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Gaussian vector fields on triangulated surfaces

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Abstract Anisotropic elasticity in the plane of the lipid membrane appears in a multitude of biophysical problems. It poses a major theoretical challenge due to the inherent curvature of fluid membranes which is coupled to the in-plane elastic deformations. Computer simulations by triangulated surfaces have proven to be very useful to resolve the complex interplay between in-plane ordering of membranes and membrane conformations. In the present work we have developed a procedure for realistic representations of Gaussian models with in-plane vector degrees of freedoms on a triangulated surface. The method opens possibilities for simulations of membranes for a variety of problems involving in-plane orientational degrees of freedoms and direct correspondence to continuum models.

Keywords Membrane curvature · Anisotropic elasticity · Triangulated surface

1 Introduction

The large scale conformations of biological membranes are regulated by membrane proteins, which in a complex interplay with membrane elasticity, local curvature generation, protein interactions and conformational entropy facilitate a multitude of biological functions, e.g. protein sorting and vesicular transport. Several families of such regulating proteins are membrane nematogens, i.e. elongated peripheral proteins with an approximate π-symmetry in the plane of the membrane [1, 2]. The description of such systems is challenging since the coupling between in-plane orientational degrees of freedoms and membrane geometry is non-trivial both in analytical and numerical treatments. Recently, we presented a Monte Carlo simulation techniques based on Dynamical Triangulated Surfaces, which addresses some of these problems [3]. While the direct coupling between membrane curvature and orientational degrees of freedoms is relatively straight forward in this approach, the indirect coupling induced by the in-plane orientational elasticity is more cumbersome. The in-plane elasticity is relevant at high lateral concentration of the membrane nematogens, which will tend to line up and order in the plane of the membrane due to interactions and excluded volume effects similarly to the nematic liquid crystals in 3D. In general membrane mediated interactions between anisotropic membrane inclusions induces such indirect couplings between membrane curvature and lateral ordering. In a mean-field treatment the overall rotational symmetry is spontaneously broken and Goldstones theorem dictates that the in-plane elasticity of the nematic membrane is governed by terms quadratic in the gradients of orientational order parameter. Simple considerations leads to the following Hamiltonian

$$\mathcal{H} = \frac{K_1}{2}\oint \mathrm{d}A(\mathrm{Div}(\mathbf{m}))^2 + \frac{K_3}{2}\oint \mathrm{d}A(\mathrm{Div}(\mathbf{m}^{\perp}))^2 \qquad (1)$$

which is the so called Franks elastic free energy for a nematic liquid crystal in 2D [4]. The elastic constants K_1 and K_3 have the dimension of energy. $\mathbf{m}$ is a unit vector giving the orientation of the nematogens, while $\mathbf{m}^{\perp}$ is it's orthonormal compliment in the plane. The local order of the nematogens is given by the tensor field $\mathbf{Q} = \mathbf{m} \otimes \mathbf{m} - \frac{1}{2}\mathbf{1}$, which fulfill

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the symmetry requirement $\mathbf{Q}(\mathbf{m}) = \mathbf{Q}(-\mathbf{m})$. Often Eq. (1) is analyzed in the one constant approximation $K_1 = K_3 = K_A$, where it takes the form

$$\mathcal{H} = \frac{K_A}{2} \oint \mathrm{d}A(\nabla(\mathbf{m}))^2. \tag{2}$$

More generally Eq. (2) is relevant for p-atic membranes, a class of models for membranes with in-plane anisotropic elasticity, which is left invariant by rotation of its components by $\frac{2\pi}{p}$ in the plane for positive integers p [5]. For convenience, we choose the elastic constant $K_A = 1$. It is important to note that the derivatives appearing in Eqs. (1) and (2) are covariant derivatives of the vector field $\mathbf{m}$ confined to the plane of the curving surface. In a previous work by Ramakrishnan et al. [3] we gave an approximate procedure to implement Eq. (2) on triangulated surfaces, by introducing the parallel transport of vectors between neighboring vertices. This paper describes a more comprehensive discretization of Eq. (2), which posses the correct trivial continuum limit and conformal invariance. The paper is organized as follows: Sect. 2 briefly describes the triangulated surface representation of mathematical surfaces in 3D. Section 3 warms up by describing the discretization of Eq. (2) for a Gaussian scalar field. Section 5 generalizes this approach to vector fields and formulate a discretized version of Eq. (2), which obey analogous symmetry properties. However, before this program can be implemented some useful properties of parallel transport of vectors on triangulated surfaces will be developed in Sect. 4. Conclusions and perspectives are given in Sect. 6.

