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FIRST VARIATION OF THE GENERAL CURVATURE-DEPENDENT SURFACE ENERGY

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Abstract. We consider general surface energies, which are weighted integrals over a closed surface with a weight function depending on the position, the unit normal and the mean curvature of the surface. Energies of this form have applications in many areas, such as materials science, biology and image processing. Often one is interested in finding a surface that minimizes such an energy, which entails finding its first variation with respect to perturbations of the surface. We present a concise derivation of the first variation of the general surface energy using tools from shape differential calculus. We first derive a scalar strong form and next a vector weak form of the first variation. The latter reveals the variational structure of the first variation, avoids dealing explicitly with the tangential gradient of the unit normal, and thus can be easily discretized using parametric finite elements. Our results are valid for surfaces in any number of dimensions and unify all previous results derived for specific examples of such surface energies.

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1. Introduction

We consider the general weighted surface energy

$$J(\Gamma) = \int_\Gamma \gamma(x, \nu, \kappa)\, \mathrm{d}S, \tag{1.1}$$

for a smooth orientable compact $(d-1)$ dimensional surface Γ in $\mathbb{R}^d$ without boundary. The energy (1.1) is weighted by a smooth function $\gamma = \gamma(x, \nu, \kappa)$, which depends on the surface point x, the unit normal ν at x, and the mean curvature $\kappa = \sum_{i=1}^{d-1} \kappa_i$ given by the sum of the principal curvatures κ_i at x (sometimes κ is called total curvature). We derive the first variation of the energy (1.1) with respect to perturbations of the surface Γ: we first obtain a scalar strong form and next a vector weak form of the first variation. The latter reveals the variational structure of the first variation, avoids dealing explicitly with the tangential gradient of

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the unit normal, and thus can be easily discretized using parametric finite elements. We exploit further the vector formulation and describe gradient flows for (1.1) that give descent directions for minimizing (1.1).

Examples of the surface energy. Energies of the form (1.1) have attracted attention in various fields, such as materials science, biology and image processing. Setting $\gamma(x,\nu,\kappa)$ equal to specific forms in (1.1), we obtain many examples that are of practical interest in these fields. The following are some of these examples.

- *Anisotropic surface energy*: By restricting the weight γ in (1.1) to

$$\gamma = \gamma(x,\nu),$$

  we obtain the general form for anisotropic surface energy that has been the subject of extensive investigation in modeling of crystals [1,2,35,43,44,46,48] in materials science. This form has also found application in the problems of boundary detection [29] and 3d scene reconstruction [28] in image processing.

- *Willmore functional*: The special form of (1.1)

$$\gamma = \frac{1}{2}\kappa^2,$$

  models the bending energy of membranes and is significant in the study of biological vesicles [23,26,38]. We refer to the book [49] for more information. The Willmore functional is also employed as a regularization term in boundary detection problems in image processing [42].

- *Spontaneous curvature*: If the spatially-varying function $\kappa_0(x)$, so-called spontaneous curvature, describes the preferred mean curvature of an unconstrained piece of membrane, then [23,38] proposed the modified bending energy

$$\gamma = \frac{1}{2}\left(\kappa - \kappa_0(x)\right)^2.$$

  It can be used to model the effect of an asymmetry in the membrane [16] or that of an additional field, as in the theory of surfactants [12,33,36].

- *Weighted Willmore functional*: The modified form of the Willmore functional

$$\gamma = g(x)\kappa^2,$$

  has been recently proposed as a space-varying regularization term depending on the image [42]. This form is also related to the modeling of biomembranes when the concentration or composition of lipids changes spatially [7,13,47].

Other image processing applications that involve various effects of the curvature in the minimization of the energy (1.1) are in shape matching [34] and in surface restoration [14]. Also a curvature-dependent weight function $\gamma = \gamma(\kappa)$ has been used recently in [19] to achieve higher-order feature-preserving regularization in image segmentation.

Related work and main contributions. Often one is interested in a minimum or a stationary point of these energies. Therefore, the first variation of (1.1) with respect to deformations of the surface Γ becomes an essential step in this investigation. Although the first variation of (1.1) has been derived in the special cases $\gamma = \gamma(x,\nu)$ [8,27,35,44,48], $\gamma = \frac{1}{2}\kappa^2$ [49], $\gamma = g(x)\kappa^2$ [42], $\gamma = \gamma(\kappa)$ [19], a general result for (1.1) in any number of dimensions, to our knowledge, does not exist. We believe that derivation of the first variation of (1.1) in its general form is useful to scientists working on the various problems involving surface energies, such as those mentioned above, in that it makes it easier for them to experiment with different forms of $\gamma(x,\nu,\kappa)$ taylored to their applications. Still the analytical formula is only one part of the picture. Typically one would like to compute the configurations predicted by the formulas as well, and this necessitates a discretization of the analytical formula in a way suitable for numerical computations. This constitutes our motivation and leads to the following two major contributions of our work:

- *Scalar form of the first variation of energy* (1.1)*:* We derive, using shape differential calculus [15,41], the following expression for the first variation of (1.1) in the direction of the velocity field $\vec{V}$ for a $(d-1)$ dimensional surface Γ:

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \Big(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma\Big)\, \vec{V}\cdot\nu \,\mathrm{d}S. \tag{1.2}$$

Hereafter, the weight $\gamma = \gamma(x, y, z)$ is a smooth function of its three arguments, and $\gamma_x, \gamma_y, \gamma_z$ denote its partial derivatives. Moreover, given a function $f = f(x, y, z)$, the symbol $[f]$ indicates the composite function $F(x) = f(x, \nu(x), \kappa(x))$ for $x \in \Gamma$. We refer to Sections 2 and 4 for definitions of the tangential derivatives and other details. This result not only unifies existing work on various forms of the surface energy (1.1), but it also provides a concise rederivation of them. As expected [15,41], $\mathrm{d}J(\Gamma;\vec{V})$ in (1.1) depends solely on the normal velocity $V = \vec{V}\cdot\nu$, so all functions on the right-hand side are scalar. We thus call (1.2) scalar form. The merit of scalar form (1.2) is that it clearly delineates how the form of the weight function γ and the geometry of the surface Γ contribute to the first variation and related gradient descent flows. However, numerical discretization of the expression (1.2) is awkward, because the principal curvatures κ_i need to be approximated numerically. Thus we derive an alternate expression.

- *Vector form of the first variation of energy* (1.1): We derive a novel weak formulation equivalent to (1.2), which involves vector quantities as well as first order tangential derivatives and reads as follows:

$$\mathrm{d}J(\Gamma;\vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{\phi} : \nabla_\Gamma \vec{Z} - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi}\,\vec{Y} + \int_\Gamma \gamma\,\mathrm{div}_\Gamma\vec{\phi} + \int_\Gamma \gamma_x\cdot\vec{\phi}, \tag{1.3}$$

where $\vec{\phi}$ is the vector perturbation or test function (replacing $\vec{V}$ in (1.2)) and $\vec{\kappa}, \vec{Z}, \vec{Y}$ are defined by the strong relations

$$\vec{\kappa} = -\Delta_\Gamma x, \qquad \vec{Z} = \gamma_z\nu, \qquad \vec{Y} = \gamma_y,$$

which can also be imposed weakly. Expression (1.3) reveals the variational structure of the first variation, avoids dealing explicitly with $\sum\kappa_i^2 = |\nabla_\Gamma\nu|^2$, and is amenable to direct discretization by C^0 parametric finite element methods. The latter is a key advantage of (1.3) over (1.2). Nonetheless, we stress that the expression (1.3) is derived from (1.2) (using tensor calculus) and could not be obtained without deriving (1.2) first (using shape differential calculus). The result (1.3) is inspired by and extends the works of Rusu [37], Dziuk [20], and Bonito *et al.* [9]; expression (1.3) reduces to that in [9] for the Willmore functional. A related expression for the case of $\gamma = \gamma(\kappa)$ was derived by Droske and Bertozzi in [19]. We discuss how to utilize (1.3) to compute a gradient flow for (1.1).

We should stress that the background required to derive these results are minimal, unlike some related results in literature requiring significant knowledge of certain specialized areas, such as Riemannian geometry. In our case, it suffices that the reader be familiar with basic geometric concepts only, such as the normal and curvature of a surface. Otherwise our paper is mostly self-contained and our derivations rely on multivariable calculus and elementary tensor algebra.

Some critical issues that we do not address in this paper are the existence, uniqueness and regularity of the minimizers of the surface energy (1.1). The energy (1.1) is too general (because of the arbitrariness of the weight function $\gamma(x, \nu, \kappa)$) for us to make a comprehensive investigation of these issues. Thus, such an analysis is not in the scope of this paper. There does exist work in literature addressing these issues in the case of Willmore functional. For these, we refer to the papers [6,21,30–32,39,40].

Outline of the paper. The rest of the paper is organized as follows. In Section 2, we introduce the basic tools from shape differential calculus; we refer to [15,41] for details. These tools form the basis for the computations in later sections. In Section 3, we derive auxiliary results of geometric nature *via* the distance function to Γ. In Section 4, we use those results to prove (1.2) and obtain the first variation for specific forms of $\gamma(x, \nu, \kappa)$. In Section 5, we derive (1.3) upon changing scalar quantities in (1.2) with vector quantities, and examine the special case $\gamma = g(x)(\kappa - \kappa_0(x))^2$. In Section 6 we formulate gradient flows based on either (1.2) or (1.3), the latter giving a novel variational formula for the L^2-gradient flow of (1.1). In Section 7, we recapitulate our main results.

