Bogomol’nyi decomposition for vesicles of arbitrary genus

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Abstract. We apply the Bogomol’nyi technique, which is usually invoked in the study of solitons or models with topological invariants, to the case of elastic energy of vesicles. We show that spontaneous bending contribution caused by any deformation from metastable bending shapes falls in two distinct topological sets: shapes of spherical topology and shapes of non-spherical topology experience respectively a deviatoric bending contribution à la Fischer and a mean curvature bending contribution à la Helfrich. In other words, topology may be considered to describe bending phenomena. Besides, we calculate the bending energy per genus and the bending closure energy regardless of the shape of the vesicle. As an illustration we briefly consider geometrical frustration phenomena experienced by magnetically coated vesicles.

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Our motivation is to amplify on the observation of vesicles with arbitrary low genus (number of holes/handles) exhibiting conformal diffusion (spontaneous conformal transformation), namely existence of two conservation laws for vesicles [1–6]. The genus is a topological invariant: a quantity conserved under smooth transformations which does not depend on the static or dynamic equations of the system under consideration. In contrast, conformal diffusion provides evidence that the system Hamiltonian is invariant under conformal transformations. Whereas the Noether theorem [7, 8] may be used to treat the latter invariance law in order to compute the corresponding conserved current and constant charge, the Bogomol’nyi technique enables one to treat successfully various models with topological invariants. In this Letter we focus on the topological conservation law only; we defer the conformal diffusion to future articles.

To obtain the Bogomol’nyi relationships we write down for vesicles of arbitrary genus a bending Hamiltonian as a covariant functional invariant under conformal transformations which depends on their shape only and which is suitable for the Bogomol’nyi decomposition. Applying the converse of the remarkable theorem of Gauss enables us to construct such an Hamiltonian. Instead of describing shapes by their Monge representation (i.e., their surface equation) as customary, we characterize shapes by their metric tensor and their shape tensor: the total integral of the shape tensor self-product is our successful candidate. Then the Bogomol’nyi
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technique reveals the topological nature of bending phenomena while differential geometry extends forward the Bogomol’nyi relationships. In particular we show that any deformation of the non-trivial metastable shapes spontaneously leads to a deviatoric bending contribution à la Fischer [13–15] for shapes of spherical topology and to a mean curvature bending contribution (up to a conformal transformation of the ambient space) à la Helfrich [2, 3, 16] for shapes of non-spherical topology: our approach exhibits that the bending contribution expression depends on the shape topology —our main result concisely contained in formulae (20), (21) and (26).

Before describing the bending energy of vesicles, we first succinctly recall the Bogomol’nyi technique [Eqs. (1)–(8) below] through the nonlinear \( \sigma \)-model [9, 10, 17]. More precisely we consider spin fields on curved surfaces \( S \) with the nonlinear \( \sigma \)-model as interaction [18–21]:

\[
\mathcal{H}_{mag} = \frac{1}{2} J \int_{S} \sqrt{g} \, d\Omega \, g^{ij} h_{\alpha \beta} \partial_{i} n^{\alpha} \partial_{j} n^{\beta},
\]

where the order parameter \( n^{\alpha} \) corresponds to a point on the two-sphere \( S^2 \) and the phenomenological parameter \( J \) to the coupling energy between neighbouring spins. The metric tensors \( g_{ij} \) and \( h_{\alpha \beta} \) describe respectively the support manifold \( S \) (i.e., the underlying geometry) and the order parameter manifold \( S^2 \): as customary, \( g \) represents the determinant \( \det(g_{ij}) \) and \( \sqrt{g} \, d\Omega \) the area element. Assuming homogeneous boundary conditions, when applicable, allows one to map each boundary to a point, then the support manifolds \( S \) are topologically equivalent to the torus \( T_{g} \) of genus \( g \). Consequently, the order parameter field \( n^{\alpha} \) effects the mapping of the compactified support \( T_{g} \) to the two-sphere \( S^2 \) which is classified by the cohomotopy group \( \Pi^2(T_{g}) \) isomorphic to the set of integers \( \mathbb{Z} \) [22]: two spin configurations belonging to distinct classes cannot be smoothly deformed into one another. Since there exists an infinite number of classes that map the torus \( T_{g} \) of genus \( g \) to the two-sphere \( S^2 \), for each compactified surface \( S \) the space of spin configurations splits into an infinite number of distinct components, each characterized by a definite topological invariant. Here the topological invariant is the degree of mapping \( Q \) which is expressed in terms of the order parameter field \( n^{\alpha} \) as

