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

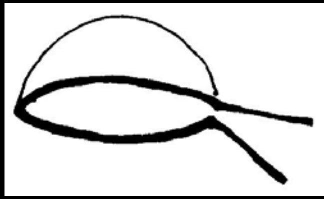
- The 1st order variation of free energy → equilibrium shapes
- The 2nd order variation of free energy→ mechanical stabilities

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)

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

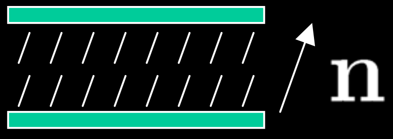
Laplace operator

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

❖ Willmore (1982) problem of surfaces

- Lipid bilayers as smectic-A liquid crystals

❖ Frank energy of liquid crystal (1958)



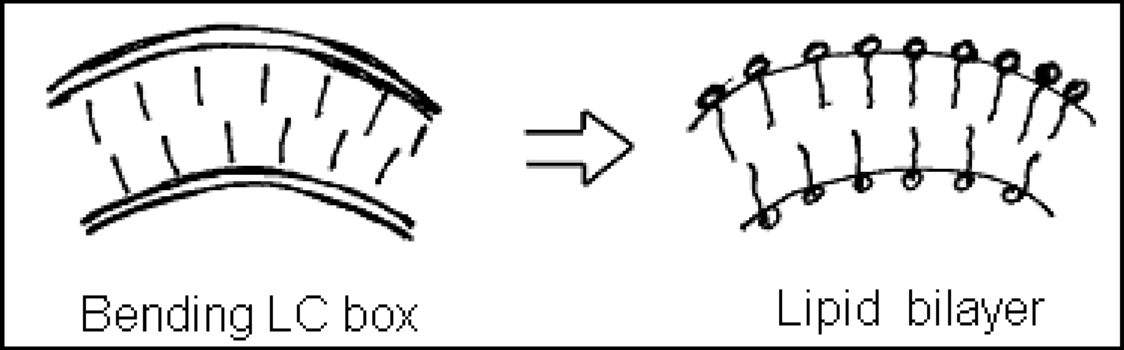
$$F = \int g_{LC} dV$$

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

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

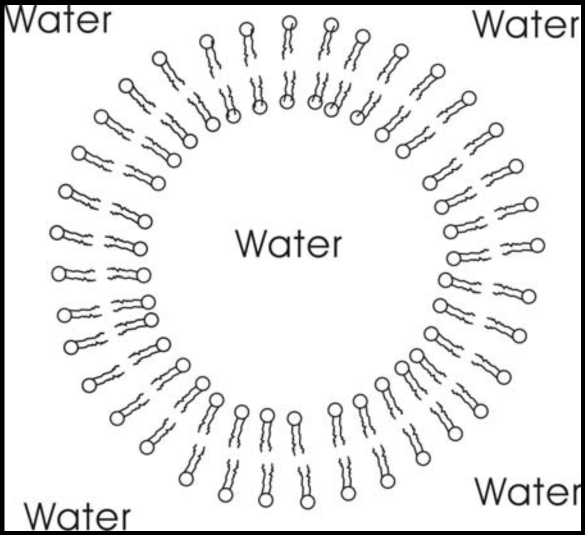
$$F = \int \mathcal{E}\, dA \qquad \mathcal{E} = \frac{k_c}{2}(2H + c_0)^2 + \bar{k}K$$

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

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

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

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



$$\delta F = 0$$

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

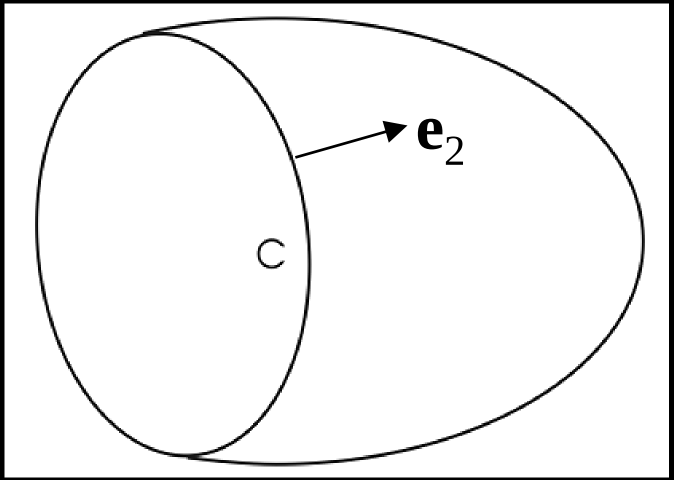
$$k_c = 0 \Rightarrow \Delta p - 2\lambda H = 0 \text{ (Young-Laplace equation)}$$

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

Willmore surfaces

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

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



$$\delta F = 0$$

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

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

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

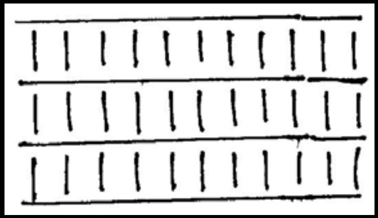
$$\left[\frac{k_c}{2}(2H + c_0)^2 + \bar{k} K + \lambda + \gamma k_g\right]\Bigg|_C = 0$$

[Tu & Ou-Yang (2003)]

