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Hamilton's equations for a fluid membrane: axial symmetry

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Abstract

Consider a homogeneous fluid membrane, or vesicle, described by the Helfrich–Canham energy, quadratic in the mean curvature. When the membrane is axially symmetric, this energy can be viewed as an ‘action’ describing the motion of a particle; the contours of equilibrium geometries are identified with particle trajectories. A novel Hamiltonian formulation of the problem is presented which exhibits the following two features: (i) the second derivatives appearing in the action through the mean curvature are accommodated in a natural phase space and (ii) the intrinsic freedom associated with the choice of evolution parameter along the contour is preserved. As a result, the phase space involves momenta conjugate not only to the particle position but also to its velocity, and there are constraints on the phase space variables. This formulation provides the groundwork for a field theoretical generalization to arbitrary configurations, with the particle replaced by a loop in space.

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Phospholipid molecules self-assemble in water to form vesicles or membranes [1, 2]. The vesicles are very thin compared to their size so that it is sensible to describe them as surfaces of negligible thickness. Moreover, the vesicle behaves as a two-dimensional fluid: there is no resistance to shear so that the molecules move freely in the plane of the membrane. In a theoretical model of lipid vesicles, this means that the energy can depend *only* on the geometry of this surface. The leading term in the energy is proportional to the integrated square of the mean curvature, penalizing bending [3–5]. The molecular details are essentially irrelevant.

The ‘shape equation’, describing equilibrium geometries [6, 7], is a fourth-order nonlinear PDE. With axial symmetry, the PDE reduces to a nonlinear ODE which, in turn, possesses a first integral [8, 9]. Indeed, it is possible to interpret the energy as an action describing

the motion of a particle. Geometrical contours can be identified with particle trajectories. Building on Deuling and Helfrich's pioneering work in the early 1970s [10], axisymmetric solutions of the shape equation describing an isolated vesicle were pretty well understood by the mid-1990s (see the reviews [11–13]).

Without the symmetry we are less well off. However, with increasing computer power, impressive results can be achieved; Monte Carlo and dynamical triangulation (see, e.g., [14, 15]) will minimize the energy for us. In the latter case, the program Surface Evolver was designed with exactly this sort of problem in mind [16].

At this level, the shape equation is consigned to the status of a curiosity. However, there is a lot of information encoded in the shape equation which can be accessed without having to solve it explicitly. For example, it is not widely known that the shape equation can be cast as a conservation law for the stresses prevailing within the membrane [9]. These stresses are completely geometrical. They transmit forces. It would be difficult to understand the nature of these forces without taking the shape equation apart. In this respect, a computation scheme to solve the shape equation would be a useful complement to energy minimization. The mechanical analogue of the axially symmetric shape equation is most naturally formulated as a Hamiltonian initial value problem. There is no obstacle, in principle, to setting up a field theoretical generalization: instead of a point particle take a closed loop; motion of the loop will generate a surface. Unfortunately, the existing Hamiltonian approaches to solving the axially symmetric shape equation, that use arclength along the contour as a parameter, are tailored very specifically to the symmetry, so they are not very helpful.

In this paper, we present a novel Hamiltonian formulation of the axially symmetric shape equation which takes no shortcuts home. It will, however, admit a field theoretical generalization with the particle replaced by a loop in space [17]. This formulation will involve two key features:

(i) When axial symmetry is relaxed there is no single privileged parameter analogous to arclength along the contour. The formalism should therefore respect the intrinsic freedom associated with the choice of evolution parameter.

(ii) A point that tends to go unnoticed in the axially symmetric context is that the action involves not only first derivatives (velocities) but also second derivatives (accelerations), a feature that is somewhat challenging from a Newtonian point of view. With axial symmetry, the problem is simply sidestepped by introducing the turning angle along the contour (a velocity) as an intermediate variable; with respect to this variable, the action involves no derivative higher than first. What amounts to the same thing, only without the sleight of hand, is to introduce the natural phase space that is appropriate for the Hamiltonian formulation of a theory based on an action involving accelerations: introduce momenta not only canonically conjugate to the particle position, but also to its velocity.