\[
Q = \frac{1}{8\pi} \int_{S} \sqrt{g} \, d\Omega \, e^{ij} f_{\alpha \beta} \partial_{i} n^{\alpha} \partial_{j} n^{\beta},
\]

with \( e^{ij} \) and \( f_{\alpha \beta} \) the antisymmetric tensors associated with the support manifold \( S \) and the target (i.e., the order parameter) manifold \( S^2 \), respectively. In spherical coordinates the total integral (2) immediately reads as the winding number. Note that the topological conservation law arises from the nature of the order parameter field \( n^{\alpha} \) only. Henceforth we demonstrate how the Bogomol’nyi technique enables one to study topological spin configurations subject to the magnetic Hamiltonian (1). By introducing the self-dual tensors

\[
T_{\pm \alpha} \equiv \frac{1}{\sqrt{2}} \left[ \partial_{i} n_{\alpha} \mp e_{ir} f_{\alpha \kappa} \partial^{r} n^{\kappa} \right],
\]

which satisfy the precious inequalities [9, 10]

\[
T_{\pm \alpha} T^{\pm \alpha} \geq 0,
\]

the magnetic Hamiltonian (1) density decomposes as

\[
\frac{1}{2} \partial_{i} n_{\alpha} \partial^{i} n^{\alpha} = \frac{1}{4} T_{\pm \alpha} T^{\pm \alpha} \pm \frac{1}{4} e^{ij} f_{\alpha \beta} \partial_{i} n^{\alpha} \partial_{j} n^{\beta}.
\]
Integrating the previous decompositions (3) over the support manifold \( S \) and inserting the formula (2) lead us to rewrite the magnetic Hamiltonian (1) in each topological class specified by the winding number \( Q \) in the form

\[
H_{\text{mag}} = \frac{1}{2} J \int_{S} \sqrt{g} \, d\Omega \, T_{\pm\alpha} T_{\pm\alpha} + 4\pi J \, |Q|,
\]

with \((\pm)\) the sign of \( Q \). Readily from the precious inequalities (4), the magnetic Hamiltonian (1) yields

\[
H_{\text{mag}} \geq 4\pi J \, |Q|.
\]

Moreover, in each topological class, the lowest value of the magnetic energy is actually attained when the self-dual tensor \( T_{\pm\alpha} \) vanishes. In other words, according to the definition (3), the metastable order parameter fields \( n^\alpha \), which actually saturate the Bogomol’nyi bound (6), satisfy the first-order self-dual differential (or Bogomol’nyi) equation multiplet

\[
\partial_i n^\alpha = \pm e^r f^{\alpha\kappa} \partial_r n^\kappa.
\]

Clearly the Bogomol’nyi decomposition reveals the underlying topology: (i) the inequality (7) claims that the minimum minimorum of the Hamiltonian in each topological class is proportional to the topological invariant; (ii) the metastable configurations which actually saturate the Hamiltonian satisfy something simpler than the usual (Euler-Lagrange) equations and no explicit solution is needed to compute their energy; (iii) from the computation emerges a self-dual symmetry; (iv) the decomposition (6) clarifies the stability of the topological configurations and exhibits a spontaneous energy contribution due to any deformation from metastable configurations; (v) a deviatoric (or strain-like) tensor \( T_{\pm\alpha} \) is constructed. Usually not explored, the last two features will appear very relevant below.

Now, we focus on vesicles of arbitrary genus. The large separation of length scales between the membrane thickness of vesicles and their overall size allows us to describe each vesicle as a surface manifold \( S \) embedded in the tridimensional space \( \mathbb{R}^3 \). As a result, initially we focus only on the energy induced by the surface manifold \( S \) itself. On the other hand, the corresponding Hamiltonian has to be invariant under conformal transformations and suitable for the Bogomol’nyi technique. Nonetheless, we must first choose how to represent the surface manifold \( S \): we invoke the converse of the remarkable theorem of Gauss [12]. Let \( S(x^k) \) be a surface manifold with arbitrary intrinsic coordinates \( (x^k) \) embedded in the tridimensional ambient space \( \mathbb{A}^3 \), then there uniquely exist a metric tensor \( g_{ij}(x^k) \) and a shape tensor \( b_{ij}(x^k) \) related by a definite equation multiplet; the converse is true except for the exact position of the surface \( S \) in the ambient space \( \mathbb{A}^3 \). Then, with a different notation, we concisely express the remarkable theorem as

\[
S(x^k) \subset \mathbb{A}^3 \iff \left( g_{ij}(x^k), b_{ij}(x^k) \right).
\]