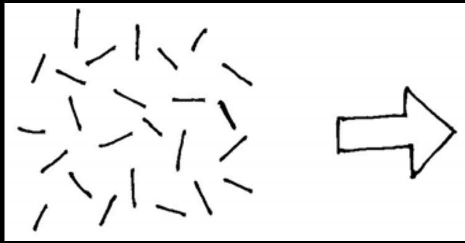
Focal conic structures in SmA LC

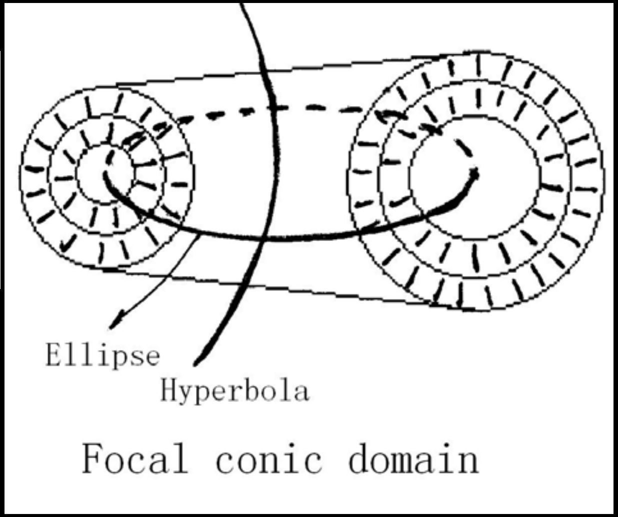
- Puzzle

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

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

$$\delta F = 0 \quad \Downarrow$$

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

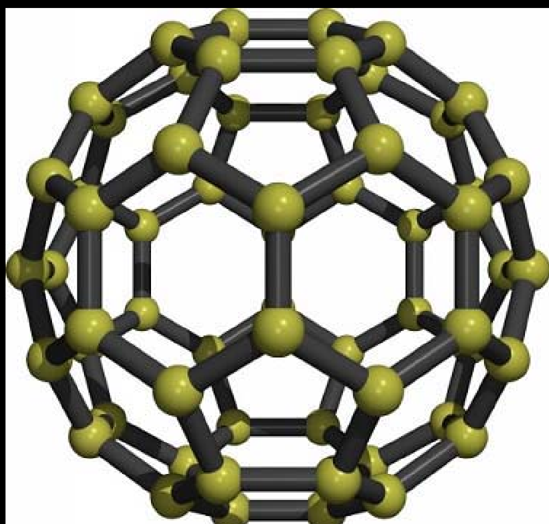
$$(\nabla^2/2 + 2H^2 - K)\partial \mathcal{E}/\partial H + (\nabla \cdot \tilde{\nabla} + 2KH)\partial \mathcal{E}/\partial K - 2H\mathcal{E} = 0$$

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

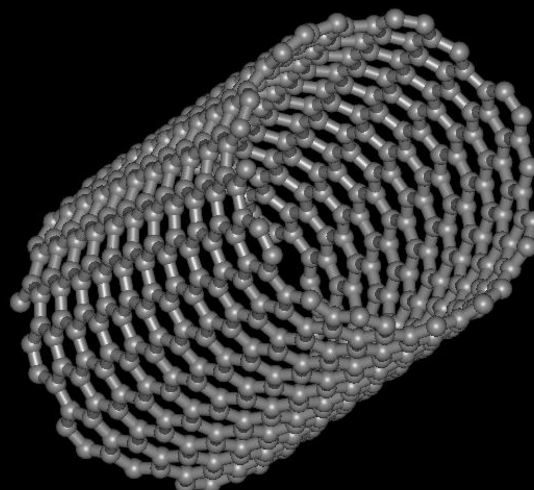
Solving both Eqs. gives good explanation of FCD. [PRE **52** (1995) 2095]