Even if axial symmetry were to be our final goal, there are benefits to this apparently unnecessarily complicated formalism: both the momenta and the constraints possess physical meaning and Hamilton's equations will evolve physical initial data in a remarkably straightforward way. As we will show, once the Hamiltonian formulation of the shape equation has been set up, modulo the tuning of suitable initial conditions that will produce a geometry that closes smoothly, its implementation is straightforward.

We model a lipid vesicle as a two-dimensional surface Σ . The surface is described locally by the embedding $\mathbf{x} = \mathbf{X}(u^a)$, where \mathbf{x} are local coordinates in space, $u^a = (u^1, u^2)$ local coordinates on the surface, and the position functions $\mathbf{X}(u^a)$ are three functions of two variables. We denote by $\mathbf{e}_a = \partial_a \mathbf{X} = \partial \mathbf{X} / \partial u^a$ the two tangent vectors to the surface. The metric induced on Σ is given by their inner product, $g_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$. 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 $K = g^{ab}K_{ab}$, where g^{ab} is the inverse of the induced metric g_{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 G , i.e., $\mathcal{R} = 2G = 2c_1c_2$.

We consider the Helfrich–Canham geometric model, or bilayer coupling model, for a fluid lipid vesicle, with energy

$$F[\mathbf{X}] = \frac{\kappa}{2} \int dA K^2 + \beta \int dA K + \sigma A - PV, \quad (1)$$

where the constant κ is the bending rigidity, $dA = \sqrt{g} d^2u$ denotes the infinitesimal area element on the surface and g is the determinant of the induced metric g_{ab} . The constants β , σ , P are Lagrange multipliers enforcing the constraints of constant total mean curvature (or constant area difference between the layers), constant area and constant enclosed volume V , respectively [18]. A refinement, known as the ADE model, imposes a non-local constraint involving the square of the area difference [19–21]. Our considerations can be extended to this and other geometrical models for membranes. Note that the volume can be written as a surface integral:

$$V = \frac{1}{3} \int dA \mathbf{n} \cdot \mathbf{X}. \quad (2)$$

We have not included a term corresponding to the Gaussian bending, $F_G[\mathbf{X}] = \kappa_G \int dA \mathcal{R}$, since it is a topological invariant by the Gauss–Bonnet theorem, and, as such, it does not contribute to the determination of equilibrium configurations. The energy (1) is invariant under rigid motions, translations and rotations, of the surface in the ambient space. It also possesses a local symmetry: invariance under reparametrizations.

The vanishing of the first variation of the energy (1), with respect to variations of the position functions $\mathbf{X}(u^a) \rightarrow \mathbf{X}(u^a) + \delta\mathbf{X}(u^a)$, gives the shape equation [6, 7, 9, 22]

$$\kappa \left[-\nabla^2 K - \frac{K}{2}(K^2 - 2\mathcal{R}) \right] + \beta\mathcal{R} + \sigma K - P = 0, \quad (3)$$

where ∇^2 denotes the surface Laplacian. This fourth-order nonlinear PDE determines the equilibrium configurations of lipid vesicles. There is only one equilibrium condition, whereas naively one would have expected three. Reparametrization invariance informs us that two linear combinations of these three equations, corresponding to tangential deformations, must vanish identically [23]. The only physical deformations are those normal to the surface.

Let us now specialize to axially symmetric configurations. The embedding of an axially symmetric configuration can be written as

$$\mathbf{x} = \mathbf{X}(u^a) = \mathbf{X}(t, \phi) = \begin{pmatrix} R(t) \cos \phi, \\ R(t) \sin \phi, \\ Z(t) \end{pmatrix}, \quad (4)$$

where t is an arbitrary parameter along the contour of the surface at fixed ϕ . Any space vector \mathbf{V} can be written in adapted components as

$$\mathbf{V}(t, \phi) = \begin{pmatrix} V_R(t) \cos \phi, \\ V_R(t) \sin \phi, \\ V_Z(t) \end{pmatrix}, \quad (5)$$

