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Helfrich–Canham bending energy as a constrained nonlinear sigma model

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Abstract
The Helfrich–Canham bending energy is identified with a nonlinear sigma model for a unit vector. The identification, however, is dependent on one additional constraint: that the unit vector be constrained to lie orthogonal to the surface. The presence of this constraint adds a source to the divergence of the stress tensor for this vector so that it is not conserved. The stress tensor which is conserved is identified and its conservation shown to reproduce the correct shape equation.

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Consider an embedded two-dimensional surface in three-dimensional space. The positive definite geometrical invariant,

$$F[\mathbf{X}] = \frac{1}{2}\int \mathrm{d}A\, K_{ab}K^{ab}, \tag{1}$$

is a measure of the energy associated with the bending of the surface. The embedding is described by three functions $\mathbf{X} = X^i$ of two variables $\xi^a (i, j, \ldots, = 1, 2, 3; a, b, \ldots, = 1, 2)$. The extrinsic curvature tensor K_{ab} is then defined by

$$K_{ab} = \mathbf{e}_b \cdot \nabla_a \mathbf{n} = K_{ba}, \tag{2}$$

where $\mathbf{e}_a = \partial\mathbf{X}/\partial\xi^a = \nabla_a\mathbf{X}$ are the two tangent vectors to the surface and $\mathbf{n}$ is the unit normal. Indices are raised with g^{ab}, the inverse of the induced metric $g_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$. $\mathrm{d}A = \sqrt{g}d^2\xi$ is the area measure induced on the surface by $\mathbf{X}$, with $g = \det g_{ab}$.

For a two-dimensional surface, $F[\mathbf{X}]$ is invariant under ambient space conformal transformations. Since its introduction by Willmore [1], it has cropped up in a number of contexts. These range from elasticity theory [2], to cellular biophysics where it models the bending energy of phospholipid membranes and is known as the Helfrich–Canham Hamiltonian [3–5], to its Lorentzian generalization describing the action defined on the two-dimensional world sheet of a relativistic string propagating in spacetime, proposed by

Polyakov to model colour flux tubes in QCD [6–8]. We will couch our discussion in terms of Euclidean surfaces.

The vanishing of the first variation of $F[\mathbf{X}]$ under an infinitesimal deformation of the embedding functions, $\mathbf{X} \to \mathbf{X} + \delta\mathbf{X}$, produces the shape equation [9, 10]

$$-\nabla^2 K + \tfrac{1}{2} K (K^2 - 2K_{ab}K^{ab}) = 0, \tag{3}$$

where ∇^2 is the surface Laplacian and $K = g^{ab} K_{ab}$ is the mean extrinsic curvature. We remark that the shape equation is of fourth order in derivatives of the shape functions. Let us also note that, a fact that will be used below, the shape equation can be written as a conservation law [11, 12],

$$\nabla_a \mathbf{f}^a = 0, \tag{4}$$

where the stress tensor $\mathbf{f}^a$ is

$$\mathbf{f}^a = K\big(K^{ab} - \tfrac{1}{2} K g^{ab}\big)\,\mathbf{e}_b - (\nabla^a K)\mathbf{n}. \tag{5}$$

In this paper, we would like to explore the fact that it is possible to rewrite the quadratic appearing in (1) in the form

$$K_{ab}K^{ab} = (\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n}), \tag{6}$$

an identity which follows immediately from the definition of K_{ab} and use of the completeness of the basis $\{\mathbf{e}_a, \mathbf{n}\}$, $g^{ab} e^i_a e^j_b = \delta^{ij} - n^i n^j$. This identity associates bending energy with non-vanishing gradients of the normal vector; it appears to map the bending energy into a nonlinear sigma model living on the curved geometry of the surface (see, e.g., chapter 14 of [13]):

$$F_\sigma[\mathbf{n}] = \frac{1}{2}\int \mathrm{d}A[(\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n}) + \lambda(\mathbf{n}^2 - 1)], \tag{7}$$

with λ a Lagrange multiplier that enforces the constraint that $\mathbf{n}$ be a unit vector. The Euler–Lagrange equations that follow from the vanishing of the first variation of $F_\sigma[\mathbf{n}]$ under $\mathbf{n} \to \mathbf{n} + \delta\mathbf{n}$ are

$$-\nabla^2 \mathbf{n} + \lambda \mathbf{n} = 0, \tag{8}$$

together with the constraint $\mathbf{n}^2 = 1$. Using this constraint, the Lagrange multiplier is identified as $\lambda = -(\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n})$, so that the Euler–Lagrange equations take the form

$$-\nabla^2 \mathbf{n} - (\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n})\mathbf{n} = 0. \tag{9}$$

These equations are integrable [14]; this fact is one motivation for investigating possible links with the bending energy (1).

