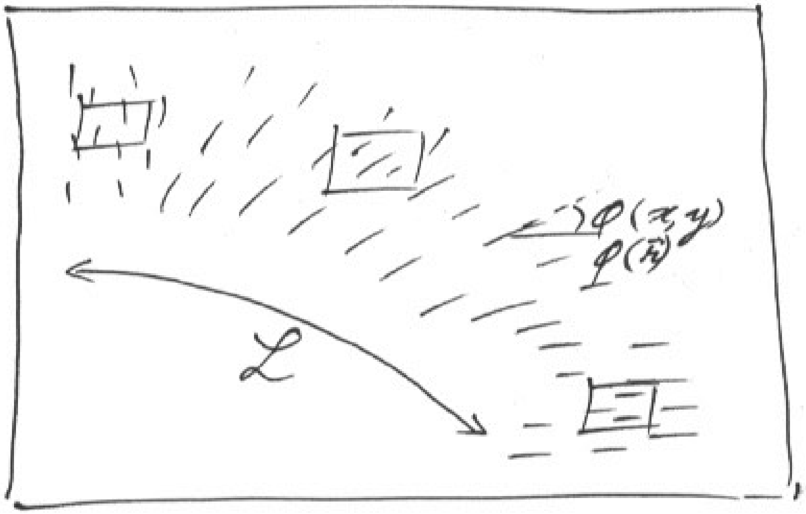
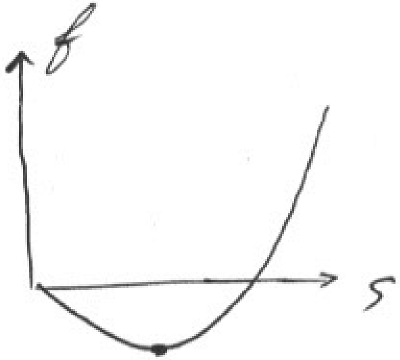




2d system $\varphi(x,y)$

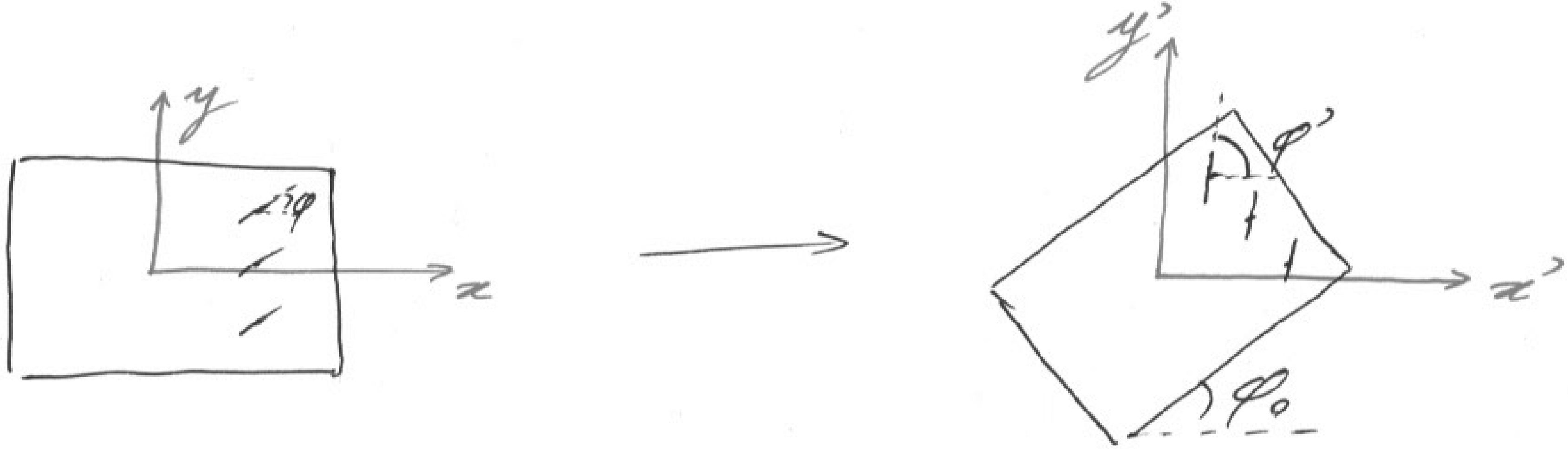
$$F = \int \Big[\alpha(\varphi) + \beta_i(\varphi(\vec{r}))\,(\nabla_i \varphi(\vec{r})) + \gamma_{ij}(\varphi(\vec{r}))\,(\nabla_i \varphi(\vec{r}))(\nabla_j \varphi(\vec{r})) + O(\nabla^3) \Big]\, dx\, dy$$

3.1.1) $\mathcal{L} \gg$ any molecular size.