2. Shape differential calculus

In this section, we introduce the tools that we need to take shape derivatives. Shape differentiation enables us to derive the first variation of the energy (1.1) with respect to perturbations of the surface Γ. Our starting point for this is the velocity method as described in Section 2.2; velocity fields are used to deform the surface Γ. Then the shape derivative, described in Section 2.3, is used to quantify the change in the surface energy with respect to deformations induced by the velocity field. Shape differentiation is a well-developed and convenient procedure to compute the first variation of shape functionals, functionals that depend on shapes, such as curves or surfaces. For more information on shape differentiation using the velocity method, we refer to the book [15] by Delfour and Zolésio. From this point on, our emphasis will be on the shape derivative of the general surface energy (1.1), the first variation being just a consequence. Note that another approach commonly used in differential geometry literature is to parametrize the surface and to use charts, then to compute the first variation of the energy in the parameter domain. We find that our approach based on shape differentiation results in more concise derivations and requires less background knowledge.

Now we define some of the notation used in the paper. Given $d \times d$ matrices A and B, we define the product $A : B = A_{ij} B_{ij}$. The symbol $\otimes$ denotes the tensor product operation for two vectors and is defined by $(v \otimes w)_{ij} = v_i w_j$. Here we use the Einstein convention, that repeated indices denote summation over those indices.

Given a scalar function $f = f(x, y, z)$ defined for $x \in U$ a tubular neighborhood of Γ, $y \in \mathbb{R}^d$ and $z \in \mathbb{R}$, we denote

$$f_x = (f_{x_1}, \ldots, f_{x_d})^T = \nabla f, \qquad f_y = (f_{y_1}, \ldots, f_{y_d})^T, \qquad f_z,$$

the partial derivatives of f. We also define the second derivatives by $f_{xx} (= D^2 f)$, f_{yy}, f_{zz}, $f_{xy}, \ldots, f_{zy}$, which are the matrices of the derivatives, for example,

$$(f_{xx})_{ij} = f_{x_i x_j}, \quad i = 1, \ldots, d, \; j = 1, \ldots, d.$$

The Laplacian of f is given by $\Delta f = f_{x_1 x_1} + \ldots + f_{x_d x_d}$.

We are interested in the composite function $f(x, \nu, \kappa)$ for $x \in \Gamma$, $\nu \in S^{d-1}$ the unit normal at x, and $\kappa \in \mathbb{R}$ the mean curvature at x, as well as

$$F(x) = f(x, \nu(x), \kappa(x)),$$

for $x \in U$, and $\nu(x), \kappa(x)$ suitable extensions off the surface Γ. In contrast to the space gradient ∇f, we define the *total gradient* of f by

$$\nabla[f] = \nabla F(x) = (f_{x_i} + f_{y_k} \nu_{k, x_i} + f_z \kappa_{x_i})_{i=1}^d.$$

It is critical to note the difference between ∇f *and* $\nabla[f]$ *to follow the derivations in the paper without any confusion. Similarly we have* $\Delta[f] = \operatorname{div}[\nabla[f]]$ *acting on all components of* f *(compare with* Δf *above).*

The notation for the third derivatives of f follows the same conventions.

2.1. **Tangential differentiation**

Let us be given $h \in C^2(\Gamma)$ and a smooth extension $\tilde{h}$ of h, $\tilde{h} \in C^2(U)$ and $\tilde{h}|_\Gamma = h$ on Γ where U is a tubular neighborhood of Γ in $\mathbb{R}^d$. Then the *tangential gradient* $\nabla_\Gamma h$ of h is defined as follows:

$$\nabla_\Gamma h = \big(\nabla \tilde{h} - \partial_\nu \tilde{h}\ \nu\big)|_\Gamma,$$

where ν denotes the unit normal vector to Γ. For $\vec{W} \in [C^1(\Gamma)]^d$ properly extended to a neighborhood of Γ, we define the *tangential divergence* of $\vec{W}$ by

$$\mathrm{div}_\Gamma \vec{W} = \big(\mathrm{div}\vec{W} - \nu^T D\vec{W}\nu\big)|_\Gamma, \tag{2.1}$$

where $D\vec{W}$ denotes the Jacobian matrix of $\vec{W}$. Similarly we define the tangential gradient $\nabla_\Gamma \vec{W}$ of $\vec{W}$, which is a matrix whose ith row is the tangential gradient $\nabla_\Gamma \vec{W}_i$ of the ith component of $\vec{W}$. Finally, the *tangential Laplacian* or *Laplace-Beltrami operator* Δ_Γ on Γ is defined as follows:

$$\Delta_\Gamma h = \mathrm{div}_\Gamma(\nabla_\Gamma h) = \big(\Delta \tilde{h} - \nu^T D^2 \tilde{h}\nu - \kappa\ \partial_\nu \tilde{h}\big)|_\Gamma. \tag{2.2}$$

In Section 3, we will present the formulas for the tangential derivatives of functions that depend on ν and κ.

2.2. **The velocity method**

We consider now a hold-all domain $\mathcal{D}$, which contains the surface Γ, and a vector field $\vec{V}$ defined on $\mathcal{D}$, which is used to define the continuous sequence of perturbed surfaces $\{\Gamma_t\}_{t\geq 0}$, with $\Gamma_0 := \Gamma$. Each point $x \in \Gamma_0$ is continuously deformed by an ordinary differential equation (ODE) defined by a smooth field $\vec{V}$. The parameter which controls the amplitude of the deformation is denoted by t.

We consider the system of autonomous ODEs for small enough T

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \vec{V}(x(t)), \quad \forall t \in [0,T], \qquad x(0) = X, \tag{2.3}$$

where $X \in \Gamma_0 = \Gamma$. This defines the mapping

$$x(t,\cdot) : X \in \Gamma \to x(t,X) \in \mathbb{R}^d, \tag{2.4}$$

and also the perturbed sets

$$\Gamma_t = \{x(t,X) : \quad X \in \Gamma_0\}. \tag{2.5}$$

We recall that the family of perturbed sets has its regularity preserved for $\vec{V}$ smooth enough [41]: if Γ_0 is of class C^r, then for any $t \in [0,T]$, Γ_t is also of class C^r.

2.3. **Derivative of shape functionals**

Let $J(\Gamma)$ be a shape functional, namely a map that associates to manifolds Γ in $\mathbb{R}^d$ of co-dimension 1 a real number. The Eulerian derivative, or *shape derivative*, of the functional $J(\Gamma)$ at Γ in the direction of the vector field $\vec{V}$, is defined as the limit

$$\mathrm{d}J(\Gamma;\vec{V}) = \lim_{t\to 0} \frac{1}{t}\big(J(\Gamma_t) - J(\Gamma)\big). \tag{2.6}$$

The shape derivative is the primary tool used in this paper to derive the first variation of surface energies. For more information on the concept of shape derivatives (including the definition and other properties), we refer to the book [15] by Delfour and Zolésio.

We now recall a series of results from shape differential calculus in $\mathbb{R}^d$. We start with the shape derivative of surface integrals of functions that do not depend on the geometry.

Lemma 2.1 ([41], Prop. 2.50 and (2.145))**.** *Let* $\psi \in W^{2,1}(\mathbb{R}^d)$ *and* Γ *be of class* C^2*. Then the functional* $J(\Gamma) = \int_\Gamma \psi \mathrm{d}S$ *is shape differentiable and the derivative*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \big(\nabla\psi\cdot\vec{V} + \psi\mathrm{div}_\Gamma\vec{V}\big)\mathrm{d}S = \int_\Gamma \big(\partial_\nu\psi + \psi\kappa\big)V\mathrm{d}S, \tag{2.7}$$

depends on the normal component $V = \vec{V}\cdot\nu$ *of the velocity* $\vec{V}$*.*

Let us now consider more general functionals $J(\Gamma)$. We are interested in computing shape derivatives for functionals of the form

$$J(\Gamma) = \int_\Gamma \varphi(x,\Gamma)\mathrm{d}S, \tag{2.8}$$

where φ maps the position $x \in \Gamma$ and manifold $\Gamma \subset \mathbb{R}^d$ of co-dimension 1 into the real numbers. The dependence of φ on Γ can be in various ways. For example, φ might depend on a function u that is the solution of a partial differential equation defined inside Γ [11,17,25]. In this paper we consider $\varphi = \gamma(x,\nu,\kappa)$ depending on the normal ν and the mean curvature κ at $x \in \Gamma$. To handle the computation of the shape derivatives of such functionals we need to take care of the derivative of φ with respect to Γ. For this we recall the notions of *material derivative* and *shape derivative*.

Definition 2.2 ([41], Prop. 2.71)**.** The *material derivative* $\dot\varphi(\Gamma;\vec{V})$ of φ at Γ in direction $\vec{V}$ is defined as follows

$$\dot\varphi(\Gamma;\vec{V}) = \lim_{t\to 0}\frac{1}{t}\big(\varphi(x(t,\cdot),\Gamma_t) - \varphi(\cdot,\Gamma_0)\big), \tag{2.9}$$

where the mapping $x(t,\cdot)$ is defined as in (2.4).

