1 Free Bulk Energy Densities on Surfaces

1.1 General Requirements

The bulk (or elastic) free energy is the functional

$$F[\mathbf{p}] = \int_{\mathcal{S}} f(\mathbf{p}, \nabla\mathbf{p})\, \mathrm{d}\mathcal{S}\,, \tag{1}$$

where ∇ is a metric compatible connection, like the covariant derivation, and $\mathbf{p}$ the director field, with $\mathrm{Im}(\mathbf{p}) = \mathbb{S}^2$. To represent the physical features of the material, the density f must be

frame-indifferent: The energy per unit volume must be same in any (rigid) frames, this means, that the push-forwards of $\mathbf{p}$ and $\mathbf{P} := \nabla\mathbf{p}$ along the (automorphic) transformation $\mathbf{R} : T\mathcal{S} \to T\mathcal{S}$ fulfill the identity

$$f(\mathbf{p}, \mathbf{P}) = f(\mathbf{R}_*\mathbf{p}, \mathbf{R}_*\mathbf{P}) = f(\mathbf{R}\mathbf{p}, \mathbf{R}\mathbf{P}\mathbf{R}^{-1})\,. \tag{2}$$

$\mathbf{R}$ is an element of $\mathrm{SO}(T\mathcal{S})$, because $\mathbf{p}$ has to stay a unit vector, i. e., with a canonical defined metric invariant tensor transpose it holds $\mathbf{R}^{-1} = \mathbf{R}^T$.

material-symmetric: Nematic liquid crystals do not change his behavior under reflection, therefor we must extend (2) with $\mathbf{R} \in \mathrm{O}(T\mathcal{S})$.

even: By the nematic interpretation of the director, we cannot distinguish the head from the tail of p. Hence, we also must require

$$f(\mathbf{p}, \nabla\mathbf{p}) = f(-\mathbf{p}, -\nabla\mathbf{p})\,. \tag{3}$$

positiv definit f must be zero in the undistorted state except on a finite set of defect locations to hold geometrical conditions for the director field, see e. g., Hairy-Ball-Theorem. All other states must produce a positive energy on all subsets of $\mathcal{S}$, i. e.,

$$f(\mathbf{p}, \mathbf{P}) \geq 0\,. \tag{4}$$

2 The two dimensional case

Let be $\mathcal{S}$ a two dimensional (smooth) manifold without boundaries and a metric tensor $g = g_{ij} dx^i \otimes dx^j$, referring to the two local covariant basis vectors ∂_i. g^{ij} denote the components of g^{-1} and $|g|$ the determinant of g. For the connection, we use the covariant derivative defined on contravariant coordinates, i. e.,

$$p^i{}_{|j} = \nabla_j p^i = \partial_j p^i + \Gamma_{jk}{}^i p^k\,, \tag{5}$$

with the Christoffel tensor

$$\Gamma_{jk}{}^{i} = g^{il}\Gamma_{jkl} = \frac{1}{2}g^{il}\left(\partial_j g_{kl} + \partial_k g_{jk} - \partial_l g_{jk}\right) . \tag{6}$$

∇ is metric compatible, therefore we can rise and lower the indices for $p^{i}{}_{|j} = P^{i}{}_{j}$ in the common way.

The rotation map $\mathbf{R} \in \mathrm{SO}(T\mathcal{S})$ can be construct by variating the tangential vector pb and its hodge dual $*\mathbf{p} = (*\mathbf{p}^{\flat})^{\sharp}$ around an counterclockwise angle $\phi \in [0, 2\pi)$ and combine the results linear with respect to the length preserving, i. e.,

$$\mathbf{R}_{\phi}\mathbf{p} := \cos\phi\mathbf{p} + \sin\phi(*\mathbf{p}) . \tag{7}$$

In this interpretation $\mathbf{R} := \mathbf{R}_{\phi} \in (\mathcal{T}^{1}{}_{1} \cap \mathrm{SO})(T\mathcal{S})$ is a (1,1)-tensor with coordinates (by testing and contraction of the basis contra- and covectors)

$$R^{i}{}_{j} = (R\partial_i)(dx^j) = \langle R\partial_i, \partial_j\rangle . \tag{8}$$

For $\mathbf{R}$ holds the identity

$$\mathbf{R}^{-1} = \mathbf{R}^{T} := {}^{\sharp}\left({}^{\flat}\mathbf{R}\right)^{T} = ((\mathbf{R}^{\sharp})^{T})^{\flat} \tag{9}$$

and in coordinates $\left(\mathbf{R}^{T}\right)^{i}{}_{j} = \left\{R_{j}{}^{i}\right\}^{i}{}_{j}$. For a better readability and to preclude confusions in the summation convention we roughly write $R_{j}{}^{i}$ without the brackets and keep in mind, that $R_{j}{}^{i}$ are components of a tensor in $\mathcal{T}^{1}{}_{1}$ and not in $\mathcal{T}_{1}{}^{1}$ and therefor we can write

$$\left(\mathbf{R}\mathbf{R}^{T}\right)^{i}{}_{j} = R^{i}{}_{k}R_{j}{}^{k} = \delta^{i}{}_{j} . \tag{10}$$

