Variational Problems in Elastic Theory of Biomembranes, Smectic-A Liquid Crystals, and Carbon Related Structures

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Outline

- Introduction to several problems in the elasticity of biomembranes, smectic-A liquid crystal, and carbon related structures
- Variational problems on 2D surface
- Morphological problems of lipid bilayers
- Elasticity and stability of cell membranes
- Summary

Introduction

Basic concept

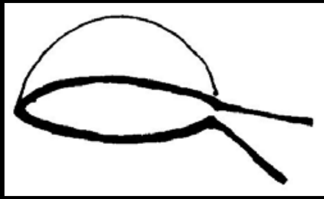
- The 1st order variation of free energy → equilibrium shapes
- The 2nd order variation of free energy→ mechanical stabilities

History

- Fluid films

❖ Soap films ---- minimal surfaces， Plateau (1803)

$$F = \lambda \int dA, \delta F = 0 \Rightarrow H = 0$$



❖ Soap bubble ---- sphere, Young (1805), Laplace (1806)

$$F = \Delta p \int dV + \lambda \oint dA, \ (\Delta p = p_o - p_i)$$

$$\delta F = 0 \Rightarrow H = \Delta p / 2\lambda = \text{Const.}$$

"An embedded surface with constant mean curvature in E^3 must be a spherical surface"---Alexandrov (1950's)

- Solid shells

❖ Possion (1821):

$$F = \oint H^2 dA$$

❖ Schadow (1922)

$$\nabla^2 H + 2H(H^2 - K) = 0$$

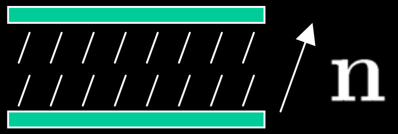
Laplace operator

$$\nabla^2 = \frac{1}{\sqrt{g}} \frac{\partial}{\partial u^i} \left(\sqrt{g} g^{ij} \frac{\partial}{\partial u^j} \right)$$

❖ Willmore (1982) problem of surfaces

- Lipid bilayers as smectic-A liquid crystals

  ❖ Frank energy of liquid crystal (1958)



LC box

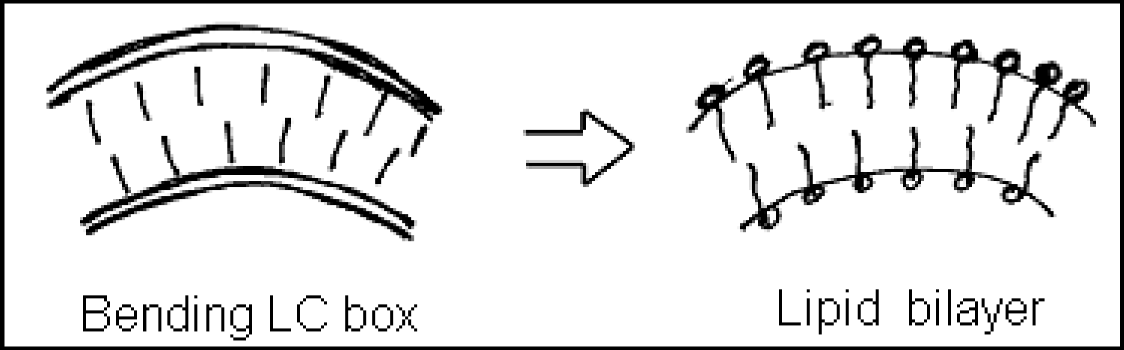
$$F = \int g_{LC} dV$$

$$\begin{aligned} g_{LC} &= \frac{k_1}{2}[(\nabla \cdot \mathbf{n} - s_0)^2 + (\nabla \times \mathbf{n})^2] \\ &- k_2(\nabla \cdot \mathbf{n})(\mathbf{n} \cdot \nabla \times \mathbf{n}) + \frac{k_3}{2}(\nabla \mathbf{n} : \nabla \mathbf{n}) \end{aligned}$$

k_1, k_2, k_3: Elastic constants

s_0: Spontaneous splay

❖ Helfrich energy of lipid bilayer (1973)