$\nabla^n \varphi \simeq \mathcal{L}^{-n}$

So as $\mathcal{L} \to \infty$ term of higher order in ∇ become negligible.

3.1.2)



rotate $\vec{r}$ and $\hat{n}$

$$\begin{cases} \varphi' = \varphi + \varphi_0 \\ x' = \cos\varphi_0 \cdot x - \sin\varphi_0 \cdot y \\ y' = \sin\varphi_0 \cdot x + \cos\varphi_0 \cdot y \end{cases}$$

i.e. $$\begin{pmatrix} x' \\ y' \end{pmatrix} = \ell \begin{pmatrix} x \\ y \end{pmatrix}$$

3.13)
$$F_0 = \int \alpha\,[\varphi(x,y)]\,dx\,dy$$

under the transform. $\varphi(x,y) \longrightarrow \varphi'(x',y')$

$dx\,dy \rightarrow dx'dy'$

$$F_0' = \int \left[\alpha\left(\varphi'(x',y')\right)\right] dx'dy'$$

$$dx'dy' = \underbrace{|e|}_{=1}\,dx\,dy$$

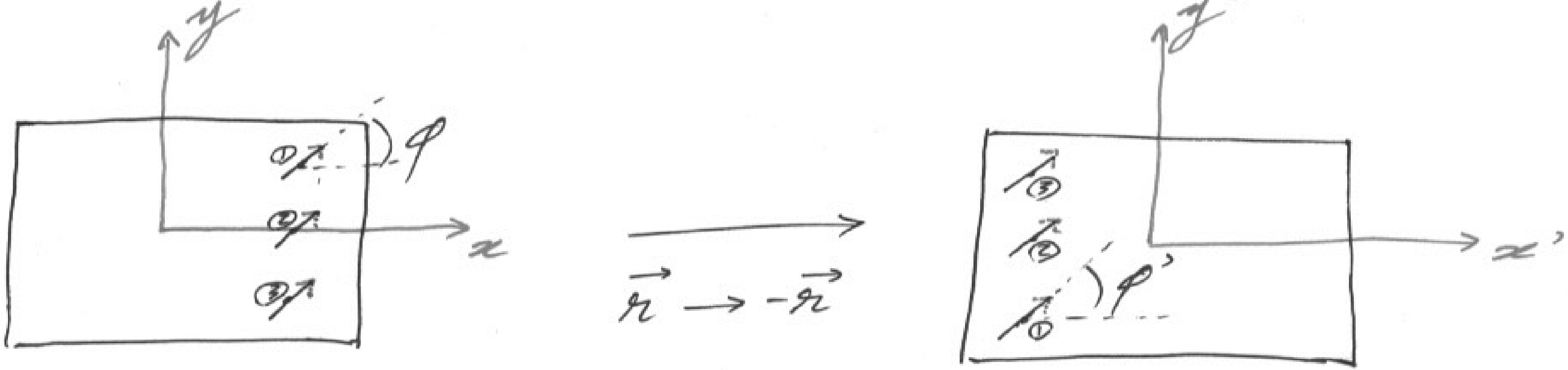
$$F_0' = \int \alpha\,[\varphi(x,y)+\varphi_0]\;dx\,dy$$

And $\forall \varphi$ $F_0 = F_0'$ requires

$$\forall \varphi, \varphi_0 \qquad \alpha(\varphi) = \alpha(\varphi+\varphi_0)$$

i.e. α is a constant, and can be disregarded.

