Local elastic stability for nematic liquid crystals

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1 Introduction

Nematic liquid crystals (NLC) are sensitive to the external magnetic and electric field. One of the well known phenomenon is Freedericksz's transition. Figure 1 shows the schematic of the Freedericksz transition. The NLC is confined between two plates which induce strong planar anchoring. Initially, the director n is parallel to the e_x . The system is then probed with magnetic or electric field. For a weak electric field E the director is not distorted and hence remains parallel to the x-axis. However, when a strong electric field which is greater than the threshold electric field E_t is applied then the director rotates by an angle θ in the x - y plane. Similarly, if the diamagnetic anisotropy of the of the NLC is positive, then the director rotates in the x - y plane on the application of sufficiently strong magnetic field. This is also celled splay-Freedericksz distortion.

[Lonberg and Meyer, 1985] observed a new type of transition for NLC composed of very long particles. They found that the distortion of director is not uniform but a periodic splay-twist distortion (see Fig. 2). This happens for materials in which the splay elastic constant K_1 is much bigger than the twist elastic constant K_2 and hence periodic distortion will have lower free energy than the uniform distortion since it avoids splay. They showed that for periodic splay-twist distortion to have lower free energy, the inequality $r < r_c$, where $r = K_2/K_1$ and $r_c = 0.303$, must hold. [Miraldi et al., 1986] further generalized the result for the weak anchoring. They showed that r_c may be changed over a wide range by controlling the surface conditions and sample thickness. [Lavrentovich and Pergamenshchik, 1990] obtained a periodic distortion even in the absence of external fields in thin hybrid nematic layers. A hybrid nematic layer has the easy axis (preferred direction of director) tangent to the lower surface (planar anchoring) and nearly normal at the free upper surface (homeotropic anchoring). The periodic structure was formed because the boundary conditions on the layer surfaces were different and degenerated. The stability analysis revealed that the critical condition for periodic distortion depended on saddle-splay elastic constant K_4 . [Sparavigna et al., 1991] also investigated the ocurrence of periodic stripes in the hybrid nematic layers with planar anchoring stronger than the homeotropic anchoring. For the thickness d lower than the critical thickness d_a , since the planar anchoring is strong, the director assumes a uniform distribution. For $d > d_a$, the uniform state is replaced by a hybrid aperiodic alignment (HAN) or a periodic deformed structure (PHAN). [Sparavigna et al., 1994] studied the PHAN-HAN transition for an elastic isotopic nematics $(K_1 = K_2 = K_3 = K)$ in the absence of an external field. They showed that PHAN arises at a critical thickness $d_p < d_a$ for wide range of K_4 .

The transitions described above are of second order and thus they can be predicted by conducting the local stability analysis of the elastic free-energy functional \mathcal{F} . This has usually been done in two ways in the literature. First way is to do the linear stability analysis of the Euler-Lagrange equation of \mathcal{F} . The second

way is to calculate the second variation $\delta^2 \mathcal{F}$ and then explore the sign of $\delta^2 \mathcal{F}$ near ground state (the state in which the director is uniform). The director \boldsymbol{n} is represented in a way such that the constraint on its length is automatically satisfied ($\boldsymbol{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, where θ is the angle between \boldsymbol{n} and z axis and $\phi = \arctan(n_x/n_y)$).

Both these methods have some limitations. The first one can accurately determine the transition condition but can't determine whether the the transition is periodic or not. The second method introduces approximations such as the wave number of the perturbing modes are small and hence is not general. Therefore, we use a third approach. Calculating the second variation of $\delta^2 \mathcal{F}$ is not a trivial task. First because finding an exact expression of $\delta^2 \mathcal{F}$ requires long computation and second difficulty is in determining whether the expression is positive definite or not. Our general procedure is as follows: (i) \boldsymbol{n} is perturbed by keeping the constraint $|\boldsymbol{n}| = 1$ valid upto 2nd order and (ii) the sign of $\delta^2 \mathcal{F}$ is computed by finding the least eigen value of a linear problem. The advantages of this method are illustrated in [Rosso et al., 2004].

2 The variational formulation

2.1 Total free energy

Total free energy of the NLC contains both the bulk free energy and the surface free energy. The Frank expression for the elastic energy density of deformed NLC in the bulk is given by

$$f = \frac{1}{2} \left\{ K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 \right\} - (K_2 + K_4) \nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}),$$
(1)

where K_1, K_2, K_3 and $(K_2 + K_4)$ are called splay, twist, bend and saddle-splay elastic constants, respectively [Barbero and Evangelista, 2006]. The last term contributes only through the surface owing to the divergence theorem and the energy associated with it is called surfacelike. This term can further be simplified as

$$\nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}) = \nabla \cdot (n_i n_{j,j} \boldsymbol{e}_i + \boldsymbol{n} \otimes \varepsilon_{ijk} n_{j,i} \boldsymbol{e}_k) \qquad \left(\text{where } n_{i,j} = \frac{\partial n_i}{\partial n_j} \right)$$
$$= \nabla \cdot (n_i n_{j,j} \boldsymbol{e}_i + \varepsilon_{lkm} \varepsilon_{ijk} n_l n_{j,i} \boldsymbol{e}_m)$$
$$= n_{i,i} n_{j,j} + n_i n_{j,ji} + \varepsilon_{lkm} \varepsilon_{ijk} n_{l,m} n_{j,i} + \varepsilon_{lkm} \varepsilon_{ijk} n_l n_{j,im}$$
$$= n_{i,i} n_{j,j} + n_i n_{j,ji} + (\delta_{im} \delta_{jl} - \delta_{jm} \delta_{li}) n_{l,m} n_{j,i} + (\delta_{mi} \delta_{jl} - \delta_{jm} \delta_{li}) n_l n_{j,im}$$
$$= n_{i,i} n_{j,j} + n_i n_{j,ji} + (n_{j,i} n_{j,i} - n_{i,j} n_{j,i}) + (n_j n_{j,ii} - n_i n_{j,ij})$$
$$= n_{i,i} n_{j,j} - n_{i,j} n_{j,i} + n_{j,i} n_{j,i} + n_j n_{j,ii} \qquad (n_{j,ji} = n_{j,ij}). \qquad (2)$$

The director \boldsymbol{n} is a unit vector hence,

$$\mathbf{n} \cdot \mathbf{n} = 1 \implies n_i n_i = 1$$
differentiating,
$$n_{i,jj} n_i = 0$$
differentiating again,
$$n_{i,jj} n_i + n_{i,j} n_{i,j} = 0.$$
(3)

Also,

$$(\nabla \boldsymbol{n})^2 = \nabla \boldsymbol{n} \nabla \boldsymbol{n} = (n_{i,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j)(n_{k,l} \boldsymbol{e}_k \otimes \boldsymbol{e}_l) = n_{i,k} n_{k,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j$$

$$\implies tr((\nabla \boldsymbol{n})^2) = n_{i,j} n_{j,i}, \qquad (4)$$

where tr is the trace of a tensor. Substituting (3) and (4) in (2), we obtain

$$\nabla \cdot (\mathbf{n} \nabla \cdot \mathbf{n} + \mathbf{n} \times \nabla \times \mathbf{n}) = (\nabla \cdot \boldsymbol{n})^2 - tr((\nabla \boldsymbol{n})^2), \tag{5}$$

which when substituted in (1), yields

$$f_{Frank} = \frac{1}{2} \left\{ K_1(\nabla \cdot \mathbf{n})^2 + K_2(\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + K_3(\mathbf{n} \times \nabla \times \mathbf{n})^2 \right\} + (K_2 + K_4)(tr((\nabla \boldsymbol{n})^2) - (\nabla \cdot \boldsymbol{n})^2).$$
(6)

The elastic energy due to twist can also be simplified further as

$$(\boldsymbol{n} \cdot \nabla \times \boldsymbol{n})^2 = (n_i \varepsilon_{jki} n_{k,j})^2 = \varepsilon_{ijk} \varepsilon_{lmp} n_i n_{k,j} n_l n_{p,m}$$

$$= \left\{ \delta_{il} (\delta_{jm} \delta_{kp} - \delta_{jp} \delta_{km}) - \delta_{im} (\delta_{jl} \delta_{kp} - \delta_{jp} \delta_{kl}) + \delta_{ip} (\delta_{jl} \delta_{km} - \delta_{jm} \delta_{kl}) \right\} n_i n_{k,j} n_l n_{p,m}$$

$$= n_i n_{k,j} n_i n_{k,j} - n_i n_{k,j} n_i n_{j,k} - n_i n_{k,j} n_j n_{k,i} + n_i n_{k,j} n_k n_{j,i} + n_i n_{k,j} n_j n_{i,k} - n_i n_{k,j} n_k n_{i,j}$$
using the result from (3) $(n_i n_{i,j} = 0)$

$$= n_i n_{k,j} n_i n_{k,j} - n_i n_{k,j} n_i n_{j,k} - n_i n_{k,j} n_j n_{k,i}$$

also, using
$$n_i n_i = 1$$

$$= n_{k,j}n_{k,j} - n_{k,j}n_{j,k} - n_in_{k,j}n_jn_{k,i}$$

$$= n_{k,j}n_{k,j} - n_{k,j}n_{j,k} - n_{k,j}n_jn_{k,i}n_i$$

$$= \nabla \boldsymbol{n} : \nabla \boldsymbol{n} - tr((\nabla \boldsymbol{n})^2) - |(\nabla \boldsymbol{n})\boldsymbol{n}|^2.$$
(7)

Similarly the bend energy can be simplified as

$$\boldsymbol{n} \times \nabla \times \boldsymbol{n} \Big|^{2} = \left| \varepsilon_{lim} \varepsilon_{jki} n_{l} n_{k,j} \boldsymbol{e}_{m} \right|^{2} = \left| (\delta_{jm} \delta_{lk} - \delta_{jl} \delta_{km}) n_{l} n_{k,j} \boldsymbol{e}_{m} \right|^{2}$$
$$= \left| n_{k} n_{k,j} \boldsymbol{e}_{j} - n_{j} n_{k,j} \boldsymbol{e}_{k} \right|^{2}$$
$$= \left| - n_{j} n_{k,j} \boldsymbol{e}_{k} \right|^{2} = \left| (\nabla \boldsymbol{n}) \boldsymbol{n} \right|^{2} \qquad (n_{k} n_{k,j} = 0 \text{ from (3)}). \tag{8}$$

Substituting (7) and (8) in (6), we get the final form of the frank free energy density

$$f = \frac{1}{2} \left\{ K_1(\nabla \cdot \mathbf{n})^2 + K_2 \left(|\nabla \mathbf{n}|^2 - tr((\nabla n)^2) \right) + (K_3 - K_2) |(\nabla n)n|^2 \right\} + (K_2 + K_4) \left(tr((\nabla n)^2) - (\nabla \cdot n)^2 \right).$$
(9)

In the absence of any external field, the bulk free energy of NLC is given by

$$\mathcal{F}_b := \int_{\mathcal{B}} f dV, \tag{10}$$

where \mathcal{B} is the region occupied by the NLC.