Carbon related structures

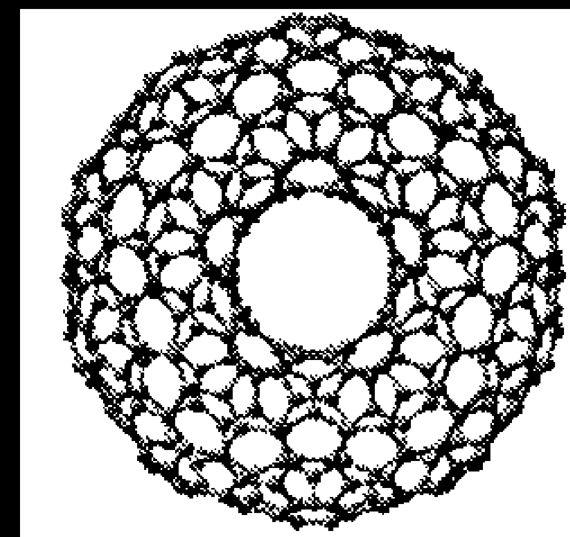
- Three typical structures



C_{60}



SWNT



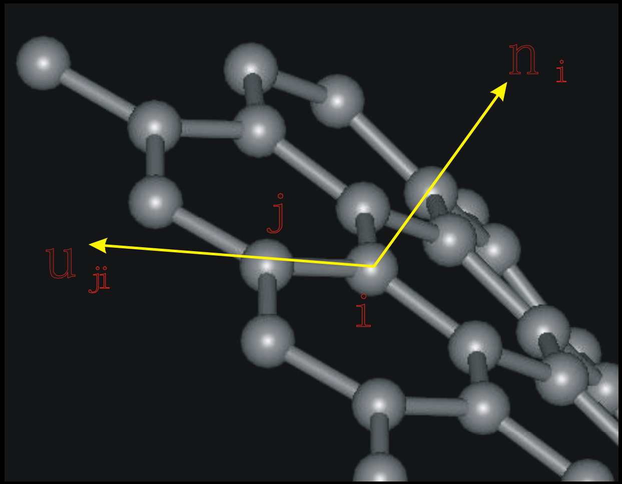
Carbon Torus

- Curvature energy of curved single graphitic layer

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

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

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



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

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

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

- Understanding three typical structures

Surface energy per area

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

$$\delta F = 0$$

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

$$\lambda = 0\text{: } \mathrm{C}_{60},\ \mathrm{Torus}$$

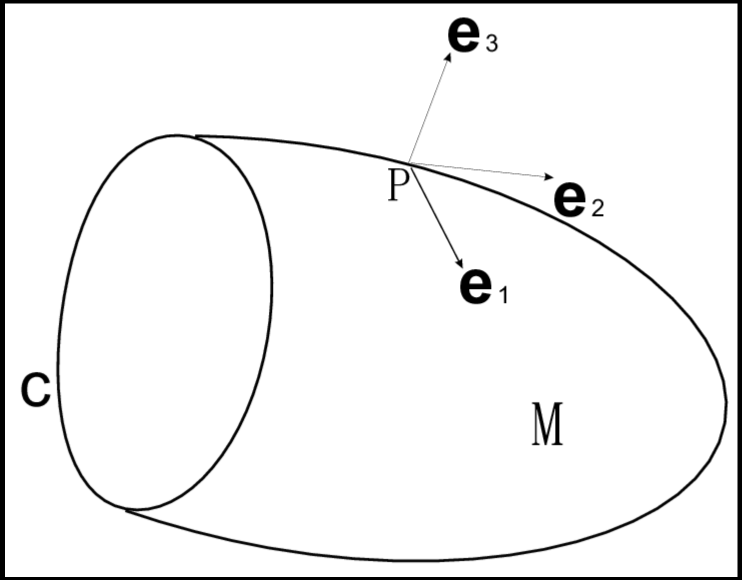
$$R^2 = k_c/2\lambda\text{: } \mathrm{SWNT}$$

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

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

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

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

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:

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

Hodge * and Gaussian mapping

- Hodge *

Basic properties:

$$*f = f\omega_1 \wedge \omega_2;$$

$$*\omega_1 = \omega_2, *\omega_2 = -\omega_1;$$

$$d * df = \nabla^2 f\omega_1 \wedge \omega_2$$

The second Green identity:

$$\int_M (fd * dh - hd * df) = \int_{\partial M} (f * dh - h * df)$$

[Westenholz *Differential Forms in Mathematical Physics*]

- Gaussian mapping

Gaussian mapping $\mathcal{G}: M \to S^2; \mathcal{G}(\mathbf{r}) = \mathbf{e}_3(\mathbf{r})$

Induced mapping $\mathcal{G}^\star : \Lambda^1 \to \Lambda^1$

$$\mathcal{G}^\star \omega_1 = \omega_{13},\ \mathcal{G}^\star \omega_2 = \omega_{23}$$

Define new differential operator $\tilde{d} = \mathcal{G}^\star d$

Define $\tilde{*}$: $\tilde{*}\omega_{13} = \omega_{23}, \tilde{*}\omega_{23} = -\omega_{13}$

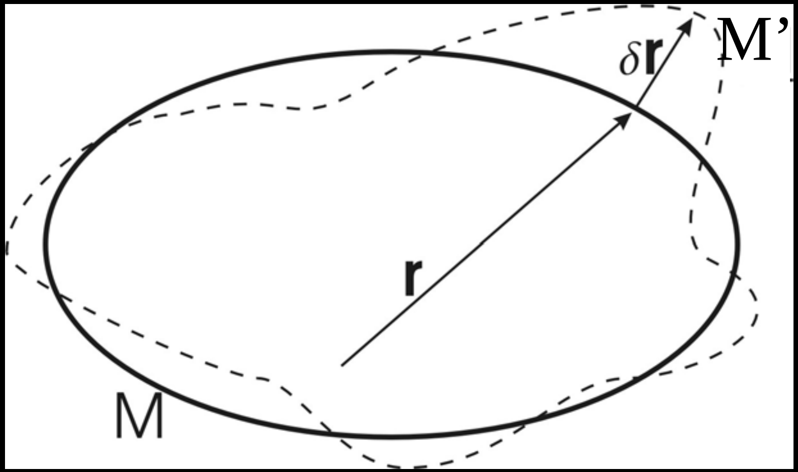
Lemma: $\int_M (f d\tilde{*}\tilde{d}h - h d\tilde{*}\tilde{d}f) = \int_{\partial M} (f\tilde{*}\tilde{d}h - h\tilde{*}df)$

Define $\nabla \cdot \tilde{\nabla}$: $d\tilde{*}\tilde{d}f = \nabla \cdot \tilde{\nabla} f \omega_1 \wedge \omega_2$

Variational theory of surface

- What is surface variation?

Each point undergoes an infinitesimal displacement



$$\delta \mathbf{r} = \delta_1 \mathbf{r} + \delta_2 \mathbf{r} + \delta_3 \mathbf{r}$$

$$\delta_i \mathbf{r} = \underbrace{\Omega_i \mathbf{e}_i}_{\text{Not use Einstein summation convention}} \quad (i = 1, 2, 3)$$

- Variation of general function on a surface

If f is a generalized function of $\mathbf{r}$ (including scalar function, vector function, and r-form dependent on point $\mathbf{r}$), define

$$\delta_i^{(q)} f = (q!)\mathcal{L}^{(q)}[f(\mathbf{r}+\delta_i\mathbf{r}) - f(\mathbf{r})] \quad (i = 1, 2, 3; q = 1, 2, 3, \cdots)$$

q-order variation of f

$$\delta^{(q)} f = (q!)\mathcal{L}^{(q)}[f(\mathbf{r}+\delta\mathbf{r}) - f(\mathbf{r})] \quad (q = 1, 2, 3, \cdots)$$

$\mathcal{L}^{(q)}[\cdots]$: $\Omega_1^{q_1}\Omega_2^{q_2}\Omega_3^{q_3}$ in Taylor series
$q_1 + q_2 + q_3 = q$
q_1, q_2, q_3 being non-negative integers.

