mathbf{X}} \cdot \dot{\mathbf{X}}')] \mathbf{P} - (\dot{\mathbf{X}}^2 h^{-1} \mathbf{P})' - \lambda_2 \mathbf{P} + \frac{\mathsf{P}}{3} \mathbf{X} \times \dot{\mathbf{X}}. \tag{82}$$

Modulo the other Hamilton's equations, which establish the relationships between the dynamical variables appearing on the rhs, this is the shape equation (4) cast in canonical form. We will show this explicitly in the next section. Note that (81) assumes the form of a continuity equation. The origin of the source term is the explicit dependence of the Hamiltonian H on $\mathbf{X}$ appearing in the volume when the pressure P is non-vanishing.

To summarize, Hamilton equations (78), (79), (80) and (81) together with the primary constraints (66), (67), and the secondary constraints (71), (72), provide an alternative formulation of the shape equation (4). Just as it does for the Einstein equations in general relativity, this formulation calls for a change of perspective. We started with a surface satisfying the shape equation. There is now no surface, only a curve.

The recipe for reconstructing a surface is simple: (i) We choose any closed curve in space $(\mathbf{X}(0, u))$. (ii) We are free to specify its velocity $\dot{\mathbf{X}}(0, u)$. At this point we have defined a basis in space adapted to the curve given by the tangent to the curve, $\mathbf{X}'(0, u)$, $\dot{\mathbf{X}}(0, u)$ and their cross product, proportional to the unit normal $\mathbf{n}(0, u)$. The remaining initial data on this curve must be consistent with the constraints. (iii) To satisfy the primary constraints (66) and (67), the momentum $\mathbf{P}$ is chosen to be orthogonal both to $\dot{\mathbf{X}}$ and to the tangent to the curve $\mathbf{X}'$. (iv) The momentum $\mathbf{p}$ is constrained by the secondary constraints (71) and (72) which

determine its two tangential components in terms of the initial data we have already specified. (Note that $\mathbf{p}$ must also be consistent with the integrability condition associated with a closed curve given by (54)). (v) We choose appropriate values for the two functions λ_1 and λ_2—this corresponds to a choice of coordinates. As we show in the next section, they are proportional to the tangential components of $\ddot{\mathbf{X}}$. (vi) We now let the system evolve according to Hamilton's equations. An equilibrium surface $\mathbf{X}(u, t)$ satisfying the shape equation will be generated.

7. Shape equation from Hamilton's equations with constraints

In this section, we show how the Hamilton equations, together with the constraints, combine to reproduce the shape equation (4).

The second Hamilton equation (79) identifies $\mathbf{P}$ and the form of the Lagrange multipliers. We dot (79) with the normal $\mathbf{n}$, and we use the primary constraints (66), (67), to obtain

$$N^3 \mathbf{P} \cdot \mathbf{n} = \kappa \sqrt{h} (\ddot{\mathbf{X}} \cdot \mathbf{n} - J) - N^2 \sqrt{h} \beta. \tag{83}$$

As the primary constraints tell us that $\mathbf{P}$ is purely normal to the surface, using the expression (13) for the mean curvature K, we recover the expression (44) for $\mathbf{P}$.

To obtain the form of the Lagrange multipliers we dot (79) with $\dot{\mathbf{X}}$ and $\mathbf{X}'$, and again use the primary constraints (66), (67), so that we find

$$\lambda_1 = \frac{\dot{\mathbf{X}} \cdot \ddot{\mathbf{X}}}{\dot{\mathbf{X}}^2}, \tag{84}$$

$$\lambda_2 = h^{-1} \mathbf{X}' \cdot \ddot{\mathbf{X}} - N_\parallel \lambda_1 = \frac{N}{\sqrt{h} \dot{\mathbf{X}}^2} \mathbf{n} \times \dot{\mathbf{X}} \cdot \ddot{\mathbf{X}}. \tag{85}$$

The first tells us that λ_1 has the geometrical meaning of the affine connection along the integral curve of $\dot{\mathbf{X}}$; the second that λ_2 is proportional to the tangential component of the acceleration $\ddot{\mathbf{X}}$ orthogonal to the velocity $\dot{\mathbf{X}}$. Therefore, for this higher derivative system, the components of the acceleration tangential to the surface are arbitrary; they are the gauge part of the evolution, whereas the normal component is proportional to the momentum $\mathbf{P}$. In the case of a soap bubble, the Lagrange multipliers were proportional to the components of the velocity—this is its natural higher order generalization.