so that on the plane $\phi = 0$ it reduces to a two-dimensional t -dependent vector with components $\{V_R(t), V_Z(t)\}$. The basis adapted to the surface is given by the two tangent vectors $\mathbf{e}_t = \partial\mathbf{X}/\partial t = \dot{\mathbf{X}}$ and $\mathbf{e}_\phi = \partial\mathbf{X}/\partial\phi$, together with the unit normal vector

$$\mathbf{n}(t, \phi) = \frac{1}{N} \begin{pmatrix} \dot{Z}(t) \cos \phi, \\ \dot{Z}(t) \sin \phi, \\ -\dot{R}(t) \end{pmatrix}, \quad (6)$$

where we introduce the function

$$N = \sqrt{\dot{R}^2 + \dot{Z}^2}. \quad (7)$$

Note that arclength l along the contour is defined infinitesimally by $dl = N dt$. The induced metric and the extrinsic curvature tensor assume the form

$$g_{ab} = \begin{pmatrix} N^2 & 0 \\ 0 & R^2 \end{pmatrix}, \quad K_{ab} = \frac{1}{N} \begin{pmatrix} \dot{R}\ddot{Z} - \dot{Z}\ddot{R} & 0 \\ 0 & R\dot{Z} \end{pmatrix}. \quad (8)$$

For the mean curvature and the scalar curvature it follows that

$$K = g^{ab} K_{ab} = \frac{R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + N^2\dot{Z}}{RN^3}, \quad \mathcal{R} = \frac{2\dot{Z}(\dot{R}\ddot{Z} - \dot{Z}\ddot{R})}{RN^4}. \quad (9)$$

The Helfrich–Canham energy (1) specialized to axially symmetric configurations, in terms of an arbitrary parameter t , is

$$F[\mathbf{X}] = 2\pi \int dt L(R, Z, \dot{R}, \dot{Z}, \ddot{R}, \ddot{Z}), \quad (10)$$

where the Lagrangian function is

$$L(R, Z, \dot{R}, \dot{Z}, \ddot{R}, \ddot{Z}) = \frac{\kappa}{2} \frac{[R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2]^2}{RN^5} + \beta \frac{R}{N^2} (\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \beta\dot{Z} + \sigma RN - \frac{P}{3} R(R\dot{Z} - Z\dot{R}). \quad (11)$$

We now treat this energy as an action determining the motion of a fictitious particle in the two-dimensional configuration space $\{R, Z\}$. The arbitrary parameter t will play the role of time. The Lagrangian function involves the squared acceleration of this fictitious particle; it enters quadratically due to bending, and linearly due to the constraint of constant total mean curvature. The only serious nonlinearity is the dependence of the Lagrangian on the velocity $\{\dot{R}, \dot{Z}\}$. The factors of R, N ensure that the action is invariant under reparametrizations of t , all that remains of the reparametrization invariance of the energy (1) once we specialize to axially symmetry. The only dependence on Z is through the volume, if $P \neq 0$.

The axially symmetric version of the shape equation can be obtained either by direct specialization of the general shape equation (3) or as the vanishing of the Euler–Lagrange derivative of the energy (10) (see the appendix)

$$\mathcal{E}_i = \frac{d^2}{dt^2} \left(\frac{\partial L}{\partial \ddot{Q}^i} \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{Q}^i} \right) + \frac{\partial L}{\partial Q^i}, \quad (12)$$

where $Q^i = \{R, Z\}$. Each gives a copy of the shape equation. As noted below, there is only a single shape equation.

Two features of the dynamical system defined by the action (10) complicate its Hamiltonian formulation: the energy depends on second derivatives of the configuration variables, the position functions; and because we have chosen to work in an arbitrary parametrization, there is a local symmetry—reparametrization invariance. The implications

of the latter will become apparent only after we have obtained the canonical Hamiltonian. First, we must construct the phase space.