3.1.5)



For a nematic (apolar particles) $F_1 = F_1'$ with

$$\varphi'(x',y') = \varphi(x,y) \qquad x' = -x \qquad \Longrightarrow \quad \vec{\nabla}' = -\vec{\nabla}$$

$$y' = -y$$

$$F_1' = \int \beta_i(\varphi'(x',y'))\, \nabla_i' \varphi'\, dx'dy'$$

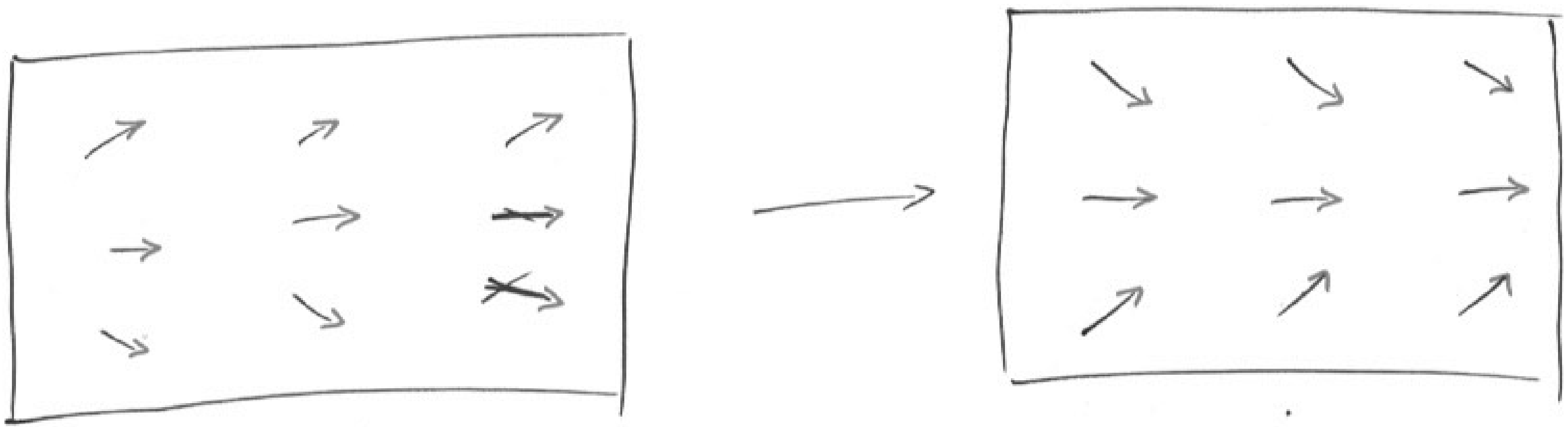
$$= \int \beta_i(\varphi(x,y))\, (-\nabla_i \varphi(x,y))\, \underbrace{|J|}_{=1}\, dx\, dy$$

$$= \int -\beta_i(\varphi(x,y))\, (\nabla_i \varphi(x,y))\, dx\, dy = F_1 = \int \beta_i(\varphi)\, \nabla_i \varphi\, dx\, dy$$

$\forall \varphi(\vec{x}) \quad F_1' = F_1$ implies

$$\forall \varphi \qquad \beta_i(\varphi)\cdot\nabla_i\varphi = -\beta_i(\varphi)\cdot\nabla_i\varphi$$

i.e. $\beta_i = 0$.



3.2.1)

$$F_2 = \int \underline{\gamma_{ij}(\varphi)\nabla_i\varphi\nabla_j\varphi} + \underline{\tilde{\gamma}_{ij}(\varphi)\nabla_i\nabla_j\varphi}$$

$$\tilde{F}_2 = \int \tilde{\gamma}_{ij}(\varphi)\ \nabla_i\nabla_j\varphi\ dx\,dy$$

$$= \underbrace{\oint \tilde{\gamma}_{ij}(\varphi)\ \nabla_j\varphi\ d\vec{s}_i}_{\text{Boundary term (negl.)}} - \int \left[\nabla_i\tilde{\gamma}_{ij}(\varphi)\right]\cdot\nabla_j\varphi\ dx\,dy$$

$$= \int \underbrace{\left(-\frac{\partial\tilde{\gamma}_{ij}}{\partial\varphi}\right)}_{\gamma\text{-like.}}\cdot\nabla_i\varphi\ \nabla_j\varphi\ dx\,dy$$

3.2.2) Rotation as in 3.1.2

$$\nabla_i' = \frac{\partial}{\partial r_i'} = \underbrace{\frac{\partial r_j}{\partial r_i'}}_{} \frac{\partial}{\partial r_j}$$

The tensor $\frac{\partial r_j}{\partial r_i'}$ is equal to $\ell_{ij}(\varphi_0) = \ell^T_{ji}$