Definition 2.3 ([41], Defs. 2.85, 2.88)**.** For surface functions $\varphi(\Gamma):\Gamma\to\mathbb{R}$, the shape derivative at Γ in the direction $\vec{V}$ is defined as

$$\varphi'(\Gamma;\vec{V}) = \dot\varphi(\Gamma;\vec{V}) - \nabla_\Gamma\varphi\cdot\vec{V}|_\Gamma. \tag{2.10}$$

Theorem 2.4 ([41], Sects. 2.31, 2.33)**.** *Let* $\varphi = \phi(x,\Gamma)$ *be given so that the material derivative* $\dot\varphi(\Gamma;\vec{V})$ *and the shape derivative* $\varphi'(\Gamma;\vec{V})$ *exist. Then, the functional* $J(\Gamma)$ *in* (2.8) *is shape differentiable and we have*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \varphi'(\Gamma;\vec{V})\mathrm{d}S + \int_\Gamma \kappa\varphi V\mathrm{d}S,$$

whereas if $\varphi = \psi(\cdot,\Omega)|_\Gamma$ *(*ψ *defined off the surface* Γ *and is a function of the domain* Ω *enclosed by* Γ*), then we obtain*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \psi'(\Omega;\vec{V})|_\Gamma\mathrm{d}S + \int_\Gamma \big(\partial_\nu\psi + \kappa\psi\big)V\mathrm{d}S, \tag{2.11}$$

where $V = \vec{V}\cdot\nu$ *is the normal component of the velocity* $\vec{V}$*.*

3. The distance function and basic geometry

In this section we employ the signed distance function to Γ to derive a few geometric results, which are useful later to obtain the first variation of the surface energy (1.1). The signed distance function $b(x)$ to the surface Γ is defined as

$$b(x,\Gamma) = \begin{cases} \mathrm{dist}(x,\Gamma) & \text{for } x \in \mathbb{R}^d - \Omega \\ 0 & \text{for } x \in \Gamma \\ -\mathrm{dist}(x,\Gamma) & \text{for } x \in \Omega \end{cases} \tag{3.1}$$

where

$$\mathrm{dist}(x,\Gamma) = \inf_{y\in\Gamma}|y-x|.$$

The signed distance representation of Γ allows us to extend ν and κ smoothly in a tubular neighborhood of Γ. We will exploit the following identities [15], Chapter 8

$$\nu = \nabla b(x)|_\Gamma, \quad \kappa = \Delta b(x)|_\Gamma, \quad \nabla_\Gamma \nu = D^2 b(x)|_\Gamma. \tag{3.2}$$

Extension of $\nu, \kappa, \nabla_\Gamma \nu$ using the signed distance function is critical for the results in this section. Moreover, the shape derivative of b with respect to $\vec{V}$ is given by [24], Section 3

$$b'(\Gamma; \vec{V}) = -V. \tag{3.3}$$

Our derivations for Lemmas 3.2–3.4 hold only for parallel surfaces defined by the signed distance function.

Lemma 3.1 ([24], Sect. 3)**.** *The shape derivatives of the normal ν and the mean curvature κ of a surface Γ of class C^2 with respect to velocity $\vec{V} \in C^2$ are given by*

$$\nu' = \nu'(\Gamma; \vec{V}) = -\nabla_\Gamma V, \tag{3.4}$$

$$\kappa' = \kappa'(\Gamma; \vec{V}) = -\Delta_\Gamma V, \tag{3.5}$$

where $V = \vec{V} \cdot \nu$ is the normal component of the velocity.

Proof. We use the shape derivative (3.3) of the signed distance function. Note the following

$$0 = (1)' = (\nabla b \cdot \nabla b)' = 2\nabla b' \cdot \nabla b,$$

which gives

$$\nu' = \nabla b'|_\Gamma = \nabla_\Gamma b'|_\Gamma + \nabla b'|_\Gamma \cdot \nu\nu = \nabla_\Gamma b'|_\Gamma = -\nabla_\Gamma V.$$

Similarly we compute

$$\kappa' = \Delta b'|_\Gamma = \mathrm{div}(\nabla b')|_\Gamma = (\mathrm{div}_\Gamma(\nabla b') + \underbrace{\nabla b^T D^2 b' \nabla b}_{=0})|_\Gamma = -\mathrm{div}_\Gamma(\nabla_\Gamma V) = -\Delta_\Gamma V.$$

One can easily show that the term $\nabla b^T D^2 b' \nabla b$ is zero by taking the gradient of $\nabla b' \cdot \nabla b = 0$,

$$\nabla(\nabla b' \cdot \nabla b) = D^2 b' \nabla b + D^2 b \nabla b' = 0,$$

so that

$$\nabla b D^2 b' \nabla b = -\nabla b D^2 b \nabla b' = -\nabla b' D^2 b \nabla b = 0.$$

Note that $0 = \nabla(1) = \nabla(\nabla b \cdot \nabla b) = 2D^2 b \nabla b$. □

Lemma 3.2. *The normal derivative of the mean curvature of a surface Γ of class C^3 is given by*

$$\partial_\nu \kappa = -\sum_i \kappa_i^2 \tag{3.6}$$

where κ_i denote the principal curvatures of the surface. For a two-dimensional surface in 3d, this is equal to

$$\partial_\nu \kappa = -(\kappa_1^2 + \kappa_2^2) = -(\kappa^2 - 2\kappa_G)$$

where $\kappa_G = \kappa_1 \kappa_2$ denotes the Gauss curvature.

Proof. To prove this result, we will work with the signed distance representation $b(x)$ of Γ, defined by (3.1). We proceed as follows

$$\begin{aligned}0 &= \Delta(1) = \Delta(\nabla b \cdot \nabla b) = \partial_{x_i}\partial_{x_i}(b_{x_j} b_{x_j}) \\ &= \partial_{x_i}(b_{x_j x_i} b_{x_j} + b_{x_j} b_{x_j x_i}) = 2\partial_{x_i}(b_{x_j} b_{x_j x_i}) \\ &= 2(b_{x_j x_i} b_{x_j x_i} + b_{x_i x_i x_j}) b_{x_j}) \\ &= 2\left(D^2 b : D^2 b + \nabla(\Delta b)\cdot\nabla b\right).\end{aligned}$$

Then

$$\partial_\nu \kappa = \nabla(\Delta b)\cdot \nabla b|_\Gamma = -|D^2 b|^2|_\Gamma = -|\nabla_\Gamma \nu|^2 = -\sum_i \kappa_i^2,$$

where $|\cdot|$ denotes the Frobenius norm of a matrix. To get this result we used the fact that squared Frobenius norm of a square matrix is equal to the sum of the squares of its eigenvalues, and that the eigenvalues of $\nabla_\Gamma \nu$ are zero and the principal curvatures κ_i. □

Lemma 3.3. *The normal and the mean curvature of a surface Γ of class C^3 satisfy the following PDE*

$$\Delta_\Gamma \nu = -|\nabla_\Gamma \nu|^2 \nu + \nabla_\Gamma \kappa \tag{3.7}$$

Proof. We derive the PDE (3.7) using the signed distance function extensions (3.2) of the geometric terms. We recall $|\nabla b|^2 = \nabla b \cdot \nabla b = 1$, which we differentiate twice

$$0 = \partial_{x_k x_k}(1) = \partial_{x_k x_i}(b_{x_l} b_{x_l}) = 2\partial_{x_k}(b_{x_l x_k} b_{x_l}) = 2(b_{x_l x_k x_k} b_{x_l} + b_{x_l x_k} b_{x_l x_k}).$$

We change the order of derivatives in $b_{x_l x_k x_k}$ and obtain the following,

$$b_{x_k x_k x_l} b_{x_l} = -b_{x_k x_l} b_{x_k x_l}. \tag{3.8}$$

Now we compute $\nabla_\Gamma \kappa = (\nabla\Delta b - \nabla\Delta b\cdot\nabla b\nabla b)|_\Gamma$.

$$\begin{aligned}(\nabla\Delta b - \nabla\Delta b\cdot\nabla b\nabla b)_i &= \partial_{x_i} b_{x_k x_k} - (\partial_{x_j} b_{x_k x_k}) b_{x_j} b_{x_i} = b_{x_k x_k x_i} - b_{x_k x_k x_j} b_{x_j} b_{x_i} \\ &= b_{x_i x_k x_k} + b_{x_k x_l} b_{x_k x_l} b_{x_i} = \Delta b_{x_i} + |D^2 b|^2 b_{x_i}.\end{aligned}$$

We restrict to the surface Γ and obtain

$$\nabla_\Gamma \kappa = (\Delta\nabla b + |D^2 b|^2 \nabla b)|_\Gamma = \Delta_\Gamma \nu + |\nabla_\Gamma \nu|^2 \nu.$$

This concludes the proof. □

Lemma 3.4. *Let the scalar function $f = f(x,\nu,\kappa)$ and the vector function $\vec{W} = \vec{W}(x,\nu,\kappa)$ on a C^4 surface be given such that $f \in C^2$ and $\vec{W} \in C^1$. Then the explicit formulas for the (total) tangential gradient $\nabla_\Gamma[f]$, the (total) tangential divergence $\mathrm{div}_\Gamma[\vec{W}]$ and the (total) tangential Laplacian $\Delta_\Gamma[f]$ are given by the following*

$$\nabla_\Gamma[f(x,\nu,\kappa)] = \nabla_\Gamma f + \nabla_\Gamma \nu f_y + f_z \nabla_\Gamma \kappa, \tag{3.9}$$

$$\mathrm{div}_\Gamma[\vec{W}(x,\nu,\kappa)] = \mathrm{div}_\Gamma \vec{W} + \vec{W}_y : \nabla_\Gamma \nu + \vec{W}_z \cdot \nabla_\Gamma \kappa, \tag{3.10}$$

$$\begin{aligned}\Delta_\Gamma[f(x,\nu,\kappa)] = {} & \Delta_\Gamma f + f_y\cdot(\nabla_\Gamma\kappa + \nu\Sigma\kappa_i^2) + (\nabla_\Gamma \nu f_{yy}) : \nabla_\Gamma \nu^T \\ & + f_z \Delta_\Gamma \kappa + f_{zz}|\nabla_\Gamma \kappa|^2 + (f_{xy} + f_{yx}^T) : \nabla_\Gamma \nu \\ & + (f_{xz} + f_{zx})\cdot\nabla_\Gamma\kappa + (f_{yz} + f_{zy})\cdot(\nabla_\Gamma \nu \nabla_\Gamma \kappa),\end{aligned} \tag{3.11}$$

where $\nabla_\Gamma f, \mathrm{div}_\Gamma \vec{W}, \Delta_\Gamma f$ *denote the partial derivatives* (*see Sect.* 2 *for the distinction between the partial derivatives* $\nabla_\Gamma f, \mathrm{div}_\Gamma \vec{W}, \Delta_\Gamma f$ *and the total derivatives* $\nabla_\Gamma[f], \mathrm{div}_\Gamma[\vec{W}], \Delta_\Gamma[f]$).

Proof. Expressions (3.9)–(3.11) can be derived using the chain rule for tangential derivatives. However, we present a concise proof of (3.9) and (3.10) using the signed distance function, because it provides a more transparent derivation.