2 Triangulated surfaces

The triangulated surface is a closed, piece-wise flat, oriented surface constituted of $2(N - \chi)$ triangles intersecting in N vertices and $3(N - \chi)$ edges. Here χ is the Euler characteristics of the surface with $\chi = 2$ for a spherical surface topology. The purpose of forming triangulated surfaces in statistical mechanical simulations of membrane properties, is primarily to analyze the large-scale conformational properties of membrane models [6]. The triangulated surface establish a framework to discretize the continuum models or serve as microscopic models of cooperative properties of membranes in analogy to conventional lattice simulations in statistical mechanics. In the present modelling work all the surface properties are stored in the vertices, e.g. the surface positions and normals are given as $\mathbf{X}_i$ and $\mathbf{N}_i$ for vertices $i = 1, \ldots, N$. Furthermore, the curvature properties in the neighborhood of a vertex are described by a shape operator S_i, represented as a symmetric 2-tensor in the tangent plane TP_i. The eigenvalues of S_i are the local principal curvatures and the associated principal directions provide a local orthonormal frame of reference of TP_i (Darboux frame). The details of the calculation of the shape operator are described in [3]. This approach allow us to define $\mathbf{m}_i \in TP_i$ the local unit director in a vertex representing the local orientation of the in-plane vector field.

3 Scalar field theory on a triangular surface

Before addressing the problem of calculating the energy of a Gaussian in-plane vector field on a triangulated surface, let us make a brief revisit in the corresponding problem for a Gaussian scalar field ϕ. For a choice of coordinates the energy for a ϕ configuration on a closed surface with area A takes the form

$$\mathcal{H}[\phi] = \frac{1}{2} \oint_A \mathrm{d}^2\alpha \sqrt{\det(g)} g^{\mu\nu} \partial_\mu \phi \partial_\nu \phi. \tag{3}$$

On a triangulated surface, we can now calculated Eq. (3) as the sum of the contributions from the triangular faces. We consider an oriented triangle Δ given by the vector positions in space $\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$ of the three vertices following the orientation. Any position on the triangular face can then be expressed in terms of the barycentric coordinates α_1, α_2 where

$$\mathbf{X}(\alpha_1, \alpha_2) = \alpha_1 \mathbf{X}_1 + \alpha_2 \mathbf{X}_2 + (1 - \alpha_1 - \alpha_2)\mathbf{X}_3. \tag{4}$$

The partial derivatives of $\mathbf{X}(\alpha_1, \alpha_2)$ can easily be calculated as

$$\partial_\nu \mathbf{X} = \mathbf{X}_\nu - \mathbf{X}_3 = \mathbf{X}_{\nu,3}, \quad \nu = 1, 2 \tag{5}$$

and thus the metrical tensor

$$g_{\mu\nu} = \partial_\nu \mathbf{X} \cdot \partial_\mu \mathbf{X} = \begin{pmatrix} (\mathbf{X}_{1,3})^2 & \mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3} \\ \mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3} & (\mathbf{X}_{2,3})^2 \end{pmatrix}. \tag{6}$$

Similarly we can calculate the inverse metrical tensor

$$g^{\mu\nu} = \left(g^{-1}\right)_{\mu\nu} = \frac{1}{\det(g)} \begin{pmatrix} (\mathbf{X}_{2,3})^2 & -\mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3} \\ -\mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3} & (\mathbf{X}_{1,3})^2 \end{pmatrix} \tag{7}$$

where the determinant $\det(g)$ is related to the area A_Δ of the triangle:

$$\det(g) = (\mathbf{X}_{2,3})^2 (\mathbf{X}_{1,3})^2 - (\mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3})^2 = (2A_\Delta)^2. \tag{8}$$