The most direct approach to handling the presence of the second derivatives $\{\ddot{R}, \ddot{Z}\}$ is to extend the phase space: we treat not only the position variables $\{R, Z\}$ but also their velocities $\{\dot{R}, \dot{Z}\}$ as configuration variables and introduce conjugate momenta for both sets of variables. (A brief summary of the Hamiltonian formulation of higher derivative systems is provided in the appendix.) The momenta $\{P_R, P_Z\}$ conjugate to the velocities $\{\dot{R}, \dot{Z}\}$ are, respectively,

$$P_R = \frac{\partial L}{\partial \dot{R}} = -\kappa \frac{\dot{Z}}{N^5} [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2] - \beta \frac{R\dot{Z}}{N^2}, \quad (13)$$

$$P_Z = \frac{\partial L}{\partial \dot{Z}} = \kappa \frac{\dot{R}}{N^5} [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2] + \beta \frac{R\dot{R}}{N^2}. \quad (14)$$

We note that the vector $\{P_R, P_Z\}$ is directed along the normal to the contour, and that its bending part is proportional to the mean curvature [17]. Note also that the vector $\{P_R, P_Z\}$ depends at most on second derivatives of $\{R, Z\}$.

The momenta $\{p_R, p_Z\}$ conjugate to $\{R, Z\}$ are, respectively,

$$\begin{aligned} p_R &= \frac{\partial L}{\partial \dot{R}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \ddot{R}} \right) \\ &= -\frac{5\kappa \dot{R} [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2]^2}{2RN^7} + \frac{\kappa (R\ddot{Z} + 2\dot{R}\dot{Z}) [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2]}{RN^5} \\ &\quad - \frac{2\beta R \dot{R} (\dot{R}\ddot{Z} - \dot{Z}\ddot{R})}{N^4} + \frac{\beta R \ddot{Z}}{N^2} + \frac{\sigma R \dot{R}}{N} + \frac{P}{3} RZ - \dot{P}_R, \end{aligned} \quad (15)$$

$$\begin{aligned} p_Z &= \frac{\partial L}{\partial \dot{Z}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \ddot{Z}} \right) \\ &= -\frac{5\kappa \dot{Z} [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2]^2}{2RN^7} + \frac{\kappa (-R\ddot{R} + \dot{R}^2 + 3\dot{Z}^2) [R(\dot{R}\ddot{Z} - \dot{Z}\ddot{R}) + \dot{Z}N^2]}{RN^5} \\ &\quad - \frac{2\beta R \dot{Z} (\dot{R}\ddot{Z} - \dot{Z}\ddot{R})}{N^4} - \frac{\beta R \ddot{R}}{N^2} + \frac{\sigma R \dot{Z}}{N} + \beta - \frac{P}{3} R^2 - \dot{P}_Z. \end{aligned} \quad (16)$$

Despite the unpromising appearance of these expressions, in [17] we will see that the vector $\{p_R, p_Z\}$ is the projection of the stress tensor associated with the membrane along the unit tangent to the contour. There is a direct physical significance attached. Note that this vector has a dependence, through the derivatives of $\{P_R, P_Z\}$, on the third derivatives of $\{R, Z\}$.

We have now identified the appropriate phase space for the system defined by the energy (10): the position of a particle in two dimensions $\{R, Z\}$, and its conjugate momenta $\{p_R, p_Z\}$, given by (15), (16), together with the velocity $\{\dot{R}, \dot{Z}\}$ and its conjugate momenta $\{P_R, P_Z\}$, given by (13), (14). Intuitively, the position is conjugate to its third derivative; the velocity is conjugate to the second derivative of the position. As we will see below, however, not all of this phase space is accessible: reparametrization invariance will imply constraints.