The third Hamilton equation (80) identifies the form of the momentum $\mathbf{p}$, as given by (49). To see this is not immediate. To facilitate the comparison, we first consider (49). We use the Gauss–Weingarten equation (26), and the expression (44) for $\mathbf{P}$, to obtain for $\mathbf{p}$

$$\mathbf{p} = \sqrt{h} l_a \left[\kappa \left(\frac{1}{2} K^2 g^{ab} - 2K K^{ab} \right) + \beta (K g^{ab} - 2K^{ab}) \right] \mathbf{e}_b - \dot{\mathbf{P}} + 2(N_\parallel \mathbf{P})'$$
$$- \left[N_\parallel{}' + \frac{N^2}{\sqrt{h}} l^a \nabla_a \left(\frac{\sqrt{h}}{N} \right) \right] \mathbf{P} + \sigma \sqrt{h} \mathbf{l} - \frac{\mathsf{P}}{3} \mathbf{X} \times \mathbf{X}'. \tag{86}$$

Now using the completeness relation on the surface $g^{ab} = l^a l^b + t^a t^b$, we have that

$$K^{ab} l_a \mathbf{e}_b = K \mathbf{l} + \frac{1}{hN} [(\mathbf{n} \cdot \mathbf{X}'') \dot{\mathbf{X}} - (\mathbf{n} \cdot \dot{\mathbf{X}}') \mathbf{X}'], \tag{87}$$

and inserting this expression into (86) we obtain the alternative expression for $\mathbf{p}$

$$\mathbf{p} = \sqrt{h} \kappa \left\{ -\frac{3}{2} K^2 \mathbf{l} - 2h^{-1} N^{-1} K [(\mathbf{n} \cdot \mathbf{X}'') \dot{\mathbf{X}} - h^{-1} N^{-1} (\mathbf{n} \cdot \dot{\mathbf{X}}') \mathbf{X}'] \right\}$$
$$- \beta \{ \sqrt{h} K \mathbf{l} + 2h^{-1/2} N^{-1} [(\mathbf{n} \cdot \mathbf{X}'') \dot{\mathbf{X}} - (\mathbf{n} \cdot \dot{\mathbf{X}}') \mathbf{X}'] \} - \dot{\mathbf{P}} + 2(N_\parallel \mathbf{P})'$$
$$- \left[N_\parallel{}' + \frac{N^2}{\sqrt{h}} l^a \nabla_a \left(\frac{\sqrt{h}}{N} \right) \right] \mathbf{P} + \sigma \sqrt{h} \mathbf{l} - \frac{\mathsf{P}}{3} \mathbf{X} \times \mathbf{X}'. \tag{88}$$

Using the information gathered from the second Hamilton equation (79), i.e. (44) for the momentum $\mathbf{P}$, and (84) for the Lagrange multiplier λ_1, it is a simple matter of algebra to see that the third Hamilton equation (80) coincides with the expression (88) for $\mathbf{p}$.

Finally, the fourth Hamilton equation (81) is (56), that we have derived in section 4 from the conservation of the stress tensor at equilibrium. To see this requires using the specific form $\mathbf{P}$, λ_1, λ_2 in the expression (82) for the current $\mathbf{m}$, and comparison with the right-hand side of the alternative expression (57).

8. Concluding remarks

In this paper, we have presented a Hamiltonian formulation of the shape equation for arbitrary, not necessarily axisymmetric, configurations of lipid vesicles. In this description the surface geometry is reconstructed from a closed curve. This is possible because the conserved internal stresses which underpin the equilibrium geometry are transmitted across closed curves; the shape equation is a conservation law for these stresses.