The energy density in Δ can now be evaluated. The partial derivatives of $\phi(\alpha_1, \alpha_2)$ become

$$\partial_\nu \phi = \phi_\nu - \phi_3 = \phi_{\nu,3}, \quad \nu = 1, 2 \tag{9}$$

and thus the energy density in Δ

$$\partial_\mu \phi g^{\mu\nu} \partial_\nu \phi = \frac{1}{\det(g)} \Big((\mathbf{X}_{2,3})^2 (\phi_{1,3})^2 - 2\mathbf{X}_{1,3}\mathbf{X}_{2,3}\phi_{1,3}\phi_{2,3} + (\mathbf{X}_{1,3})^2 (\phi_{2,3})^2 \Big) \tag{10}$$

$$\partial_\mu \phi g^{\mu\nu} \partial_\nu \phi = \frac{1}{(2A_\Delta)^2} \left(\mathbf{X}_{2,3}\phi_{1,3} - \mathbf{X}_{1,3}\phi_{2,3} \right)^2 \tag{11}$$

$$\partial_\mu \phi g^{\mu\nu} \partial_\nu \phi = \frac{1}{(2A_\Delta)^2} \left(\phi_1 \mathbf{X}_{2,3} + \phi_2 \mathbf{X}_{3,1} + \phi_3 \mathbf{X}_{1,2} \right)^2, \tag{12}$$

Equations (10), (11) and (12) are all very useful relations. By the substitution $\phi_{12} = \phi_1 - \phi_2 = \phi_{13} - \phi_{23}$ the mixed term in Eq. (10) can be replaced by $-2\phi_{13}\phi_{23} = (\phi_{12})^2 - (\phi_{13})^2 - (\phi_{23})^2$.

$$\begin{aligned} \partial_\mu \phi g^{\mu\nu} \partial_\nu \phi &= \frac{1}{(2A_\Delta)^2} \Big(\mathbf{X}_{2,3} \cdot \mathbf{X}_{2,1} (\phi_{1,3})^2 + \mathbf{X}_{1,3} \cdot \mathbf{X}_{1,2} (\phi_{2,3})^2 \\ &\quad + \mathbf{X}_{1,3} \cdot \mathbf{X}_{2,3} (\phi_{1,2})^2 \Big) \\ &= \frac{1}{2A_\Delta} \Big(\cot(\beta_{31}) (\phi_{3,1})^2 \\ &\quad + \cot(\beta_{23}) (\phi_{2,3})^2 + \cot(\beta_{12}) (\phi_{1,2})^2 \Big) \end{aligned} \tag{13}$$

Here we have used that $\mathbf{X}_{1,2} = \mathbf{X}_{1,3} - \mathbf{X}_{2,3}$. The angles $\beta_{31}, \beta_{23}, \beta_{12}$ are the interior triangular angles opposing the edges (31), (23) and (12) in Δ.

Adding all the contributions from the triangular faces gives the following discretization of Eq. (3)

$$\mathcal{H}[\phi_i] = \frac{1}{2} \sum_i \sum_{j \in i} \frac{\cot(\beta_{ij}) + \cot(\beta_{ji})}{2} (\phi_{i,j})^2 \tag{14}$$

β_{ij} and β_{ji} are the two triangular angles across the link (ij). This relation was obtained by Itzykson and Drouffe, who also generalized it to pseudo-scalar fields (reviewed in [7]). There may be homogeneous terms involved in the energy expression, like a ϕ^2 term, but they have a trivial implementation on a triangulated surface as single vertex properties. A striking feature of Eq. (14) is that the conformal invariance of Eq. (3) is preserved in the discretized version since all angle preserving deformations of the triangulization leaves it unchanged. Note, that although the numerical calculation of Eq. (14) involves many steps, they are all very simple algebraic operations. Also, the informations about the surface is stored as properties of vertex points of the triangulated surface, while the approximated energy is evaluated from simple linear interpolation of the fields and surface positions in the triangular simplices and the induced metric on these faces. In the following we will attempt to extend this expression to triangulated surfaces with in-plane orientational fields.