Our next step is to construct the Hamiltonian on the phase space. Because the Lagrangian depends on second derivatives of $\{R, Z\}$, the definition of the canonical Hamiltonian H_0 involves the Legendre transformation with respect to the accelerations $\{\ddot{R}, \ddot{Z}\}$ as well as the velocities, $\{\dot{R}, \dot{Z}\}$ (see the appendix), as

$$H_0(P_R, p_R, \dot{R}, R; P_Z, p_Z, \dot{Z}, Z) = P_R \ddot{R} + P_Z \ddot{Z} + p_R \dot{R} + p_Z \dot{Z} - L(R, Z, \dot{R}, \dot{Z}, \ddot{R}, \ddot{Z}). \quad (17)$$

The definition of the momenta $\{P_R, P_Z\}$ is used to express the higher derivatives configuration variables $\{\ddot{R}, \ddot{Z}\}$ in terms of the phase space variables $P_R, P_Z, \dot{R}, \dot{Z}, Z, R$. Unlike a lower order Hamiltonian system, the terms $p_R \dot{R}, p_Z \dot{Z}$ are left alone; they are already in canonical form.

To facilitate the elimination of $\{\ddot{R}, \ddot{Z}\}$ in (17), we square (13) and (14), defining the momenta $\{P_R, P_Z\}$, and add to give

$$R^2(\dot{R}\ddot{Z} - \dot{Z}\ddot{R})^2 = \frac{N^8}{\kappa^2} \left[\left(P_R + \kappa \frac{\dot{Z}^2}{N^3} + \beta \frac{R\dot{Z}}{N^2} \right)^2 + \left(P_Z - \kappa \frac{\dot{Z}\dot{R}}{N^3} - \beta \frac{R\dot{R}}{N^2} \right)^2 \right]. \quad (18)$$

It follows that the canonical Hamiltonian is expressed in terms of the phase space variables as

$$H_0 = p_R \dot{R} + p_Z \dot{Z} + \frac{N^3}{2\kappa R} \left[\left(P_R + \kappa \frac{\dot{Z}^2}{N^3} + \beta \frac{R\dot{Z}}{N^2} \right)^2 + \left(P_Z - \kappa \frac{\dot{Z}\dot{R}}{N^3} - \beta \frac{R\dot{R}}{N^2} \right)^2 \right] - \frac{\kappa \dot{Z}^2}{2RN} - \beta \dot{Z} - \sigma RN + \frac{P}{3} R(R\dot{Z} - Z\dot{R}). \quad (19)$$

This Hamiltonian is quadratic in $\{P_R, P_Z\}$ and linear in $\{p_R, p_Z\}$.

We have dealt with the first difficulty, the higher order nature of the system defined by (10); now we face the second one, the presence of a local symmetry. In this higher derivative model, the presence of reparametrization invariance implies that the Hessian of the Lagrangian with respect to the second derivatives is degenerate; and it is impossible to invert for the accelerations in terms of their conjugate momenta. The Hessian is

$$H_{ij} = \frac{\partial^2 L}{\partial \ddot{Q}^i \partial \ddot{Q}^j} = \frac{\kappa R}{N^5} \begin{pmatrix} \dot{Z}^2 & -\dot{R}\dot{Z} \\ -\dot{R}\dot{Z} & \dot{R}^2 \end{pmatrix}, \quad (20)$$

with $Q^i = \{R, Z\}$, and we see that its determinant vanishes. This means that at any value of the parameter t the phase space variables are not all independent, they are connected by constraints. The first (or primary) constraint is easily identified from the definition of the higher momenta (13), (14) as

$$C = P_R \dot{R} + P_Z \dot{Z} = 0. \quad (21)$$

This is simply the statement that the vector $\{P_R, P_Z\}$ is directed along the normal to the contour. As we will see, this is equivalent to the fact that the tangential component of the acceleration is gauge: the parametrization we choose will fix this component.

The Hamiltonian that generates the motion is given by adding this constraint to the canonical Hamiltonian,

$$H = H_0 + \lambda C; \quad (22)$$

the Lagrange multiplier λ is an arbitrary function of t that enforces the constraint (21).