Let be $\mathbf{v}$ an arbitrary tangential vector and $\phi_{\mathbf{v}}$ denote the counterclockwise angle from $\mathbf{p}$ to $\mathbf{v}$. We can describe the reflection at the line along $\mathbf{v}$ as $\mathbf{S}_{\mathbf{v}} = \mathbf{R}_{2\phi_{\mathbf{v}}}$, therefor $\mathbf{S}_{\mathbf{v}}$ is odd, i. e.,

$$\mathbf{S}_{\mathbf{v}}(-\mathbf{p}) = \mathbf{R}_{2\phi_{\mathbf{v}}}(-\mathbf{p}) = -\mathbf{R}_{2\phi_{\mathbf{v}}}\mathbf{p} = -\mathbf{S}_{\mathbf{v}}\mathbf{p} . \tag{11}$$

Furthermore, it is valid, that $\mathbf{S}_{\mathbf{v}}^{-1} = \mathbf{S}_{\mathbf{v}}$, because

$$\begin{aligned}
\mathbf{S}_{\mathbf{v}}^{2}\mathbf{p} &= \mathbf{R}_{2(\pi-\phi_{\mathbf{v}})}\mathbf{R}_{2\phi_{\mathbf{v}}}\mathbf{p} && (12)\\
&= \mathbf{S}_{\mathbf{v}}\left[\cos(2\phi_{\mathbf{v}})\mathbf{p} + \sin(2\phi_{\mathbf{v}})(*\mathbf{p})\right] && (13)\\
&= \cos(2\phi_{\mathbf{v}})\left[\cos(2\phi_{\mathbf{v}})\mathbf{p} + \sin(2\phi_{\mathbf{v}})(*\mathbf{p})\right] - \sin(2\phi_{\mathbf{v}})\left[\cos(2\phi_{\mathbf{v}})(*\mathbf{p}) - \sin(2\phi_{\mathbf{v}})\mathbf{p}\right] && (14)\\
&= \mathbf{p} . && (15)
\end{aligned}$$

Lemma 1. *For the bulk free energy density f holds $f(\mathbf{p}, \mathbf{P}) = f(-\mathbf{p}, \mathbf{P})$.*

Proof. With the material-symmetry, the oddness (11) and $\mathbf{S}_{\mathbf{v}}^{-1} = \mathbf{S}_{\mathbf{v}}$, we obtain

$$f(\mathbf{p}, \mathbf{P}) = f(\mathbf{S}_{\mathbf{v}}\mathbf{p}, \mathbf{S}_{\mathbf{v}}\mathbf{P}\mathbf{S}_{\mathbf{v}}) = f((-\mathbf{S}_{\mathbf{v}})(-\mathbf{p}), (-\mathbf{S}_{\mathbf{v}})\mathbf{P}(-\mathbf{S}_{\mathbf{v}})) = f(-\mathbf{p}, \mathbf{P}) \tag{16}$$

□

Theorem 1. *With the symmetry lemma above and the evenness of f, it is valid, that*

$$f(\mathbf{p},\mathbf{P}) = f(-\mathbf{p},\mathbf{P}) = f(\mathbf{p},-\mathbf{P}) = f(-\mathbf{p},-\mathbf{P})\,. \tag{17}$$

With this property of the energy density, a expansion of f contains only terms of $\mathbf{p}$ and $\mathbf{P}$ of even order. Therefor we obtain a necessary condition for the bulk free energy density, which is sufficiently for the evenness, material-symmetry and positive definiteness Proberties. A development of f up to second order must be of the form

$$f(\mathbf{p},\mathbf{P}) = L^{(2)}_{i_1 i_2} p^{i_1} p^{i_2} + L^{(4)}_{i_1\dots i_4} P^{i_1 i_2} P^{i_3 i_4} + L^{(6)}_{i_1\dots i_6} p^{i_1} p^{i_2} P^{i_3 i_4} P^{i_5 i_6}\,, \tag{18}$$

with symmetric and positive definite tensors $\mathbf{L}^{(m)} \in \mathcal{T}^0{}_m(T\mathcal{S})$. Die Eigenschaft s.p.d. zu sein muss noch quantisiert werden. Die gerade anzahligen Tensorstufen legen aber nahe, dass sich das kanonisch über das freie Produkt abwälzen lässt, wobei hierbei eine Art „Vorzeichenregel bzgl des Produktes“ zu beobachten ist, zb. ist das freie Produkt zweier negativ definiter Tensoren positiv definit. Analoges hat sich auch bei der Symmetrieeigenschaft gezeigt. The main problem is to determine all $\mathbf{L}^{(m)}$ with a maximum of freeness, so that f fulfill the requirements of the free bulk energy density. Die oben genannte Quantisierung der s.p.d. Tensoren sollte auf ein $\mathbb{R}$-Vektorraum führen. Die Frank-Oseen Dichte legt das nahe. Das wäre der Schlüssel, da nur noch über die endliche Basis geprüft werden müsste. Heiße Kandidaten für den $\mathbf{L}^{(4)}$ finden sich in der unteren Folgerung zur Frank-Oseen-Dichte. We know by restricting the three dimensional Frank-Oseen-Energy-Density f_{FO} to the two dimensional surface, that