4 Parallel transport of vectors on a triangular surface

The above considerations do not work directly for vector fields in the plane of the membrane. The main problem is that the derivatives in Eq. (2) involve the comparison of vectors in the tangent planes at different surface positions. The covariant derivative $\nabla_{\mathbf{q}} \mathbf{m}(\mathbf{X}) \simeq (T_{\mathbf{X}+\mathbf{q}\to\mathbf{X}}(\mathbf{m}(\mathbf{X}+\mathbf{q})) - \mathbf{m}(\mathbf{X}))/|\mathbf{q}|$ where $\mathbf{q} \in TP_{\mathbf{X}}$ and $T_{\mathbf{X}+\mathbf{q}\to\mathbf{X}}$ represents the parallel transport of tangent vectors from surface position $\mathbf{X}+\mathbf{q}$ to $\mathbf{X}$. In [3] we suggested a simple scheme for performing parallel transport in a neighborhood of a triangulated surface. Consider two neighboring vertex points i and j with tangent planes TP_i and TP_j and given vertex positions and associated normals: $(\mathbf{X}_i, \mathbf{N}_i)$ and $(\mathbf{X}_j, \mathbf{N}_j)$. Let $\mathbf{m}_i \in TP_i$ be a vector in the tangent plane of i. The approximative parallel transport of $\mathbf{m}_i$ along a geodesic curve, which starts out in vertex i and end up in vertex j is given by

$$T_{i\to j} : TP_i \to TP_j \tag{15}$$

$$\mathbf{m}_i \to T_{i\to j}(\mathbf{m}_i) = M(\mathbf{N}_j, \mathbf{N}_i, \mathbf{X}_{ji}) \mathbf{m}_i \tag{16}$$

here $M(\mathbf{N}_j, \mathbf{N}_i, \mathbf{X}_{ji})$ is the matrix which is facilitating the mapping. In the following this rotation matrix will be identified. According to Levi–Civita the in-plane orientation with respect a geodesic curve is invariant under parallel transport. Here, the orientation of the geodesic path between i and j will be approximated as the projections of $\mathbf{X}_{ji}$ on the planes TP_i and TP_j characterized by the unit vectors:

$$\hat{\mathbf{r}}_i = \frac{\mathbf{X}_{ji} - (\mathbf{N}_i \cdot \mathbf{X}_{ji}) \mathbf{N}_i}{|\mathbf{X}_{ji} - (\mathbf{N}_i \cdot \mathbf{X}_{ji}) \mathbf{N}_i|} \tag{17}$$

$$\hat{\mathbf{r}}_j = \frac{\mathbf{X}_{ji} - (\mathbf{N}_j \cdot \mathbf{X}_{ji}) \mathbf{N}_j}{|\mathbf{X}_{ji} - (\mathbf{N}_j \cdot \mathbf{X}_{ji}) \mathbf{N}_j|} \tag{18}$$

Similarly, their 90 degree rotated vectors in TP_i and TP_j can be defined:

$$\begin{aligned} \hat{\mathbf{r}}_i^\perp &= \mathbf{N}_i \times \hat{\mathbf{r}}_i \\ \hat{\mathbf{r}}_j^\perp &= \mathbf{N}_j \times \hat{\mathbf{r}}_j \end{aligned} \tag{19}$$

Vector $\mathbf{m}_i \in TP_i$ can now be expressed in the new basis $(\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_i^\perp)$ for TP_i as

$$\mathbf{m}_i = (\mathbf{m}_i \cdot \hat{\mathbf{r}}_i) \hat{\mathbf{r}}_i + (\mathbf{m}_i \cdot \hat{\mathbf{r}}_i^\perp) \hat{\mathbf{r}}_i^\perp \tag{20}$$

In Levi-Civita parallelism both the length of $\mathbf{m}_i$ and the orientation with respect to the geodesic path are preserved during parallel transport, i.e. the coordinates are the same in the basis $(\hat{\mathbf{r}}_j, \hat{\mathbf{r}}_j^\perp)$ for TP_j:

$$T_{i\to j}(\mathbf{m}_i) = (\mathbf{m}_i \cdot \hat{\mathbf{r}}_i)\hat{\mathbf{r}}_j + (\mathbf{m}_i \cdot \hat{\mathbf{r}}_i^{\perp})\hat{\mathbf{r}}_j^{\perp} = \left((\hat{\mathbf{r}}_j \otimes \hat{\mathbf{r}}_i) + \left(\hat{\mathbf{r}}_j^{\perp} \otimes \hat{\mathbf{r}}_i^{\perp}\right)\right)\mathbf{m}_i \tag{21}$$