The functions $f, \vec{W}$ are not necessarily defined off the surface Γ, nor are the normal ν and the mean curvature κ. We need to extend these smoothly to a tubular neighborhood of the surface Γ. For this, we use the signed distance function extensions (3.2) of ν and κ. Moreover, we define the smooth extensions $\tilde{f}$, $\tilde{W}$ of $f, \vec{W}$ by

$$f(x,\nu,\kappa) = \tilde{f}(x,\nabla b,\Delta b)|_\Gamma, \qquad \vec{W}(x,\nu,\kappa) = \tilde{W}(x,\nabla b,\Delta b)|_\Gamma.$$

We will perform the algebra on $\tilde{f}$, $\tilde{W}$ for the derivations, then restrict the results to the surface Γ and obtain the tangential derivatives (3.9), (3.10). We continue to refer to $\tilde{f}, \tilde{W}$ by $f, \vec{W}$ respectively for convenience.

We start by computing the first derivative of f.

$$\nabla[f(x,\nabla b,\Delta b)] = \nabla f + D^2 b f_y + f_z \nabla\Delta b, \tag{3.12}$$

from which we can compute

$$\begin{aligned}\nabla[f(x,\nabla b,\Delta b)] - \nabla[f(x,\nabla b,\Delta b)]\cdot\nabla b\nabla b &= (\nabla f + D^2 b f_y + f_z\nabla\Delta b) - (\nabla f + D^2 b f_y + f_z \nabla\Delta b)\cdot\nabla b\nabla b\\ &= (\nabla f - \nabla f\cdot\nabla b\nabla b) + D^2 b f_y + f_z(\nabla\Delta b - \nabla\Delta b\cdot\nabla b\nabla b).\end{aligned}$$

Note that $(D^2 b f_y)\cdot\nabla b\nabla b$ vanishes as $D^2 b\nabla b = 0$. Then we restrict $\nabla[f(x,\nabla b,\Delta b)]$ to Γ and obtain

$$\nabla_\Gamma[f(x,\nu,\kappa)] = \nabla_\Gamma f + \nabla_\Gamma \nu f_y + f_z \nabla_\Gamma\kappa.$$

Now we derive the formula for the tangential divergence by

$$\mathrm{div}_\Gamma[\vec{W}(x,\nu,\kappa)] = \left(\partial_{x_i}[W^i(x,\nabla b,\Delta b)] - b_{x_i}\partial_{x_i}[W^j(x,\nabla b,\Delta b)]b_{x_j}\right)|_\Gamma.$$

We compute

$$\begin{aligned}&\partial_{x_i}[W^i(x,\nabla b,\Delta b)] - b_{x_i}\partial_{x_i}[W^j(x,\nabla b,\Delta b)]b_{x_j}\\ &\qquad = W^i_{x_i} + W^i_{y_k} b_{x_k x_i} + W^i_z(\Delta b)_{x_i} - b_{x_i}W^j_{x_i}b_{x_j} - b_{x_j}W^j_{y_k}b_{x_k x_i}b_{x_i} - b_{x_i}W^j_z(\Delta b)_{x_i}b_{x_j}\\ &\qquad = W^i_{x_i} - b_{x_i}W^j_{x_i}b_{x_j} + W^i_{y_k}b_{x_k x_i} + W^i_z((\Delta b)_{x_i} - (\Delta b)_{x_j}b_{x_j}b_{x_i}),\end{aligned}$$

whose restriction to Γ results in

$$\mathrm{div}_\Gamma[\vec{W}(x,\nu,\kappa)] = \mathrm{div}_\Gamma\vec{W} + \vec{W}_y : \nabla_\Gamma\nu + \vec{W}_z\cdot\nabla_\Gamma\kappa.$$

We now use the chain rule for tangential derivatives to handle (3.11). The tangential Laplacian $\Delta_\Gamma[f]$ is given by

$$\Delta_\Gamma[f] = \mathrm{div}_\Gamma[\nabla_\Gamma[f]] = \mathrm{div}_\Gamma[\nabla_\Gamma f + \nabla_\Gamma\nu f_y + f_z\nabla_\Gamma\kappa]. \tag{3.13}$$

We introduce the notation for

$$\partial^i_\Gamma f = f_{x_i} - f_{x_k}\nu_k\nu_i, \qquad \partial^{ij}_\Gamma f = \partial^j_\Gamma\partial^i_\Gamma f$$

and proceed to compute the three terms in (3.13)

$$\begin{aligned}
\mathrm{div}_\Gamma[\nabla_\Gamma f] =&\partial_\Gamma^k[\partial_\Gamma^k f] = \partial_\Gamma^{kk} f + \partial_\Gamma^k f_{y_l} \partial_\Gamma^k \nu_l + \partial_\Gamma^k f_z \partial_\Gamma^k \kappa \\
=&\Delta_\Gamma f + \nabla_\Gamma \nu : \nabla_\Gamma f_y + \nabla_\Gamma f_z \cdot \nabla_\Gamma \kappa, \\
\mathrm{div}_\Gamma[\nabla_\Gamma \nu f_y] =&\partial_\Gamma^k[\partial_\Gamma^k \nu_l f_{y_l}] = \partial_\Gamma^{kk}\nu_l f_{y_l} + \partial_\Gamma^k \nu_l \partial_\Gamma^k [f_{y_l}] \\
=&\partial_\Gamma^{kk}\nu_l f_{y_l} + \partial_\Gamma^k \nu_l \partial_\Gamma^k f_{y_l} + \partial_\Gamma^k \nu_l f_{y_l y_m} \partial_\Gamma^k \nu_m + \partial_\Gamma^k \nu_l f_{y_l z} \partial_\Gamma^k \kappa \\
=&\Delta_\Gamma \nu \cdot f_y + \nabla_\Gamma \nu : \nabla_\Gamma f_y + \nabla_\Gamma \nu : (f_{yy} \nabla_\Gamma \nu^T) + \nabla_\Gamma \kappa^T \nabla_\Gamma \nu f_{yz} \\
=&\nabla_\Gamma \kappa \cdot f_y - |\nabla_\Gamma \nu|^2 f_y \cdot \nu + \nabla_\Gamma \nu : \nabla_\Gamma f_y + \nabla_\Gamma \nu : (f_{yy} \nabla_\Gamma \nu^T) + f_{yz}^T \nabla_\Gamma \nu \nabla_\Gamma \kappa, \qquad \text{(using (3.7))} \\
\mathrm{div}_\Gamma[f_z \nabla_\Gamma \kappa] =&f_z \Delta_\Gamma \kappa + \nabla_\Gamma [f_z] \cdot \nabla_\Gamma \kappa \\
=&f_z \nabla_\Gamma \kappa + \nabla_\Gamma f_z \cdot \nabla_\Gamma \kappa + f_{zy}^T \nabla_\Gamma \nu \nabla_\Gamma \kappa + f_{zz} |\nabla_\Gamma \kappa|^2.
\end{aligned}$$

We substitute these three terms back in (3.13), use the fact $|\nabla_\Gamma \nu|^2 = \Sigma \kappa_i^2$, and obtain the formula (3.11). □

Proposition 3.5 ([15], Sect. 8.5.5, (5.27))**.** *For a function $f \in C^1(\Gamma)$ and a vector $\vec{\omega} \in C^1(\Gamma)^d$, we have the following tangential Green's formula*

$$\int_\Gamma f \mathrm{div}_\Gamma \vec{\omega} + \nabla_\Gamma f \cdot \vec{\omega} \mathrm{d}S = \int_\Gamma \kappa f \vec{\omega} \cdot \nu \mathrm{d}S. \tag{3.14}$$

4. First variation of the surface energy: scalar form

Now we present the main result of our paper: the first shape derivative of the general weighted surface energy

$$J(\Gamma) = \int_\Gamma \gamma(x, \nu, \kappa) \mathrm{d}S. \tag{4.1}$$

Theorem 4.1 (scalar form)**.** *The first shape derivative of the general weighted surface energy (4.1) with $\gamma = \gamma(x, \nu, \kappa)$ at Γ in the direction of velocity $\vec{V}$ is given by*

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma -\gamma_y \cdot \nabla_\Gamma V - \gamma_z \Delta_\Gamma V + \Big(\gamma\kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma\Big) V \mathrm{d}S, \tag{4.2}$$

or

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma \Big(\mathrm{div}_\Gamma[\gamma_y] - \Delta_\Gamma[\gamma_z] + (\gamma - \gamma_y \cdot \nu)\kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma\Big) V \mathrm{d}S, \tag{4.3}$$

where $V = \vec{V} \cdot \nu$ and we have

$$\mathrm{div}_\Gamma[\gamma_y] = \mathrm{div}_\Gamma \gamma_y + \gamma_{yy} : \nabla_\Gamma \nu + \gamma_{yz} \cdot \nabla_\Gamma \kappa, \tag{4.4}$$

and

$$\begin{aligned}
\Delta_\Gamma[\gamma_z] \quad = \quad & \Delta_\Gamma \gamma_z + \gamma_{zy} \cdot (\nabla_\Gamma \kappa + \nu \Sigma \kappa_i^2) + (\nabla_\Gamma \nu \gamma_{zyy}) : \nabla_\Gamma \nu^T \\
& + \gamma_{zz} \Delta_\Gamma \kappa + \gamma_{zzz} |\nabla_\Gamma \kappa|^2 + (\gamma_{zxy} + \gamma_{zyx}^T) : \nabla_\Gamma \nu \\
& + (\gamma_{zxz} + \gamma_{zzx}) \cdot \nabla_\Gamma \kappa + (\gamma_{zyz} + \gamma_{zzy}) \cdot (\nabla_\Gamma \nu \nabla_\Gamma \kappa).
\end{aligned} \tag{4.5}$$