Basic properties

(i) $\delta_i^{(q)}$ and $\delta^{(q)}$ $(i = 1, 2, 3; q = 1, 2, \cdots)$ are linear operators;

(ii) $\delta_1^{(1)}$, $\delta_2^{(1)}$, $\delta_3^{(1)}$ and $\delta^{(1)}$ are commutative with each other;

(iii) $\delta_i^{(q+1)} = \delta_i^{(1)}\delta_i^{(q)}$ and $\delta^{(q+1)} = \delta^{(1)}\delta^{(q)}$,
thus we can safely replace $\delta_i^{(1)}$, $\delta_i^{(q)}$, $\delta^{(1)}$, and $\delta^{(q)}$ by
δ_i, δ_i^q, δ, and δ^q $(q = 2, 3, \cdots)$, respectively;

(iv) For functions f and g,
$\delta_i[f(\mathbf{r}) \circ g(\mathbf{r})] = \delta_i f(\mathbf{r}) \circ g(\mathbf{r}) + f(\mathbf{r}) \circ \delta_i g(\mathbf{r})$,
where $\circ$ represents the ordinary production,
vector production or exterior production;

(v) $\delta_i f[g(\mathbf{r})] = (\partial f/\partial g)\delta_i g$; (vi) $\delta^q = (\delta_1 + \delta_2 + \delta_3)^q$.

- Variational equation of frame

$$\delta_l \mathbf{e}_i = \Omega_{lij}\mathbf{e}_j, \Omega_{lij} = -\Omega_{lji} \qquad d\delta_l = \delta_l d$$

$$\boxed{\begin{aligned} \delta_1\omega_1 &= d\Omega_1 - \omega_2\Omega_{121}, \\ \delta_1\omega_2 &= \Omega_1\omega_{12} - \omega_1\Omega_{112}, \\ \Omega_{113} &= a\Omega_1, \quad \Omega_{123} = b\Omega_1 \end{aligned}}$$

$$\boxed{\begin{aligned} \delta_2\omega_1 &= \Omega_2\omega_{21} - \omega_2\Omega_{221}, \\ \delta_2\omega_2 &= d\Omega_2 - \omega_1\Omega_{212}, \\ \Omega_{213} &= b\Omega_2, \quad \Omega_{223} = c\Omega_2 \end{aligned}}$$

$$\boxed{\begin{aligned} &\delta_3\omega_1 = \Omega_3\omega_{31} - \omega_2\Omega_{321}, \\ &\delta_3\omega_2 = \Omega_3\omega_{32} - \omega_1\Omega_{312}, \\ &d\Omega_3 = \Omega_{313}\omega_1 + \Omega_{323}\omega_2; \end{aligned}}$$

$$\boxed{\delta_l\omega_{ij} = d\Omega_{lij} + \Omega_{lik}\omega_{kj} - \omega_{ik}\Omega_{lkj}}$$

Variational problem on closed surface

- Functional

$$\mathcal{F} = \int_M \mathcal{E}(2H[\mathbf{r}], K[\mathbf{r}])dA + \Delta p \int_V dV$$

$$\delta\mathcal{F} = \delta_1\mathcal{F} + \delta_2\mathcal{F} + \delta_3\mathcal{F}$$

- Lemmas

$$\delta_3 dA = -(2H)\Omega_3 dA \qquad \delta_3 \int_V dV = \int_M \Omega_3 dA$$

$$\delta_3(2H)dA = 2(2H^2 - K)\Omega_3 dA + d * d\Omega_3$$

$$\delta_3 K dA = 2KH\Omega_3 dA + d\tilde{*}\tilde{d}\Omega_3 \qquad \delta_1\mathcal{F} = \delta_2\mathcal{F} = 0$$

- Euler-Lagrange equation

$$\left[\left(\nabla^2 + 4H^2 - 2K\right)\frac{\partial}{\partial(2H)} + \left(\nabla\cdot\tilde{\nabla} + 2KH\right)\frac{\partial}{\partial K} - 2H\right]\mathcal{E} + \Delta p = 0.$$

$$\mathcal{E} = \frac{k_c}{2}(2H + c_0)^2 + \bar{k}K + \lambda$$

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

- Second order variation

if $\partial \mathcal{E}/\partial K = \bar{k} = const.$

$$\begin{aligned}
\delta^2\mathcal{F} &= (\delta_1^2 + \delta_2^2 + \delta_3^2 + 2\delta_1\delta_2 + 2\delta_1\delta_3 + 2\delta_2\delta_3) \\
&= \int_M \Omega_3^2 \left[(4H^2 - 2K)^2 \frac{\partial^2 \mathcal{E}_H}{\partial(2H)^2} - 4HK\frac{\partial \mathcal{E}_H}{\partial(2H)} + 2K\mathcal{E}_H - 2Hp\right] dA \\
&\quad + \int_M \Omega_3 \nabla^2 \Omega_3 \left[4H\frac{\partial \mathcal{E}_H}{\partial(2H)} + 4(2H^2 - K)\frac{\partial^2 \mathcal{E}_H}{\partial(2H)^2} - \mathcal{E}_H\right] dA \\
&\quad - \int_M \frac{4\partial \mathcal{E}_H}{\partial(2H)} \Omega_3 \nabla \cdot \tilde{\nabla}\Omega_3 dA + \int_M \frac{\partial^2 \mathcal{E}_H}{\partial(2H)^2}(\nabla^2\Omega_3)^2 dA \\
&\quad + \int_M \frac{\partial \mathcal{E}_H}{\partial(2H)} \left[\nabla(2H\Omega_3) \cdot \nabla\Omega_3 - 2\nabla\Omega_3 \cdot \tilde{\nabla}\Omega_3\right] dA
\end{aligned}$$

$$\mathcal{E}_H = \mathcal{E} - \bar{k}K$$

Variational problem on open surface

- Functional

$$\mathcal{F} = \int_M \mathcal{E}(2H[\mathbf{r}], K[\mathbf{r}])dA + \int_C \Gamma(k_n, k_g)ds$$

- Euler-Lagrange equation

Equilibrium surface equation

$$(\nabla^2 + 4H^2 - 2K)\frac{\partial \mathcal{E}}{\partial(2H)} + (\nabla \cdot \tilde{\nabla} + 2KH)\frac{\partial \mathcal{E}}{\partial K} - 2H\mathcal{E} = 0$$