$\cancel{\partial r}$ $$\begin{pmatrix} r_1' \\ r_2' \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\varphi_0 & \sin\varphi_0 \\ -\sin\varphi_0 & \cos\varphi_0 \end{pmatrix}}_{=\ell} \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}$$

$$\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \underbrace{\begin{pmatrix} \cos\varphi_0 & -\sin\varphi_0 \\ \sin\varphi_0 & \cos\varphi_0 \end{pmatrix}}_{\ell^T} \begin{pmatrix} r_1' \\ r_2' \end{pmatrix}$$

$$\frac{\partial r_1}{\partial r_1'} = \cos\varphi_0 = \ell_{11}$$

etc...

$$\frac{\partial r_2}{\partial r_1'} = -\sin\varphi_0 = (\ell^T)_{21} = \ell_{12}$$

Thus $\nabla_i' = \ell_{ij}(\varphi_0)\,\nabla_j$

$\vec{r}_i' = \ell_{ij}(\varphi_0)\,\vec{r}_j$

$$F' = \int \gamma_{ij}(\varphi+\varphi_0)\,[\ell_{ik}(\varphi_0)\cdot\nabla_k(\varphi+\varphi_0)]\cdot[\ell_{j\ell}(\varphi_0)\,\nabla_\ell(\varphi+\varphi_0)]\,dx\,dy$$

$$= \int [\ell_{ki}(-\varphi_0)\,\gamma_{ij}(\varphi+\varphi_0)\,\ell_{j\ell}(\varphi_0)]\,(\nabla_k\varphi)(\nabla_\ell\varphi)\,dx\,dy$$

exchanging dummy indices $i \leftrightarrow k \quad j \leftrightarrow \ell$:

$$F' = \int [\ell_{ik}(-\varphi_0)\,\gamma_{k\ell}(\varphi+\varphi_0)\,\ell_{\ell j}(\varphi_0)]\,\nabla_i\varphi\,\nabla_j\varphi\,dx\,dy$$

So $F = F'$

$\forall \varphi, \varphi_0 \qquad \gamma_{ij}(\varphi) = \ell_{ik}(-\varphi_0)\,\gamma_{k\ell}(\varphi+\varphi_0)\,\ell_{\ell j}(\varphi_0)$

$\gamma(\varphi+\varphi_0) = \gamma(\varphi) + \delta\gamma$

3.2.3) For small φ_0, the r.h.s reads

$$\begin{pmatrix} 1 & \varphi_0 \\ -\varphi_0 & 1 \end{pmatrix} \begin{pmatrix} \gamma_{11} + \delta\gamma_{11} & \gamma_{12} + \delta\gamma_{12} \\ \gamma_{21} + \delta\gamma_{21} & \gamma_{22} + \delta\gamma_{22} \end{pmatrix} \begin{pmatrix} 1 & -\varphi_0 \\ \varphi_0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \varphi_0 \\ -\varphi_0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \gamma_{11} + \delta\gamma_{11} + \varphi_0\gamma_{12} & -\varphi_0\gamma_{11} + \gamma_{12} + \delta\gamma_{12} \\ \gamma_{21} + \delta\gamma_{21} + \varphi_0\gamma_{22} & -\varphi_0\gamma_{21} + \gamma_{22} + \delta\gamma_{22} \end{pmatrix}$$

$$= \begin{pmatrix} \gamma_{11} + \delta\gamma_{11} + \varphi_0\gamma_{12} + \varphi_0\gamma_{21} & -\varphi_0\gamma_{11} + \gamma_{12} + \delta\gamma_{12} + \varphi_0\gamma_{22} \\ -\varphi_0\gamma_{11} + \gamma_{21} + \delta\gamma_{21} + \varphi_0\gamma_{22} & -\varphi_0\gamma_{12} - \varphi_0\gamma_{21} + \gamma_{22} + \delta\gamma_{22} \end{pmatrix}$$

$$= \begin{pmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{pmatrix}$$

has to be

$$\delta \gamma_{11} + \varphi_0 (\gamma_{12} + \gamma_{21}) = 0$$

$$\delta \gamma_{12} + \varphi_0 (\gamma_{22} - \gamma_{11}) = 0$$

$$\delta \gamma_{21} + \varphi_0 (\gamma_{22} - \gamma_{11}) = 0$$

$$\delta \gamma_{22} - \varphi_0 (\gamma_{12} + \gamma_{21}) = 0$$

And

$$\frac{\delta \gamma_{11}}{\varphi_0} = \frac{d \gamma_{11}}{d \varphi}(\varphi)$$

yields Eq. (9).