Apart from the bulk energy which depends on the molecular shape and on the molecular interactions, NLC also interacts with the surface and hence has surface energy \mathcal{F}_a . The anchoring is defined as the phenomenon of orientation of liquid crystal by the surface. The anchoring direction or easy direction is the direction of spontaneous orientation of n on the surface. The anchoring energy \mathcal{F}_a is taken to be in the form

$$\mathcal{F}_a := \int_{\partial \mathcal{B}} g(\boldsymbol{n}) dA = \int_{\partial \mathcal{B}} \boldsymbol{n} \cdot \boldsymbol{A} \boldsymbol{n} dA, \tag{11}$$

where A is symmetric second rank tensor which for simplicity is assumed to be piecewise constant on $\partial \mathcal{B}$. The total free energy therefore is the summation of bulk and anchoring energy,

$$\mathcal{F}[\mathcal{B}] = \mathcal{F}_b[\mathcal{B}] + \mathcal{F}_a[\partial \mathcal{B}]. \tag{12}$$

2.2 First variation

Making the first variation of \mathcal{F} go to zero, we can get the Euler-Lagrange equation for \mathcal{F} , which will give us the equilibrium conditions for \boldsymbol{n} . Our goal is to do the stability analysis of this extremal for which we will need the second variation of \mathcal{F} . Let us consider the variation of \boldsymbol{n} of the form

$$\boldsymbol{n}_{\varepsilon}(\boldsymbol{x}) := \boldsymbol{n} + \varepsilon \boldsymbol{\phi}(\boldsymbol{x}) + \varepsilon^2 \boldsymbol{\psi}(\boldsymbol{x})$$
(13)

such that $\boldsymbol{n}_{\varepsilon} \cdot \boldsymbol{n}_{\varepsilon} = 1 + \mathcal{O}(\boldsymbol{\varepsilon}^{3})$. This condition on substitution of (13) gives,

$$\boldsymbol{n}_{\varepsilon} \cdot \boldsymbol{n}_{\varepsilon} = 1 + \mathcal{O}(\varepsilon^3) = 1 + \varepsilon \boldsymbol{\phi} \cdot \boldsymbol{n} + \varepsilon^2 \boldsymbol{\phi} \cdot \boldsymbol{\phi} + \varepsilon^2 \boldsymbol{\psi} \cdot \boldsymbol{n} + \mathcal{O}(\varepsilon^3)$$

and hence gives these two extra conditions,

$$\boldsymbol{\phi} \cdot \boldsymbol{n} = 0, \tag{14}$$

$$\boldsymbol{\psi} \cdot \boldsymbol{n} = -\frac{1}{2} \boldsymbol{\phi} \cdot \boldsymbol{\phi}. \tag{15}$$

It can be seen from (15) that taking second order variation $\psi = 0$, will result in $\phi = 0$, and thus for attaining the required accuracy on the constraint, we need to retain both the term. Alternatively, if the director is represented by the two angles as mentioned in the previous section, then the constraint is automatically satisfied. A second method that is found in the literature is

$$\boldsymbol{n}_{\varepsilon} = \frac{\boldsymbol{n} + \varepsilon \boldsymbol{\phi}}{|\boldsymbol{n} + \varepsilon \boldsymbol{\phi}|}.$$
(16)

This when simplified and expanded for small ε becomes,

$$n_{\varepsilon} = \frac{n + \varepsilon \phi}{|n + \varepsilon \phi|} = \frac{n + \varepsilon \phi}{\sqrt{(n + \varepsilon \phi) \cdot (n + \varepsilon \phi)}}$$

= $\frac{n + \varepsilon \phi}{\sqrt{(1 + 2\varepsilon \phi \cdot n + \varepsilon^2 \phi \cdot \phi)}}$
= $(n + \varepsilon \phi) \left(1 - \frac{1}{2}(2\varepsilon \phi \cdot n + \varepsilon^2 \phi \cdot \phi) + \frac{1}{8}(2\varepsilon \phi \cdot n + \varepsilon^2 \phi \cdot \phi)^2\right) + \mathcal{O}(\varepsilon^3)$
= $n + \varepsilon \left(\phi - (\phi \cdot n)n\right) + \varepsilon^2 \left(\frac{1}{2}(-\phi \cdot \phi + (\phi \cdot n)^2)n + (\phi \cdot n)\phi\right) + \mathcal{O}(\varepsilon^3)$ (17)

Now, if we assume condition (14) holds then,

$$n_{\varepsilon} = n + \varepsilon \phi - \varepsilon^{2} \frac{1}{2} (\phi \cdot \phi) n + \mathcal{O}(\varepsilon^{3})$$

$$n_{\varepsilon} = n + \varepsilon \phi + \varepsilon^{2} \psi + \mathcal{O}(\varepsilon^{3})$$
(18)
where,
$$\psi \cdot n = -\frac{1}{2} \phi \cdot \phi.$$

Thus these two representation are equivalent if restricted to second order accuracy and conditions (14) and (15) are satisfied.

Using, (13), we can express $\nabla \boldsymbol{n}_{\varepsilon}$ as,

$$\nabla \boldsymbol{n}_{\varepsilon} = \nabla \boldsymbol{n} + \varepsilon \nabla \phi + \varepsilon^2 \nabla \psi \tag{19}$$

The first variation of the functional \mathcal{F} can be calculated as,

$$\begin{split} \delta \mathcal{F} &= \frac{d}{d\varepsilon} \mathcal{F}(\boldsymbol{n}_{\varepsilon}, \nabla \boldsymbol{n}_{\varepsilon}) \Big|_{\varepsilon=0} = \frac{d}{d\varepsilon} \mathcal{F}_{b}(\boldsymbol{n}_{\varepsilon}, \nabla \boldsymbol{n}_{\varepsilon}) \Big|_{\varepsilon=0} + \frac{d}{d\varepsilon} \mathcal{F}_{a}(\boldsymbol{n}_{\varepsilon}) \Big|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon} \int_{B} f(\boldsymbol{n}_{\varepsilon}, \nabla \boldsymbol{n}_{\varepsilon}) dV \Big|_{\varepsilon=0} + \frac{d}{d\varepsilon} \int_{\partial \mathcal{B}} g(\boldsymbol{n}_{\varepsilon}) dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial f}{\partial \boldsymbol{n}_{\varepsilon}} \cdot \frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon} + \frac{\partial f}{\partial \nabla \boldsymbol{n}_{\varepsilon}} : \frac{d\nabla \boldsymbol{n}_{\varepsilon}}{d\varepsilon} dV \Big|_{\varepsilon=0} + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial \boldsymbol{n}_{\varepsilon}} \cdot \frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon} dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial f}{\partial \boldsymbol{n}_{\varepsilon}} \cdot (\phi + 2\varepsilon\psi) + \frac{\partial f}{\partial \nabla \boldsymbol{n}_{\varepsilon}} : (\nabla\phi + 2\varepsilon\nabla\psi) dV \Big|_{\varepsilon=0} + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial \boldsymbol{n}_{\varepsilon}} \cdot (\phi + 2\varepsilon\psi) dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial f}{\partial \boldsymbol{n}} \cdot \phi + \frac{\partial f}{\partial \nabla \boldsymbol{n}} : \nabla \phi dV + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial \boldsymbol{n}} \cdot \phi dA. \end{split}$$
(20)

The first variation $\delta \mathcal{F}$ can be further simplified using the following relation for an arbitrary tensor T and arbitrary vector a

$$\boldsymbol{T}: \nabla \boldsymbol{a} = T_{ij} \frac{\partial a_i}{\partial x_j} = \frac{\partial}{\partial x_j} (T_{ij} a_i) - \frac{\partial}{\partial x_j} (T_{ij}) a_i = \nabla \cdot (\boldsymbol{T}^T \boldsymbol{a}) - \boldsymbol{a} \cdot \nabla \cdot (\boldsymbol{T}).$$
(22)

Substituting the above relation in (21) gives

$$\begin{split} \delta \mathcal{F} &= \int_{\mathcal{B}} \frac{\partial f}{\partial \boldsymbol{n}} \cdot \boldsymbol{\phi} + \nabla \cdot \left(\frac{\partial f}{\partial \nabla \boldsymbol{n}}^{T} \boldsymbol{\phi} \right) - \boldsymbol{\phi} \cdot \nabla \cdot \frac{\partial f}{\partial \nabla \boldsymbol{n}} dV + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial \boldsymbol{n}} \cdot \boldsymbol{\phi} dA. \\ &= \int_{\mathcal{B}} \left(\frac{\partial f}{\partial \boldsymbol{n}} - \nabla \cdot \frac{\partial f}{\partial \nabla \boldsymbol{n}} \right) \cdot \boldsymbol{\phi} + \nabla \cdot \left(\frac{\partial f}{\partial \nabla \boldsymbol{n}}^{T} \boldsymbol{\phi} \right) dV + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial \boldsymbol{n}} \cdot \boldsymbol{\phi} dA. \end{split}$$

Using the divergence theorem, the above equation can be written in two parts as

$$\begin{split} \delta \mathcal{F} &= \int_{\mathcal{B}} \left(\frac{\partial f}{\partial n} - \nabla \cdot \frac{\partial f}{\partial \nabla n} \right) \cdot \phi dV + \int_{\partial \mathcal{B}} \frac{\partial f}{\partial \nabla n}^{T} \phi \cdot \mathbf{N} dA + \int_{\partial \mathcal{B}} \frac{\partial g}{\partial n} \cdot \phi dA \\ &= \int_{\mathcal{B}} \left(\frac{\partial f}{\partial n} - \nabla \cdot \frac{\partial f}{\partial \nabla n} \right) \cdot \phi dV + \int_{\partial \mathcal{B}} \left(\frac{\partial f}{\partial \nabla n} \mathbf{N} + \frac{\partial g}{\partial n} \right) \cdot \phi dA \\ &= \int_{\mathcal{B}} \mathbf{p}(\mathbf{n}, \nabla \mathbf{n}) \cdot \phi dV + \int_{\partial \mathcal{B}} \mathbf{q}(\mathbf{n}, \nabla \mathbf{n}) \cdot \phi dA, \end{split}$$
(23)

where

$$\boldsymbol{p}(\boldsymbol{n}, \nabla \boldsymbol{n}) = \frac{\partial f}{\partial \boldsymbol{n}} - \nabla \cdot \frac{\partial f}{\partial \nabla \boldsymbol{n}} \qquad \text{and} \qquad \boldsymbol{q}(\boldsymbol{n}, \nabla \boldsymbol{n}) = \frac{\partial f}{\partial \nabla \boldsymbol{n}} \boldsymbol{N} + \frac{\partial g}{\partial \boldsymbol{n}} \qquad (24)$$

and N is the outward unit normal. To calculate p and q, we can use the form of free energy given by equation (9) and (11). To simplify the expressions further, we will need the following results

$$\begin{aligned} \frac{\partial}{\partial \mathbf{n}} \nabla \cdot \mathbf{n} &= \frac{\partial}{\partial n} tr(\nabla \mathbf{n}) = 0 \\ \frac{\partial}{\partial \nabla \mathbf{n}} (\nabla \cdot \mathbf{n})^2 &= 2\nabla \cdot \mathbf{n} \frac{\partial}{\partial \nabla \mathbf{n}} tr(\nabla \mathbf{n}) = 2\nabla \cdot \mathbf{n} \frac{\partial}{\partial \nabla \mathbf{n}} \mathbf{I} : \nabla \mathbf{n} = 2\nabla \cdot \mathbf{n} \mathbf{I} \\ \frac{\partial}{\partial \nabla \mathbf{n}} |\nabla \mathbf{n}|^2 &= \frac{\partial}{\partial \nabla \mathbf{n}} \nabla \mathbf{n} : \nabla \mathbf{n} = 2\nabla \mathbf{n} \\ \frac{\partial}{\partial \nabla \mathbf{n}} tr((\nabla \mathbf{n})^2) &= \frac{\partial}{\partial \nabla \mathbf{n}} \nabla \mathbf{n} \nabla \mathbf{n} : \mathbf{I} = \frac{\partial}{\partial \nabla \mathbf{n}} \nabla \mathbf{n} : \nabla \mathbf{n}^T = \frac{\partial}{\partial n_{i,j}} n_{k,l} n_{l,k} \mathbf{e}_l \otimes \mathbf{e}_j \\ &= \delta_{ik} \delta_{jl} n_{l,k} \mathbf{e}_l \otimes \mathbf{e}_l + \delta_{il} \delta_{jk} n_{k,l} \mathbf{e}_l \otimes \mathbf{e}_l = (n_{j,i} + n_{j,i}) \mathbf{e}_l \otimes \mathbf{e}_l = 2\nabla \mathbf{n}^T \\ \frac{\partial}{\partial \mathbf{n}} |(\nabla \mathbf{n}) \mathbf{n}|^2 &= \frac{\partial}{\partial \mathbf{n}} (\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{n}) \mathbf{n} = \frac{\partial}{\partial \mathbf{n}} (\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{n} = \frac{\partial}{\partial n_i} [(\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jk} n_k n_j \mathbf{e}_i \\ &= [(\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jk} \delta_{ik} n_j \mathbf{e}_i + [(\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jk} \delta_{ij} n_k \mathbf{e}_i \\ &= [(\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jl} n_j \mathbf{e}_i + [(\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jk} \delta_{ij} n_k \mathbf{e}_i \\ &= ((\nabla \mathbf{n})^T (\nabla \mathbf{n})]_{jl} n_j \mathbf{e}_i + [(\nabla \mathbf{n})^T (\nabla \mathbf{n})] \mathbf{n} \\ &= 2(\nabla \mathbf{n})^T (\nabla \mathbf{n}) \mathbf{n} \\ &= \frac{\partial}{\partial \nabla \mathbf{n}} (\nabla \mathbf{n}) \mathbf{n} \cdot (\nabla \mathbf{n}) \mathbf{n} = \frac{\partial}{\partial \nabla \mathbf{n}} (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{n} = \frac{\partial}{\partial \nabla \mathbf{n}} (\nabla \mathbf{n}) \mathbf{n} \cdot \mathbf{n} \\ &= \frac{\partial}{\partial n_{i,j}} n_{p,m} n_l n_m \mathbf{e}_i \otimes \mathbf{e}_j = \delta_{ip} \delta_{jl} n_{p,m} n_l n_m \mathbf{e}_i \otimes \mathbf{e}_j + n_{p,l} \delta_{ip} \delta_{jm} n_l n_m \mathbf{e}_i \otimes \mathbf{e}_j \\ &= n_{i,m} n_j n_m \mathbf{e}_i \otimes \mathbf{e}_j + n_{i,l} n_l n_j \mathbf{e}_i \otimes \mathbf{e}_j = \nabla \mathbf{n} (\mathbf{n} \otimes \mathbf{n}) + \nabla \mathbf{n} (\mathbf{n} \otimes \mathbf{n}) \\ &= 2\nabla \mathbf{n} (\mathbf{n} \otimes \mathbf{n}) \\ \frac{\partial}{\partial \mathbf{n}} \mathbf{n} \cdot \mathbf{A} \mathbf{n} = \frac{\partial}{\partial n_i} A_{jk} n_j n_k \mathbf{e}_i = A_{jk} \delta_{ij} n_k \mathbf{e}_i + A_{jk} \delta_{ik} n_j \mathbf{e}_i = A_{ik} n_k \mathbf{e}_i + A_{ji} n_j \mathbf{e}_i \\ &= (\mathbf{A} + \mathbf{A}^T) \mathbf{n} = 2\mathbf{A} \mathbf{n}$$
 (A = A^T). (25)