- Boundary conditions

$$\mathbf{e}_2 \cdot \nabla \left[\frac{\partial \mathcal{E}}{\partial (2H)} \right] + \mathbf{e}_2 \cdot \tilde{\nabla} \left(\frac{\partial \mathcal{E}}{\partial K} \right) - \frac{d}{ds} \left(\tau_g \frac{\partial \mathcal{E}}{\partial K} \right) + \frac{d^2}{ds^2} \left(\frac{\partial \Gamma}{\partial k_n} \right) + \frac{\partial \Gamma}{\partial k_n} (k_n^2 - \tau_g^2)$$
$$+ \tau_g \frac{d}{ds} \left(\frac{\partial \Gamma}{\partial k_g} \right) + \frac{d}{ds} \left(\tau_g \frac{\partial \Gamma}{\partial k_g} \right) - \left(\Gamma - \frac{\partial \Gamma}{\partial k_g} k_g \right) k_n \bigg|_C = 0,$$

$$- \frac{\partial \mathcal{E}}{\partial (2H)} - k_n \frac{\partial \mathcal{E}}{\partial K} + \frac{\partial \Gamma}{\partial k_g} k_n - \frac{\partial \Gamma}{\partial k_n} k_g \bigg|_C = 0,$$
$$\frac{d^2}{ds^2} \left(\frac{\partial \Gamma}{\partial k_g} \right) + K \frac{\partial \Gamma}{\partial k_g} - k_g \left(\Gamma - \frac{\partial \Gamma}{\partial k_g} k_g \right) + 2(k_n - H) k_g \frac{\partial \Gamma}{\partial k_n}$$

$$- \tau_g \frac{d}{ds} \left(\frac{\partial \Gamma}{\partial k_n} \right) - \frac{d}{ds} \left(\tau_g \frac{\partial \Gamma}{\partial k_n} \right) - \mathcal{E} \bigg|_C = 0.$$

Morphological problems of lipid bilayers

Lipid vesicles

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

- Sphere $$\Delta p R^2 + 2\lambda R - k_c c_0 (2 - c_0 R) = 0$$

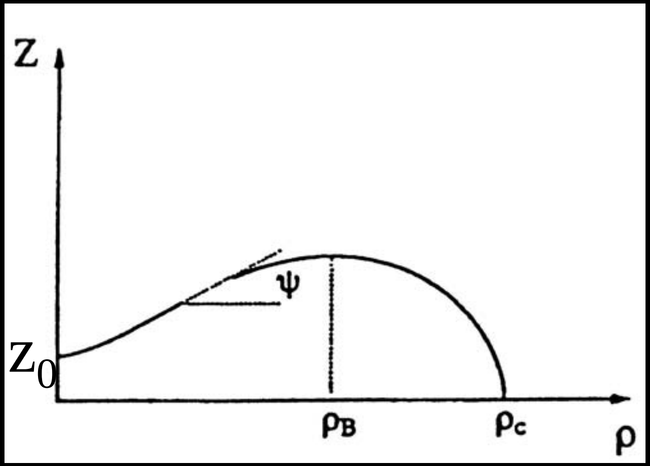
1 root: If $(2\lambda + k_c c_0^2)^2 + 8 \Delta p k_c c_0 = 0$

2 roots: If $(2\lambda + k_c c_0^2)^2 + 8 \Delta p k_c c_0 > 0$

- Red blood cell---biconcave shape

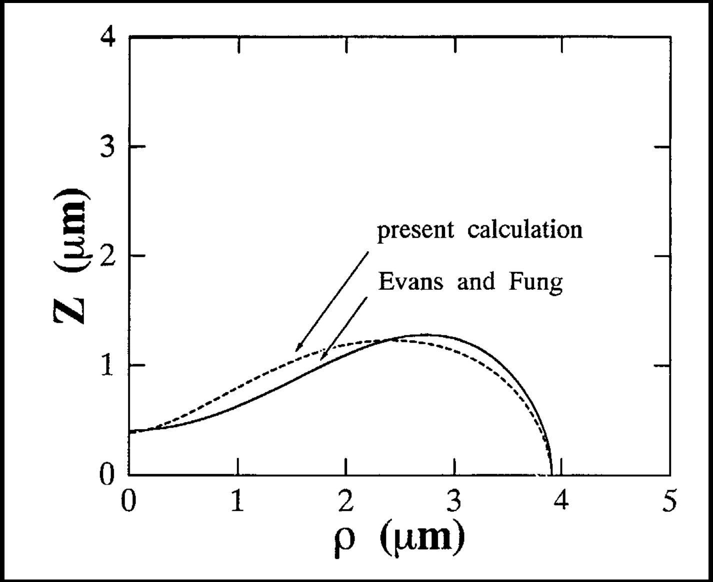
$$z = z_0 + \int_0^{\rho} \tan\psi(\rho')d\rho'$$

$$\sin\psi(\rho) = c_0\rho\ln(\rho/\rho_B), c_0 < 0$$

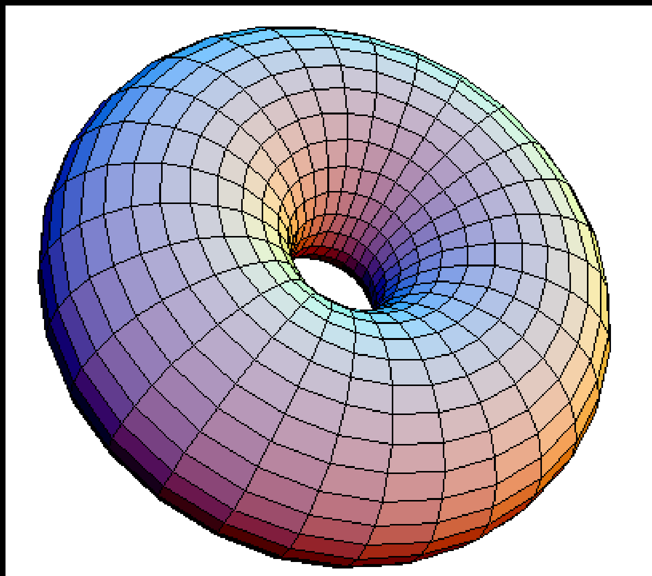


[Ou-Yang, Hu J.G., & Liu J.X. 1992]