The geometrical meaning of the couple \((g_{ij}, b_{ij})\) in (8) is revealed by introducing both the infinitesimal tangential displacement \( d\mathbf{T} \) over the surface manifold \( S \) and the infinitesimal normal displacement \( d\mathbf{N} \) to the surface manifold \( S \) inside the ambient space \( \mathbb{A}^3 \); we have

\[
d\mathbf{T} \cdot d\mathbf{T} = g_{ij}(x^k) \, dx^i dx^j, \quad (10a)
\]
\[
d\mathbf{N} \cdot d\mathbf{T} = b_{ij}(x^k) \, dx^i dx^j. \quad (10b)
\]
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In differential geometry, the quadratic differential forms (10\(a\)) and (10\(b\)) are referred to as the first and second fundamental forms, respectively. Furthermore, the Riemann tensor, which measures how much a manifold is curved, reduces to

\[ R_{klmn} = K \left[ g_{km}g_{ln} - g_{kn}g_{lm} \right], \quad (11) \]

where the Gaussian curvature \( K \) depends only on the metric tensor \((g_{ij})\) and its first and second derivatives: such an entity is called a bending invariant or is said to be intrinsic \([12,23]\). When the surface manifold \( S \) is embedded in a curved tridimensional ambient space \( \mathbb{A}^3 \), then the intrinsic curvature \( K \) splits as

\[ K = G + \tilde{K}, \quad (12) \]

where the extrinsic curvature \( G \) satisfies

\[ G = \frac{1}{2} e_{ij} e^{kl} b_{ik} b_{jl}, \quad (13) \]

whereas the sectional curvature \( \tilde{K} \) characterizes the ambient space. For example, the sectional curvature \( \tilde{K} \) vanishes for the flat space \( \mathbb{R}^3 \) and is equal to one for the three-sphere \( S^3 \). We complete this brief overview by stating the Gauss-Bonnet theorem \([23,24]\):

\[ \int_{S \subset \mathbb{A}^3} \sqrt{g} \, d\Omega \, K = -4\pi (g + e - 1) \quad (14) \]

with \( S_{g,e} \) a surface manifold topologically equivalent to a closed surface manifold of genus \( g \) less \( e \) points (ends) embedded in \( \mathbb{A}^3 \).

With this background, we now assume the bending Hamiltonian as the following functional

\[ H_b = \frac{k}{2} \int_{S \subset \mathbb{R}^3} \sqrt{g} \, d\Omega \, g^{ij} b_{ik} b_{jl}, \quad (15) \]

where the phenomenological parameter \( k \) describes the bending rigidity. Since the total integral in (13) is known to be invariant under conformal transformations \([25,26]\), it remains to show that our assumption fits the Bogomol’nyi technique as desired. To begin, note that the bending Hamiltonian \( H_b \) formula (15) stresses the similitude with the magnetic Hamiltonian \( H_{mag} \) (1). Then the self-dual deviatoric tensors are defined as

\[ B^\pm_{ijkl} \equiv \frac{1}{\sqrt{2}} \left[ b_{ij} \mp e_{ik} e_{jl} b^{kl} \right] \quad (16) \]

which yield the precious relationships

\[ B^\pm_{ijkl} B^\pm_{ijkl} = (\lambda \mp \lambda \lambda)^2 \geq 0 \quad (17) \]

where \( \lambda \) and \( \lambda \) denote the eigenvalues of the shape tensor \( (b_{ij}) \), namely the principal curvatures of the surface (or support) manifold \( S \). Here the decompositions (5) read

\[ \frac{1}{2} b_{ij} b^{ij} = \frac{1}{2} B^\pm_{ijkl} B^\pm_{ijkl} \pm G. \quad (18) \]

By inserting the previous decomposition (18) in the formula (13) and recognizing the total curvature (14), the bending Hamiltonian \( H_b \) (15) decomposes as

\[ H_b = \frac{k}{2} \int_{S_{g,e} \subset \mathbb{R}^3} \sqrt{g} \, d\Omega \, B^\pm_{ijkl} B^\pm_{ijkl} \mp 4\pi k (g + e - 1). \quad (19) \]
Note that we have used the fact that, according to (12), the extrinsic curvature $G$ and the intrinsic curvature $K$ are equal when the ambient space is flat ($\bar{K} = 0$). Existence theorems select the correct value for the sign ($\pm$) and the proper topological classes for vesicles as follows. From the precious relationships (17) it is evident that the surface manifolds $S$ which actually saturate the Bogomol’nyi decomposition (19) are the totally umbilical surfaces ($\bar{K} = \lambda$) and the minimal surfaces ($\bar{K} + \lambda = 0$). Since only the round two-sphere $S^2$ is totally umbilical [23,24], the decomposition with sign ($+$) is relevant only for surface manifolds $S_0$ topologically equivalent to the round two-sphere $S^2$; our first key result reads

$$\mathcal{H}_b[S_0] = \frac{1}{2}k \int_{S_0 \subset \mathbb{R}^3} \sqrt{g} \, d\Omega \, B_{ij}^+ B^{ij} + 4\pi k. \quad (20)$$