These results combined with the bulk energy density (9), gives

$$\frac{\partial f}{\partial \boldsymbol{n}} = 2(K_3 - K_2)(\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n})\boldsymbol{n}$$

$$\frac{\partial f}{\partial \nabla \boldsymbol{n}} = \left(2K_1(\nabla \cdot \boldsymbol{n})I + 2K_2\nabla \boldsymbol{n} - 2K_2\nabla \boldsymbol{n}^T + 2(K_3 - K_2)\nabla \boldsymbol{n}(\boldsymbol{n} \otimes \boldsymbol{n}) + (K_2 + K_4)(2\nabla \boldsymbol{n}^T - 2(\nabla \cdot \boldsymbol{n})\boldsymbol{I})\right)$$
(26)

Taking divergence of terms in $(26)_2$ separately, we get the following identities

$$\nabla \cdot (\nabla \cdot \boldsymbol{n} \boldsymbol{I}) = \nabla \cdot (n_{k,k} \delta_{ij} \boldsymbol{e}_i \otimes \boldsymbol{e}_j) = (n_{k,k} \delta_{ij} \boldsymbol{e}_i)_j = (n_{k,k} \boldsymbol{e}_i)_{,i} = \nabla (\nabla \cdot \boldsymbol{n})$$

$$\nabla \cdot (\nabla \boldsymbol{n}) = \nabla^2 \boldsymbol{n}$$

$$\nabla \cdot \nabla \boldsymbol{n}^T = \nabla \cdot (n_{j,i} \boldsymbol{e}_i \otimes \boldsymbol{e}_j) = (n_{j,i} \boldsymbol{e}_i)_{,j} = n_{j,ji} \boldsymbol{e}_i = \nabla (\nabla \cdot \boldsymbol{n})$$

$$\nabla \cdot \left(\nabla \boldsymbol{n} (\boldsymbol{n} \otimes \boldsymbol{n}) \right) = \nabla \cdot (n_{i,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j n_k n_l \boldsymbol{e}_k \otimes \boldsymbol{e}_l) = \nabla \cdot (n_{i,j} n_j n_l \boldsymbol{e}_i \otimes \boldsymbol{e}_l) = (n_{i,j} n_j n_l)_{,l} \boldsymbol{e}_i$$

$$= n_{i,jl} n_j n_l \boldsymbol{e}_i + n_{i,j} n_{j,l} n_l \boldsymbol{e}_i + n_{i,j} n_j n_{l,l} \boldsymbol{e}_i = (n_{i,jl} n_j + n_{i,j} n_{j,l}) n_l \boldsymbol{e}_i + n_{i,j} n_j n_{l,l} \boldsymbol{e}_i$$

$$= (n_{i,j} n_j)_{,l} \boldsymbol{e}_i + n_{i,j} n_j n_{l,l} \boldsymbol{e}_i = \nabla ((\nabla \boldsymbol{n}) \boldsymbol{n}) \boldsymbol{n} + \nabla \cdot \boldsymbol{n} (\nabla \boldsymbol{n}) \boldsymbol{n}$$
(27)

Thus, using the results (26) and (27) in (24), we obtain

$$p = \frac{\partial f}{\partial n} - \nabla \cdot \frac{\partial f}{\partial \nabla n}$$

= $2 \left\{ (K_3 - K_2) (\nabla n)^T (\nabla n) n - K_1 \nabla (\nabla \cdot n) - K_2 (\nabla^2 n - \nabla (\nabla \cdot n)) - (K_3 - K_2) (\nabla ((\nabla n) n) n + \nabla \cdot n (\nabla n) n) \right\}$
= $2 \left\{ (K_2 - K_1) \nabla (\nabla \cdot n) - K_2 \nabla^2 n + (K_3 - K_2) ((\nabla n)^T (\nabla n) n - \nabla ((\nabla n) n) n - \nabla \cdot n (\nabla n) n) \right\}$. (28)

The saddle-splay constant K_4 vanishes from the above equation and hence doesn't appear in the equilibrium equations. However, it may appear in the natural boundary conditions. Similarly, the integrand q using (24),(25) and (26) simplifies to

$$q = \frac{\partial f}{\partial \nabla n} \mathbf{N} + \frac{\partial g}{\partial n}$$

$$= \left(2K_1 (\nabla \cdot \mathbf{n}) \mathbf{I} + 2K_2 \nabla \mathbf{n} - 2K_2 \nabla \mathbf{n}^T + 2(K_3 - K_2) \nabla \mathbf{n} (\mathbf{n} \otimes \mathbf{n}) + (K_2 + K_4) (2\nabla \mathbf{n}^T - 2(\nabla \cdot \mathbf{n}) \mathbf{I}) \right) \mathbf{N} + 2\mathbf{A}\mathbf{n}$$

$$= 2 \left\{ \left(K_1 (\nabla \cdot \mathbf{n}) \mathbf{N} + K_2 \left((\nabla \mathbf{n}) - \nabla \mathbf{n}^T \right) \mathbf{N} + (K_3 - K_2) (\mathbf{n} \cdot \mathbf{N}) (\nabla \mathbf{n}) \mathbf{n} + (K_2 + K_4) \left(\nabla \mathbf{n}^T - (\nabla \cdot \mathbf{n}) \mathbf{I} \right) \mathbf{N} + \mathbf{A}\mathbf{n} \right\}$$
(29)

If n is an extremal of \mathcal{F} , then the variation $\delta \mathcal{F}$ given by (23) is zero and hence from the condition (14), we have

$$\boldsymbol{p} = 2\lambda_v \boldsymbol{n}$$
 on $\boldsymbol{\mathcal{B}}$ (30)

$$\boldsymbol{q} = 2\lambda_s \boldsymbol{n}$$
 on $\partial \mathcal{B}$, (31)

where λ_v and λ_s are Lagrange multipliers. The Lagrange multipliers appearing in the problem is due to constraint $\mathbf{n} \cdot \mathbf{n} = 1$. The equation (30) is the Euler-Lagrange equation,

$$(K_2 - K_1)\nabla(\nabla \cdot \boldsymbol{n}) - K_2\nabla^2\boldsymbol{n} + (K_3 - K_2)\left((\nabla \boldsymbol{n})^T(\nabla \boldsymbol{n})\boldsymbol{n} - \nabla((\nabla \boldsymbol{n})\boldsymbol{n})\boldsymbol{n} - \nabla \cdot \boldsymbol{n}(\nabla \boldsymbol{n})\boldsymbol{n}\right) = \lambda_v\boldsymbol{n}.$$
 (32)

For the special case of isotropy $K_1 = K_2 = K_3 = K$, the above equation simplifies to

and

$$\nabla^2 \boldsymbol{n} = -\frac{\lambda_v}{K} \boldsymbol{n},\tag{33}$$

3D Poisson's equation. The (31) is the natural boundary condition,

$$\left(K_{1}(\nabla \cdot \boldsymbol{n})\boldsymbol{N}+K_{2}\left(\nabla \boldsymbol{n}\right)-\nabla \boldsymbol{n}^{T}\right)\boldsymbol{N}+(K_{3}-K_{2})(\boldsymbol{n}\cdot\boldsymbol{N})(\nabla \boldsymbol{n})\boldsymbol{n}+(K_{2}+K_{4})\left(\nabla \boldsymbol{n}^{T}-(\nabla \cdot \boldsymbol{n})\boldsymbol{I}\right)\boldsymbol{N}+\boldsymbol{A}\boldsymbol{n}=\lambda_{s}\boldsymbol{n},$$
(34)

which for the special case of the isotropy and $K_4 = 0$, simplifies to

$$K(\nabla \boldsymbol{n})\boldsymbol{N} = (\lambda_s \boldsymbol{I} - \boldsymbol{A})\boldsymbol{n}.$$
(35)

For a uniform \boldsymbol{n} to satisfy the equations (33) and (35), the conditions required are (i) $\lambda_v = 0$ and (ii) \boldsymbol{A} has to spherical such that $\lambda_s = 1/3tr(\boldsymbol{A})$. The saddle-splay constant K_4 appears only from the boundary condition and hence instability criterion dependent on K_4 is surface driven. The condition (15) doesn't come into picture in the first variation since $\mathcal{O}(\epsilon^2)$ terms don't play any role in the first variation.