This formulation of the shape equation offers a completely new approach for constructing equilibrium configurations based on the numerical solution of Hamilton's equations. Whether its implementation turns out to be tractable, in practice, remains to be seen. There is no problem generating equilibrium surfaces: any initial data consistent with the constraints will do this. The subtlety is identifying initial data that are consistent with a surface which closes smoothly. In general, the curve will self-intersect and singularities will arise. The initial data will thus need to be tuned accordingly. This problem is a global one. Progress is likely to be limited until a second problem is tackled: what is the most appropriate choice of Lagrange multipliers for any given initial data? This will fix the parametrization of the surface. There may not be a single choice which is appropriate everywhere. In this sense, the present paper ought to be considered as a first step. Comparison with the Hamiltonian formulation of general relativity, first introduced in the sixties by Arnowitt, Deser and Misner, which provides the basic theoretical framework for the numerical solution of Einstein's equations, is not out of place. Over 40 years later, despite the extensive computational resources now at our disposal, problems not unlike those mentioned here continue to present a challenge.

Acknowledgments

Appendix A

In this appendix, we collect various geometrical formulae that are useful at intermediate stages of the calculations that we have performed. The Frenet–Serret equations for the curve $\mathcal{C}$, seen as living on Σ are, with $\nabla_s = t^a \nabla_a$:

$$\nabla_s t^a = k l^a, \tag{A.1}$$

$$\nabla_s l^a = -k t^a, \tag{A.2}$$

where k is the geodesic curvature for the curve. The Frenet–Serret equations for the curve $\mathcal{C}$ seen as living in space are

$$\nabla_s \mathbf{t} = k_1 \mathbf{l} + k_2 \mathbf{n} \tag{A.3}$$

$$\nabla_s \mathbf{l} = -k_1 \mathbf{t} + k_3 \mathbf{n} \tag{A.4}$$

$$\nabla_s \mathbf{n} = -k_2 \mathbf{t} - k_3 \mathbf{l}, \tag{A.5}$$

where $k_1 = k$ is the geodesic curvature, and k_2, k_3 are given by the projections of the surface extrinsic curvature by $k_2 = -K_{ab} t^a t^b$, $k_3 = -K_{ab} t^a l^b$.

The evolution in the parameter t of the basis $\{\mathbf{X}', \mathbf{l}, \mathbf{n}\}$ can be derived from the fact that partial derivatives commute, so that $\dot{\mathbf{X}}' = (\dot{\mathbf{X}})'$. It follows that

$$\dot{\mathbf{X}}' = (\partial_u N + N_\| k)\mathbf{l} + (\partial_u N_\| - h^{-1} N k)\mathbf{X}' + (\mathbf{n} \cdot \dot{\mathbf{X}}')\mathbf{n}, \tag{A.6}$$

$$\dot{\mathbf{l}} = -h^{-1}(N' + N_\| k)\mathbf{X}' + N^{-1}[(\mathbf{n} \cdot \ddot{\mathbf{X}}) - N_\|(\mathbf{n} \cdot \dot{\mathbf{X}}')]\mathbf{n}, \tag{A.7}$$

$$\dot{\mathbf{n}} = -h^{-1}(\mathbf{n} \cdot \dot{\mathbf{X}}')\mathbf{X}' - N^{-1}[(\mathbf{n} \cdot \ddot{\mathbf{X}}) - N_\|(\mathbf{n} \cdot \dot{\mathbf{X}}')]\mathbf{l}. \tag{A.8}$$

Note that

$$\partial_t \sqrt{h} = -\sqrt{h} N k + \sqrt{h} \partial_u N_\|. \tag{A.9}$$

The acceleration is

$$\ddot{\mathbf{X}} = (\dot{N}_\| - h^{-1} N \partial_u N + N_\| \partial_u N_\| - 2h^{-1} N N_\| k)\mathbf{X}' + (\dot{N} + N_\| \partial_u N + N_\|^2 k)\mathbf{l} - (\mathbf{n} \cdot \ddot{\mathbf{X}})\mathbf{n}. \tag{A.10}$$

We also note the identities

$$\nabla_a l^a = -k \tag{A.11}$$

$$\nabla_a t^a = N^{-1} \nabla_s N. \tag{A.12}$$

Appendix B

In this appendix, we show how the secondary constraints (71), (72) follow from the conservation in time of the primary constraints (66), (67). The first thing to note is that the primary constraints are in involution under the Poisson bracket (69),

$$\{C_1, C_2\} = C_2 \approx 0, \tag{B.1}$$

where the symbol $\approx$ denotes equality modulo the constraints themselves.