For SmA LC, in the limit of thin thickness

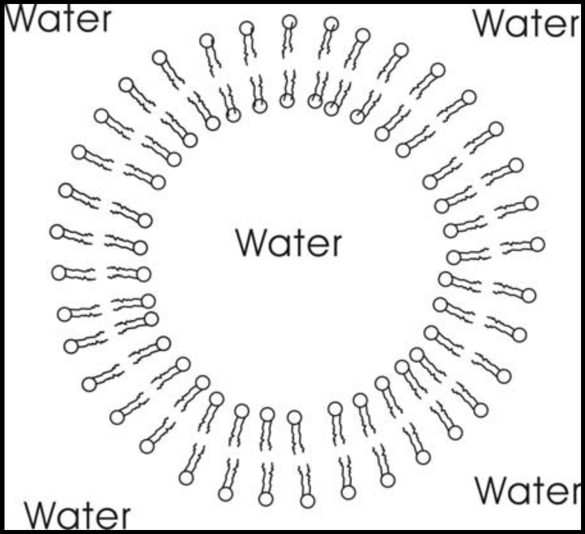
$$F = \int \mathcal{E} dA \qquad \mathcal{E} = \frac{k_c}{2}(2H + c_0)^2 + \bar{k}K$$

$$k_c = (k_1 + k_3)t,\ \bar{k} = -k_3 t$$

$$c_0 = \frac{k_1 s_0}{(k_1+k_3)t}: \text{ Spontaneous curvature}$$

❖ Shape equation of lipid vesicles, Ou-Yang & Helfrich (1987)

$$F = \Delta p \int dV + \lambda \oint dA + \oint \mathcal{E} dA$$



$$\delta F = 0$$

$$\Delta p - 2\lambda H + k_c \nabla^2 (2H) + k_c (2H + c_0)(2H^2 - c_0 H - 2K) = 0$$

$$k_c = 0 \Rightarrow \Delta p - 2\lambda H = 0 \text{ (Young-Laplace equation)}$$

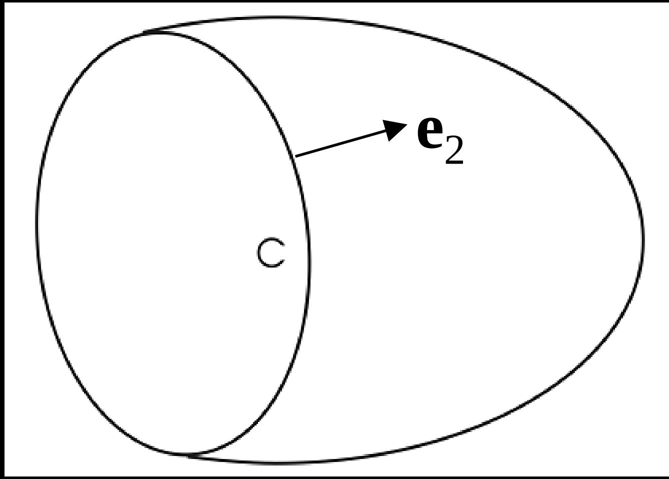
$$\Delta p = 0, \lambda = 0, c_0 = 0 \Rightarrow \nabla^2 H + 2H(H^2 - K) = 0$$

Willmore surfaces

❖ Open lipid vesicles, Capovilla, Guven, & Santiago (2002)

$$F = \lambda \int dA + \int \mathcal{E} dA + \gamma \oint_C ds$$

$$\delta F = 0$$



$$k_c(2H + c_0)(2H^2 - c_0 H - 2K) - 2\lambda H + k_c \nabla^2 (2H) = 0$$

$$\left[k_c(2H + c_0) + \bar{k} k_n\right]\Big|_C = 0$$

$$\left[-2k_c \frac{\partial H}{\partial \mathbf{e}_2} + \gamma k_n + \bar{k} \frac{d\tau_g}{ds}\right]\Bigg|_C = 0$$

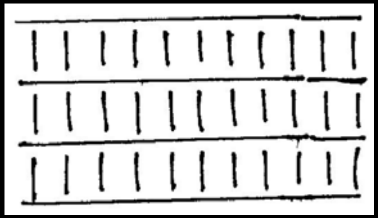
$$\left[\frac{k_c}{2}(2H + c_0)^2 + \bar{k} K + \lambda + \gamma k_g\right]\Bigg|_C = 0$$