If $\mathbf{n}$ happens to be the unit normal to some surface, then the fact that $\nabla_a \mathbf{n} = K_{ab} g^{bc} \mathbf{e}_c$, and the Codazzi–Mainardi identities $\nabla_a K^{ab} = \nabla^b K$, allow us to rewrite the Euler–Lagrange equations in a geometrical form as $\nabla_a K = 0$. Clearly, this is not even a distant relative of the shape equation (3). It is of second order in derivatives of $\mathbf{n}$ and of third order in derivatives of $\mathbf{X}$. Despite this fact, unfortunately, this erroneous identification has been made frequently in the literature; not by Polyakov, though, who was well aware of the pitfalls of a hasty identification (see section 10.4 of [7]). What $F_\sigma[\mathbf{n}]$ fails to do is to capture the fact that $\mathbf{n}$ is normal to the surface. If $\mathbf{n}$ may point in any direction, then $F_\sigma[\mathbf{n}]$ describes a Heisenberg ferromagnet on the surface. On the other hand, if we wish to describe the bending energy, the unit vector $\mathbf{n}$ must also satisfy the constraints

$$\mathbf{n} \cdot \mathbf{e}_a = 0. \tag{10}$$

If the surface is fixed, **n** is also; if **n** is allowed to vary, the surface must respond accordingly. This leads to an interesting reformulation of the bending energy. We introduce the novel functional, with additional constraints,

$$F[\mathbf{n}, \mathbf{e}_a, \mathbf{X}] = \int \mathrm{d}A \left[\frac{1}{2}(\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n}) + \frac{\lambda}{2}(\mathbf{n}^2 - 1) + \lambda^a (\mathbf{n} \cdot \mathbf{e}_a) + \mathbf{f}^a \cdot (\mathbf{e}_a - \nabla_a \mathbf{X}) \right]. \tag{11}$$

The normalization $\mathbf{n}^2 = 1$ and orthogonality constraints (10) are implemented using the Lagrange multipliers λ and λ^a, respectively. The latter constraints may be thought of as a frustration of the nonlinear sigma model. They would be simple enough to implement if the $\mathbf{e}_a$ were any two fixed vector fields. The fact that the vectors $\mathbf{e}_a$ are the tangent vectors to the surface, however, couples **n** not only to them, but also through them to the embedding functions **X** themselves; this connection is captured in the final set of constraints in (11). This model is a special case of a general construction introduced by one of us in [12], where the issue of implementing the necessary integrability conditions needed for the surface to exist is sidestepped.

The Euler–Lagrange equations for $\mathbf{n}, \mathbf{e}_a$ and **X**, that follow from the vanishing of the first variation of $F[\mathbf{n}, \mathbf{e}_a, \mathbf{X}]$, together are completely equivalent to the shape equation (3). Moreover, the Lagrange multipliers $\mathbf{f}^a$ appearing in (11) coincide with the stress tensor (5)—this justifies the abuse of notation. How the shape equation comes out is rather interesting. First, the Euler–Lagrange equation for the embedding functions **X** provides the conservation law (4), $\nabla_a \mathbf{f}^a = 0$, since **X** appears only in the last constraint. The equations for **n** and $\mathbf{e}_a$ determine the form of the Lagrange multipliers $\mathbf{f}^a$: for **n** we have

$$-\nabla^2 \mathbf{n} + \lambda \mathbf{n} + \lambda^a \mathbf{e}_a = 0, \tag{12}$$

and for $\mathbf{e}_a$, when the constraints are enforced,

$$\mathbf{f}^a = T^{ab} \mathbf{e}_b - \lambda^a \mathbf{n}, \tag{13}$$

where we identify the stress tensor associated with an unconstrained nonlinear sigma model for **n** on the background intrinsic geometry of the surface

$$T^{ab} = (\nabla^a \mathbf{n}) \cdot (\nabla^b \mathbf{n}) - \tfrac{1}{2} g^{ab} (\nabla^c \mathbf{n}) \cdot (\nabla_c \mathbf{n}). \tag{14}$$

If $\lambda^a = 0$, (12) reproduces the Euler–Lagrange equations for a nonlinear sigma model (8). The normal projection of (12) gives, as before, $\lambda = -(\nabla_a \mathbf{n}) \cdot (\nabla^a \mathbf{n})$, or λ is (minus) the energy density; taking into account the constraint (10), its tangential counterparts give

$$\lambda^a = \mathbf{e}^a \cdot \nabla^2 \mathbf{n} = \nabla^b (\mathbf{e}^a \cdot \nabla_b \mathbf{n}) = \nabla^b K^a{}_b = \nabla^a K. \tag{15}$$