which gives a compact formulation of the parallel transport Eq. (16) between neighboring tangent planes. It is trivial that $T_{i\to j}(\mathbf{m}_i)$ is an unique, norm-preserving and linear mapping from TP_i to TP_j, since Eq. (21) is simply a rotation. Equation (21) can easily be extended to general in-plane vectors and tensors. Take e.g. a 2-tensor $\mathbf{Q}_i = Q_{\alpha,\beta}\mathbf{e}_\alpha \otimes \mathbf{e}_\beta \in TP_i \times TP_i$, where $\mathbf{e}_1, \mathbf{e}_2$ is an orthonormal basis set of TP_i and $Q_{\alpha,\beta}$ is the coordinates of the tensor. Then

$$T_{i\to j}(\mathbf{Q}_i) = Q_{\alpha,\beta}T_{i\to j}(\mathbf{e}_\alpha) \otimes T_{i\to j}(\mathbf{e}_\beta) \tag{22}$$

An interesting property of Eq. (21) is that it can be composed of parallel transport along $\mathbf{X}_{ji}$. Let $\mathbf{X}_i + s\mathbf{X}_{ji}$ with $s \in]0,1[$ be the position of some point i' along the edge between vertices i and j. To this position we can assign a plane, e.g. the triangular face given by a normal vector $\mathbf{N}_\Delta$. Parallel translations from i to i' are thus given by matrices:

$$M(\mathbf{N}_\Delta, \mathbf{N}_i, s\mathbf{X}_{ji}) = \left(\hat{\mathbf{r}}_{ji} \otimes \hat{\mathbf{r}}_i\right) + \left(\hat{\mathbf{r}}_{ji}^{\perp} \otimes \hat{\mathbf{r}}_i^{\perp}\right) \tag{23}$$

and from i' to j:

$$M(\mathbf{N}_j, \mathbf{N}_\Delta, s\mathbf{X}_{ji}) = \left(\hat{\mathbf{r}}_j \otimes \hat{\mathbf{r}}_{ji}\right) + \left(\hat{\mathbf{r}}_j^{\perp} \otimes \hat{\mathbf{r}}_{ji}^{\perp}\right) \tag{24}$$

where we have defined $\hat{\mathbf{r}}_{ji} = \frac{\mathbf{X}_{ji}}{|\mathbf{X}_{ji}|}$. The combined parallel transport from i to j along $\mathbf{X}_{ji}$ via i' thus takes the form

$$\begin{aligned} M(\mathbf{N}_j, \mathbf{N}_\Delta, s\mathbf{X}_{ji})M(\mathbf{N}_\Delta, \mathbf{N}_i, s\mathbf{X}_{ji}) &= \left(\left(\hat{\mathbf{r}}_j \otimes \hat{\mathbf{r}}_{ji}\right) + \left(\hat{\mathbf{r}}_j^{\perp} \otimes \hat{\mathbf{r}}_{ji}^{\perp}\right)\right) \\ &\quad \left(\left(\hat{\mathbf{r}}_{ji} \otimes \hat{\mathbf{r}}_i\right) + \left(\hat{\mathbf{r}}_{ji}^{\perp} \otimes \hat{\mathbf{r}}_i^{\perp}\right)\right) \\ &= \left(\hat{\mathbf{r}}_j \otimes \hat{\mathbf{r}}_i\right) + \left(\hat{\mathbf{r}}_j^{\perp} \otimes \hat{\mathbf{r}}_i^{\perp}\right) \\ &= M(\mathbf{N}_j, \mathbf{N}_i, \mathbf{X}_{ji}) \end{aligned} \tag{25}$$

The last statement follows from the property of dyadic products:

$$(\mathbf{a} \otimes \mathbf{b})(\mathbf{c} \otimes \mathbf{d}) = (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \otimes \mathbf{d}) \tag{26}$$

Note that the composition rule Eq. (25) is independent of the choice of s. It will make it possible in a consistent manner to give the vectors $\mathbf{m}_i$ stored in vertex i a meaning in the neighboring triangular faces, which will be useful for the formulation of a discrete energy expressions for Eq. (2).

5 Vector field theory on a triangular surface

In the derivation of the discretized surface formulation of the scalar field theory Eq. (3) the metrical properties of the surface was induced from the imbedding 3D Euclidean space. Practically, this was done by approximating the surface by locally flat triangles, where the induced metric is trivial. In the following the same route for the Gaussian energy expression Eq. (2) involving the lateral vector field $\mathbf{m}$ will be utilized.