The time derivative of the first primary constraint (66) is

$$\dot{C}_1 = \{C_1, H\} \approx \{C_1, H_0\} = \mathbf{P} \cdot \frac{\delta H_0}{\delta \mathbf{P}} - \dot{\mathbf{X}} \cdot \frac{\delta H_0}{\delta \dot{\mathbf{X}}}. \tag{B.2}$$

We need to evaluate the functional derivatives of the canonical Hamiltonian functional (64). For the functional derivative of the canonical Hamiltonian with respect to $\mathbf{P}$, we immediately have

$$\frac{\delta H_0}{\delta \mathbf{P}} = \frac{N^3}{\kappa \sqrt{h}} \mathbf{P} + \left(J + N^2 \frac{\beta}{\kappa} \right) \mathbf{n}. \tag{B.3}$$

In order to evaluate the functional derivative of H_0 with respect to the velocity $\dot{\mathbf{X}}$, we hold $\mathbf{X}$ fixed, and consider the variation with respect to $\dot{\mathbf{X}}$ of the geometric quantities that appear in the canonical Hamiltonian:

$$\delta N = \mathbf{l} \cdot \delta \dot{\mathbf{X}}, \qquad \delta N_\| = h^{-1} \mathbf{X}' \cdot \delta \dot{\mathbf{X}}, \qquad \delta \mathbf{n} = -N^{-1}(\mathbf{n} \cdot \delta \dot{\mathbf{X}})\mathbf{l}.$$

For the part of the mean curvature that does not depend on the acceleration $\ddot{\mathbf{X}}$, defined as J in (14), it follows that

$$\delta J = h^{-1}\{2(\mathbf{n}\cdot\dot{\mathbf{X}}')\mathbf{X}' + N^{-1}[\dot{\mathbf{X}}^2(\mathbf{l}\cdot\mathbf{X}'') - 2N_{\parallel}h(\mathbf{l}\cdot\dot{\mathbf{X}}')]\mathbf{n} - 2(\mathbf{n}\cdot\mathbf{X}'')\dot{\mathbf{X}}\}\cdot\delta\dot{\mathbf{X}} + 2N_{\parallel}\mathbf{n}\cdot(\delta\dot{\mathbf{X}})'.$$

Using these expressions we have

$$\begin{aligned}
\frac{\delta H_0}{\delta\dot{\mathbf{X}}} &= \mathbf{p} + \left[\frac{3N^2}{2\kappa\sqrt{h}}\mathbf{P}^2 + \frac{2N\beta}{\kappa}(\mathbf{P}\cdot\mathbf{n}) + \frac{\beta^2\sqrt{h}}{2\kappa} - \sigma\sqrt{h}\right]\mathbf{l} + 2h^{-1}(\mathbf{n}\cdot\dot{\mathbf{X}}')(\mathbf{P}\cdot\mathbf{n})\mathbf{X}' \\
&\quad - 2[N_{\parallel}(\mathbf{P}\cdot\mathbf{n})\mathbf{n}]' + h^{-1}N^{-1}(\mathbf{P}\cdot\mathbf{n})[\dot{\mathbf{X}}^2(\mathbf{l}\cdot\mathbf{X}'' - 2N_{\parallel}h(\mathbf{l}\cdot\dot{\mathbf{X}}'))]\mathbf{n} \\
&\quad - 2h^{-1}(\mathbf{n}\cdot\mathbf{X}'')(\mathbf{P}\cdot\mathbf{n})\dot{\mathbf{X}} + \frac{\mathsf{P}}{3}\mathbf{X}\times\mathbf{X}'.
\end{aligned} \tag{B.4}$$

We can simplify this expression using the completeness relation $\delta^{ij} = n^i n^j + l^i l^j + h^{-1}\dot{X}^i\dot{X}^j$, so that, modulo the constraints, $(\mathbf{P}\cdot\mathbf{n})\mathbf{n}\approx\mathbf{P}$. Hence