[Tu & Ou-Yang (2003)]

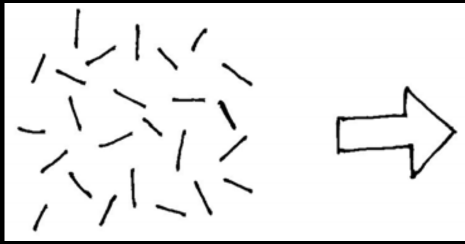
Focal conic structures in SmA LC

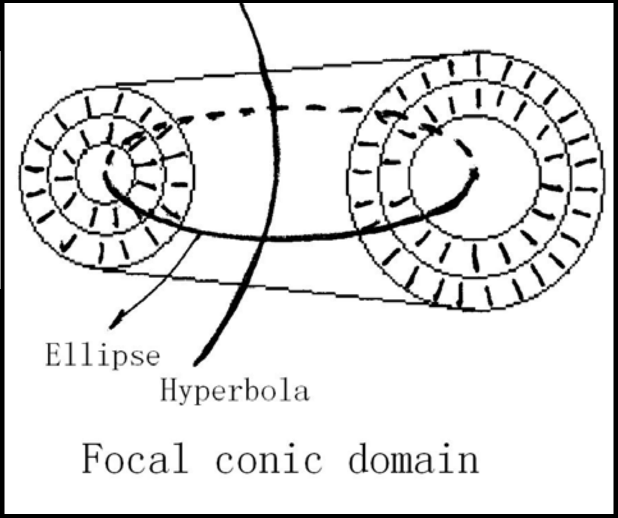
- Puzzle

The configuration of min. energy in SmA LC:



Dupin cyclides are usually formed when LC cools from Isotropic phase to SmA:





G. Friedel, Annls. Phys. **18** (1922) 273

- Bragg, Nature **133** (1934) 445.
  "Why the cyclides are preferred to other geometrical structures under the preservation of the interlayer spacing?"

- Naito, Okuda, Ou-Yang, PRL **70** (1993) 2912; PRE **52** (1995) 2095.
  "The Gibbs free energy difference between Isotropic and SmA phases must be balanced by the curvature elastic energy of SmA layers."

- General variational problem on a surface

Curvature — Volume — Surface — Thickness

$$F = F_C + F_V + F_A = \oint \mathcal{E}(H, K, t)\,dA$$

$$\delta F = 0$$

$$\oint (\partial\mathcal{E}/\partial t)\,dA = 0$$

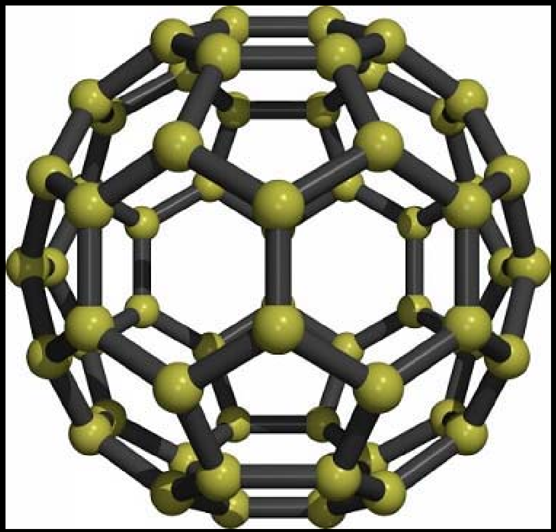
$$(\nabla^2/2 + 2H^2 - K)\partial\mathcal{E}/\partial H + (\nabla\cdot\tilde{\nabla} + 2KH)\partial\mathcal{E}/\partial K - 2H\mathcal{E} = 0$$

$$\nabla\cdot\tilde{\nabla} = \frac{1}{\sqrt{g}}\frac{\partial}{\partial u^i}\left(\sqrt{g}KL^{ij}\frac{\partial}{\partial u^j}\right)$$