Proof. We use Theorem 2.4 with $\psi = \gamma(x, \nu, \kappa)$. Then we have

$$\psi'(\Gamma; \vec{V}) = \gamma_y \cdot \nu' + \gamma_z \kappa' = -\gamma_y \cdot \nabla_\Gamma V - \gamma_z \Delta_\Gamma V,$$

using (3.4) and (3.5). We also compute $\partial_\nu[\gamma(x,\nu,\kappa)]$:

$$\begin{aligned}\partial_\nu\left[\gamma(x,\nu,\kappa)\right] &= \partial_\nu\gamma(x,\nu,\kappa)+\gamma_y(x,\nu,\kappa)D\nu\nu+\gamma_z(x,\nu,\kappa)\partial_\nu\kappa\\ &= \partial_\nu\gamma(x,\nu,\kappa)-\gamma_z(x,\nu,\kappa)\sum\kappa_i^2.\end{aligned}$$

The second line follows from Lemma 3.2 and the fact that $D\nu\nu=0$. Then substituting ψ' and $\partial_\nu\psi$ in (2.11) we have

$$\mathrm{d}J(\Gamma;\vec{V})=-\int_\Gamma \gamma_y\cdot\nabla_\Gamma V+\gamma_z\Delta_\Gamma V\mathrm{d}S+\int_\Gamma\left(\partial_\nu\gamma-\gamma_z\sum\kappa_i^2+\gamma\kappa\right)V\mathrm{d}S.$$

Integrating the first integral by parts with tangential Green's formula (3.14), we obtain

$$\mathrm{d}J(\Gamma;\vec{V})=\int_\Gamma\left(-\mathrm{div}_\Gamma[\gamma_y]-\gamma_y\cdot\nu\kappa-\Delta_\Gamma[\gamma_z]+\partial_\nu\gamma-\gamma_z\sum\kappa_i^2+\gamma\kappa\right)V\mathrm{d}S.$$

We can readily compute $\mathrm{div}_\Gamma[\gamma_y]$ and $\Delta_\Gamma[\gamma_z]$ using Lemma (3.4). □

Remark 4.2. We can compare the results (4.2) and (4.3) with the one obtained in [19] for the case of $\gamma=\gamma(\kappa)$. The three terms in the middle of equation (4.3) are shared. In our case, the dependence of γ on x and ν adds the first and the last terms in the integral (4.3). More importantly, the simultaneous dependence on x,ν,κ results in much richer structure in the tangential derivatives $\mathrm{div}_\Gamma[\gamma_y]_\Gamma$ and $\Delta_\Gamma[\gamma_z]$ and we elucidate the structure of these terms in detail using Lemma 3.4. In contrast to [19], which requires significant knowledge of Riemannian geometry for its derivations, we make use of shape differential calculus based on signed distance functions representations. This results in a more transparent and self-contained derivation using mostly multivariable calculus, without requiring substantial background in Riemannian geometry.

Given the first shape derivative for the general weighted surface energy (4.1), we can easily compute the shape derivatives for the special cases mentioned in the introduction.

Anisotropic surface energy. The anisotropic surface energy is given by setting $\gamma=\gamma(x,\nu)$ in (4.1). Energies of this form have been used to model anisotropic crystalline surface energy in material science [1,2,35,43,44,46,48], and for boundary detection [29], 3d scene reconstruction [27] in image processing. In the following we obtain the first variation in a very concise way as a corollary of Theorem 4.1.

Corollary 4.3. *The first shape derivative of the surface energy* (4.1) *for* $\gamma=\gamma(x,\nu)$ *(with no curvature dependence) at* Γ *in the direction of* $\vec{V}$ *is given by*

$$\begin{aligned}\mathrm{d}J(\Gamma;\vec{V}) &= \int_\Gamma(\kappa\gamma+\partial_\nu\gamma)V-\gamma_y\cdot\nabla_\Gamma V\mathrm{d}S\\ &= \int_\Gamma((\gamma-\gamma_y\cdot\nu)\kappa+\partial_\nu\gamma+\mathrm{div}_\Gamma[\gamma_y])V\mathrm{d}S,\end{aligned}$$

where $V=\vec{V}\cdot\nu$ *and* $\mathrm{div}_\Gamma[\gamma_y]=\mathrm{div}_\Gamma\gamma_y+\gamma_{yy}:\nabla_\Gamma\nu$.

Proof. As γ does not depend on κ, we have $\gamma_z=0$ and $\gamma_{yz}=0$. Dropping these terms from (4.3) and (4.4) respectively, we easily obtain the results for the case $\gamma=\gamma(x,\nu)$. □

Remark 4.4. In the materials science literature [2,10,35,44,46,48], one is often interested in the anisotropic surface energy and its first variation

$$J(\Gamma)=\int_\Gamma\gamma(\nu)\mathrm{d}S,\qquad \mathrm{d}J(\Gamma;\vec{V})=\int_\Gamma\kappa_\gamma V\mathrm{d}S,\tag{4.6}$$

where $\gamma : S^{d-1} \to \mathbb{R}^+$ is a smooth function, positively homogeneous of degree 1, that is, $\gamma(\lambda y) = |\lambda|\gamma(y)$ for $\lambda \in \mathbb{R}$ (implying $\gamma_y(y) \cdot y = \gamma(y)$), and the anisotropic mean curvature κ_γ and the Cahn-Hoffman vector ν_γ are defined by

$$\kappa_\gamma = \mathrm{div}_\Gamma[\nu_\gamma], \qquad \nu_\gamma = \gamma_y(\nu).$$

As we have $\partial_\nu \gamma = 0$ and $\gamma - \gamma_y \cdot \nu = 0$ from homogeneity of γ, we see that the first variation of the anisotropic energy (4.6) follows trivially from Corollary (4.3)

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma (\kappa(\gamma - \gamma_y \cdot \nu) + \partial_\nu \gamma + \mathrm{div}_\Gamma[\gamma_y]) V \mathrm{d}S = \int_\Gamma \kappa_\gamma V \mathrm{d}S.$$

Isotropic energy with curvature. We also consider the case with $\gamma = \gamma(x, \kappa)$, where the weight does not depend on the normal ν. This form generalizes several curvature-dependent surface energy models used in material science, biology and image processing [7,12–14,22,26,33,34,36,42,47]. The first variation for energies of this general form is not given in the literature to the best of our knowledge.

Corollary 4.5. *The first shape derivative of the surface energy* (4.1) *for* $\gamma = \gamma(x, \kappa)$ *(with no normal dependence) at* Γ *in the direction of velocity* $\vec{V}$ *is given by*

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma \left(-\Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z \sum \kappa_i^2 + \partial_\nu \gamma \right) V \mathrm{d}S, \tag{4.7}$$

where $V = \vec{V} \cdot \nu$ *and*

$$\Delta_\Gamma[\gamma_z] = \Delta_\Gamma \gamma_z + \gamma_{zz} \Delta_\Gamma \kappa + \gamma_{zzz} |\nabla_\Gamma \kappa|^2 + (\gamma_{zxz} + \gamma_{zzx}) \cdot \nabla_\Gamma \kappa. \tag{4.8}$$

Proof. As γ does not depend on ν, we have $\gamma_y = 0$, consequently $\mathrm{div}_\Gamma[\gamma_y] = 0$ in (4.3). Also we have $\gamma_{zy} = 0$, $\gamma_{zxy} = \gamma_{zyx} = 0$, so that (4.5) simplifies to (4.8). □

Weighted Willmore functional. We can use Corollary 4.5 to compute the shape derivative for a weighted Willmore functional, with $\gamma = \frac{1}{2} g(x)\kappa^2$. This functional has been used as a regularization term for boundary detection problems in image processing [42]. It is also useful for modeling of biomembranes when composition or concentration of lipids in the membrane varies spatially [7,13,47].

Corollary 4.6. *The first shape derivative of the surface energy* (4.1) *for* $\gamma = \frac{1}{2} g(x)\kappa^2$ *at* Γ *in the direction of velocity* $\vec{V}$ *(with* $V = \vec{V} \cdot \nu$*) is given by*

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma \left(-g\Delta_\Gamma \kappa - 2g_x \cdot \nabla_\Gamma \kappa + \frac{1}{2} g\kappa^3 - \Delta_\Gamma g \kappa + \frac{1}{2} \partial_\nu g \kappa^2 - g\kappa \sum \kappa_i^2 \right) V \mathrm{d}S. \tag{4.9}$$

Proof. To prove this, we use the equations (4.7) and (4.8) from Corollary 4.5. We have $\gamma_x = \frac{1}{2} g_x \kappa^2$, $\gamma_z = g\kappa$, $\gamma_{zz} = g$, $\gamma_{zzz} = 0$, $\gamma_{zx} = g_x \kappa$, $\gamma_{zxz} = \gamma_{zzx} = g_x$. Consequently

$$\Delta_\Gamma[\gamma_z] = \Delta_\Gamma g \kappa + g \Delta_\Gamma \kappa + 2g_x \cdot \nabla_\Gamma \kappa,$$

in (4.8). Substituting this in (4.7), we obtain the result (4.9). □

Willmore functional. Now we compute the shape derivative of the Willmore functional, with $\gamma = \frac{1}{2}\kappa^2$. This has been used to model bending energy of membranes [26], also to impose regularity in surface restoration [14] and boundary detection [42] problems in image processing.

Corollary 4.7. *The first shape derivative of the Willmore functional, namely energy* (4.1) *with* $\gamma = \frac{1}{2}\kappa^2$*, at* Γ *in the direction of* $\vec{V}$ *(with* $V = \vec{V}\cdot\nu$*) is given by*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \left(-\Delta_\Gamma\kappa + \frac{1}{2}\kappa^3 - \kappa\sum\kappa_i^2\right) V\,\mathrm{d}S. \tag{4.10}$$

For surfaces in 3*d, this is equal to*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \left(-\Delta_\Gamma\kappa - \frac{1}{2}\kappa^3 + 2\kappa\kappa_G\right) V\,\mathrm{d}S, \tag{4.11}$$

where $\kappa_G = \kappa_1\kappa_2$ *is the Gauss curvature.*

Proof. The proof follows easily from Corollary 4.6 by setting $g = 1$. To obtain the result for surfaces in 3d, we use Lemma 3.2. □

Spontaneous curvature. As our final result in this section, we consider $\gamma = \frac{1}{2}(\kappa - \kappa_0(x))^2$, where $\kappa_0(x)$ is the spontaneous curvature and is space-dependent. The spontaneous curvature describes the preferred mean curvature of an unconstrained piece of membrane and was proposed in [23,38] as part of a modified bending energy. It can be used to model the asymmetry in a membrane [16] or the net effect of an additional field, as in the theory of surfactants [12,33,36].