$$\begin{aligned}
f_{FO}(\mathbf{p},\nabla\mathbf{p}) &= K_1(\mathrm{Div}\mathbf{p})^2 + K_3(\mathrm{Rot}\mathbf{p})^2 && (19)\\
&= K_1 p^i{}_{|i} p^j{}_{|j} + K_3 p^i{}_{|j}\left(p_i{}^{|j} - p^j{}_{|i}\right) && (20)\\
&= K_1 \delta^{i_2}{}_{i_1}\delta^{i_4}{}_{i_3} P^{i_1}{}_{i_2} P^{i_3}{}_{i_4} + K_3\left(\delta^{i_3}{}_{i_1}\delta^{i_2}{}_{i_4} P^{i_1}{}_{i_2} P_{i_3}{}^{i_4} - \delta^{i_4}{}_{i_1}\delta^{i_2}{}_{i_3} P^{i_1}{}_{i_2} P^{i_3}{}_{i_4}\right) && (21)\\
&= \left(K_1 g_{i_1 i_2} g_{i_3 i_4} + K_3\left(g_{i_1 i_3} g_{i_2 i_4} - g_{i_1 i_4} g_{i_2 i_3}\right)\right) P^{i_1 i_2} P^{i_3 i_4}\,, && (22)
\end{aligned}$$

with free parameters $K_1, K_3 \geq 0$.

Conclusion 1. *The prototype density* (18) *is equal to f_{FO}, if for the (metric independent) Levi-Civita symbols $\varepsilon_{ij} = \varepsilon^{ij}$ apply to $L^{(2)}_{i_1 i_2} = 0$, $L^{(4)}_{i_1\dots i_4} = K_1 g_{i_1 i_2} g_{i_3 i_4} + K_3 |g| \varepsilon_{i_1 i_2}\varepsilon_{i_3 i_4}$ and $L^{(6)}_{i_1\dots i_6} = 0$, i. e.,*

$$\mathbf{L}_{FO} := \mathbf{L}^{(4)} = K_1 g\otimes g + K_3 |g| \varepsilon\otimes\varepsilon \in \mathcal{T}^0{}_4(T\mathcal{S}) \tag{23}$$

*is the only coefficients tensor, which have an interest in the prototype density. We call $\mathbf{L}_{FO}$ the **Frank-Oseen tensor**.*

Proof. The main work is done by (22). (For a better readability, we use (i,j,k,l) as indices, instead of (i_1,i_2,i_3,i_4).) Hence, we only have to show that $g_{ik}g_{jl} - g_{il}g_{jk} = |g|\varepsilon_{ij}\varepsilon_{kl}$. By rising some indices, we obtain

$$g_{ik}g_{jl} - g_{il}g_{jk} = g_{mk}g_{nl}\left(\delta_i{}^m\delta_j{}^n - \delta_i{}^n\delta_j{}^m\right) = g_{mk}g_{nl}\varepsilon_{ij}\varepsilon^{mn}\,. \tag{24}$$

The Levi-Civita symbols are related to the volume form $\mu = \sqrt{|g|}dx^1 \wedge dx^2$ by the (metric dependent) Levi-Civita tensor

$$E_{ij} := \sqrt{|g|}\varepsilon_{ij} = \mu(\partial_i, \partial_j)\,. \tag{25}$$

In addition by rising the indices it holds $E^{ij} = \frac{1}{\sqrt{|g|}}\varepsilon^{ij}$. Therefor, we finally get

$$g_{ik}g_{jl} - g_{il}g_{jk} = g_{mk}g_{nl}E_{ij}E^{mn} = E_{ij}E_{kl} = |g|\varepsilon_{ij}\varepsilon_{kl}\,. \tag{26}$$

□

This leads us to write the Frank-Oseen energy density in the (bilinear?) form

$$\begin{aligned} f_{FO}(\mathbf{p}, \mathbf{P}) = f_{FO}(\mathbf{P}) &= \mathbf{P} : \mathbf{L}_{F0} : \mathbf{P} & (27)\\ &= \left(K_1 g_{i_1 i_2} g_{i_3 i_4} + K_3 |g| \varepsilon_{i_1 i_2} \varepsilon_{i_3 i_4}\right) P^{i_1 i_2} P^{i_3 i_4}\,. & (28) \end{aligned}$$

Theorem 2. *The two dimensional Frank-Oseen energy density is a bulk free energy density.*

Proof. By Conclusion 1 we only have to proof the frame-indifferent, i. e., $f_{FO}(\mathbf{RPR}^T) = f_{FO}(\mathbf{P})$. The 2-tensor contraction, i. e., the trace, is frame-indifferent, because

$$\left(\mathbf{RPR}^T\right)^i{}_i = R^i{}_k P^k{}_l R_i{}^l = \delta^l{}_k P^k{}_l = P^l{}_l\,. \tag{29}$$

Hence, $\mathbf{P} : (g \otimes g) : \mathbf{P} = P^i{}_i P^j{}_j$ is also frame-indifferent. □