It is noticeable that any deformation of the metastable bending configurations for shapes of spherical topology spontaneously leads to a deviatoric bending contribution à la Fischer [13–15]: to the best of our knowledge, there is no direct derivation in the literature for such a bending contribution suggested first by Fischer [13]. Since within the flat ambient space $\mathbb{R}^3$ there is no closed minimal surface ($e = 0$) whereas minimal surfaces of genus $g$ ($g \geq 0$) with $e$ ends ($e \geq 2$) do exist [24], the decomposition with sign ($-$) is relevant only for surface manifolds $S_{g,e}$ topologically equivalent to such minimal surfaces $S_{g,e}$; our second key result immediately reads

$$\mathcal{H}_b[S_{g,e}] = \frac{1}{2}k \int_{S_{g,e} \subset \mathbb{R}^3} \sqrt{g} \, d\Omega \, B_{ij}^- B^{-ij} + 4\pi k (g + e - 1). \quad (21)$$

Here any deformation of the metastable bending configurations spontaneously leads to a mean curvature (or anti-deviatoric) bending contribution à la Helfrich [16] widely employed to describe bending phenomena [1–3]. Note that the minimal surface $S_{0,2}$, namely the catenoid, is the elementary neck used to build or analyze numerically vesicles of arbitrary genus $g$ [23,24]. We cannot proceed much further unless we invoke an assertion due to Chen which claims [23,24]

$$\int_{S \subset \mathbb{R}^3} \sqrt{g} \, d\Omega \, \frac{1}{2} b_{ij} b^{ij} = \int_{\varepsilon(S) \subset \varepsilon(\mathbb{R}^3)} \sqrt{g^\varepsilon} \, d\Omega^\varepsilon \, \left[ \frac{1}{2} b^\varepsilon_{ij} b^{\varepsilon ij} + \bar{K}^\varepsilon \right], \quad (22)$$

where $\varepsilon$ corresponds to an arbitrary conformal transformation. Consequently the bending Hamiltonian $\mathcal{H}_b$ [13] extends as

$$\mathcal{H}_b = \frac{1}{2}k \int_{\varepsilon(S) \subset \varepsilon(\mathbb{R}^3)} \sqrt{g^\varepsilon} \, d\Omega^\varepsilon \, \left[ b^\varepsilon_{ij} b^{\varepsilon ij} + 2\bar{K}^\varepsilon \right]. \quad (23)$$

It is easily seen that the extended bending Hamiltonian $\mathcal{H}_b$ (23) decomposes as

$$\mathcal{H}_b = \frac{1}{2}k \int_{\varepsilon(S_{g,e}) \subset \varepsilon(\mathbb{R}^3)} \sqrt{g^\varepsilon} \, d\Omega^\varepsilon \, b^{\pm ij}_{ij} B^{\pm ij} + 4\pi k (g + e - 1) + 2k c^\pm_{\varepsilon}$$

with $C^+_{\varepsilon} = 0$ and $C^-_{\varepsilon} = \int_{\varepsilon(S_{g,e}) \subset \varepsilon(\mathbb{R}^3)} \sqrt{g^\varepsilon} \, d\Omega^\varepsilon \, \bar{K}^\varepsilon. \quad (24)$

Consequently, the Chen assertion (24) strongly suggests to apply existence theorems for minimal surfaces living in curved tridimensional space $\mathbb{R}^3$. To illustrate this point, we will establish Bogomol’nyi relationships for closed surfaces. A theorem due to
Lawson claims that there exist closed minimal surfaces $\xi_{m,n}$ of arbitrary genus $g = mn$ in the three-sphere $S^3$ ($\tilde{K} = 1$); $\xi_{0,n}$ is the round two-sphere $S^2$, $\xi_{1,1}$ the flat torus (i.e., the Clifford torus). Furthermore, the Willmore-Kusner conjecture [28-31] asserts that the surfaces $\xi_{g,1}$ actually minimize the functional $C^e$ in (24): we may have

$$\Lambda_g \equiv \inf_{S_{g,0} \subset \mathbb{R}^3} \left[ \int_{c(S_{g,0}) \subset c(\mathbb{R}^3)} \sqrt{g^2} \, d\Omega^t \tilde{K}^t \right] = \int_{\xi_{g,1} \subset S^3} \sqrt{7} \, d\Omega. \quad (25)$$