Corollary 4.8. *The first shape derivative of the Willmore functional with spontaneous curvature, namely energy* (4.1) *with* $\gamma = \frac{1}{2}(\kappa - \kappa_0(x))^2$ *at* Γ *in the direction of velocity* $\vec{V}$ *(with* $V = \vec{V}\cdot\nu$*) is given by*

$$\mathrm{d}J(\Gamma;\vec{V}) = \int_\Gamma \left(-\Delta_\Gamma(\kappa-\kappa_0) + \frac{1}{2}\kappa(\kappa-\kappa_0)^2 - (\kappa-\kappa_0)\left(\sum\kappa_i^2 + \partial_\nu\kappa_0\right)\right) V\,\mathrm{d}S.$$

Proof. This follows from Corollary 4.5. We first compute the derivatives of γ: $\gamma_x = (\kappa_0)_x(\kappa_0 - \kappa)$, $\gamma_z = (\kappa - \kappa_0)$, $\partial_\nu\gamma = (\kappa_0 - \kappa)\partial_\nu\kappa_0$, $\gamma_{zx} = -(\kappa_0)_x$, $\gamma_{zz} = 1$, $\gamma_{zxz} = 0$, $\gamma_{zzx} = 0$, $\gamma_{zzz} = 0$. Thus we have

$$\Delta_\Gamma[\gamma_z] = \Delta_\Gamma\gamma_z + \gamma_{zz}\Delta_\Gamma\kappa = -\Delta_\Gamma\kappa_0 + \Delta_\Gamma\kappa = \Delta_\Gamma(\kappa - \kappa_0),$$

which we substitute back in (4.3). Rearrangement of the terms yields the result. □

5. First variation of the surface energy: vector form

In this section we derive the weak formulation (1.3) for the general surface energy (1.1). Expression (1.3) entails only first tangential derivatives and does not explicitly require computing $\nabla_\Gamma\nu$, and so $\sum_i \kappa_i^2 = |\nabla_\Gamma\nu|^2$. This is advantageous and will be exploited later in Section 6.

We start by rewriting the shape derivative (4.3) of (1.1) at Γ with respect to perturbation $\vec{\phi}$ (with the normal component $\phi = \vec{\phi}\cdot\nu$) upon integrating by parts:

$$\mathrm{d}J(\Gamma;\vec{\phi}) = \int_\Gamma -\gamma_y\cdot\nabla_\Gamma\phi + \nabla_\Gamma[\gamma_z]\cdot\nabla_\Gamma\phi + \left(\gamma\kappa - \gamma_z|\nabla_\Gamma\nu|^2 + \partial_\nu\gamma\right)\phi\,\mathrm{d}S. \tag{5.1}$$

To obtain the alternate formula (1.3) we replace scalar quantities in (5.1) by the corresponding vector quantities. The following lemma is used to convert the second term.

Lemma 5.1. *Given $f, \phi \in H^1(\Gamma)$ and the vector functions $\vec{f}, \vec{\phi}$, related to f, ϕ by $\vec{f} = f\nu$, $\phi = \vec{\phi}\cdot\nu$, we can rewrite the H^1 scalar product of f, ϕ as follows*

$$\begin{aligned}\int_\Gamma \nabla_\Gamma f\cdot\nabla_\Gamma\phi = \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma\vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} \\ + \int_\Gamma f|\nabla_\Gamma\nu|^2\phi - \int_\Gamma f\nabla_\Gamma\kappa\cdot\vec{\phi}.\end{aligned} \tag{5.2}$$

Proof. First note that $\nabla_\Gamma f$ is equal to

$$\nabla_\Gamma f = \nabla_\Gamma(\vec{f}\cdot\nu) = \nabla_\Gamma\vec{f}^T\nu + \nabla_\Gamma\nu^T\vec{f} = \nabla_\Gamma\vec{f}^T\nu + f\nabla_\Gamma\nu\nu = \nabla_\Gamma\vec{f}^T\nu \tag{5.3}$$

because of the symmetry of $\nabla_\Gamma\nu$ and the fact that ∇_Γ is orthogonal to ν. Using (5.3), we can rewrite $\nabla_\Gamma f\cdot\nabla_\Gamma\phi$,

$$\begin{aligned}\nabla_\Gamma f\cdot\nabla_\Gamma\phi &= \nabla_\Gamma\vec{f}^T\nu\cdot\nabla_\Gamma(\vec{\phi}\cdot\nu) = \nabla_\Gamma\vec{f}^T\nu\cdot(\nabla_\Gamma\vec{\phi}^T\nu + \nabla_\Gamma\nu^T\vec{\phi}) \\ &= (\nabla_\Gamma\vec{f}^T\nu)\cdot(\nabla_\Gamma\vec{\phi}^T\nu) + (\nabla_\Gamma\vec{f}^T\nu)\cdot(\nabla_\Gamma\nu^T\vec{\phi}) \\ &= (\nu\otimes\nu)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} + \nabla_\Gamma f\cdot(\nabla_\Gamma\nu^T\vec{\phi}).\end{aligned}$$

We integrate over the surface Γ,

$$\int_\Gamma \nabla_\Gamma f\cdot\nabla_\Gamma\phi = \int_\Gamma (\nu\otimes\nu)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} + \int_\Gamma \nabla_\Gamma f\cdot(\nabla_\Gamma\nu^T\vec{\phi}).$$

We use the identity $I - \nu\otimes\nu = \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)$ to rewrite the integral

$$\int_\Gamma \nabla_\Gamma f\cdot\nabla_\Gamma\phi = \int_\Gamma (I - \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} + \int_\Gamma \nabla_\Gamma f\cdot(\nabla_\Gamma\nu^T\vec{\phi}). \tag{5.4}$$

Now we take the second integral on the right hand side of (5.4) and integrate by parts using tangential Green's formula (3.14)

$$\int_\Gamma \nabla_\Gamma f\cdot(\nabla_\Gamma\nu^T\vec{\phi}) = -\int_\Gamma f\,\mathrm{div}_\Gamma(\nabla_\Gamma\nu^T\vec{\phi}) = -\int_\Gamma f\nabla_\Gamma\nu : \nabla_\Gamma\vec{\phi} - \int_\Gamma f\Delta_\Gamma\nu\cdot\vec{\phi}. \tag{5.5}$$

To obtain (5.5), we carried out the differentiation with div_Γ and used the symmetry of $\nabla_\Gamma\nu$ and the fact that $\mathrm{div}_\Gamma\nabla_\Gamma\nu = \Delta_\Gamma\nu$. We will rewrite $f\,\nabla_\Gamma\nu : \nabla_\Gamma\vec{\phi}$ in (5.5). First we compute

$$\begin{aligned}\nabla_\Gamma\vec{f} &= \nabla_\Gamma(f\nu) = f\nabla_\Gamma\nu + \nu\otimes\nabla_\Gamma f \\ &= f\nabla_\Gamma\nu + \nu\otimes\nabla_\Gamma\vec{f}^T\nu = f\nabla_\Gamma\nu + (\nu\otimes\nu)\nabla_\Gamma\vec{f},\end{aligned}$$

using equation (5.3), whence we obtain

$$\begin{aligned}f\,\nabla_\Gamma\nu : \nabla_\Gamma\vec{\phi} &= \Big(\nabla_\Gamma\vec{f} - (\nu\otimes\nu)\nabla_\Gamma\vec{f}\Big) : \nabla_\Gamma\vec{\phi} = (I - \nu\otimes\nu)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} \\ &= \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi},\end{aligned}$$

which we substitute in (5.5),

$$\int_\Gamma \nabla_\Gamma f\cdot\nabla_\Gamma\nu^T\vec{\phi} = -\int_\Gamma \frac{1}{2}(\nabla_\Gamma x + \nabla_\Gamma x^T)\nabla_\Gamma\vec{f} : \nabla_\Gamma\vec{\phi} - \int_\Gamma f\Delta_\Gamma\nu\cdot\vec{\phi}. \tag{5.6}$$

We substitute (5.6) in (5.4) and obtain

$$\int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T) \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma f \Delta_\Gamma \nu \cdot \vec{\phi}. \tag{5.7}$$

The last integral in (5.7) can be split into two parts by substituting $\vec{\phi} = \phi\nu + \nabla_\Gamma x \vec{\phi}$. We write

$$f \Delta_\Gamma \nu \cdot \vec{\phi} = f\phi \Delta_\Gamma \nu \cdot \nu + f \Delta_\Gamma \nu \cdot \nabla_\Gamma x \vec{\phi},$$

whence

$$f \Delta_\Gamma \nu \cdot \vec{\phi} = -f\phi |\nabla_\Gamma \nu|^2 + f \nabla_\Gamma \kappa \cdot \vec{\phi}. \tag{5.8}$$

We have used the fact that $\Delta_\Gamma \nu = -|\nabla_\Gamma \nu|^2 \nu + \nabla_\Gamma \kappa$ from Lemma 3.3. Finally substituting (5.8) in (5.7) yields

$$\begin{aligned}\int_\Gamma \nabla_\Gamma f \cdot \nabla_\Gamma \phi = \int_\Gamma \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} - \int_\Gamma (\nabla_\Gamma x + \nabla_\Gamma x^T) \nabla_\Gamma \vec{f} : \nabla_\Gamma \vec{\phi} \\ + \int_\Gamma f |\nabla_\Gamma \nu|^2 \phi - \int_\Gamma f \nabla_\Gamma \kappa \cdot \vec{\phi}.\end{aligned}$$

This concludes the proof. □

Now, with the following theorem, we introduce the alternate vector form of the shape derivative (5.1).