Let us consider the oriented triangle Δ again now equipped with the vector field $\tilde{\mathbf{m}}(\alpha_1, \alpha_2) \perp \mathbf{N}_\Delta$ where (α_1, α_2) are the barycentric coordinates as defined in Sect. 3. A simple interpolation for the field on Δ apply

$$\tilde{\mathbf{m}}(\alpha_1, \alpha_2) = \alpha_1\tilde{\mathbf{m}}_1 + \alpha_2\tilde{\mathbf{m}}_2 + (1 - \alpha_1 - \alpha_2)\tilde{\mathbf{m}}_3 \tag{27}$$

where $\tilde{\mathbf{m}}_1$, $\tilde{\mathbf{m}}_2$ and $\tilde{\mathbf{m}}_3$ are the vectors at the three corners of the triangle all perpendicular to the triangle normal $\mathbf{N}_\Delta$. Discussion on how to fix these corner vectors for a model with vectors defined in the vertex tangent planes will be postponed to the end of the section. First, we repeat the calculation of Sect. 3, now with a vector field model formulated with the barycentric coordinate system:

$$\begin{aligned} \mathcal{H}_\Delta &= \frac{1}{2}\int_\Delta \mathrm{d}^2\alpha\sqrt{g}g^{\mu\nu}g^{\delta\rho}D_\mu\tilde{\mathbf{m}}_\delta D_\nu\tilde{\mathbf{m}}_\rho \\ &= \frac{1}{2}\int_\Delta \mathrm{d}^2\alpha\sqrt{g}g^{\mu\nu}D_\mu\tilde{\mathbf{m}}D_\nu\tilde{\mathbf{m}} \end{aligned} \tag{28}$$

The second equation in Eq. (28) is valid since we are free to choose the basis set for the vector field (and the metric) and the triangular patch is flat. The whole program for the scalar field carried out in Sect. 3 can be repeated for the vector field on the triangular patch.

$$\begin{aligned} \mathcal{H}_\Delta &= \frac{1}{2}\int_\Delta \mathrm{d}\alpha^2\sqrt{g}g^{\mu\nu}D_\mu\tilde{\mathbf{m}}D_\nu\tilde{\mathbf{m}} \\ &= \frac{1}{4A_\Delta}\left(\cot(\beta_{13})(\tilde{\mathbf{m}}_{1,3})^2 + \cot(\beta_{23})(\tilde{\mathbf{m}}_{2,3})^2 \right. \\ &\quad \left. + \cot(\beta_{12})(\tilde{\mathbf{m}}_{1,2})^2\right) \end{aligned} \tag{29}$$

where

$$D_\nu\tilde{\mathbf{m}} = \partial_\nu\tilde{\mathbf{m}} = \tilde{\mathbf{m}}_\nu - \tilde{\mathbf{m}}_3 = \tilde{\mathbf{m}}_{\nu,3}. \quad \nu = 1,2 \tag{30}$$

and $\tilde{\mathbf{m}}_{1,2} = \tilde{\mathbf{m}}_{1,3} - \tilde{\mathbf{m}}_{2,3}$. This shows that we can calculate the orientational energy of the vector field on a triangle based on knowledge of the triangular geometry and the vectors at the corners. For the link (12) we thus need to calculate $(\tilde{\mathbf{m}}_{1,2})^2 = (\tilde{\mathbf{m}}_2 - \tilde{\mathbf{m}}_1)^2$. To proceed, the three corner vectors $\tilde{m}_i \perp \mathbf{N}_\Delta$, $i = 1,2,3$ of Δ must be fixed. From the analysis of Sect. 4 it is clear that $\tilde{\mathbf{m}}_1 = M(\mathbf{N}_1, \mathbf{N}_\Delta, \mathbf{R}_{21})\mathbf{m}_1$ is the parallel transported vector $\mathbf{m}_1 \in TP_1$ at vertex 1 to the plane of the triangle Δ along the link direction $\hat{\mathbf{r}}_{21}$ (and anywhere else on the flat triangular face). $\tilde{\mathbf{m}}_1$ can thus be expressed as a rotation of $\mathbf{m}_1$, the in-plane vector under investigation. This definition is consistent with the composition rule for parallel transport Eq. (25), e.g. $T_{1\to 2}\mathbf{m}_1 = M(\mathbf{N}_2, \mathbf{N}_\Delta, s\mathbf{X}_{21})\tilde{\mathbf{m}}_1$. Similarly, we choose the other corner vectors of Δ, like $\tilde{\mathbf{m}}_2 = M(\mathbf{N}_2, \mathbf{N}_\Delta, \mathbf{R}_{12})\mathbf{m}_2$. The inner products in Eq. (29) can now be calculated.