2.3 The second variation

To compute the stability of solutions given by the (32) and (34), we need to calculate the second variation of \mathcal{F} ,

$$\begin{split} \delta^{2}\mathcal{F} &= \frac{d^{2}\mathcal{F}}{d\varepsilon^{2}}\Big|_{\varepsilon=0} = \frac{d^{2}}{d\varepsilon^{2}}\mathcal{F}_{b}(\boldsymbol{n}_{\varepsilon},\nabla\boldsymbol{n}_{\varepsilon}) + \frac{d^{2}}{d\varepsilon^{2}}\mathcal{F}_{a}(\boldsymbol{n}_{\varepsilon})\Big|_{\varepsilon=0} \\ &= \frac{d^{2}}{d\varepsilon^{2}}\int_{\mathcal{B}}f(\boldsymbol{n}_{\varepsilon},\nabla\boldsymbol{n}_{\varepsilon})dV\Big|_{\varepsilon=0} + \frac{d^{2}}{d\varepsilon^{2}}\int_{\partial\mathcal{B}}g(\boldsymbol{n}_{\varepsilon})dA\Big|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon}\Big\{\frac{d}{d\varepsilon}\int_{\mathcal{B}}f(\boldsymbol{n}_{\varepsilon},\nabla\boldsymbol{n}_{\varepsilon})dV\Big\}\Big|_{\varepsilon=0} + \frac{d}{d\varepsilon}\Big\{\frac{d}{d\varepsilon}\int_{\partial\mathcal{B}}g(\boldsymbol{n}_{\varepsilon},)dA\Big\}\Big|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon}\Big\{\int_{\mathcal{B}}\frac{\partial f}{\partial\boldsymbol{n}_{\varepsilon}}\cdot\frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon} + \frac{\partial f}{\partial\boldsymbol{\nabla}\boldsymbol{n}_{\varepsilon}}:\frac{d\nabla\boldsymbol{n}_{\varepsilon}}{d\varepsilon}dV\Big\}\Big|_{\varepsilon=0} + \frac{d}{d\varepsilon}\Big\{\int_{\partial\mathcal{B}}\frac{\partial g}{\partial\boldsymbol{n}_{\varepsilon}}\cdot\frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon}dA\Big\}\Big|_{\varepsilon=0} \\ &= \frac{d}{d\varepsilon}\Big\{\int_{\mathcal{B}}\frac{\partial f}{\partial\boldsymbol{n}_{\varepsilon}}\cdot(\phi+2\varepsilon\psi) + \frac{\partial f}{\partial\boldsymbol{\nabla}\boldsymbol{n}_{\varepsilon}}:(\nabla\phi+2\varepsilon\nabla\psi)dV\Big\}\Big|_{\varepsilon=0} + \frac{d}{d\varepsilon}\Big\{\int_{\partial\mathcal{B}}\frac{\partial g}{\partial\boldsymbol{n}_{\varepsilon}}\cdot(\phi+2\varepsilon\psi)dA\Big\}\Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}}p_{1}(\boldsymbol{n},\nabla\boldsymbol{n},\phi,\nabla\phi,\psi,\nabla\psi)dV + \int_{\partial\mathcal{B}}q_{1}(\boldsymbol{n},\phi,\psi)dA, \end{split}$$

$$(36)$$

where

$$p_{1}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}, \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) = \frac{d}{d\varepsilon} \left\{ \frac{\partial f}{\partial \boldsymbol{n}_{\varepsilon}} \cdot (\boldsymbol{\phi} + 2\varepsilon \boldsymbol{\psi}) + \frac{\partial f}{\partial \nabla \boldsymbol{n}_{\varepsilon}} : (\nabla \boldsymbol{\phi} + 2\varepsilon \nabla \boldsymbol{\psi}) \right\} \bigg|_{\varepsilon=0}$$

and
$$q_{1}(\boldsymbol{n}, \boldsymbol{\phi}, \boldsymbol{\psi}) = \frac{d}{d\varepsilon} \left\{ \frac{\partial g}{\partial \boldsymbol{n}_{\varepsilon}} \cdot (\boldsymbol{\phi} + 2\varepsilon \boldsymbol{\psi}) \right\} \bigg|_{\varepsilon=0}.$$
 (37)

Expressions for p_1 and q_1 can further be simplified separately by using chain rule for differentiation and substituting extremum condition (30) and (31). The expression for p_1 becomes

$$\begin{split} p_{1}(\boldsymbol{n},\nabla\boldsymbol{n},\phi,\nabla\phi,\psi,\nabla\psi)) &= \frac{\partial^{2}f}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}}\frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon}\cdot(\phi+2\varepsilon\psi) + \frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}}:\frac{d\nabla\boldsymbol{n}_{\varepsilon}}{d\varepsilon}\cdot(\phi+2\varepsilon\psi) + 2\frac{\partial f}{\partial\boldsymbol{n}_{\varepsilon}}\cdot\psi + \\ & \frac{\partial^{2}f}{\partial\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}\frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon}:(\nabla\phi+2\varepsilon\nabla\psi) + \frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}:\frac{d\nabla\boldsymbol{n}_{\varepsilon}}{d\varepsilon}:(\nabla\phi+2\varepsilon\nabla\psi) + 2\frac{\partial f}{\partial\nabla\boldsymbol{n}_{\varepsilon}}:\nabla\psi\bigg|_{\varepsilon=0}, \\ &= \frac{\partial^{2}f}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}}:(\phi+2\varepsilon\psi)\otimes(\phi+2\varepsilon\psi) + \frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}}:(\nabla\phi+2\varepsilon\nabla\psi)\cdot(\phi+2\varepsilon\psi) + 2\frac{\partial f}{\partial\boldsymbol{n}_{\varepsilon}}\cdot\psi + \\ & \frac{\partial^{2}f}{\partial\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}(\phi+2\varepsilon\psi):(\nabla\phi+2\varepsilon\nabla\psi) + \frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}:(\nabla\phi+2\varepsilon\nabla\psi):(\nabla\phi+2\varepsilon\nabla\psi) + 2\frac{\partial f}{\partial\nabla\boldsymbol{n}_{\varepsilon}}:\nabla\psi\bigg|_{\varepsilon=0}, \\ &= \frac{\partial^{2}f}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}}:(\phi\otimes\phi+\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}}:(\nabla\phi)\cdot\phi+2\frac{\partial f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}:(\nabla\phi) + \frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}_{\varepsilon}\partial\nabla\boldsymbol{n}_{\varepsilon}}:(\nabla\phi) + 2\frac{\partial f}{\partial\nabla\boldsymbol{n}_{\varepsilon}}:\nabla\psi\bigg|_{\varepsilon=0}, \end{split}$$

$$= \frac{\partial^2 f}{\partial n \partial n} : \phi \otimes \phi + 2 \frac{\partial^2 f}{\partial \nabla n \partial n} : (\nabla \phi) \cdot \phi + 2 \frac{\partial f}{\partial n} \cdot \psi + \frac{\partial^2 f}{\partial \nabla n \partial \nabla n} : (\nabla \phi) : (\nabla \phi) + 2 \frac{\partial f}{\partial \nabla n} : \nabla \psi.$$

$$= 2 \left(\frac{\partial f}{\partial n} \cdot \psi + \frac{\partial f}{\partial \nabla n} : \nabla \psi \right) + \frac{\partial^2 f}{\partial n \partial n} : \phi \otimes \phi + 2 \frac{\partial^2 f}{\partial \nabla n \partial n} : (\nabla \phi) \cdot \phi + \frac{\partial^2 f}{\partial \nabla n \partial \nabla n} : (\nabla \phi) : (\nabla \phi) \quad (38)$$

First term in the above equation is linear in the variation ψ and is similar to the integrand of the volume integral in (21) (replacing ϕ with ψ). Therefore, it can also be simplified using the divergence relation (22). To avoid the repetition, we skip this derivation. All other terms in (38) are of quadratic order. Therefore, we can represent the above equation by separating linear and quadratic term as

$$p_1(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}, \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) = l_p(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) + Q_p(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}),$$
(39)

where

$$l_p(\boldsymbol{n},
abla \boldsymbol{n}, \boldsymbol{\psi},
abla \boldsymbol{\psi}) = 2igg(rac{\partial f}{\partial \boldsymbol{n}} \cdot \boldsymbol{\psi} + rac{\partial f}{\partial
abla \boldsymbol{n}} :
abla \boldsymbol{\psi}igg)$$

and

$$Q_p(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \frac{\partial^2 f}{\partial \boldsymbol{n} \partial \boldsymbol{n}} : \boldsymbol{\phi} \otimes \boldsymbol{\phi} + 2 \frac{\partial^2 f}{\partial \nabla \boldsymbol{n} \partial \boldsymbol{n}} : (\nabla \boldsymbol{\phi}) \cdot \boldsymbol{\phi} + \frac{\partial^2 f}{\partial \nabla \boldsymbol{n} \partial \nabla \boldsymbol{n}} : (\nabla \boldsymbol{\phi}) : (\nabla \boldsymbol{\phi}).$$
(40)

Similarly the integrand q_1 of the surface integral becomes,

$$q_{1}(\boldsymbol{n},\boldsymbol{\phi},\boldsymbol{\psi}) = \frac{\partial^{2}g}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}} \frac{d\boldsymbol{n}_{\varepsilon}}{d\varepsilon} \cdot (\boldsymbol{\phi} + 2\varepsilon\boldsymbol{\psi}) + 2\frac{\partial g}{\partial\boldsymbol{n}_{\varepsilon}} \cdot \boldsymbol{\psi} \bigg|_{\varepsilon=0}$$
$$= \frac{\partial^{2}g}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}} : (\boldsymbol{\phi} + 2\varepsilon\boldsymbol{\psi}) \otimes (\boldsymbol{\phi} + 2\varepsilon\boldsymbol{\psi}) + 2\frac{\partial g}{\partial\boldsymbol{n}_{\varepsilon}} \cdot \boldsymbol{\psi} \bigg|_{\varepsilon=0}$$
$$= \frac{\partial^{2}g}{\partial\boldsymbol{n}_{\varepsilon}\partial\boldsymbol{n}_{\varepsilon}} : \boldsymbol{\phi} \otimes \boldsymbol{\phi} + 2\frac{\partial g}{\partial\boldsymbol{n}_{\varepsilon}} \cdot \boldsymbol{\psi}, \tag{41}$$

which again when separated in linear and quadratic form becomes

$$q_1(\boldsymbol{n}, \boldsymbol{\phi}, \boldsymbol{\psi}) = l_q(\boldsymbol{n}, \boldsymbol{\psi}) + Q_q(\boldsymbol{n}, \boldsymbol{\phi}), \qquad (42)$$

where

$$l_q(\boldsymbol{n}, \boldsymbol{\psi}) = 2 \frac{\partial g}{\partial \boldsymbol{n}_{\varepsilon}} \cdot \boldsymbol{\psi} \quad \text{and} \quad Q_q(\boldsymbol{n}, \boldsymbol{\phi}) = \frac{\partial^2 g}{\partial \boldsymbol{n}_{\varepsilon} \partial \boldsymbol{n}_{\varepsilon}} : \boldsymbol{\phi} \otimes \boldsymbol{\phi}.$$
(43)

Therefore, the second variation $\delta^2 \mathcal{F}$ can now be written as

$$\delta^{2} \mathcal{F} = \int_{\mathcal{B}} l_{p}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\psi}, \nabla \boldsymbol{\psi}) dV + \int_{\partial \mathcal{B}} l_{q}(\boldsymbol{n}, \boldsymbol{\psi}) dA + \int_{\mathcal{B}} Q_{p}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV + \int_{\partial \mathcal{B}} Q_{q}(\boldsymbol{n}, \boldsymbol{\phi}) dA.$$
(44)

As mentioned earlier, the linear term in the above equation matches exactly with the first variation (21) if we replace ϕ with ψ . Therefore, following the similar procedure, we obtain

$$\delta^{2} \mathcal{F} = 2 \left\{ \int_{\mathcal{B}} \boldsymbol{p}(\boldsymbol{n}, \nabla \boldsymbol{n}) \cdot \boldsymbol{\psi} dV + \int_{\partial \mathcal{B}} \boldsymbol{q}(\boldsymbol{n}, \nabla \boldsymbol{n}) \cdot \boldsymbol{\psi} dA \right\} + \int_{\mathcal{B}} Q_{p}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV + \int_{\partial \mathcal{B}} Q_{q}(\boldsymbol{n}, \boldsymbol{\phi}) dA.$$
(45)

Note that the factor of 2 is missing in [Rosso et al., 2004]. Also, the quadratic term Q_q in [Rosso et al., 2004] depends on $\nabla \phi$ and ∇n , which can be achieved by using divergence theorem in the third term of the equation. The exact expressions for p and q are given in (28) and (29). Also, since the second variation is calculated on the extremals, we can substitute (30) and (31) in the above equation to get

$$\delta^{2}\mathcal{F} = 4\left\{\int_{\mathcal{B}}\lambda_{v}\boldsymbol{n}\cdot\boldsymbol{\psi}dV + \int_{\partial\mathcal{B}}\lambda_{s}\boldsymbol{n}\cdot\boldsymbol{\psi}dA\right\} + \int_{\mathcal{B}}Q_{p}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi})dV + \int_{\partial\mathcal{B}}Q_{q}(\boldsymbol{n},\boldsymbol{\phi})dA.$$
 (46)

which on the application of constraint (15), becomes

$$\delta^{2}\mathcal{F} = -2\left\{\int_{\mathcal{B}}\lambda_{v}|\boldsymbol{\phi}|^{2}dV + \int_{\partial\mathcal{B}}\lambda_{s}|\boldsymbol{\phi}|^{2}dA\right\} + \int_{\mathcal{B}}Q_{p}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi})dV + \int_{\partial\mathcal{B}}Q_{q}(\boldsymbol{n},\boldsymbol{\phi})dA.$$
(47)