The Poisson bracket appropriate for this higher derivative model is, for any two phase space functions f, g (see the appendix),

$$\{f, g\} = \frac{\partial f}{\partial \dot{R}} \frac{\partial g}{\partial P_R} + \frac{\partial f}{\partial R} \frac{\partial g}{\partial p_R} + \frac{\partial f}{\partial \dot{Z}} \frac{\partial g}{\partial P_Z} + \frac{\partial f}{\partial Z} \frac{\partial g}{\partial p_Z} - (f \leftrightarrow g); \quad (23)$$

the time derivative of a phase space function f is given by the Poisson bracket with the Hamiltonian (22)

$$\dot{f} = \{f, H\} = \{f, H_0\} + \lambda \{f, C\}. \quad (24)$$

We have identified a constraint C on the phase space variables. This is not the whole story, however. Even if $C = 0$ initially, we are not guaranteed that it continues to hold. Consistency requires that $C = 0$ be preserved by the evolution: a short calculation gives

$$\dot{C} = \{C, H_0\} = -H_0. \quad (25)$$

Thus, we need to impose the secondary constraint

$$H_0 = 0; \quad (26)$$

the canonical Hamiltonian itself must vanish, the hallmark of reparametrization invariance. Here, it shows up as a secondary constraint. Clearly, $\dot{H}_0 = 0$. There are no other (tertiary) constraints. As a constraint, $H_0 = 0$ specifies the tangential part of the vector $\{p_R, p_Z\}$ in terms of the remaining dynamical variables.

The Hamiltonian function (22) generating the dynamics is a linear combination of two constraints. Hamilton's equations will reproduce the equilibrium condition given by the vanishing of the Euler–Lagrange derivative (12).

The first pair of equations is

$$\frac{dR}{dt} = \frac{\partial H}{\partial p_R} = \dot{R}, \quad (27)$$

$$\frac{dZ}{dt} = \frac{\partial H}{\partial p_Z} = \dot{Z}, \quad (28)$$

since $\{p_R, p_Z\}$ appear in the Hamiltonian only in the combination $p_R \dot{R} + p_Z \dot{Z}$. These equations tell us how the vector $\{R, Z\}$ evolves; in this formalism they are model independent.

The second pair of equations is

$$\frac{d\dot{R}}{dt} = \ddot{R} = \frac{\partial H}{\partial P_R} = \frac{N^3}{\kappa R} \left(P_R + \kappa \frac{\dot{Z}^2}{N^3} + \beta \frac{R\dot{Z}}{N^2} \right) + \lambda \dot{R}, \quad (29)$$

$$\frac{d\dot{Z}}{dt} = \ddot{Z} = \frac{\partial H}{\partial P_Z} = \frac{N^3}{\kappa R} \left(P_Z - \kappa \frac{\dot{Z}\dot{R}}{N^3} - \beta \frac{R\dot{R}}{N^2} \right) + \lambda \dot{Z}. \quad (30)$$

They tell us how $\{\dot{R}, \dot{Z}\}$ evolves. They involve the Lagrange multiplier λ explicitly.

Just as (27) and (28), encode the definition of the canonical variables $\{\dot{R}, \dot{Z}\}$ as the time derivatives of $\{R, Z\}$, one would expect these equations to encode the definition of the momenta $\{P_R, P_Z\}$ in terms of $\{R, Z\}$, $\{\dot{R}, \dot{Z}\}$ and $\{\ddot{R}, \ddot{Z}\}$.

Let us first express the Lagrange multiplier λ in terms of the acceleration. We multiply (29) by \dot{R} and (30) by \dot{Z} and we add. Using the constraint (21), we identify

$$\lambda = \frac{\dot{R}\ddot{R} + \dot{Z}\ddot{Z}}{N^2} = \frac{\dot{N}}{2N^2}. \quad (31)$$

It vanishes in a parametrization by arclength. Geometrically, it is the affine connection for the planar curve described by $\{R(t), Z(t)\}$; the component of the acceleration tangent to the contour is pure gauge—it can be chosen arbitrarily. In particular, it can be chosen to vanish. If the expression (31) for λ is fed back into (29) and (30), we find that they reproduce the forms (13) and (14) for P_R and P_Z , respectively. We do, however, have to use the primary constraint.