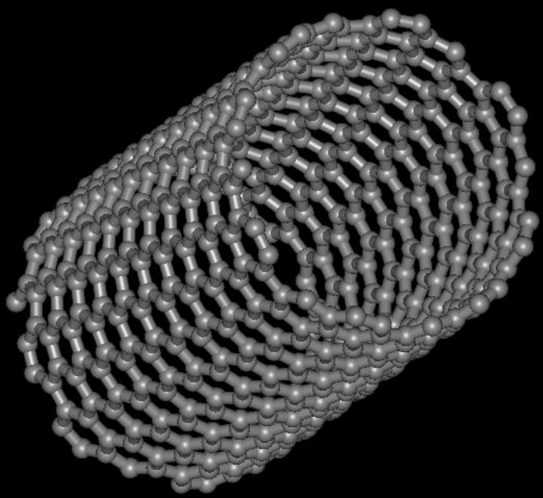
Solving both Eqs. gives good explanation of FCD. [PRE **52** (1995) 2095]

Carbon related structures

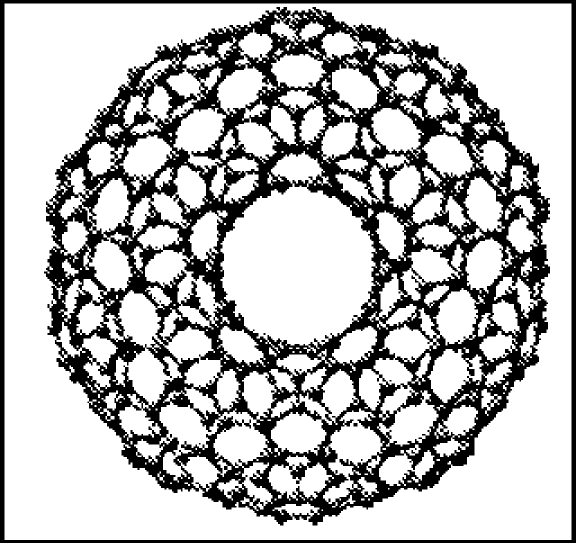
- Three typical structures



C_{60}



SWNT



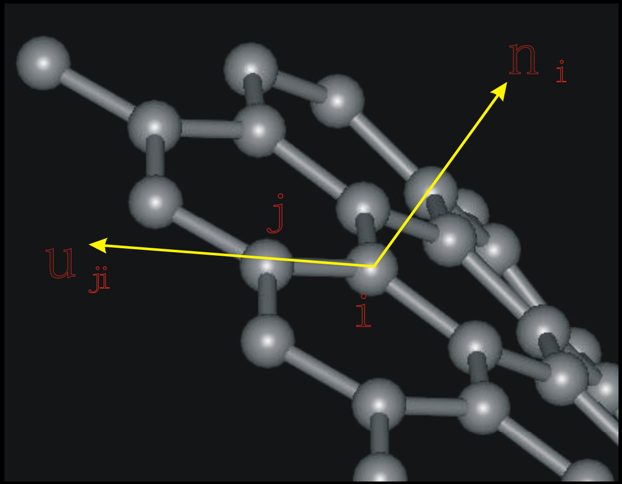
Carbon Torus

- Curvature energy of curved single graphitic layer

❖ Lattice model [Lenosky et al. Nature **355** (1992) 333]

$$E = \epsilon_1 \sum_i \left(\sum_{(j)} \mathbf{u}_{ij} \right)^2 + \epsilon_2 \sum_{(ij)} (1 - \mathbf{n}_i \cdot \mathbf{n}_j) + \epsilon_3 \sum_{(ij)} (\mathbf{n}_i \cdot \mathbf{u}_{ij})(\mathbf{n}_j \cdot \mathbf{u}_{ji})$$

$$(\epsilon_1, \epsilon_2, \epsilon_3) = (0.96, 1.29, 0.05)\ \text{eV}$$



❖ Continuum limit [Ou-Yang etal. PRL **78** (1997) 4055]

$$E = \int \left[\tfrac{1}{2} k_c (2H)^2 + \bar{k} K \right] dA$$

$$k_c = (18\epsilon_1 + 24\epsilon_2 + 9\epsilon_3) r_0^2 / (32\Omega) = 1.17\text{eV}$$
$$\bar{k}/k_c = -(8\epsilon_2 + 3\epsilon_3)/(6\epsilon_1 + 8\epsilon_2 + 3\epsilon_3) = -0.645$$