The term inside the curly braces is negative if both the Lagrange multipliers are negative and hence the first term will be positive. However, to compute the sign of $\delta^2 \mathcal{F}$, we still need to resolve the sign of quadratic terms. Also, note that the quadratic terms Q_p and Q_q does not depend on the second variation ψ of n and hence the second variation of \mathcal{F} can be expressed in the term of ϕ only. The use of divergence identity (22) in the expression for Q_p , (40), gives

$$Q_{p}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi}) = \frac{\partial^{2}f}{\partial\boldsymbol{n}\partial\boldsymbol{n}}:\boldsymbol{\phi}\otimes\boldsymbol{\phi} + 2\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}\partial\boldsymbol{n}}:(\nabla\boldsymbol{\phi})\cdot\boldsymbol{\phi} + \nabla\cdot\left\{\left(\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}\partial\nabla\boldsymbol{n}}:(\nabla\boldsymbol{\phi})\right)^{T}\boldsymbol{\phi}\right\} - \boldsymbol{\phi}\cdot\nabla\cdot\left(\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}\partial\nabla\boldsymbol{n}}:(\nabla\boldsymbol{\phi})\right).$$
(48)

By using the divergence theorem in the quadratic part of $\delta^2 \mathcal{F}$, we get

$$\int_{\mathcal{B}} Q_p(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV + \int_{\partial \mathcal{B}} Q_q(\boldsymbol{n}, \boldsymbol{\phi}) dA = \int_{\mathcal{B}} Q_b(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV + \int_{\partial \mathcal{B}} Q_a(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dA, \quad (49)$$

where

$$Q_{b}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi}) = \frac{\partial^{2}f}{\partial\boldsymbol{n}\partial\boldsymbol{n}}:\boldsymbol{\phi}\otimes\boldsymbol{\phi} + \boldsymbol{\phi}\cdot\left\{2\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}\partial\boldsymbol{n}}:(\nabla\boldsymbol{\phi}) - \nabla\cdot\left(\frac{\partial^{2}f}{\partial\nabla\boldsymbol{n}\partial\nabla\boldsymbol{n}}:(\nabla\boldsymbol{\phi})\right)\right\}$$

and

$$Q_a(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \frac{\partial^2 g}{\partial \boldsymbol{n} \partial \boldsymbol{n}} : \boldsymbol{\phi} \otimes \boldsymbol{\phi} + \left\{ \left(\frac{\partial^2 f}{\partial \nabla \boldsymbol{n} \partial \nabla \boldsymbol{n}} : (\nabla \boldsymbol{\phi}) \right) \boldsymbol{N} \right\} \cdot \boldsymbol{\phi}.$$
(50)

Lets first look at the quadratic term Q_b of the volume integral. We will require the results of the (25)-(27) for simplification. From the first equation in (26), we have

$$\frac{\partial f}{\partial \boldsymbol{n}} = 2(K_3 - K_2)(\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n}) \boldsymbol{n}$$
(51)

Differentiating w.r.t \boldsymbol{n} , we get

$$\frac{\partial^2 f}{\partial \boldsymbol{n} \partial \boldsymbol{n}} = 2(K_3 - K_2) \frac{\partial}{\partial \boldsymbol{n}} (\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n}) \boldsymbol{n}.$$
(52)

Again using (51) and differentiating w.r.t to ∇n , we obtain

$$\frac{\partial^2 f}{\partial \nabla \boldsymbol{n} \partial \boldsymbol{n}} = 2(K_3 - K_2) \frac{\partial}{\partial \nabla \boldsymbol{n}} (\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n}) \boldsymbol{n}$$
(53)

Similarly, from the second equation in the (26), we have

$$\frac{\partial f}{\partial \nabla \boldsymbol{n}} = \left(2K_1 (\nabla \cdot \boldsymbol{n}) \boldsymbol{I} + 2K_2 \nabla \boldsymbol{n} - 2K_2 \nabla \boldsymbol{n}^T + 2(K_3 - K_2) \nabla \boldsymbol{n} (\boldsymbol{n} \otimes \boldsymbol{n}) + (K_2 + K_4) (2\nabla \boldsymbol{n}^T - 2(\nabla \cdot \boldsymbol{n}) \boldsymbol{I}) \right),$$
(54)

Differentiating the above expression with respect to ∇n , we get

$$\frac{\partial^2 f}{\partial \nabla \boldsymbol{n} \partial \nabla \boldsymbol{n}} = 2K_1 \frac{\partial}{\partial \nabla \boldsymbol{n}} (\nabla \cdot \boldsymbol{n}) \boldsymbol{I} + 2K_2 \frac{\partial}{\partial \nabla \boldsymbol{n}} \nabla \boldsymbol{n} - 2K_2 \frac{\partial}{\partial \nabla \boldsymbol{n}} \nabla \boldsymbol{n}^T + 2(K_3 - K_2) \frac{\partial}{\partial \nabla \boldsymbol{n}} \nabla \boldsymbol{n} (\boldsymbol{n} \otimes \boldsymbol{n}) + (K_2 + K_4) \left(2 \frac{\partial}{\partial \nabla \boldsymbol{n}} \nabla \boldsymbol{n}^T - 2 \frac{\partial}{\partial \nabla \boldsymbol{n}} (\nabla \cdot \boldsymbol{n}) \boldsymbol{I} \right).$$
(55)

Each term in the above equations can be simplified as shown below

$$\frac{\partial}{\partial n} (\nabla n)^{T} (\nabla n) n = \frac{\partial}{\partial n_{i}} (n_{k,j} n_{k,l} n_{l} e_{j}) \otimes e_{i} = n_{k,j} n_{k,l} \delta_{li} e_{j} \otimes e_{i} = n_{k,j} n_{k,l} e_{j} \otimes e_{l} = (\nabla n)^{T} (\nabla n)$$

$$\frac{\partial}{\partial \nabla n} (\nabla n)^{T} (\nabla n) n = \frac{\partial}{\partial n_{i,m}} (n_{k,j} n_{k,l} n_{l} e_{j}) \otimes e_{i} \otimes e_{m} = (\delta_{ik} \delta_{jm} n_{k,l} n_{l} + n_{k,j} \delta_{ik} \delta_{lm} n_{l}) e_{j} \otimes e_{i} \otimes e_{m}$$

$$= n_{i,l} n_{l} e_{j} \otimes e_{i} \otimes e_{j} + n_{i,j} n_{l} e_{j} \otimes e_{i} \otimes e_{l}$$

$$\frac{\partial}{\partial \nabla n} \nabla \cdot n I = \frac{\partial}{\partial n_{i,j}} (n_{k,k} e_{l} \otimes e_{l}) \otimes e_{i} \otimes e_{j} = \delta_{ik} \delta_{jk} e_{l} \otimes e_{l} \otimes e_{j} = e_{i} \otimes e_{j} \otimes e_{j} \otimes e_{j}$$

$$\frac{\partial}{\partial \nabla n} \nabla n = \frac{\partial}{\partial n_{i,j}} n_{k,l} e_{k} \otimes e_{l} \otimes e_{i} \otimes e_{j} = \delta_{ik} \delta_{jl} e_{k} \otimes e_{l} \otimes e_{j} = e_{i} \otimes e_{j} \otimes e_{i} \otimes e_{j}$$

$$\frac{\partial}{\partial \nabla n} \nabla n^{T} = \frac{\partial}{\partial n_{i,j}} n_{l,k} e_{k} \otimes e_{l} \otimes e_{i} \otimes e_{j} = \delta_{il} \delta_{jk} e_{k} \otimes e_{l} \otimes e_{j} = e_{j} \otimes e_{i} \otimes e_{j}$$

$$\frac{\partial}{\partial \nabla n} \nabla n^{T} = \frac{\partial}{\partial n_{i,j}} n_{l,k} e_{k} \otimes e_{l} \otimes e_{i} \otimes e_{j} = \delta_{il} \delta_{jk} e_{l} \otimes e_{l} \otimes e_{j} = e_{j} \otimes e_{i} \otimes e_{j} \otimes e_{j}$$

$$\frac{\partial}{\partial \nabla n} \nabla n^{T} = \frac{\partial}{\partial n_{i,j}} n_{l,k} e_{k} \otimes e_{l} \otimes e_{j} = \delta_{il} \delta_{jk} e_{l} \otimes e_{l} \otimes e_{j} = e_{j} \otimes e_{i} \otimes e_{j}$$

$$\frac{\partial}{\partial \nabla n} \nabla n(n \otimes n) = \frac{\partial}{\partial n_{i,j}} (n_{k,l} n_{l} n_{m}) e_{k} \otimes e_{m} \otimes e_{j} \otimes e_{j} = \delta_{ik} \delta_{jl} n_{l} n_{m} e_{k} \otimes e_{m} \otimes e_{j} \otimes e_{j} \otimes e_{j} \otimes e_{j} \otimes e_{j} \otimes e_{j} \otimes e_{j}$$

$$= n_{j} n_{m} e_{i} \otimes e_{m} \otimes e_{j} \otimes e_{j}.$$
(56)

By substituting the results of (56) in (52), (53) and (55), we obtain

$$\frac{\partial^2 f}{\partial n \partial n} = 2(K_3 - K_2)(\nabla n)^T (\nabla n)$$

$$\frac{\partial^2 f}{\partial \nabla n \partial n} = 2(K_3 - K_2)(n_{i,l}n_l e_j \otimes e_i \otimes e_j + n_{i,j}n_l e_j \otimes e_i \otimes e_l)$$

$$\frac{\partial^2 f}{\partial \nabla n \partial \nabla n} = 2K_1 e_i \otimes e_i \otimes e_j \otimes e_j + 2K_2 e_i \otimes e_j \otimes e_i \otimes e_j - 2K_2 e_j \otimes e_i \otimes e_i \otimes e_j + 2(K_3 - K_2)n_j n_m e_i \otimes e_m \otimes e_i \otimes e_j + 2(K_2 + K_4)(e_j \otimes e_i \otimes e_i \otimes e_j - e_i \otimes e_i \otimes e_j \otimes e_j). \quad (57)$$

Finally substituting these second order derivatives of f in $(50)_1$, we get the quadratic function Q_b as

$$Q_{b}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi}) = 2(K_{3}-K_{2})\left\{ (\nabla\boldsymbol{n})^{T}(\nabla\boldsymbol{n}):\boldsymbol{\phi}\otimes\boldsymbol{\phi} + 2(n_{i,l}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j} + n_{i,j}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{l}):(\nabla\boldsymbol{\phi})\cdot\boldsymbol{\phi}\right\}$$
$$-2\nabla\cdot\left\{ \left(K_{1}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j} + K_{2}(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j} - \boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}) + (K_{3}-K_{2})n_{j}n_{m}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{m}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j} + (K_{2}+K_{4})(\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j} - \boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j})\right):\nabla\boldsymbol{\phi}\right\}\cdot\boldsymbol{\phi}$$

$$(58)$$

The expression of Q_b includes fourth order tensors. They are separately evaluated below

$$(\nabla \boldsymbol{n})^T (\nabla \boldsymbol{n}) : \boldsymbol{\phi} \otimes \boldsymbol{\phi} = n_{k,i} n_{k,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j : \phi_l \phi_m \boldsymbol{e}_l \otimes \boldsymbol{e}_m = n_{k,i} n_{k,j} \phi_l \phi_m \delta_{il} \delta_{jm} = n_{k,i} n_{k,j} \phi_i \phi_j$$
$$= n_{k,i} \phi_i n_{k,j} \phi_j = (\nabla \boldsymbol{n}) \boldsymbol{\phi} \cdot (\nabla \boldsymbol{n}) \boldsymbol{\phi} = |(\nabla \boldsymbol{n}) \boldsymbol{\phi}|^2,$$

$$\begin{aligned} (n_{i,l}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}+n_{i,j}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{l}):(\nabla\phi)\cdot\phi &=(n_{i,l}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}+n_{i,j}n_{l}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{l}):\phi_{m,p}\boldsymbol{e}_{m}\otimes\boldsymbol{e}_{p}\cdot\phi \\ &=(\phi_{i,j}n_{i,l}n_{l}+\phi_{i,l}n_{i,j}n_{l})\boldsymbol{e}_{j}\cdot\phi \\ &=\left((\nabla\phi)^{T}(\nabla\boldsymbol{n})\boldsymbol{n}+(\nabla\boldsymbol{n})^{T}(\nabla\phi)\boldsymbol{n}\right)\cdot\phi \\ &=(\nabla\boldsymbol{n})\boldsymbol{n}\cdot(\nabla\phi)\phi+(\nabla\phi)\boldsymbol{n}\cdot(\nabla\boldsymbol{n})\phi \end{aligned}$$