The third pair of equations is

$$\begin{aligned} \frac{dP_R}{dt} = -\frac{\partial H}{\partial \dot{R}} = -p_R - \lambda P_R - \frac{3\dot{R}N}{2\kappa R} (P_R^2 + P_Z^2) + \frac{P_Z\dot{Z}}{R} - \frac{\beta^2 R\dot{R}}{2\kappa N} \\ + \frac{\beta}{\kappa N} [P_Z(2\dot{R}^2 + \dot{Z}^2) - P_R\dot{R}\dot{Z}] + \sigma \frac{R\dot{R}}{N} + \frac{P}{3} RZ, \end{aligned} \quad (32)$$

$$\begin{aligned} \frac{dP_Z}{dt} = -\frac{\partial H}{\partial \dot{Z}} = -p_Z - \lambda P_Z - \frac{3\dot{Z}N}{2\kappa R} (P_R^2 + P_Z^2) + \frac{P_Z\dot{R}}{R} - \frac{2P_R\dot{Z}}{R} - \frac{\beta^2 R\dot{Z}}{2\kappa N}, \\ - \frac{\beta}{\kappa N} [P_R(\dot{R}^2 + 2\dot{Z}^2) - P_Z\dot{R}\dot{Z}] + \sigma \frac{R\dot{Z}}{N} - \frac{P}{3} R^2. \end{aligned} \quad (33)$$

They tell us how the vector $\{P_R, P_Z\}$ evolves. One would expect these equations to encode the definition of the momenta p_R and p_Z given by (15) and (16). To show this is not entirely straightforward. It is necessary to use the information gathered in the previous Hamilton equations, namely the form of $\{P_R, P_Z\}$ and of λ .

Finally, the fourth pair of equations is

$$\frac{dp_R}{dt} = -\frac{\partial H}{\partial R} = \frac{N^3}{2\kappa R^2}(P_R^2 + P_Z^2) + \frac{P_R \dot{Z}^2}{R^2} - \frac{P_Z \dot{R}\dot{Z}}{R^2} - \frac{\beta^2 N}{2\kappa} + \sigma N - \frac{P}{3}(2R\dot{Z} - Z\dot{R}), \quad (34)$$

$$\frac{dp_Z}{dt} = -\frac{\partial H}{\partial Z} = \frac{P}{3}R\dot{R}. \quad (35)$$

They tell us how $\{p_R, p_Z\}$ evolve. With these equations, we reproduce the vanishing of the Euler–Lagrange derivative (12). One sees that the latter of the two equations has the obvious first integral

$$\mathcal{J} = p_Z - \frac{P}{6}R^2 = \text{const}. \quad (36)$$

The first integral of the axially symmetric shape equation [8, 9] emerges naturally within this framework.

The recipe to construct an axially symmetric equilibrium configuration is as follows. Choose initial data: at $t = 0$, take a point on the plane, specified by its position vector $\{R, Z\}$, choose a velocity vector $\{\dot{R}, \dot{Z}\}$ (this encodes the initial direction of the contour); next choose a vector $\{P_R, P_Z\}$, orthogonal to the velocity (so as to satisfy the primary constraint (21)); finally choose the momentum $\{p_R, p_Z\}$ with a tangential component consistent with the secondary constraint $H_0 = 0$ where H_0 is given by equation (19). These are our physical degrees of freedom.

This initial data set is evolved using Hamilton’s equations. An equilibrium surface contour $\{R(t), Z(t)\}$ will be generated. The contour itself will not depend on the choice of the Lagrange multiplier λ (or equivalently the choice of the parameter t).

Our discussion has only mentioned briefly one major point: tuning. One will need to get the initial conditions right to produce a surface that closes smoothly. The difficulty is that generating the appropriate geometry will require solving a two-point boundary value problem with specific conditions on the canonical variables at the endpoints to ensure closure, and, as previous work on the subject shows [24–27], this involves fine-tuning the initial conditions on these variables—it can be extremely delicate. Tuning difficulties will, of course, reappear with a vengeance when axial symmetry is relaxed. All the more reason to possess a robust formalism to hand.