Theorem 5.2 (vector form)**.** *Using a vector test function $\vec{\phi}$, with $\phi = \vec{\phi} \cdot \nu$, the shape derivative (5.1) can be rewritten as*

$$dJ(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \, \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \tag{5.9}$$

where $\vec{Y}(x) = \gamma_y(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x))$, $\vec{Z}(x) = \gamma_z(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x)) \nu(x)$.

Proof. Let us define the quantity $Z(x) := \gamma_z(x, \nu(x), \vec{\kappa}(x) \cdot \nu(x))$.
Then the shape derivative (5.1) at Γ with respect to ϕ can be written as

$$dJ(\Gamma; \phi) = -\int_\Gamma \vec{Y} \cdot \nabla_\Gamma \phi + \int_\Gamma \nabla_\Gamma Z \cdot \nabla_\Gamma \phi + \int_\Gamma \gamma \kappa \phi - \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi + \int_\Gamma \partial_\nu \gamma \phi. \tag{5.10}$$

We replace the second integral in (5.10) with the corresponding vector expression using Lemma 5.1.

$$\begin{aligned}dJ(\Gamma; \vec{\phi}) = -\int_\Gamma \vec{Y} \cdot \nabla_\Gamma \phi + \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} + \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi \\ - \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi} + \int_\Gamma \gamma \kappa \phi - \int_\Gamma Z |\nabla_\Gamma \nu|^2 \phi + \int_\Gamma \partial_\nu \gamma \phi.\end{aligned} \tag{5.11}$$

Integrals with $|\nabla_\Gamma \nu|^2$ cancel out. We apply tangential Green's formula (3.14) to the following term

$$\begin{aligned}\int_\Gamma \kappa \gamma \phi = \int_\Gamma \kappa \gamma \vec{\phi} \cdot \nu = \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma [\gamma] \cdot \vec{\phi} \\ = \int_\Gamma \gamma \mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \nabla_\Gamma \gamma \cdot \vec{\phi} + \int_\Gamma \vec{\phi}^T \nabla_\Gamma \nu \vec{Y} + \int_\Gamma Z \nabla_\Gamma \kappa \cdot \vec{\phi},\end{aligned}$$

(note that $\nabla_\Gamma[\gamma] = \nabla_\Gamma\gamma + \nabla_\Gamma\nu\gamma_y + \gamma_z\nabla_\Gamma\kappa$ from Lem. 3.4), and substitute the result back in (5.11),

$$
\begin{aligned}
\mathrm{d}J(\Gamma;\vec\phi) = &-\int_\Gamma \vec Y\cdot\nabla_\Gamma\phi + \int_\Gamma (I-(\nabla_\Gamma x+\nabla_\Gamma x^T))\nabla_\Gamma\vec\phi : \nabla_\Gamma\vec Z - \int_\Gamma Z\nabla_\Gamma\kappa\cdot\vec\phi \\
&+\int_\Gamma \gamma\mathrm{div}_\Gamma\vec\phi + \int_\Gamma \nabla_\Gamma\gamma\cdot\vec\phi + \int_\Gamma \vec\phi^T\nabla_\Gamma\nu\vec Y + \int_\Gamma Z\nabla_\Gamma\kappa\cdot\vec\phi + \int_\Gamma \partial_\nu\gamma\phi.
\end{aligned}
\tag{5.12}
$$

The integrals $\int_\Gamma Z\nabla_\Gamma\kappa\cdot\vec\phi$ cancel out.

We combine two of the integrals $\int_\Gamma \nabla_\Gamma\gamma\cdot\vec\phi + \int_\Gamma \partial_\nu\gamma\phi = \int_\Gamma \gamma_x\cdot\vec\phi$.

Also we combine the two integrals involving $\vec Y$ by

$$
-\nabla_\Gamma\phi + \vec\phi^T\nabla_\Gamma\nu = -\nabla_\Gamma(\vec\phi\cdot\nu) + \vec\phi^T\nabla_\Gamma\nu = -\nu^T\nabla_\Gamma\vec\phi - \vec\phi^T\nabla_\Gamma\nu + \vec\phi^T\nabla_\Gamma\nu = -\nu^T\nabla_\Gamma\vec\phi.
$$

Thereby we obtain

$$
\mathrm{d}J(\Gamma;\vec\phi) = \int_\Gamma (I-(\nabla_\Gamma x+\nabla_\Gamma x^T))\nabla_\Gamma\vec\phi : \nabla_\Gamma\vec Z - \int_\Gamma \nu^T\nabla_\Gamma\vec\phi\vec Y + \int_\Gamma \gamma\mathrm{div}_\Gamma\vec\phi + \int_\Gamma \nabla\gamma\cdot\vec\phi,
$$

which is the sought result. □

Remark 5.3. Note that the shape derivative (5.9) contains only first order tangential derivatives and does not include $\nabla_\Gamma\nu$. Therefore it can be easily discretized in space using a parametric finite element method with piecewise linear basis functions. We refer to [9,19,20,37] for related work.

Remark 5.4. One can write an equivalent expression for the shape derivative (5.9) by replacing $\nabla_\Gamma x + \nabla_\Gamma x^T$ with two times the projection matrix $Q = I - \nu\otimes\nu$. However we prefer to keep the current form of the shape derivative with $\nabla_\Gamma x + \nabla_\Gamma x^T$, because the goal is to enable finite element computations of the gradient flows of (1.1) using (5.9), in which case the extensions may not coincide. For the Willmore functional, the shape derivative with $\nabla_\Gamma x + \nabla_\Gamma x^T$ has been observed to result in better numerical behavior compared to the alternative with Q [9].

In the case of a quadratic energy given by $\gamma(x,\nu,\kappa) = \frac{1}{2}g(x)(\kappa - \kappa_0(x))^2$, the alternate formulation (5.9) of the shape derivative reduces to a linear form. If $g = 1$ and $\kappa_0 = 0$, then the corresponding energy is the Willmore functional and the shape derivative simplifies further and reduces to the linear form proposed in [9]. In contrast, the scheme proposed for $\gamma = \gamma(\kappa)$ in [19] reduces to Rusu's scheme [37], which depends quadratically on the curvature vector and is reported to exhibit undesirable tangential motions close to equilibrium shapes [9,20].

Theorem 5.5 (vector form for quadratic weight function)**.** *For $\gamma(x,\nu,\kappa) = \frac{1}{2}g(x)\ (\kappa-\kappa_0(x))^2$ with smooth functions g,κ_0 defined off the surface Γ, the shape derivative (5.9) of the energy (1.1) with respect to a vector-valued perturbation $\vec\phi\in H^1(\Gamma)$ can be rewritten as a linear functional of $\vec\kappa,\vec Z$*

$$
\begin{aligned}
\mathrm{d}J(\Gamma;\vec\phi) = &\int_\Gamma (I-(\nabla_\Gamma x+\nabla_\Gamma x^T))\nabla_\Gamma\vec\phi : \nabla_\Gamma\vec Z \\
&+\frac{1}{2}\int_\Gamma \mathrm{div}_\Gamma\vec\kappa\,(g\mathrm{div}_\Gamma\vec\phi + \nabla g\cdot\vec\phi) - \int_\Gamma \vec Z\cdot\nu\,(\kappa_0\mathrm{div}_\Gamma\vec\phi + \nabla\kappa_0\cdot\vec\phi) \\
&-\int_\Gamma \kappa_0\nabla g\cdot\vec\phi\,\vec\kappa\cdot\nu + \frac{1}{2}\int_\Gamma \kappa_0^2(g\mathrm{div}_\Gamma\vec\phi + \nabla g\cdot\vec\phi),
\end{aligned}
\tag{5.13}
$$

where $\vec{Z}(x) = g(x)(\kappa(x) - \kappa_0(x))\nu(x)$. *If* $g = 1$ *in* (5.13), *then* (5.13) *reduces to*

$$\begin{aligned}\mathrm{d}J(\Gamma;\vec{\phi}) = &\int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} + \frac{1}{2}\int_\Gamma \mathrm{div}_\Gamma \vec{\phi}\, \mathrm{div}_\Gamma \vec{\kappa} \\ &- \int_\Gamma \vec{Z}\cdot\nu(\kappa_0 \mathrm{div}_\Gamma \vec{\phi} + \nabla\kappa_0 \cdot \vec{\phi}) + \frac{1}{2}\int_\Gamma \kappa_0^2 \mathrm{div}_\Gamma \vec{\phi},\end{aligned} \tag{5.14}$$

which can be further simplified provided $\kappa_0 = 0$

$$\mathrm{d}J(\Gamma;\vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{\kappa} + \frac{1}{2}\int_\Gamma \mathrm{div}_\Gamma \vec{\phi}\, \mathrm{div}_\Gamma \vec{\kappa}. \tag{5.15}$$

Proof. We first write the explicit values of the weight function γ and its derivatives

$$\gamma = \frac{1}{2}g(\kappa-\kappa_0)^2, \qquad \gamma_x = \frac{\nabla g}{2}(\kappa-\kappa_0)^2 - g\nabla\kappa_0(\kappa-\kappa_0), \qquad \gamma_y = 0, \qquad \gamma_z = g(\kappa-\kappa_0).$$

We can further transform γ and γ_x

$$\begin{aligned}\gamma &= \frac{g}{2}\kappa^2 - g\kappa\kappa_0 + \frac{g}{2}\kappa_0^2 = \frac{1}{2}g\mathrm{div}_\Gamma\vec{\kappa} - \kappa_0\vec{Z}\cdot\nu - \frac{1}{2}g\kappa_0^2,\\ \gamma_x &= \frac{1}{2}\nabla g(\kappa^2 - 2\kappa\kappa_0 + \kappa_0^2) - g\nabla\kappa_0(\kappa-\kappa_0)\\ &= \frac{1}{2}\nabla g\mathrm{div}_\Gamma\vec{\kappa} - \kappa_0\nabla g\vec{\kappa}\cdot\nu + \frac{1}{2}\nabla g\kappa_0^2 - \nabla\kappa_0\vec{Z}\cdot\nu.\end{aligned}$$

Now we substitute γ and its derivatives in (5.9)

$$\begin{aligned}\mathrm{d}J(\Gamma;\vec{\phi}) = &\int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{\phi} : \nabla_\Gamma\vec{Z}\\ &+ \int_\Gamma \left(\frac{1}{2}g\mathrm{div}_\Gamma\vec{\kappa} - \kappa_0\vec{Z}\cdot\nu - \frac{1}{2}g\kappa_0^2\right)\mathrm{div}_\Gamma\vec{\phi}\\ &+ \int_\Gamma \left(\frac{1}{2}\nabla g\mathrm{div}_\Gamma\vec{\kappa} - \kappa_0\nabla g\vec{\kappa}\cdot\nu + \frac{1}{2}\nabla g\kappa_0^2 - \nabla\kappa_0\vec{Z}\cdot\nu\right)\cdot\vec{\phi}.\end{aligned}$$

Reorganizing the terms yields the equation (5.13). The results (5.14) and (5.15) follow trivially. □

6. Gradient flows

An important application of the first variation of the general surface energy (1.1), is the formulation of gradient descent flows, which are instrumental to computing the minima of (1.1). The gradient descent flows give rise to deformations of Γ that decrease its energy which, once discretized in space and time, lead to a numerical method. We present now one such formulation which is suitable for C^0 finite element space discretization. We refer to the articles [1–4,45] for more information on gradient flows.