$$\nabla\cdot\left((\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j}):\nabla\phi\right)\cdot\phi = \nabla\cdot\left((\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j}):\phi_{k,l}\boldsymbol{e}_{k}\otimes\boldsymbol{e}_{l}\right)\cdot\phi \\ &=\nabla\cdot\left(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\phi_{k,k}\right)\cdot\phi =\phi_{k,ki}\phi_{i}=(\phi_{k,k}\phi_{i})_{i}-\phi_{k,k}\phi_{i,i}=\nabla\cdot\left((\nabla\cdot\phi)\phi\right)-(\nabla\cdot\phi)^{2} \end{aligned}$$

$$\nabla \cdot \left\{ (\boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} - \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j}) : \nabla \phi \right\} \cdot \phi$$

$$= \nabla \cdot \left\{ (\boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} - \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j}) : \phi_{k,l} \boldsymbol{e}_{k} \otimes \boldsymbol{e}_{l} \right\} \cdot \phi$$

$$= \nabla \cdot (\phi_{k,l} \boldsymbol{e}_{k} \otimes \boldsymbol{e}_{l} - \phi_{l,k} \boldsymbol{e}_{k} \otimes \boldsymbol{e}_{l}) \cdot \phi = \phi_{k,ll} \phi_{k} - \phi_{l,kl} \phi_{k}$$

$$= (\phi_{k,l} \phi_{k})_{,l} - \phi_{k,l} \phi_{k,l} - (\phi_{l,k} \phi_{k})_{,l} + \phi_{l,k} \phi_{k,l}$$

$$= \nabla \cdot \left((\nabla \phi)^{T} \phi - (\nabla \phi) \phi \right) - |\nabla \phi|^{2} + tr \left((\nabla \phi)^{2} \right)$$

$$\nabla \cdot (n_j n_m \boldsymbol{e}_i \otimes \boldsymbol{e}_m \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j : \nabla \boldsymbol{\phi}) \cdot \boldsymbol{\phi} = \nabla \cdot (n_j n_m \boldsymbol{e}_i \otimes \boldsymbol{e}_m \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_j : \boldsymbol{\phi}_{k,l} \boldsymbol{e}_k \otimes \boldsymbol{e}_l) \cdot \boldsymbol{\phi}$$
$$= \nabla \cdot (n_j n_m \phi_{i,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_m) \cdot \boldsymbol{\phi} = (n_j n_m \phi_{i,j})_m \phi_i$$
$$= (n_j n_m \phi_{i,j} \phi_i)_m - (n_j n_m \phi_{i,j} \phi_{i,m})$$
$$= \nabla \cdot \left((\nabla \boldsymbol{\phi}) \boldsymbol{n} \cdot \boldsymbol{\phi} \boldsymbol{n} \right) - (\nabla \boldsymbol{\phi}) \boldsymbol{n} \cdot (\nabla \boldsymbol{\phi}) \boldsymbol{n}$$

$$\nabla \cdot \left\{ \left(\boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} - \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{j} \right) \right\} : \nabla \boldsymbol{\phi} \right\} \cdot \boldsymbol{\phi}$$

$$= \nabla \cdot \left\{ \left(\boldsymbol{e}_{j} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} - \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{j} \otimes \boldsymbol{e}_{j} \right) \right\} : \phi_{k,l} \boldsymbol{e}_{k} \otimes \boldsymbol{e}_{l} \right\} \cdot \boldsymbol{\phi}$$

$$= \nabla \cdot \left\{ \left(\phi_{k,l} \boldsymbol{e}_{l} \otimes \boldsymbol{e}_{k} - \phi_{k,k} \boldsymbol{e}_{i} \otimes \boldsymbol{e}_{i} \right) \right\} \cdot \boldsymbol{\phi} = \phi_{k,lk} \phi_{l} - \phi_{k,ki} \phi_{i} = 0$$
(59)

Substituting the above calculations in (58), we obtain the final form of the quadratic term Q_b as

$$Q_{b}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi}) = 2(K_{3}-K_{2})\left\{ |(\nabla\boldsymbol{n})\boldsymbol{\phi}|^{2} + 2(\nabla\boldsymbol{n})\boldsymbol{n}\cdot(\nabla\boldsymbol{\phi})\boldsymbol{\phi} + 2(\nabla\boldsymbol{\phi})\boldsymbol{n}\cdot(\nabla\boldsymbol{n})\boldsymbol{\phi} - \nabla\cdot\left((\nabla\boldsymbol{\phi})\boldsymbol{n}\cdot\boldsymbol{\phi}\boldsymbol{n}\right) + (\nabla\boldsymbol{\phi})\boldsymbol{n}\cdot(\nabla\boldsymbol{\phi})\boldsymbol{n}\right\} - 2\left\{ K_{1}\left(\nabla\cdot\left((\nabla\cdot\boldsymbol{\phi})\boldsymbol{\phi}\right) - (\nabla\cdot\boldsymbol{\phi})^{2}\right) + K_{2}\left(\nabla\cdot\left((\nabla\boldsymbol{\phi})^{T}\boldsymbol{\phi} - (\nabla\boldsymbol{\phi})\boldsymbol{\phi}\right) - |\nabla\boldsymbol{\phi}|^{2} + tr\left((\nabla\boldsymbol{\phi})^{2}\right)\right)\right\}$$

$$(60)$$

The second variation as written in (47) consists of two quadratic terms one due to volume integral and other one due to surface integral. These quadratic terms are rearranged in (49) using divergence theorem. The volume integral in (49) on substitution of above expression becomes

$$Q_{1} = \int_{\mathcal{B}} Q_{b}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV$$

$$= 2 \int_{\mathcal{B}} K_{1}(\nabla \cdot \boldsymbol{\phi})^{2} + K_{2} \left\{ |\nabla \boldsymbol{\phi}|^{2} - tr\left((\nabla \boldsymbol{\phi})^{2}\right) \right\} + (K_{3} - K_{2}) \left\{ |(\nabla \boldsymbol{n})\boldsymbol{\phi}|^{2} + 2(\nabla \boldsymbol{n})\boldsymbol{n} \cdot (\nabla \boldsymbol{\phi})\boldsymbol{\phi} + 2(\nabla \boldsymbol{\phi})\boldsymbol{n} \cdot (\nabla \boldsymbol{n})\boldsymbol{\phi} + |(\nabla \boldsymbol{\phi})\boldsymbol{n}|^{2} \right\} - \nabla \cdot \left\{ (K_{3} - K_{2}) \left((\nabla \boldsymbol{\phi})\boldsymbol{n} \cdot \boldsymbol{\phi}\boldsymbol{n} \right) + K_{1} \left((\nabla \cdot \boldsymbol{\phi})\boldsymbol{\phi} \right) + K_{2} \left((\nabla \boldsymbol{\phi})^{T} \boldsymbol{\phi} - (\nabla \boldsymbol{\phi})\boldsymbol{\phi} \right) \right\} dV$$

$$(61)$$

which on using the divergence relation simplifies to

$$= 2 \int_{\mathcal{B}} K_1 (\nabla \cdot \phi)^2 + K_2 \left\{ |\nabla \phi|^2 - tr \left((\nabla \phi)^2 \right) \right\} + (K_3 - K_2) \left\{ 2(\nabla n) n \cdot (\nabla \phi) \phi + |(\nabla \phi) n + (\nabla n) \phi|^2 \right\} dV$$

$$- 2 \int_{\partial \mathcal{B}} \left\{ (K_3 - K_2) \left((\nabla \phi) n \cdot \phi (n \cdot N) \right) + K_1 (\nabla \cdot \phi) (\phi \cdot N) - K_2 \left((\nabla \phi)^T \phi \cdot N + (\nabla \phi) \phi \cdot N \right) \right\} dA \quad (62)$$

Similarly the second quadratic term Q_a in the second variation can be simplified. Using the last result of (25), we calculate

$$\frac{\partial^2 g}{\partial \boldsymbol{n} \partial \boldsymbol{n}} = 2 \frac{\partial}{\partial \boldsymbol{n}} (\boldsymbol{A} \boldsymbol{n}) = 2\boldsymbol{A}, \tag{63}$$

which along with (57) when substituted in (50) gives

$$Q_{a}(\boldsymbol{n},\nabla\boldsymbol{n},\boldsymbol{\phi},\nabla\boldsymbol{\phi}) = 2\boldsymbol{A}\boldsymbol{\phi}\cdot\boldsymbol{\phi} + \left\{ \left(2K_{1}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j}+2K_{2}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}-2K_{2}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}+2(K_{3}-K_{2})n_{j}n_{m}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{m}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}+2(K_{2}+K_{4})(\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}-\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j})\right):\left(\nabla\boldsymbol{\phi}\right)\boldsymbol{N}\right\}\cdot\boldsymbol{\phi}$$

$$(64)$$

Simplifying the terms of the above equation separately we get,

$$\left(\left(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j}\right):\nabla\phi\right)\boldsymbol{N}\cdot\phi=\phi_{j,j}(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i})\boldsymbol{N}\cdot\phi=(\nabla\cdot\phi)(\boldsymbol{N}\cdot\phi)$$

$$\left(\left(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}-2K_{2}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\right):\nabla\phi\right)\boldsymbol{N}\cdot\phi=\phi_{i,j}(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j})\boldsymbol{N}\cdot\phi-\phi_{i,j}(\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i})\boldsymbol{N}\cdot\phi$$

$$=(\nabla\phi)\boldsymbol{N}\cdot\phi-(\nabla\phi)^{T}\boldsymbol{N}\cdot\phi=(\nabla\phi)^{T}\phi\cdot\boldsymbol{N}-(\nabla\phi)\phi\cdot\boldsymbol{N}$$

$$\left(n_{j}n_{m}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{m}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}:\nabla\phi\right)\boldsymbol{N}\cdot\phi=\phi_{i,j}n_{j}n_{m}(\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{m})\boldsymbol{N}\cdot\phi=\phi_{i,j}n_{j}n_{m}N_{m}(\boldsymbol{e}_{i}\cdot\phi)$$

$$=(\nabla\phi)\boldsymbol{n}\cdot\phi(\boldsymbol{n}\cdot\boldsymbol{N})$$

$$\left(\left(\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}-\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{j}\right):\nabla\phi\right)\boldsymbol{N}\cdot\phi=\left(\phi_{i,j}\boldsymbol{e}_{j}\otimes\boldsymbol{e}_{i}-\phi_{j,j}\boldsymbol{e}_{i}\otimes\boldsymbol{e}_{i}\right)\boldsymbol{N}\cdot\phi$$

$$=(\nabla\phi)^{T}\boldsymbol{N}\cdot\phi-(\nabla\cdot\phi)\boldsymbol{N}\cdot\phi=\left((\nabla\phi)\phi-(\nabla\cdot\phi)\phi\right)\cdot\boldsymbol{N}$$

$$(65)$$

Substituting, the above results in (64) we get the final form of Q_a . Using this expression in the surface integral of quadratic part of second variation (49), we get

$$Q_{2} = \int_{\partial \mathcal{B}} Q_{a}(\boldsymbol{n}, \nabla \boldsymbol{n}, \boldsymbol{\phi}, \nabla \boldsymbol{\phi}) dV$$

= $2 \int_{\partial \mathcal{B}} \boldsymbol{A} \boldsymbol{\phi} \cdot \boldsymbol{\phi} + (K_{3} - K_{2}) \left((\nabla \boldsymbol{\phi}) \boldsymbol{n} \cdot \boldsymbol{\phi} (\boldsymbol{n} \cdot \boldsymbol{N}) \right) + K_{1} (\nabla \cdot \boldsymbol{\phi}) (\boldsymbol{\phi} \cdot \boldsymbol{N}) - K_{2} \left((\nabla \boldsymbol{\phi})^{T} \boldsymbol{\phi} \cdot \boldsymbol{N} + (\nabla \boldsymbol{\phi}) \boldsymbol{\phi} \cdot \boldsymbol{N} \right)$
+ $(K_{2} + K_{4}) \left((\nabla \boldsymbol{\phi}) \boldsymbol{\phi} - (\nabla \cdot \boldsymbol{\phi}) \boldsymbol{\phi} \right) \cdot \boldsymbol{N} dA$ (66)