3.2.4) Rearrange system as

$$\partial_\varphi (\gamma_{11} + \gamma_{22}) = 0 \implies \gamma_{11} + \gamma_{22} = 2C = \text{constant}$$

$$\partial_\varphi (\gamma_{12} - \gamma_{21}) = 0 \implies \gamma_{12} - \gamma_{21} = 2D = \text{constant}.$$

$$\partial_\varphi (\gamma_{11} - \gamma_{22}) = -2(\gamma_{12} + \gamma_{21})$$

$$\partial_\varphi (\gamma_{12} + \gamma_{21}) = 2(\gamma_{11} - \gamma_{22})$$

So $\partial_\varphi^2 (\gamma_{11} - \gamma_{22}) = -4 (\gamma_{11} - \gamma_{22})$

$$\Longrightarrow \quad \gamma_{11} - \gamma_{22} = 2A \cos(2\varphi) + 2B \sin(2\varphi)$$

with A, B integration constants.

This yields:

$$\left| \begin{array}{l} \gamma_{11} = C + A\cos(2\varphi) + B\sin(2\varphi) \\ \gamma_{22} = C - A\cos 2\varphi - B\sin(2\varphi) \end{array} \right.$$

And we have $\gamma_{12} + \gamma_{21} = -\frac{1}{2}\partial_\varphi(\gamma_{11} - \gamma_{22})$, yielding

$$\gamma_{12} + \gamma_{21} = 2A\sin(2\varphi) - 2B\cos(2\varphi)$$

$$\Longrightarrow \left| \begin{array}{l} \gamma_{12} = D + A\sin(2\varphi) - B\cos(2\varphi) \\ \gamma_{21} = -D + A\sin(2\varphi) - B\cos(2\varphi) \end{array} \right.$$

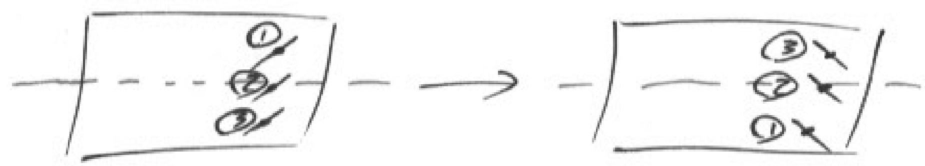
$$F = \int \gamma_{11} \nabla_x \varphi \nabla_x \varphi + (\gamma_{12} + \gamma_{21}) \nabla_x \varphi \nabla_y \varphi + \gamma_{22} \nabla_y \varphi \nabla_y \varphi \, dx\,dy$$

$$= \int \Big\{ C' \left[(\nabla_x \varphi)^2 + (\nabla_y \varphi)^2 \right]$$
$$+ \left[A \cos(2\varphi) + B \sin(2\varphi) \right] \left[(\nabla_x \varphi)^2 - (\nabla_y \varphi)^2 \right]$$
$$+ \left[2A \sin(2\varphi) - 2B \cos(2\varphi) \right] \nabla_x \varphi \nabla_y \varphi \Big\} dx\,dy$$

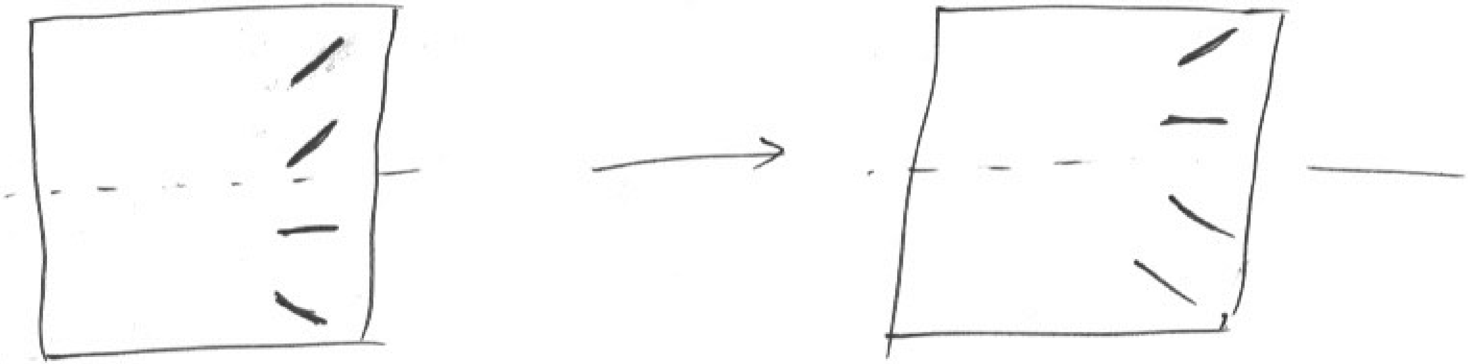
i.e. D is irrelevant.