In this paper, we have examined the construction of axially symmetric equilibrium configurations of a fluid membrane described by the Helfrich–Canham energy from a Hamiltonian point of view. If axial symmetry were our final aim this would be a heavy-handed approach to the problem. The value of all of this formalism will become apparent when we consider the generalization to non-axially symmetric configurations [17]. This will involve stepping up from the Hamiltonian dynamics of a particle to the corresponding dynamics of a field describing a closed curve in space. The membrane surface will be generated by the evolution of this curve. The details will be provided in [17].

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Appendix

For the benefit of the reader unfamiliar with the Hamiltonian formulation of higher derivative systems, we consider in this appendix the Hamiltonian description of a toy model: a particle moving in one dimension described by a Lagrangian of the form $L = L(q, \dot{q}, \ddot{q})$. The Euler–Lagrange derivative for this Lagrangian is

$$\mathcal{E} = \frac{d^2}{dt^2} \left(\frac{\partial L}{\partial \ddot{q}} \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}} \right) + \frac{\partial L}{\partial q}. \quad (\text{A.1})$$

The phase space is given by the two conjugate pairs $\{\dot{q}, P\}$ and $\{q, p\}$. The momenta conjugate to \dot{q} and q are, respectively,

$$P = \frac{\partial L}{\partial \ddot{q}}, \quad (\text{A.2})$$

$$p = \frac{\partial L}{\partial \dot{q}} - \frac{d}{dt} \left(\frac{\partial L}{\partial \ddot{q}} \right). \quad (\text{A.3})$$

The canonical Hamiltonian is constructed as the Legendre transformation with respect to both the acceleration \ddot{q} and the velocity \dot{q} as

$$H(\dot{q}, P; q, p) = P\dot{q} + p\dot{q} - L, \quad (\text{A.4})$$

where one uses the definition of the higher momentum P to express the highest derivative \ddot{q} in terms of the phase space variables P, \dot{q} and q . The term $p\dot{q}$ in the canonical Hamiltonian is left alone, since it is already in canonical form.

The Poisson bracket appropriate for this higher derivative model, for two arbitrary phase space functions f, g , is

$$\{f, g\} = \frac{\partial f}{\partial \dot{q}} \frac{\partial g}{\partial P} + \frac{\partial f}{\partial q} \frac{\partial g}{\partial p} - (f \leftrightarrow g), \quad (\text{A.5})$$

and the time derivative of a phase space function is given by this Poisson bracket with the Hamiltonian

$$\frac{df}{dt} = \{f, H\}. \quad (\text{A.6})$$

In particular, it follows that the Hamilton equations are

$$\frac{dq}{dt} = \frac{\partial H}{\partial p} = \dot{q}, \quad (\text{A.7})$$

$$\frac{d\dot{q}}{dt} = \frac{\partial H}{\partial P}, \quad (\text{A.8})$$

$$\frac{dP}{dt} = -\frac{\partial H}{\partial \dot{q}}, \quad (\text{A.9})$$

$$\frac{dp}{dt} = -\frac{\partial H}{\partial q}. \quad (\text{A.10})$$

The first equation identifies the time derivative of q with the canonical variable \dot{q} ; the second equation identifies the form of the momenta P conjugate to \dot{q} and the third equation identifies the momenta p conjugate to q modulo the definition of P . Using the first three equations, the fourth equation then reproduces the vanishing of the Euler–Lagrange derivative (A.1).

One important special case is given by a Lagrangian *linear* in the acceleration, $L = g(q, \dot{q})\ddot{q}$. In this case, the higher momentum $P = g(q, \dot{q})$ is independent of \ddot{q} so that the acceleration cannot be expressed in terms of the canonical variables. However, it is always possible to add a total derivative to the Lagrangian and obtain a Lagrangian that depends at most on \dot{q} (see, e.g., [28]).

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