We start by introducing a scalar product $b(\cdot,\cdot)$ on Γ, which induces the Hilbert space $H(\Gamma)$. Then we solve the following equation

$$\vec{V}\in H(\Gamma): \qquad b(\vec{V},\vec{\phi}) = -\mathrm{d}J(\Gamma;\vec{\phi}), \quad \forall\vec{\phi}\in H(\Gamma). \tag{6.1}$$

If $\|\cdot\|_{H(\Gamma)}$ is the norm induced by $b(\cdot,\cdot)$, then it turns out that the velocity $\vec{V}$ computed this way decreases the energy provided $\vec{V}\neq 0$

$$\mathrm{d}J(\Gamma;\vec{V}) = -b(\vec{V},\vec{V}) = -\|\vec{V}\|^2_{H(\Gamma)} < 0.$$

The choice of b depends on the problem at hand. A natural choice is the $L^2(\Gamma)$ scalar product $b(\vec{V},\vec{\phi}) = \int_\Gamma \vec{V}\cdot\vec{\phi}$, in which case the Hilbert space $H(\Gamma)$ is $L^2(\Gamma)$ Other scalar products, such as H^1 and H^{-1}, are possible, inducing $H(\Gamma) = H^1(\Gamma)$ and $H(\Gamma) = H^{-1}(\Gamma)$, and have been illustrated in [18]. The L^2 scalar product, in conjunction with the first variation (1.2), gives

$$\int_\Gamma \vec{V}\cdot\vec{\phi} = -\int_\Gamma \left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z|\nabla_\Gamma\nu|^2 + \partial_\nu\gamma\right)\vec{\phi}\cdot\nu, \quad \forall\vec{\phi}\in L^2(\Gamma),$$

or equivalently the *descent direction*

$$\vec{V} = -\left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z|\nabla_\Gamma\nu|^2 + \partial_\nu\gamma\right)\nu.$$

Space discretization of this relation *via* C^0 finite element methods yields discrete surfaces with discontinuous normals, which makes the use of $\nabla_\Gamma\nu$ problematic. A fully discrete scheme, which reconstructs a Lipschitz normal ν by local averaging and uses a semi-implicit time discretization, has been proposed in [5].

In contrast, we could resort to (1.3) for the surface energy (1.1). Then the weak formulation for the L^2 gradient flow would be given by

$$\int_\Gamma \vec{V}\cdot\vec{\phi} = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{\phi} : \nabla_\Gamma\vec{Z} - \int_\Gamma \nu^T\nabla_\Gamma\vec{\phi}\,\vec{Y} + \int_\Gamma \gamma\,\mathrm{div}_\Gamma\vec{\phi} + \int_\Gamma \gamma_x\cdot\vec{\phi}, \tag{6.2}$$

and those for mean curvature vector $\vec{\kappa}$ and auxiliary vector variables are $\vec{Y},\vec{Z}$

$$\int_\Gamma \vec{\kappa}\cdot\vec{\phi} = \int_\Gamma \nabla_\Gamma x : \nabla_\Gamma\vec{\phi}, \qquad \int_\Gamma \vec{Y}\cdot\vec{\phi} = \int_\Gamma \gamma_y\cdot\vec{\phi}, \qquad \int_\Gamma \vec{Z}\cdot\vec{\phi} = \int_\Gamma \gamma_z\vec{\phi}\cdot\nu.$$

Equation (6.2) is advantageous, because it does not require computing the derivatives of the normal ν.

If we have a quadratic weight function $\gamma = \frac{1}{2}g(\kappa-\kappa_0)^2$, then the weak formulation (6.2) reduces to an expression that is linear in $\vec{\kappa},\vec{Z}$ with no cross terms

$$\begin{aligned}\int_\Gamma \vec{V}\cdot\vec{\phi} = &\int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{\phi} : \nabla_\Gamma\vec{Z} \\ &+ \frac{1}{2}\int_\Gamma \mathrm{div}_\Gamma\vec{\kappa}\,(g\mathrm{div}_\Gamma\vec{\phi} + \nabla g\cdot\vec{\phi}) - \int_\Gamma \vec{Z}\cdot\nu\,(\kappa_0\mathrm{div}_\Gamma\vec{\phi} + \nabla\kappa_0\cdot\vec{\phi}) \\ &- \int_\Gamma \kappa_0\nabla g\cdot\vec{\phi}\,\vec{\kappa}\cdot\nu + \frac{1}{2}\int_\Gamma \kappa_0^2(g\mathrm{div}_\Gamma\vec{\phi} + \nabla g\cdot\vec{\phi}).\end{aligned} \tag{6.3}$$

For the Willmore weight $\gamma = \frac{1}{2}\kappa^2$, we obtain the even simpler system

$$\begin{aligned}&\int_\Gamma \vec{V}\cdot\vec{\phi} = -\int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T))\nabla_\Gamma\vec{\phi} : \nabla_\Gamma\vec{\kappa} + \frac{1}{2}\int_\Gamma \mathrm{div}_\Gamma\vec{\phi}\,\mathrm{div}_\Gamma\vec{\kappa}, \\ &\int_\Gamma \vec{\kappa}\cdot\vec{\phi} = \int_\Gamma \nabla_\Gamma x : \nabla_\Gamma\vec{\phi},\end{aligned} \tag{6.4}$$

which was introduced by Bonito *et al.* in [9] and was used to compute evolution of biomembranes. We also mention the related schemes [19,20,37].

7. Summary of the main results

In this paper, we consider the general surface energy (1.1), which is in the form of a surface integral with anisotropic curvature-dependent weight function $\gamma = \gamma(x, \nu, \kappa)$. This energy is used as a model in many different areas, such as material science, biology and image processing (see the introduction Sect. 1 for examples).

A critical need in practice is the characterization of minima of (1.1), as well as the development of numerical methods for their computation. For this purpose, we determine the first variation of (1.1) with respect to deformations of Γ given by velocity fields $\vec{V}$:

$$\mathrm{d}J(\Gamma; \vec{V}) = \int_\Gamma \left(\mathrm{div}_\Gamma[\gamma_y]_\Gamma - \Delta_\Gamma[\gamma_z] + \gamma\kappa - \gamma_z |\nabla_\Gamma \nu|^2 \int_\Gamma \partial_\nu \gamma \phi + \partial_\nu \gamma \right) \vec{V} \cdot \nu \,\mathrm{d}S. \tag{7.1}$$

We refer to Sections 2 and 4 for definitions of the tangential derivatives and other details. This is the first contribution of our paper.

Our second contribution is the following vector formulation equivalent to (7.1)

$$\mathrm{d}J(\Gamma; \vec{\phi}) = \int_\Gamma (I - (\nabla_\Gamma x + \nabla_\Gamma x^T)) \nabla_\Gamma \vec{\phi} : \nabla_\Gamma \vec{Z} - \int_\Gamma \nu^T \nabla_\Gamma \vec{\phi} \vec{Y} + \int_\Gamma \gamma \,\mathrm{div}_\Gamma \vec{\phi} + \int_\Gamma \gamma_x \cdot \vec{\phi}, \tag{7.2}$$

where $\vec{\phi}$ is the vector perturbation or test function and $\vec{\kappa}, \vec{Z}, \vec{Y}$ satisfy the relations

$$\vec{\kappa} = -\Delta_\Gamma x, \qquad \vec{Z} = \gamma_z \nu, \qquad \vec{Y} = \gamma_y,$$

which can also be imposed weakly. The main advantage of (7.2) over (7.1) is that it does not include $\nabla_\Gamma \nu$ and is thus suitable for direct spatial discretization by C^0 parametric finite elements. This is instrumental to implement a numerical method computing gradient descent flows for the energy (1.1). For example, in the case of L^2 gradient flows given by $\int_\Gamma \vec{V} \cdot \vec{\phi} = -\mathrm{d}J(\Gamma, \vec{\phi})$, a semi-implicit time discretization of this equation would linearize the system, and thus require only linear solves at each time step. The full expression for the L^2 gradient flow is given by (6.2). If we further assume that the weight function γ is isotropic and quadratic in κ, namely $\gamma = \frac{1}{2} g(x)(\kappa - \kappa_0(x))^2$ for some scalar function $g(x)$, then equation (6.2) reduces to (6.3), which is linear in both $\vec{\kappa}$ and $\vec{Z}$ with no cross terms. Finally, for $g(x) = 1, \kappa_0(x) = 0$, *i.e.* $\gamma = \frac{1}{2}\kappa^2$, the case of Willmore energy, equation (6.2) further simplifies to (6.4), which coincides with that obtained by Bonito *et al.* [9].

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