3.2.5) Introduce another symmetry:

$$x \to x$$
$$y \to -y$$
$$\varphi \to -\varphi$$



If molecules achiral, F doesn't change



~~Under~~ Under $y \to -y$ $\quad \varphi \to -\varphi$

C terms are invariant

A ——————

B terms change sign $\Longrightarrow$ B must vanish

$$F = \int C\left[(\nabla_x \varphi)^2 + (\nabla_y \varphi)^2\right] + A\left[\cos(2\varphi)\left((\nabla_x \varphi)^2 - (\nabla_y \varphi)^2\right) + 2\sin(2\varphi)\,(\nabla_x \varphi)(\nabla_y \varphi)\right] dx\,dy$$

Consider $\hat{n} = \begin{pmatrix} \cos\varphi \\ \sin\varphi \end{pmatrix}$

$$\vec{\nabla} \cdot \hat{n} = \nabla_x \cos\varphi + \nabla_y \sin\varphi$$

$$= -\sin\varphi \cdot \nabla_x\varphi + \cos\varphi \, \nabla_y\varphi$$

$$(\vec{\nabla} \cdot \hat{n})^2 = \sin^2\varphi \, (\nabla_x\varphi)^2 - 2\sin\varphi\cos\varphi \, \nabla_x\varphi \, \nabla_y\varphi + \cos^2\varphi \, (\nabla_y\varphi)^2$$

$$= \frac{1-\cos 2\varphi}{2} (\nabla_x\varphi)^2 - \sin(2\varphi)\,(\nabla_x\varphi)(\nabla_y\varphi) + \frac{1+\cos(2\varphi)}{2} (\nabla_y\varphi)^2$$

$$= \frac{1}{2}\left[(\nabla_x\varphi)^2 + (\nabla_y\varphi)^2\right] - \cos(2\varphi)\left[(\nabla_x\varphi)^2 - (\nabla_y\varphi)^2\right] - \sin(2\varphi)\,(\nabla_x\varphi)(\nabla_y\varphi).$$

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$$\vec{\nabla} \times \hat{n} = (\nabla_x \sin\varphi - \nabla_y \cos\varphi)\, \hat{z}$$

$$= (\cos\varphi \; \nabla_x \varphi + \sin\varphi \; \nabla_y \varphi)\, \hat{z}$$

$$\hat{n} \times (\vec{\nabla} \times \hat{n}) = \left(\begin{array}{c} \text{———} \\ \text{———} \end{array} \right)$$

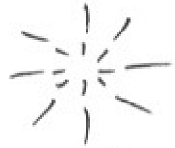
$$[\hat{n} \times (\vec{\nabla} \times \hat{n})]^2 = \frac{1}{2} \left[(\nabla_x \varphi)^2 + (\nabla_y \varphi) \right]^2 + \cos(2\varphi) \left[(\nabla_x \varphi)^2 - (\nabla_y \varphi)^2 \right] + \sin(2\varphi)\, (\nabla_x \varphi)(\nabla_y \varphi)$$

So

$$(\nabla_x \varphi)^2 + (\nabla_y \varphi)^2 = (\vec{\nabla} \cdot \vec{n})^2 + [\hat{n} \times (\vec{\nabla} \times \hat{n})]^2$$

$$\cos(2\varphi) \left[(\nabla_x \varphi)^2 - (\nabla_y \varphi)^2 \right] + \sin 2\varphi \; \nabla_x \varphi \; \nabla_y \varphi$$

$$= \frac{1}{2} \left\{ [\hat{n} \times (\vec{\nabla} \times \hat{n})]^2 - (\vec{\nabla} \cdot \vec{n})^2 \right\}$$

K_1 : splay : example: $\hat{n} = \hat{r}$ 

K_3 : bend : example $\hat{n} = \hat{x} + \varepsilon \cos\left(\frac{x}{\lambda}\right) \hat{y}$

K_2 : twist

4.10^{-21} J

size of a molecule $\simeq$ 1 nm

$$K_i \simeq J.m^{-1} \simeq k_B T / b$$

$$\simeq 4\,pN$$

3.2.8) Is it OK to assume that $S = ct$ everywhere?