$$(\tilde{\mathbf{m}}_{1,2})^2 = (\tilde{\mathbf{m}}_2 - \tilde{\mathbf{m}}_1)\cdot(\tilde{\mathbf{m}}_2 - \tilde{\mathbf{m}}_1) = (\mathbf{m}_2 - M(\mathbf{N}_2,\mathbf{N}_1,\mathbf{R}_{21})\mathbf{m}_1) \cdot (\mathbf{m}_2 - M(\mathbf{N}_2,\mathbf{N}_1,\mathbf{R}_{21})\mathbf{m}_1) \quad (31)$$

Equation (31) follows from the fact that $M(\mathbf{N}_T,\mathbf{N}_2,\mathbf{R}_{21})$ is a rotation matrix, which leaves the inner vector product invariant. Furthermore, it now follows from Eq. (25) that

$$M(\mathbf{N}_\Delta,\mathbf{N}_2,\mathbf{R}_{12})^{-1}M(\mathbf{N}_\Delta,\mathbf{N}_1,\mathbf{R}_{21}) = M(\mathbf{N}_2,\mathbf{N}_\Delta,\mathbf{R}_{12}) \times M(\mathbf{N}_\Delta,\mathbf{N}_1,\mathbf{R}_{21}) = M(\mathbf{N}_2,\mathbf{N}_1,\mathbf{R}_{21}). \quad (32)$$

Equation (29) can now be formulated in terms of vectors in the tangent planes of the vertices:

$$\begin{aligned}\mathcal{H}_\Delta &= \frac{1}{2}\int_\Delta d\alpha\sqrt{g}g^{\mu\nu}D_\mu\tilde{\mathbf{m}}D_\nu\tilde{\mathbf{m}} \\ &= \frac{1}{4A_\Delta}\Big(\cot(\beta_{13})(\tilde{\mathbf{m}}_{1,3})^2 + \cot(\beta_{23})(\tilde{\mathbf{m}}_{2,3})^2 \\ &\quad + \cot(\beta_{12})(\tilde{\mathbf{m}}_{1,2})^2\Big) \\ &= \frac{1}{4A_\Delta}\Big(\cot(\beta_{13})(\mathbf{m}_3 - T_{1\to3}(\mathbf{m}_1))^2 \\ &\quad + \cot(\beta_{23})(\mathbf{m}_3 - T_{2\to3}(\mathbf{m}_2))^2. \\ &\quad + \cot(\beta_{12})(\mathbf{m}_2 - T_{1\to2}(\mathbf{m}_1))^2\Big) \end{aligned} \quad (33)$$

which is corresponding to Eq. (13) for scalar fields. Note, that the condition of $\mathbf{m}$ as a unit vector was relaxed in Eq. (27) and in the following calculations. This is possible, since homogeneous contributions to the energy, e.g. a term $\propto (\mathbf{m}^2 - 1)^2$ or a constraint $|\mathbf{m}| = 1$, are enforced in the vertices in analogy to scalar fields (Sect. 3). Now, finally, all the contributions from the triangles can be summed and we reach a simple generalization of Eq. (14)

$$\mathcal{H}[\mathbf{m}_i] = \frac{1}{2}\sum_i\sum_{j\in i}\frac{\cot(\beta_{ij}) + \cot(\beta_{ji})}{2}(\mathbf{m}_i - T_{j\to i}(\mathbf{m}_j))^2 \quad (34)$$

6 Conclusion

This work presents the generalized discrete form of the energy for a Gaussian scalar field on a triangulated surface to Gaussian vector fields. We demonstrated the procedure for a popular energy expression for the description of the elasticity of nematic membranes Eq. (2), but it can in a straightforward manner be applied to other energy expressions involving vector fields, e.g. Eq. (1), or Gaussian tensor fields. The procedure involves parallel transport of vectors in calculations of derivatives of vector fields and will thus capture the effect of indirect coupling between Gaussian curvature and local nematic or other p-atic ordering in a membrane.

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