$$\begin{aligned}
\frac{\delta H_0}{\delta\dot{\mathbf{X}}} &\approx \mathbf{p} + \left[\frac{3N^2}{2\kappa\sqrt{h}}\mathbf{P}^2 + \frac{2N\beta}{\kappa}(\mathbf{P}\cdot\mathbf{n}) + \frac{\beta^2\sqrt{h}}{2\kappa} - \sigma\sqrt{h}\right]\mathbf{l} + 2h^{-1}(\mathbf{P}\cdot\dot{\mathbf{X}}')\mathbf{X}' - 2(N_{\parallel}\mathbf{P})' \\
&\quad + h^{-1}N^{-1}[\dot{\mathbf{X}}^2(\mathbf{l}\cdot\mathbf{X}'' - 2N_{\parallel}h(\mathbf{l}\cdot\dot{\mathbf{X}}'))]\mathbf{P} - 2h^{-1}(\mathbf{P}\cdot\mathbf{X}'')\dot{\mathbf{X}} + \frac{\mathsf{P}}{3}\mathbf{X}\times\mathbf{X}'
\end{aligned} \tag{B.5}$$

and one finds that the conservation in time of C_1 gives the vanishing of the canonical Hamiltonian density $\mathcal{H}_0$, defined by $H_0 = \oint \mathrm{d}u\,\mathcal{H}_0$:

$$\dot{C}_1 \approx -\mathcal{H}_0 = 0. \tag{B.6}$$

To see that this expression holds it is essential to recognize that

$$J(\mathbf{P}\cdot\mathbf{n}) \approx N_{\parallel}(\mathbf{P}\cdot\dot{\mathbf{X}}') - (N_{\parallel}\mathbf{P})'\cdot\dot{\mathbf{X}} - h^{-1}\dot{\mathbf{X}}^2(\mathbf{P}\cdot\mathbf{X}''), \tag{B.7}$$

where again one uses the fact that $(\mathbf{P}\cdot\mathbf{n})\mathbf{n}\approx\mathbf{P}$, and $(N_{\parallel}\mathbf{P})'\cdot\mathbf{X}'\approx -N_{\parallel}(\mathbf{P}\cdot\dot{\mathbf{X}}')$.

Similarly, the conservation in time of the second primary constraint (67) gives the secondary constraint (72):

$$\dot{C}_2 = \{C_2, H\} \approx \{C_2, H_0\} = -\mathbf{X}'\cdot\frac{\delta H_0}{\delta\dot{\mathbf{X}}} - \dot{\mathbf{X}}\cdot\mathbf{P}' \approx -S_2 = 0. \tag{B.8}$$

Appendix C

In this appendix, we fill in the details of the derivations of the third and fourth Hamilton equations (80) and (81). Consider first the third Hamilton equation, $\dot{\mathbf{P}} = -\delta H/\delta\dot{\mathbf{X}}$. We use (B.5) from appendix B, and we obtain immediately

$$\begin{aligned}
\dot{\mathbf{P}} &= -\mathbf{p} - \left[\frac{3N^2}{2\kappa\sqrt{h}}\mathbf{P}^2 + \frac{2N\beta}{\kappa}(\mathbf{P}\cdot\mathbf{n}) + \frac{\beta^2\sqrt{h}}{2\kappa} - \sigma\sqrt{h}\right]\mathbf{l} + 2\left(N_{\parallel}\mathbf{P}\right)' - 2h^{-1}(\mathbf{P}\cdot\dot{\mathbf{X}}')\mathbf{X}' \\
&\quad + h^{-1}N^{-1}[2N_{\parallel}h(\mathbf{l}\cdot\dot{\mathbf{X}}') - \dot{\mathbf{X}}^2(\mathbf{l}\cdot\mathbf{X}'')]\mathbf{P} + 2h^{-1}(\mathbf{P}\cdot\mathbf{X}'')\dot{\mathbf{X}} \\
&\quad - \frac{\mathsf{P}}{3}\mathbf{X}\times\mathbf{X}' - \lambda_1\mathbf{P}.
\end{aligned} \tag{C.1}$$

Using the secondary constraint (72) in the last term of the first line gives the third Hamilton equation in the form given in the text (80).