Modulo the constraints (10) and the definition of K_{ab}, we find that T^{ab} can be rewritten as

$$T^{ab} = K^{ac} K_c{}^b - \tfrac{1}{2} g^{ab} K^{cd} K_{cd} = K \left(K^{ab} - \tfrac{1}{2} g^{ab} K \right). \tag{16}$$

To obtain the expression on the right, we have used the Gauss–Codazzi equation for a two-dimensional surface,

$$\tfrac{1}{2} \mathcal{R} g_{ab} = K K_{ab} - K_{ac} K^c{}_b, \tag{17}$$

which expresses the Ricci scalar induced by **X**, equal to twice the Gaussian curvature, in terms of a quadratic in K_{ab}. Therefore, inserting (15) for λ^a and (16) for T^{ab} into the Euler–Lagrange equation for $\mathbf{e}_a$ (13), we reproduce the stress tensor (5). We identify λ^a as the normal stress and T^{ab} as the tangential stress in the membrane.

To arrive at the shape equation, let us return now to the conservation law (4). Using (13), we can re-express the conservation law in terms of tangential and normal components:

$$\nabla_a \lambda^a + K^{ab} T_{ab} = 0, \tag{18}$$

$$\nabla_a T^{ab} - \lambda_a K^{ab} = 0. \tag{19}$$

Using (15) for λ^a and (16) for T^{ab}, it is immediate to see that the first, normal, component coincides with the shape equation (3). The coupling of $\mathbf{n}$ to the tangents provides a source to the sigma model stress tensor: it is no longer conserved. The source is the Lagrange multiplier λ^a implementing the constraint (15). When λ^a is substituted into (19), it is identically satisfied, a feature that has its origin in the reparametrization invariance of the model. We note that the Lagrange multiplier λ does not appear in these equations. We also remark on the fact that we do not need to know how K_{ab} itself responds to a deformation of the surface in this presentation.

What is the status of the Euler–Lagrange equation for $\mathbf{n}$? Substituting λ and λ^a into (12), we obtain a purely kinematical statement about embedded geometries identifying what the projections of $\nabla^2\mathbf{n}$ are with respect to the basis vectors $\mathbf{e}_a$ and $\mathbf{n}$:

$$\nabla^2\mathbf{n} = (\nabla_a K)\,\mathbf{e}^a - K^{ab}K_{ab}\mathbf{n}. \tag{20}$$

To see this, just take a divergence of the Weingarten equations $\nabla_a\mathbf{n} = K_{ab}\mathbf{e}^b$ using the Gauss equations $\nabla_a\mathbf{e}_b = -K_{ab}\mathbf{n}$ to express $\nabla_a\mathbf{e}_b$ as a normal vector.

There is a second independent quadratic invariant in the extrinsic curvature involving the square of the mean curvature, K^2. However, it does not lend itself to a simple expression of the form (6). On the other hand, the fully contracted Gauss–Codazzi equation,

$$\mathcal{R} = K^2 - K_{ab}K^{ab}, \tag{21}$$

identifies the difference between the two quadratics with the scalar curvature, defined intrinsically, i.e., independent of the normal $\mathbf{n}$. For a two-dimensional surface, the corresponding invariant is the Gauss–Bonnet topological invariant. In higher dimensions, the difference is still independent of $\mathbf{n}$. As a result, both λ and λ^a are unchanged with respect to the values given above.

We note, in this context, that the winding number of $\mathbf{n}$ is

$$Q = \frac{1}{8\pi}\int \mathrm{d}A\,\epsilon^{ab}\epsilon_{ijk}n^i\nabla_a n^j\nabla_b n^k, \tag{22}$$

where ϵ^{ab} and ϵ^{ijk} are, respectively, the Levi-Civita tensors on the surface and in space [15]. Modulo (21), Q is just the Gauss–Bonnet invariant of the surface. Thus once the constraint is implemented, the winding number is fixed by the topology of the surface.

To summarize, it has been shown that the coupling of a sigma model to the geometry constraining the unit vector $\mathbf{n}$ to lie normal to the surface converts it into the Helfrich–Canham model—involving only the surface geometry. A lot is known about both models. One expects that this identification might allow results from one model to be imported into the other. In particular, one would expect this formulation of the Helfrich–Canham model to be potentially useful in statistical mechanics. The functional $F[\mathbf{X}, \mathbf{n}, \mathbf{e}_a]$ defined by (11) is quadratic in $\mathbf{n}$. This suggests that, in the evaluation of the partition function, $\mathbf{n}$ may be integrated out. This possible virtue of the formulation presented in this paper will be the subject of future work.

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