Readily the Bogomol’nyi decomposition for closed surfaces ($e = 0$) takes the form

$$H_b[S_g] = \frac{1}{2} k \int_{c(S_g) \subset S^3} \sqrt{g^2} \, d\Omega^t B^{ij} B^{ij} - 4\pi k (g-1) + 2k\Lambda_g, \quad (26)$$

where the conformal transformation $c$ maps $\mathbb{R}^3$ to $S^3$. Accordingly, the Bogomol’nyi technique combined with the Chen assertion [22] allows us to measure how much a surface manifold is deformed from any surface which is minimal inside a certain curved ambient space $A^3$. Thus, without loss of generality, the Willmore-Kusner conjecture [27] enables us to outline through the formula (24) our third key result: any deformation of the metastable bending configurations for shapes of non-spherical topology spontaneously leads to a mean curvature bending contribution à la Helfrich up to a conformal transformation of the ambient space. Before summarizing let us expose how the bending energy bounds (i.e., the Bogomol’nyi bounds) are governed. From the Bogomol’nyi decompositions (20), (21) and (26) the Bogomol’nyi bounds are:

$$H_b[S_{g,e}] \geq \begin{cases} 2\Lambda_g k + 4\pi k (g-1) & \text{if } g \geq 0 \text{ and } e = 0, \\ 4\pi k (g + e - 1) & \text{if } g \geq 0 \text{ and } e \geq 2. \end{cases} \quad (27)$$
Obviously the Bogomol’nyi bounds for vesicles \( \frac{27}{27} \) are proportional to the bending rigidity \( k \) and separate into two parts: a closure bending energy \( 2\Lambda_g k \) and a genus/end bending energy \( 4\pi k (g + e - 1) \). Whereas the bending energy per genus/end is straightforward to compute \( (4\pi k) \), there exists no literal formula for the Lawson sequence \( \Lambda_g \) yet: for the round two-sphere \( S^2 \) and the flat torus \( \xi_{1,1} \) the Lawson sequence \( \Lambda_g \) takes respectively as exact value \( \Lambda_0 = 4\pi \) and \( \Lambda_1 = 2\pi^2 \) (circles in Fig. 1), for higher genus we have computed numerical estimates (crosses in Fig. 1).

To summarize our key results concisely expressed in formulae (20), (21) and (26) the Bogomol’nyi technique, extended forward with existence theorems from differential geometry, allows us to show that any deformation of the non-trivial metastable shapes (which are clearly identified) generates a bending elastic energy contribution which falls in two distinct categories with respect to the topology of the shape: (i) for shapes of spherical topology a deviatoric bending contribution à la Fischer \([13, 14]\) spontaneously arises; (ii) for shapes of non-spherical topology a mean curvature bending contribution à la Helfrich \([2, 3, 16]\) (up to a conformal transformation of the ambient space) spontaneously emerges. We observe that this splitting comes from the breaking of the self-dual symmetry of the Bogomol’nyi relationships by existence theorems from differential geometry. Besides, the Bogomol’nyi relationships allow us to compute both the bending energy per genus/end and the bending closure energy for vesicles regardless of their shape.

As a further illustration, our approach leads to a clear understanding of geometrical frustration phenomena experienced by magnetically coated vesicles \([18, 21]\): the presence of the double Bogomol’nyi decomposition generates a competition between magnetic solitons and shapes which tend to saturate the magnetic energy \([1]\) and the bending energy \([13]\), respectively. More precisely, when at least one deviatoric tensor cannot vanish, the balance between the two deviatoric energies releases the frustration: hence both magnetic and geometric effects manifest in accordance with the deviatoric energies, e.g. by removing a mismatch between magnetic and geometric (or underlying support) length scales.

In conclusion, our approach gives in a rather natural manner the Bogomol’nyi relationships for vesicles: their typical features combined with existence theorems from differential geometry show that spontaneous bending deformation from metastable bending shapes splits in two distinct topological classes (shapes of spherical topology and shapes of non-spherical topology): in other words, topology may be considered to describe bending phenomena—in contradiction with customary phenomenological approaches \([4, 5]\). Furthermore, the appearance of Bogomol’nyi relationships for vesicles provides a powerful guide for understanding vesicles and enlarges the application field of the Bogomol’nyi technique (traditionally used in fields ranging from condensed matter physics to high energy physics) to elastic and geometrical phenomena in soft condensed matter.

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