Let us turn to the derivation of the fourth Hamilton equation $\dot{\mathbf{p}} = -\delta H/\delta\mathbf{X}$. Now we hold $\dot{\mathbf{X}}$ fixed, and consider a variation of the geometric quantities that appear in the canonical

Hamiltonian w.r.t. **X**:

$$\delta \mathbf{X}' = (\delta \mathbf{X})',$$

$$\delta \mathbf{l} = -N^{-1} N_\parallel [\mathbf{n} \cdot (\delta \mathbf{X})'] \mathbf{n} - h^{-1} [\mathbf{l} \cdot (\delta \mathbf{X})'] \mathbf{X}',$$

$$\delta \mathbf{n} = (N^{-1} N_\parallel \mathbf{l} - h^{-1} \mathbf{X}')[\mathbf{n} \cdot (\delta \mathbf{X})'] = N^{-1} h^{-1/2} (\mathbf{n} \times \dot{\mathbf{X}}) \mathbf{n} \cdot (\delta \mathbf{X})',$$

$$\delta N = -N_\parallel \mathbf{l} \cdot (\delta \mathbf{X})',$$

$$\delta N_\parallel = h^{-1} [N \mathbf{l} \cdot (\delta \mathbf{X})' - N_\parallel \mathbf{X}' \cdot (\delta \mathbf{X})'].$$

For the quantity J this implies

$$\delta J = 2 N h^{-1} (\mathbf{n} \cdot \dot{\mathbf{X}}') \mathbf{l} \cdot (\delta \mathbf{X})' + 2[h^{-2} \dot{\mathbf{X}}^2 (\mathbf{n} \cdot \mathbf{X}'') - N_\parallel h^{-1} (\mathbf{n} \cdot \dot{\mathbf{X}}')] \mathbf{X}' \cdot (\delta \mathbf{X})'$$

$$+ \left[2 \frac{N_\parallel^2}{N} (\mathbf{l} \cdot \dot{\mathbf{X}}') - N^{-1} N_\parallel h^{-1} \dot{\mathbf{X}}^2 (\mathbf{l} \cdot \mathbf{X}'') - 2 N_\parallel h^{-1} (\mathbf{X}' \cdot \dot{\mathbf{X}}') + h^{-2} \dot{\mathbf{X}}^2 (\mathbf{X}' \cdot \mathbf{X}'') \right] \mathbf{n} \cdot (\delta \mathbf{X})'$$

$$- h^{-1} \dot{\mathbf{X}}^2 \mathbf{n} \cdot (\delta \mathbf{X})''. \tag{C.2}$$

Using these expressions, and exploiting again the fact that $(\mathbf{P} \cdot \mathbf{n}) \mathbf{n} \approx \mathbf{P}$, we find that the fourth Hamilton equation is

$$\dot{\mathbf{p}} = -\partial_u \left\{ \left[\frac{3 N^2}{2\kappa \sqrt{h}} N_\parallel \mathbf{P}^2 + \frac{2\beta}{\kappa} N N_\parallel (\mathbf{P} \cdot \mathbf{n}) - 2 N h^{-1} (\mathbf{P} \cdot \mathbf{X}') + \sqrt{h} N_\parallel \left(\frac{\beta^2}{2\kappa} - \sigma \right) \right] \mathbf{l} \right.$$

$$+ \left[h^{-3/2} \frac{N^3}{2\kappa} \mathbf{P}^2 - h^{-2} \dot{\mathbf{X}}^2 (\mathbf{P} \cdot \mathbf{X}'') + 2 h^{-1} N_\parallel (\mathbf{P} \cdot \mathbf{X}') - h^{-1/2} N \left(\frac{\beta^2}{2\kappa} - \sigma \right) \right] \mathbf{u}$$

$$+ \frac{1}{N} [h^{-1} N_\parallel \dot{\mathbf{X}}^2 (\mathbf{l} \cdot \mathbf{X}'') - 2 N_\parallel^2 (\mathbf{l} \cdot \dot{\mathbf{X}}') + 2 N N_\parallel h^{-1} (\mathbf{X}' \cdot \dot{\mathbf{X}}') - h^{-2} N \dot{\mathbf{X}}^2 (\mathbf{X}' \cdot \mathbf{X}'')] \mathbf{P}$$

$$\left. - (\dot{\mathbf{X}}^2 h^{-1} \mathbf{P})' - \lambda_2 \mathbf{P} + \frac{\mathsf{P}}{3} \mathbf{X} \times \dot{\mathbf{X}} \right\} - \frac{\mathsf{P}}{3} N \sqrt{h} \mathbf{n}. \tag{C.3}$$

This gives the fourth Hamilton equation in the form given in the text (81).

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