- Understanding three typical structures

Surface energy per area

$$F = \int \left[\frac{1}{2}k_c(2H)^2 + \bar{k}K\right] dA + \lambda \int dA$$

$$\delta F = 0$$

$$\nabla^2 H + 2H(H^2 - K) - \lambda H/k_c = 0$$

$\lambda = 0$: C_{60}, Torus

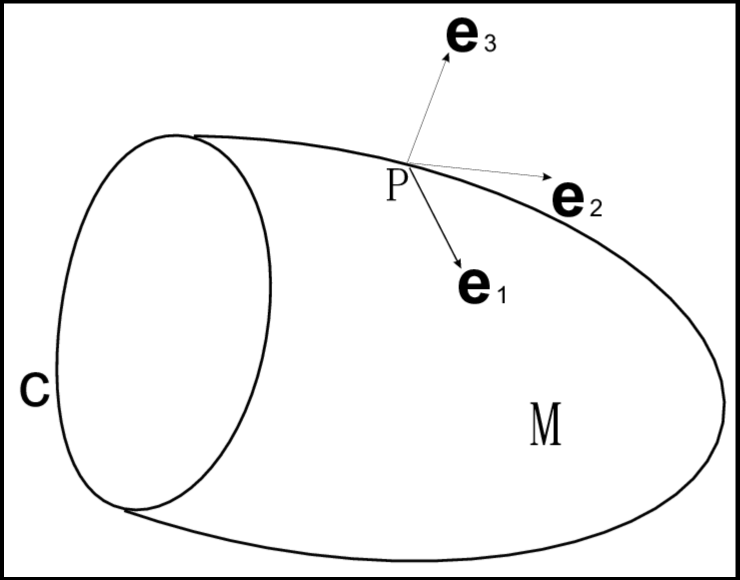
$R^2 = k_c/2\lambda$: SWNT

Variational problems on 2D surface

[JPA **37** (2004) 11407]

Surface theory in E^3

- Moving frame method



Orthogonal moving frame

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}, (i, j = 1, 2, 3)$$

$$\{P; \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$$

Pay attention to the direction of curve C

Differential of frame

$$d\mathbf{r} = \lim_{P \to P'} \overrightarrow{PP'} = \omega_1 \mathbf{e}_1 + \omega_2 \mathbf{e}_2$$

$$d\mathbf{e}_i = \omega_{ij} \mathbf{e}_j; \omega_{ij} = -\omega_{ji}, \quad (i = 1, 2, 3)$$

- Structure equations of the surface

$$dd\mathbf{r} = 0 \ \& \ dd\mathbf{e}_i = 0 \Longrightarrow$$

$$\begin{aligned} &d\omega_1 = \omega_{12} \wedge \omega_2; \\ &d\omega_2 = \omega_{21} \wedge \omega_1; \\ &\omega_1 \wedge \omega_{13} + \omega_2 \wedge \omega_{23} = 0; \\ &d\omega_{ij} = \omega_{ik} \wedge \omega_{kj} \quad (i, j = 1, 2, 3). \end{aligned}$$

$$\omega_1 \wedge \omega_{13} + \omega_2 \wedge \omega_{23} = 0 (Cartan)$$
$$\Rightarrow \omega_{13} = a\omega_1 + b\omega_2, \omega_{23} = b\omega_1 + c\omega_2$$

Curvature matrix $\begin{pmatrix} a & b \\ b & c \end{pmatrix}$

- Other formulas

Area element:

$$dA = \omega_1 \wedge \omega_2$$

1st fundamental form:

$$I = d\mathbf{r} \cdot d\mathbf{r} = \omega_1^2 + \omega_2^2$$

2nd fundamental form:

$$II = a\omega_1^2 + 2b\omega_1\omega_2 + c\omega_2^2$$

3rd fundamental form:

$$III = \omega_{31}^2 + \omega_{32}^2$$

Mean curvature:

$$H = (a + c)/2$$

Gaussian curvature:

$$K = ac - b^2$$

Gaussian Elegant Theorem:

$$d\omega_{12} = -K\omega_1 \wedge \omega_2$$

$$\Downarrow$$

Gauss–Bonnet Formula:

$$\int_M K dA + \int_C k_g ds = 2\pi\chi(M)$$