[Evans & Fung, Microvasc. Res. **4** (1972) 335]

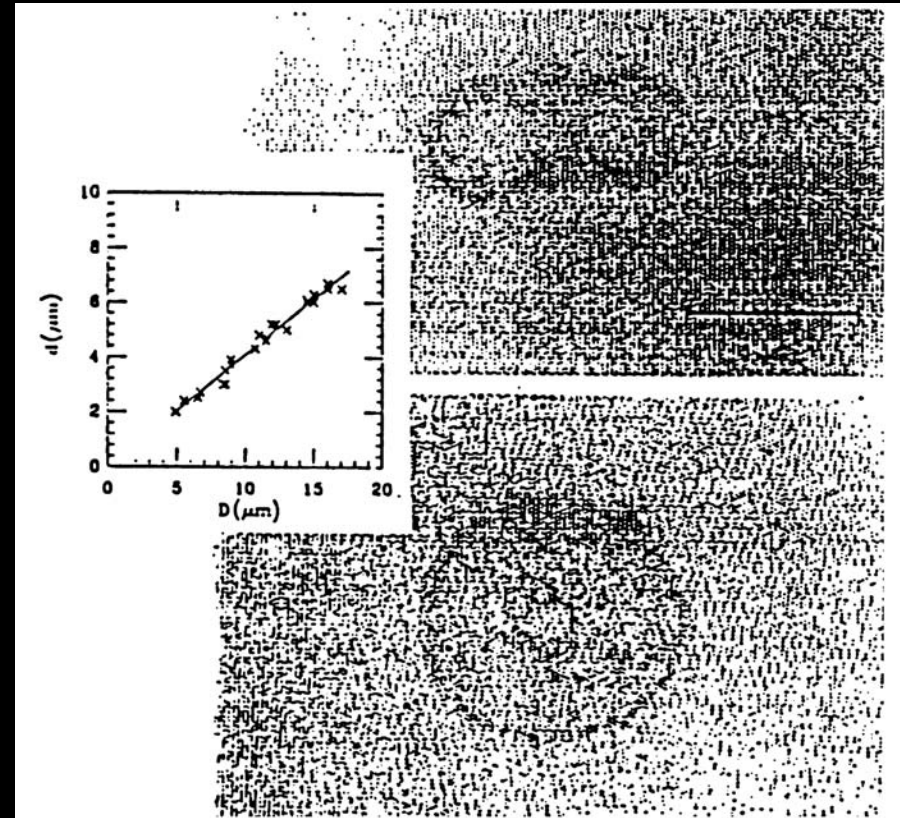


- Torus



$$R/r=\sqrt{2}$$

[Ou-Yang 1990 PRA **41** 4517]



Confirmed by experiments:

- M. Muty & D. Bensimon, PRA, 1991, 24 tori;
- A.S. Rudolph et al, Nature, 1991, in Phospholipid membrane;
- Z. Lin et al, Langmuir, 1994, in Micelles.

Open lipid bilayers

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

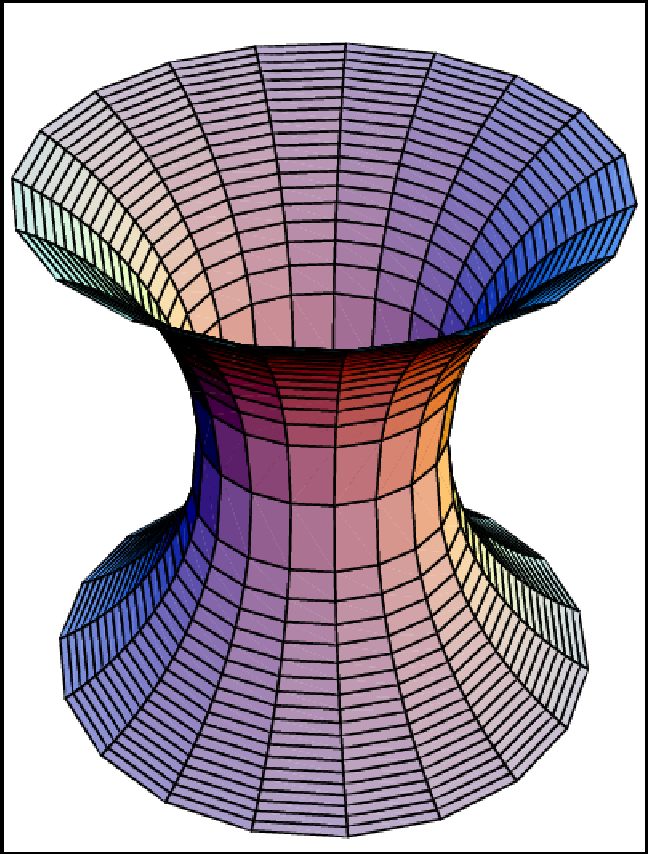
$$\left[k_c(2H + c_0) + \bar{k} k_n\right]\Big|_C = 0$$