Adding (62) and (66) gives us the quadratic part of the second variation

$$Q = Q_1 + Q_2 = 2 \int_{\mathcal{B}} K_1 (\nabla \cdot \phi)^2 + K_2 \left\{ |\nabla \phi|^2 - tr \left((\nabla \phi)^2 \right) \right\} + (K_3 - K_2) \left\{ 2(\nabla n) n \cdot (\nabla \phi) \phi + |(\nabla \phi) n + (\nabla n) \phi|^2 \right\} dV + 2 \int_{\partial \mathcal{B}} (K_2 + K_4) \left((\nabla \phi) \phi - (\nabla \cdot \phi) \phi \right) \cdot \mathbf{N} + \mathbf{A} \phi \cdot \phi dA$$
(67)

Adding the linear part to it as in (47), we get the second variation of \mathcal{F}

$$\delta^{2} \mathcal{F} = G = 2 \int_{\mathcal{B}} K_{1} (\nabla \cdot \phi)^{2} + K_{2} \left\{ |\nabla \phi|^{2} - tr \left((\nabla \phi)^{2} \right) \right\} + (K_{3} - K_{2}) \left\{ 2(\nabla n)n \cdot (\nabla \phi)\phi + |(\nabla \phi)n + (\nabla n)\phi|^{2} \right\} - \lambda_{v} |\phi^{2}| dV + 2 \int_{\partial \mathcal{B}} (K_{2} + K_{4}) \left((\nabla \phi)\phi - (\nabla \cdot \phi)\phi \right) \cdot \mathbf{N} + \mathbf{A}\phi \cdot \phi - \lambda_{s} |\phi|^{2} dA$$

$$(68)$$

The expression for G matches with that of [Rosso et al., 2004] except for the factor of 2. For the equilibrium configuration to be stable the sufficient condition is that the second variation $\delta^2 \mathcal{F}$ or equivalently G is positive subject to the constriant (14). Hence, the minimum value of G should be positive for all ϕ . The problem can now be posed in the form of finding ϕ for which the G has the minima. Hence, we will be required to find the first variation of G.

2.4 The first variation of G

Using the classical reasoning [Courant and Hilbert, 1989], we will minimze G on a unit sphere

$$\int_{\mathcal{B}} |\phi|^2 dV = 1. \tag{69}$$

This variational problem is known as secondary variational problem. The constraint functional for this problem can be written as

$$\tilde{G}(\boldsymbol{\phi}) = G(\boldsymbol{\phi}) - \mu \int_{\mathcal{B}} |\boldsymbol{\phi}|^2 dV,$$
(70)

where μ is the Lagrange multiplier. For finding the first variation of \tilde{G} , we will follow the same procedure as discussed in Sec. 2.2. Replacing \boldsymbol{n} by $\boldsymbol{\phi}$ and introducing only the first variation of $\boldsymbol{\phi}$, we get

$$\boldsymbol{\phi}_{\varepsilon} := \boldsymbol{\phi} + \varepsilon \boldsymbol{\zeta} \tag{71}$$

The first variation of the functional \tilde{G} can be calculated as,

$$\delta \tilde{G} = \frac{d}{d\varepsilon} \tilde{G}(\phi_{\varepsilon}, \nabla \phi_{\varepsilon}) \bigg|_{\varepsilon=0} = \frac{d}{d\varepsilon} \int_{B} \tilde{f}(\phi_{\varepsilon}, \nabla \phi_{\varepsilon}) dV \bigg|_{\varepsilon=0} + \frac{d}{d\varepsilon} \int_{\partial \mathcal{B}} \tilde{g}(\phi_{\varepsilon}, \nabla \phi_{\varepsilon}) dA \bigg|_{\varepsilon=0}$$

where

$$\tilde{f}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = 2 \left\{ K_1 (\nabla \cdot \boldsymbol{\phi})^2 + K_2 \left\{ |\nabla \boldsymbol{\phi}|^2 - tr \left((\nabla \boldsymbol{\phi})^2 \right) \right\} + (K_3 - K_2) \left\{ 2 (\nabla \boldsymbol{n}) \boldsymbol{n} \cdot (\nabla \boldsymbol{\phi}) \boldsymbol{\phi} + |(\nabla \boldsymbol{\phi}) \boldsymbol{n} + (\nabla \boldsymbol{n}) \boldsymbol{\phi}|^2 \right\} - \lambda_v |\boldsymbol{\phi}|^2 \right\} - \lambda_v |\boldsymbol{\phi}|^2$$

and

$$\tilde{g}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = 2 \left\{ (K_2 + K_4) \left((\nabla \boldsymbol{\phi}) \boldsymbol{\phi} - (\nabla \cdot \boldsymbol{\phi}) \boldsymbol{\phi} \right) \cdot \boldsymbol{N} + \boldsymbol{A} \boldsymbol{\phi} \cdot \boldsymbol{\phi} - \lambda_s |\boldsymbol{\phi}|^2 \right\}.$$
(72)

Unlike the case of \mathcal{F} , where the surface integral depends only on n, the surface integral in G also depends on $\nabla \phi$. However, the following observation can eliminate the dependence of \tilde{g} on $\nabla \phi$

$$\int_{\partial \mathcal{B}} \left((\nabla \phi)\phi - (\nabla \cdot \phi)\phi \right) \cdot \mathbf{N} dA = \int_{\mathcal{B}} \nabla \cdot \left((\nabla \phi)\phi - (\nabla \cdot \phi)\phi \right) dV$$
$$= \int_{\mathcal{B}} \nabla \cdot \left((\nabla \phi)\phi \right) - \nabla \cdot \left((\nabla \cdot \phi)\phi \right) dV$$

$$= \int_{\mathcal{B}} (\phi_{i,j}\phi_j)_{,i} - (\phi_{i,i}\phi_j)_{,j} dV$$

$$= \int_{\mathcal{B}} \phi_{i,ji}\phi_j + \phi_{i,j}\phi_{j,i}, i - \phi_{i,ij}\phi_j - \phi_{i,i}\phi_{j,j}) dV$$

$$= \int_{\mathcal{B}} tr \left((\nabla\phi)^2 \right) - \left(\nabla \cdot \phi \right)^2 dV.$$
(73)

Therefore, we can rewrite $\delta \tilde{G}$ as

$$\delta \tilde{G} = \frac{d}{d\varepsilon} \int_{B} \tilde{f}(\boldsymbol{\phi}_{\varepsilon}, \nabla \boldsymbol{\phi}_{\varepsilon}) dV \bigg|_{\varepsilon=0} + \frac{d}{d\varepsilon} \int_{\partial \mathcal{B}} \tilde{g}(\boldsymbol{\phi}_{\varepsilon}) dA \bigg|_{\varepsilon=0}$$

where

$$\tilde{f}(\phi,\nabla\phi) = 2\left\{K_1(\nabla\cdot\phi)^2 + K_2\left\{|\nabla\phi|^2 - tr\left((\nabla\phi)^2\right)\right\} + (K_3 - K_2)\left\{2(\nabla n)n\cdot(\nabla\phi)\phi + |(\nabla\phi)n + (\nabla n)\phi|^2\right\} - \lambda_v|\phi|^2 + (K_2 + K_4)\left(tr((\nabla\phi)^2) - (\nabla\cdot\phi)^2\right)\right\} - \mu|\phi|^2$$

and

$$\tilde{g}(\boldsymbol{\phi}) = 2 \left\{ \boldsymbol{A}\boldsymbol{\phi} \cdot \boldsymbol{\phi} - \lambda_s |\boldsymbol{\phi}|^2 \right\}.$$
(74)

Following the procedure discussed in 2.2, we find

$$\begin{split} \delta \tilde{G} &= \frac{d}{d\varepsilon} \int_{B} \tilde{f}(\phi_{\varepsilon}, \nabla \phi_{\varepsilon}) dV \Big|_{\varepsilon=0} + \frac{d}{d\varepsilon} \int_{\partial \mathcal{B}} \tilde{g}(\phi_{\varepsilon}) dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial \tilde{f}}{\partial \phi_{\varepsilon}} \cdot \frac{d\phi_{\varepsilon}}{d\varepsilon} + \frac{\partial \tilde{f}}{\partial \nabla \phi_{\varepsilon}} : \frac{d\nabla \phi_{\varepsilon}}{d\varepsilon} dV \Big|_{\varepsilon=0} + \int_{\partial \mathcal{B}} \frac{\partial \tilde{g}}{\partial \phi_{\varepsilon}} \cdot \frac{d\phi_{\varepsilon}}{d\varepsilon} dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial \tilde{f}}{\partial \phi_{\varepsilon}} \cdot \zeta + \frac{\partial \tilde{f}}{\partial \nabla \phi_{\varepsilon}} : \nabla \zeta dV \Big|_{\varepsilon=0} + \int_{\partial \mathcal{B}} \frac{\partial \tilde{g}}{\partial \phi_{\varepsilon}} \cdot \zeta + \frac{\partial \tilde{g}}{\partial \nabla \phi_{\varepsilon}} : \nabla \zeta dA \Big|_{\varepsilon=0} \\ &= \int_{\mathcal{B}} \frac{\partial \tilde{f}}{\partial \phi} \cdot \zeta + \frac{\partial \tilde{f}}{\partial \nabla \phi} : \nabla \zeta dV + \int_{\partial \mathcal{B}} \frac{\partial \tilde{g}}{\partial \phi} \cdot \zeta dA, \end{split}$$
(75)

which on the use of divergence relation in (21) yields

$$\begin{split} \delta \tilde{G} &= \int_{\mathcal{B}} \frac{\partial \tilde{f}}{\partial \phi} \cdot \boldsymbol{\zeta} + \nabla \cdot \left(\frac{\partial \tilde{f}}{\partial \nabla \phi}^{T} \boldsymbol{\zeta} \right) - \boldsymbol{\zeta} \cdot \nabla \cdot \frac{\partial \tilde{f}}{\partial \nabla \phi} dV \int_{\partial \mathcal{B}} \frac{\partial \tilde{g}}{\partial \phi} \cdot \boldsymbol{\zeta} dA \\ &= \int_{\mathcal{B}} \left(\frac{\partial \tilde{f}}{\partial \phi} - \nabla \cdot \frac{\partial \tilde{f}}{\partial \nabla \phi} \right) \cdot \boldsymbol{\zeta} + \nabla \cdot \left(\frac{\partial \tilde{f}}{\partial \nabla n}^{T} \boldsymbol{\zeta} \right) dV + \int_{\partial \mathcal{B}} \frac{\partial \tilde{g}}{\partial \phi} \cdot \boldsymbol{\zeta} dA \end{split}$$

and finally using the divergence theorem, the above equation can be written in two parts as

$$\delta \tilde{G} = \int_{\mathcal{B}} \left(\frac{\partial \tilde{f}}{\partial \phi} - \nabla \cdot \frac{\partial \tilde{f}}{\partial \nabla \phi} \right) \cdot \boldsymbol{\zeta} dV + \int_{\partial \mathcal{B}} \left(\frac{\partial \tilde{f}}{\partial \nabla \phi} \boldsymbol{N} + \frac{\partial \tilde{g}}{\partial \phi} \right) \cdot \boldsymbol{\zeta} dA$$
$$= \int_{\mathcal{B}} \tilde{\boldsymbol{p}}(\phi, \nabla \phi) \cdot \boldsymbol{\zeta} dV + \int_{\partial \mathcal{B}} \tilde{\boldsymbol{q}}(\phi, \nabla \phi) \cdot \boldsymbol{\zeta} dA, \tag{76}$$

where

$$\tilde{\boldsymbol{p}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \frac{\partial \tilde{f}}{\partial \boldsymbol{\phi}} - \nabla \cdot \frac{\partial \tilde{f}}{\partial \nabla \boldsymbol{\phi}} \qquad \text{and} \qquad \tilde{\boldsymbol{q}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \frac{\partial \tilde{f}}{\partial \nabla \boldsymbol{\phi}} \boldsymbol{N} + \frac{\partial \tilde{g}}{\partial \boldsymbol{\phi}} \qquad (77)$$

To simplify further, we need the expressions for $\partial \tilde{f}/\partial \phi$ and $\partial \tilde{f}/\partial \nabla \phi$. Note that many terms in $(74)_1$ are similar to (9) if we replace \boldsymbol{n} with ϕ . Hence the results of (25) and (27) will be useful. Following additional

results will be required to simplify new terms in (74)

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$$\frac{\partial}{\partial \phi} \left\{ (\nabla n) n \cdot (\nabla \phi) \phi \right\} = (\nabla \phi)^T (\nabla n) n$$

$$\frac{\partial}{\partial \phi} |(\nabla \phi) n + (\nabla n) \phi|^2 = \frac{\partial}{\partial \phi} \left(|(\nabla \phi) n|^2 + |(\nabla n) \phi|^2 + 2(\nabla \phi) n \cdot (\nabla n) \phi \right) = 2 \left((\nabla n)^T (\nabla n) \phi + (\nabla n)^T (\nabla \phi) n \right)$$

$$\frac{\partial}{\partial \nabla \phi} \left\{ (\nabla n) n \cdot (\nabla \phi) \phi \right\} = \frac{\partial}{\partial \phi_{l,m}} (n_{i,k} n_k \phi_{i,j} \phi_j) e_l \otimes e_m = \delta_{il} \delta_{jm} n_k n_{i,k} \phi_j e_l \otimes e_m = n_k n_{i,k} \phi_j e_i \otimes e_j = \nabla n n \otimes \phi$$

$$\frac{\partial}{\partial \nabla \phi} |(\nabla \phi) n + (\nabla n) \phi|^2 = \frac{\partial}{\partial \nabla \phi} \left(|(\nabla \phi) n|^2 + |(\nabla n) \phi|^2 + 2(\nabla \phi) n \cdot (\nabla n) \phi \right)$$

$$= \frac{\partial}{\partial \phi_{i,j}} \left(\phi_{k,l} n_l \phi_{k,m} n_m + 2\phi_{k,l} n_l n_{k,m} \phi_m \right) e_i \otimes e_j$$

$$= (\delta_{ik} \delta_{lj} n_l \phi_{k,m} n_m + \delta_{ik} \delta_{jm} n_l \phi_{k,l} n_m + 2\delta_{ik} \delta_{lj} n_l n_{k,m} \phi_m) e_i \otimes e_j$$

$$= 2(n_j \phi_{i,m} n_m + n_l \phi_{i,l} n_j + 2n_j n_{i,m} \phi_m) e_i \otimes e_j$$

$$= 2(\nabla \phi n + \nabla n \phi) \otimes n$$
(78)

Using (25),(27) and the above results we get the derivatives of \tilde{f} as,

$$\frac{\partial \tilde{f}}{\partial \phi} = 4(K_3 - K_2) \left((\nabla \phi)^T (\nabla n) n + (\nabla n)^T (\nabla n) \phi + (\nabla n)^T (\nabla \phi) n \right) - 4\lambda_v \phi - 2\mu \phi$$

$$\frac{\partial \tilde{f}}{\partial \nabla \phi} = \left(2K_1 (\nabla \cdot \phi) I + 2K_2 \nabla \phi - 2K_2 \nabla \phi^T + 4(K_3 - K_2) \left(\nabla n (n \otimes \phi) + (\nabla \phi n + \nabla n \phi) \otimes n \right) + (K_2 + K_4) (2\nabla \phi^T - 2(\nabla \cdot \phi) I) \right)$$

$$\frac{\partial \tilde{g}}{\partial \phi} = 2 \left(A \phi - 2\lambda_s \phi \right)$$
(79)

The expression $(27)_4$ can be written in a general form for any three vectors ${\pmb a}, {\pmb b}, {\pmb c}$ as

$$\nabla \cdot \left(\nabla \boldsymbol{a}(\boldsymbol{b} \otimes \boldsymbol{c}) \right) = \nabla \cdot (a_{i,j} \boldsymbol{e}_i \otimes \boldsymbol{e}_j b_k c_l \boldsymbol{e}_k \otimes \boldsymbol{e}_l)$$

$$= \nabla \cdot (a_{i,j} b_j c_l \boldsymbol{e}_i \otimes \boldsymbol{e}_l)$$

$$= (a_{i,j} b_j c_l)_l \boldsymbol{e}_i$$

$$= a_{i,jl} b_j c_l \boldsymbol{e}_i + a_{i,j} b_{j,l} c_l \boldsymbol{e}_i + a_{i,j} b_j c_{l,l} \boldsymbol{e}_l$$

$$= (a_{i,jl} b_j + a_{i,j} b_{j,l}) c_l \boldsymbol{e}_i + a_{i,j} b_j c_{l,l} \boldsymbol{e}_l$$

$$= (a_{i,j} b_j)_{,l} c_l \boldsymbol{e}_i + a_{i,j} b_j c_{l,l} \boldsymbol{e}_l$$

$$= \nabla ((\nabla \boldsymbol{a}) \boldsymbol{b}) \boldsymbol{c} + \nabla \cdot \boldsymbol{c} (\nabla \boldsymbol{a}) \boldsymbol{b}.$$
(80)

Using in the above identity, we obtain following useful expressions

$$\nabla \cdot \left(\nabla \boldsymbol{n}(\boldsymbol{n} \otimes \boldsymbol{\phi}) \right) = \nabla ((\nabla \boldsymbol{n})\boldsymbol{n})\boldsymbol{\phi} + \nabla \cdot \boldsymbol{\phi}(\nabla \boldsymbol{n})\boldsymbol{n}$$
$$\nabla \cdot \left(\nabla \boldsymbol{\phi}(\boldsymbol{n} \otimes \boldsymbol{n}) \right) = \nabla ((\nabla \boldsymbol{\phi})\boldsymbol{n})\boldsymbol{n} + \nabla \cdot \boldsymbol{n}(\nabla \boldsymbol{\phi})\boldsymbol{n}$$
$$\nabla \cdot \left(\nabla \boldsymbol{n}(\boldsymbol{\phi} \otimes \boldsymbol{n}) \right) = \nabla ((\nabla \boldsymbol{n})\boldsymbol{\phi})\boldsymbol{n} + \nabla \cdot \boldsymbol{n}(\nabla \boldsymbol{n})\boldsymbol{\phi}$$
(81)

Finally substituting (79) in (77) and using (81), we obtain

$$\tilde{p}(\phi, \nabla \phi) = 2(K_3 - K_2) \left((\nabla \phi)^T (\nabla n) n + (\nabla n)^T (\nabla n) \phi + (\nabla n)^T (\nabla \phi) n \right) - 4\lambda_v \phi - 2\mu \phi - 2K_1 \nabla (\nabla \cdot \phi) - 2K_2 \left(\nabla^2 \phi - \nabla (\nabla \cdot \phi) \right) - 4(K_3 - K_2) \left(\nabla ((\nabla n) \phi) n + \nabla \cdot n (\nabla n) \phi + \nabla ((\nabla \phi) n) n + \nabla \cdot n (\nabla \phi) n + \nabla ((\nabla n) n) \phi + \nabla \cdot \phi (\nabla n) n \right) \right)$$

$$= 2 \left\{ (K_2 - K_1) \nabla (\nabla \cdot \phi) - K_2 \nabla^2 \phi + 2(K_3 - K_2) \left((\nabla \phi)^T (\nabla n) n + (\nabla n)^T (\nabla n) \phi + (\nabla n)^T (\nabla \phi) n - \nabla ((\nabla n) n) \phi - \nabla \cdot \phi (\nabla n) n - [\nabla ((\nabla n) \phi) + \nabla ((\nabla \phi) n)] n - \nabla \cdot n [(\nabla \phi) n + (\nabla n) \phi] \right) - 2\lambda_v \phi - \mu \phi \right\}$$

$$(82)$$

and

$$\tilde{\boldsymbol{q}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \left(2K_1(\nabla \cdot \boldsymbol{\phi})I + 2K_2\nabla \boldsymbol{\phi} - 2K_2\nabla \boldsymbol{\phi}^T + 4(K_3 - K_2)\left(\nabla \boldsymbol{n}(\boldsymbol{n} \otimes \boldsymbol{\phi}) + (\nabla \boldsymbol{\phi}\boldsymbol{n} + \nabla \boldsymbol{n} \boldsymbol{\phi}) \otimes \boldsymbol{n}\right) \\ + (K_2 + K_4)(2\nabla \boldsymbol{\phi}^T - 2(\nabla \cdot \boldsymbol{\phi})\boldsymbol{I})\right)\boldsymbol{N} + 2(\boldsymbol{A}\boldsymbol{\phi} - 2\lambda_s\boldsymbol{\phi}) \\ = 2\left\{K_1(\nabla \cdot \boldsymbol{\phi})\boldsymbol{N} + K_2(\nabla \boldsymbol{\phi} - \nabla \boldsymbol{\phi}^T)\boldsymbol{N} + 2(K_3 - K_2)\left(\nabla \boldsymbol{n}\boldsymbol{n}(\boldsymbol{\phi} \cdot \boldsymbol{N}) + (\nabla \boldsymbol{\phi}\boldsymbol{n} + \nabla \boldsymbol{n} \boldsymbol{\phi})\boldsymbol{n} \cdot \boldsymbol{N}\right) \\ + (K_2 + K_4)(\nabla \boldsymbol{\phi}^T\boldsymbol{N} - (\nabla \cdot \boldsymbol{\phi})\boldsymbol{N}) + (\boldsymbol{A}\boldsymbol{\phi} - 2\lambda_s\boldsymbol{\phi})\right\}$$
(83)

The expression for $\tilde{\boldsymbol{p}}$ in [Rosso et al., 2004] differs from (82) since it has one term $(\nabla \boldsymbol{\phi})^T (\nabla \boldsymbol{n}) \boldsymbol{n}$ missing and a factor of 2 missing. Also, the expression for $\tilde{\boldsymbol{q}}$ in [Rosso et al., 2004] differs from (83) since it has two terms $(\nabla \boldsymbol{\phi} \boldsymbol{n} + \nabla \boldsymbol{n} \boldsymbol{\phi}) \boldsymbol{n} \cdot \boldsymbol{N}$ missing and a factor of 2 missing. At extremum $\delta \tilde{G}$ should be zero. Also, from (14), we have

$$\boldsymbol{\phi}_{\varepsilon} \cdot \boldsymbol{n} = 0 \implies \boldsymbol{\zeta} \cdot \boldsymbol{n} = 0 \tag{84}$$

therefore the Euler-Lagrange equation becomes

$$\tilde{\boldsymbol{p}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \nu_v \boldsymbol{n} \tag{85}$$

and natural boundary condition becomes

$$\tilde{\boldsymbol{q}}(\boldsymbol{\phi}, \nabla \boldsymbol{\phi}) = \nu_s \boldsymbol{n},\tag{86}$$

where ν_v and ν_s are new Lagrange multipliers. The eigen value problem (85) and (86) and the minima of G are closely related. The minimum value attained by G on the manifold (69) is equal to the minimum eigen value μ_{min} for which there is a solution to these equations [Rosso et al., 2004],[Courant and Hilbert, 1989, pp.399]. This implies that the director field is locally stable whenever the minimum eigen value μ_{min} of (81) and (82) is positive.

Conclusion

A local elastic stability criterion for NLC is derived by calculating the minima of second variation of free energy functional over the manifold (69). The constraint that the length of the director is unity is satisfied till $\mathcal{O}(\varepsilon^3)$. The local stability criteria reduces to the condition that the minimum eigen value of system of equations (81) and (82) is positive. The form of equations differs slightly from what derived by [Rosso et al., 2004].

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Figure 1: The schematic diagram for Freedericksz's tranistion. E is the electric field and n is the director. Source: Wikipedia



Figure 2: Schematic representation of (a) the uniform splay-Freedericksz's transition and (b) the periodic splay-twist distortion. Source:[Lonberg and Meyer, 1985]

Tables