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

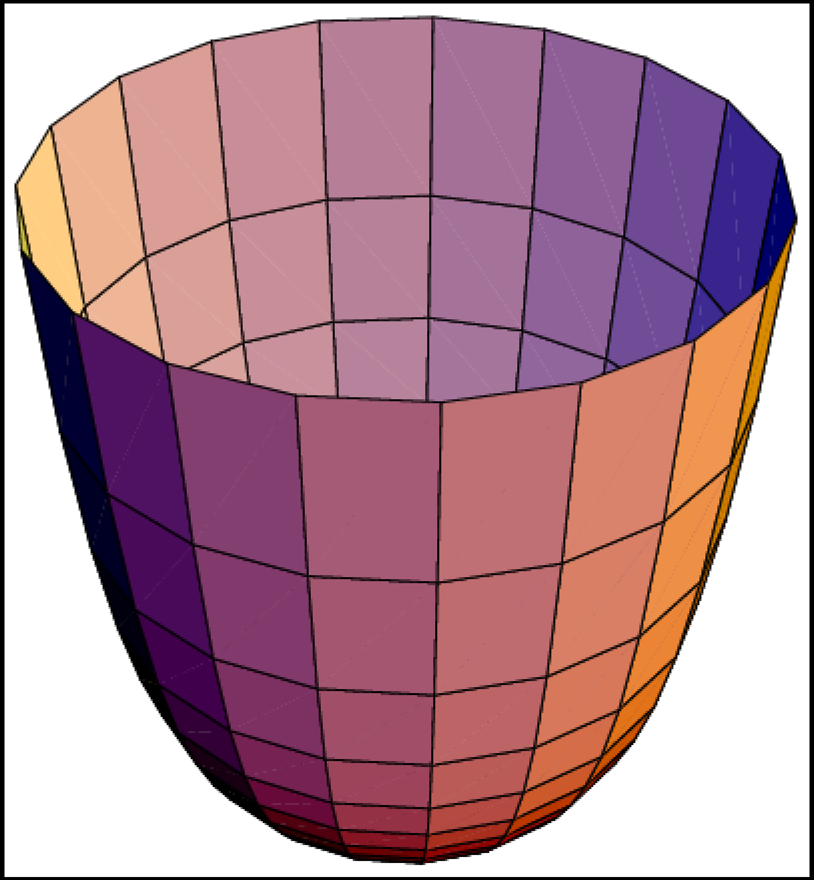
$$\left[\frac{k_c}{2}(2H + c_0)^2 + \bar{k} K + \lambda + \gamma k_g\right]\Bigg|_C = 0$$

- No axisymmetric constant mean curvature surface with edges

- Central part of the torus



- Cuplike membrane



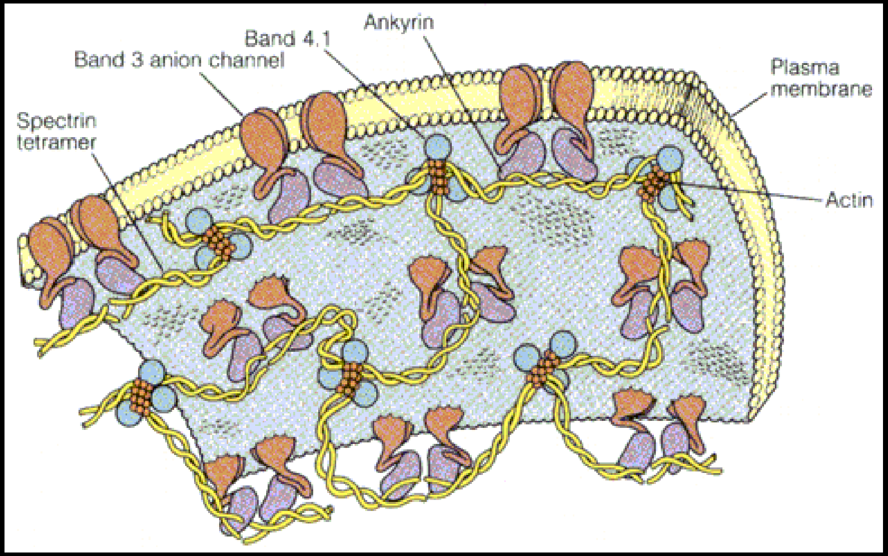
[Tu & Ou-Yang PRE **68** (2003) 61915]

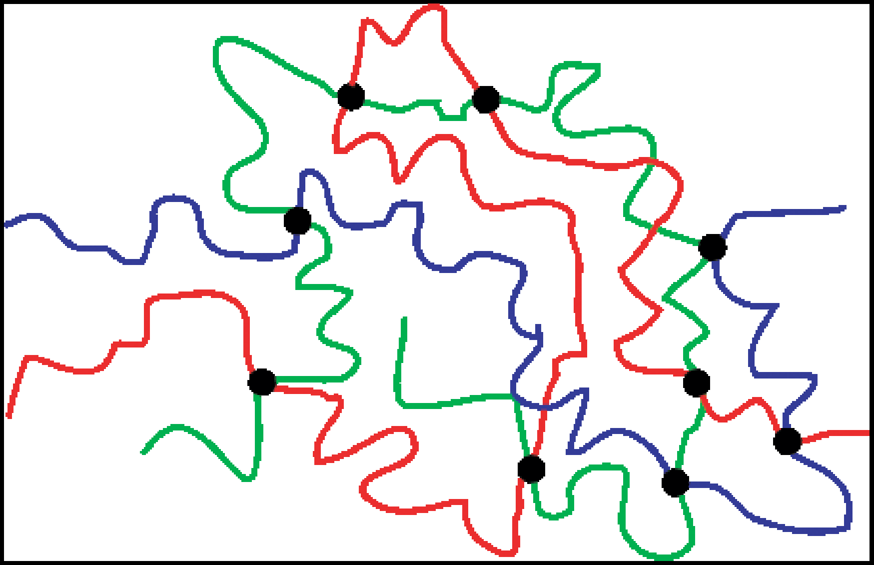
Elasticity and stability of cell membranes

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

Simplified model

- Cell membrane=lipid bilayer+membrane skeleton
- Membrane skeleton = cross-linking protein network = rubber membrane





[Schematic structure of MSK (left) and rubber (right) at molecular levels]

Free energy

$$\mathcal{F} = \int_M (\mathcal{E}_d + \mathcal{E}_H) dA + p \int_V dV$$

$$\mathcal{E}_H = (k_c/2)(2H + c_0)^2 + \lambda$$

$$\mathcal{E}_d = (k_d/2)[(2J)^2 - Q]$$

$$2J = \varepsilon_{11} + \varepsilon_{22},\ Q = \varepsilon_{11}\varepsilon_{22} - \varepsilon_{12}^2$$

Small deformation; remain to the second order terms

shape equation and in-plane strain equations

- Shape equation

$$p - 2H(\lambda + k_d J) + k_c(2H + c_0)(2H^2 - c_0 H - 2K)$$
$$+ k_c \nabla^2 (2H) - \frac{k_d}{2}(a\varepsilon_{11} + 2b\varepsilon_{12} + c\varepsilon_{22}) = 0$$

- In-plane strain equations

$$k_d[-d(2J) \wedge \omega_2 - \frac{1}{2}(\varepsilon_{11} d\omega_2 - \varepsilon_{12} d\omega_1) + \frac{1}{2} d(\varepsilon_{12}\omega_1 + \varepsilon_{22}\omega_2)] = 0$$
$$k_d[d(2J) \wedge \omega_1 - \frac{1}{2}(\varepsilon_{12} d\omega_2 - \varepsilon_{22} d\omega_1) - \frac{1}{2} d(\varepsilon_{11}\omega_1 + \varepsilon_{12}\omega_2)] = 0$$

- Special example: spherical cell membrane with homogenous strains

$$\varepsilon_{12} = 0,\ \varepsilon_{11} = \varepsilon_{22} = \varepsilon = \text{constant};$$

$$pR^2 + (2\lambda + 3k_d\varepsilon)R + k_c c_0(c_0 R - 2) = 0$$

R is the radius of the spherical surface

Mechanical stability

- 2nd order variation of free energy (sphere)

$$\Omega_1\omega_1 + \Omega_2\omega_2 = d\Omega + *d\chi$$ (Hodge decomposed theorem)

$$\delta^2\mathcal{F} = G_1 + G_2$$

$$\begin{aligned} G_1 &= \int \Omega_3^2(3k_d/R^2 + 2k_c c_0/R^3 + p/R)dA \\ &+ \int \Omega_3\nabla^2\Omega_3(k_c c_0/R + 2k_c/R^2 + pR/2)dA + \int k_c(\nabla^2\Omega_3)^2 dA \\ &+ \frac{3k_d}{R}\int \Omega_3\nabla^2\Omega dA + k_d\int \left(\nabla^2\Omega\right)^2 dA + \frac{k_d}{2R^2}\int \Omega\nabla^2\Omega dA \\ G_2 &= \frac{k_d}{4}\int (\nabla^2\chi)^2 dA + \frac{k_d}{2R^2}\int \chi\nabla^2\chi dA \geq 0 \end{aligned}$$

- Expansion of spherical harmonic functions

$$\Omega_3 = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} a_{lm} Y_{lm}(\theta, \phi), \; a_{lm}^* = (-1)^m a_{l,-m}$$

$$\Omega = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} b_{lm} Y_{lm}(\theta, \phi), \; b_{lm}^* = (-1)^m b_{l,-m}$$

$$\begin{aligned} G_1 \;=\; & \sum_{l=0}^{\infty} \sum_{m=0}^{l} 2|a_{lm}|^2 \{3k_d + [l(l+1) - 2][l(l+1)k_c/R^2 - k_c c_0/R - pR/2] \\ & - \sum_{l=0}^{\infty} \sum_{m=0}^{l} \frac{3k_d}{R} l(l+1)(a_{lm}^* b_{lm} + a_{lm} b_{lm}^*) \\ & + \sum_{l=0}^{\infty} \sum_{m=0}^{l} \frac{k_d}{R^2} \left[2l^2(l+1)^2 - l(l+1)\right] |b_{lm}|^2 \end{aligned}$$

Quadratic form

Critical pressure

If $p < p_l = \frac{3k_d}{[2l(l+1)-1]R} + \frac{2k_c[l(l+1)-c_0R]}{R^3} \quad (l = 2, 3, \cdots)$

then G_1 is positive definite.

$$p_c = \min\{p_l\} = \begin{cases} \frac{3k_d}{11R} + \frac{2k_c[6-c_0R]}{R^3} < \frac{k_c[23-2c_0R]}{R^3}, & (3k_dR^2 < 121k_c) \\ \\ \frac{2\sqrt{3k_dk_c}}{R^2} + \frac{k_c}{R^3}(1-2c_0R), & (3k_dR^2 > 121k_c) \end{cases}$$

- k_d=0, $p_c = \frac{2k_c(6-c_0R)}{R^3}$, ~ spherical lipid vesicle [Ou-Yang & Helfrich 1987 *PRL* 59 2486]

- Classic shell: c_0=0, $k_d \sim Yh$, $k_c \sim Yh^3$, $R >> h$, $p_c \sim Yh^2/R^2$

- Membrane skeleton enhances the mechanical stability of cell membranes, at least for spherical shape

Taking typical data of cell membrane,
$k_c \sim 20 k_B T$ [Duwe *et al.* 1990 *J. Phys. Fr.* **51** 945],
$k_d \sim 6 \times 10^{-4} k_B T/nm^2$ [Lenormand *et al.* 2001 *Biophys. J.* **81** 43],
$h \sim 4nm$, $R \sim 1\mu m$, $c_0 R \sim 1$, we have $p_c \sim 2$ Pa.
If not considering k_d, we have $p_c \sim 0.2$ Pa.

Summary

- Several problems in the elasticity of biomembranes, smectic-A liquid crystal, and carbon related structures are discussed
- Variational problems on 2D surface are dealt with exterior differential forms
- Elasticity and stability of lipid bilayer and cell membrane are calculated and compared with each other.

Acknowledgement

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Thank you for your attention!