Free Energy Representation for surfaces w/ fluid symmetry

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Sources:

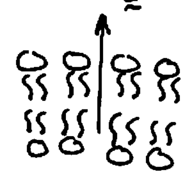
1. Steigmann, D.J. Fluid films w/ curvature elasticity. Arch. Rational Mech. Anal. 150 (1999) 127-152 (mostly section 4, 135-140)

2. Jenkins, J.T. The equations of mechanical equilibrium of a model membrane. SIAM J. Appl. Math Vol32 #4 1977

3. Prof. Healey's notes on 1

Free Energy Representation for surfaces w/ fluid symmetry

Motivation: Lipid Membranes

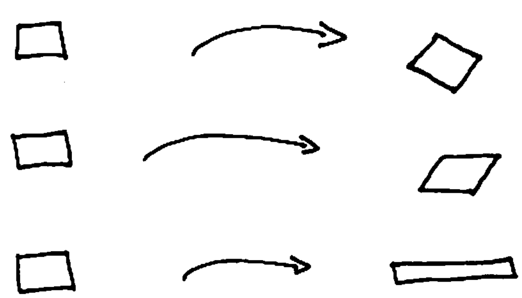


- phosphate hydrophilic heads
- fatty acid hydrophobic tails
- Function
  - protective barrier
  - transport bio-matter
- Constraints
  - director remains normal to surface $\qquad \underset{\sim}{a}_\alpha \cdot \underset{\sim}{d} = 0$
  - director has unit length $\underset{\sim}{d} \cdot \underset{\sim}{d} = 1 \qquad \underset{\sim}{d} = \underset{\sim}{n}$
- Symmetry
  - unimodular transformations in surface plane
    - density preserving
    - 2-D fluid

$$\underline{\underline{H}} : T_X \longrightarrow T_X \quad \ni \quad \det \underline{\underline{H}} = 1$$

where T_X is tangent plane of ref. config.

Ex



rotation

shear

elongation

Rationale:

- Lipids free to move relative to eachother
- Hydrophobic interactions enforce density preservation

Claim: Surfaces w/ fluid symmetry have free energy of the form

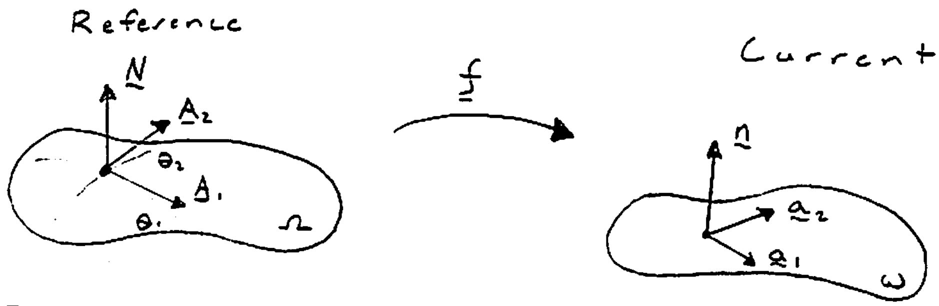
$$\mathcal{W} = \mathcal{W}(J, H, K)$$

where $J \equiv \sqrt{\frac{a}{A}}$ area ratio, $H = \frac{1}{2}\,\mathrm{tr}\,\underline{\underline{b}}$ mean curvature (curvature tensor)

$K = \det \underline{\underline{b}}$ Gaussian curvature

Hit Parade

$$\text{(Hyp)}\quad \mathcal{W}(\underline{\underline{F}}, \underline{\underline{b}}) \xrightarrow{(MO)} \underline{\Phi}(\underline{\underline{C}}, \underline{\underline{K}}) \xrightarrow{(MS)} \mathcal{I}(J, H, K)$$



$\Omega \subset \mathbb{R}^2$

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embedded in $\mathbb{E}^3$

$\underline{X} = \underline{X}(\theta^\alpha) \qquad \alpha = 1, 2 \qquad \underline{x} = \underline{f}(\underline{X}(\theta^\alpha))$

$$\theta^\alpha \rightarrow \theta^\alpha + \varepsilon \lambda^\alpha$$

$$\frac{d\underline{x}}{d\theta^\alpha}\lambda^\alpha = \frac{d}{d\varepsilon}\Big[\underline{f}(\underline{X}(\theta^\alpha + \varepsilon\lambda^\alpha))\Big]\Big|_{\varepsilon = 0}$$

$$= \frac{\partial \underline{f}}{\partial \underline{X}} \frac{\partial \underline{X}}{\partial \theta^\alpha} \lambda^\alpha$$

$$\Rightarrow \boxed{\underline{a}_\alpha = \underline{\underline{F}}\,\underline{A}_\alpha}$$

$\underline{a}_\alpha \equiv \frac{d\underline{x}}{d\theta^\alpha} \qquad \underline{A}_\alpha \equiv \frac{\partial \underline{X}}{\partial \theta^\alpha}$

$\underline{\underline{F}} \equiv \nabla \underline{f} : \quad T_{\underline{X}} \longrightarrow T_{x}$

Surface component of deformation

$$\underline{\underline{F}} = \underline{a}_\alpha \otimes \underline{A}^\alpha$$

$$\underline{N} = \frac{\underline{A}_1 \times \underline{A}_2}{|\underline{A}_1 \times \underline{A}_2|}$$

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given by tangent vectors due to $\underline{a}_\nu \cdot \underline{d} = 0$

Effect of change in normal direction

$$\Theta^\beta \to \Theta^\beta + \varepsilon \lambda^\beta$$

$$\underline{a}_{\alpha,\beta} \lambda^\beta = \frac{d}{d\varepsilon}\left[\frac{\partial \underline{f}}{\partial \underline{X}}\left(\underline{X}(\Theta^\beta + \varepsilon\lambda^\beta)\right) \frac{\partial \underline{X}}{\partial \Theta^\alpha}\left(\underline{X}(\Theta^\beta + \varepsilon\lambda^\beta)\right)\right]\Bigg|_{\varepsilon=0}$$

$$= \frac{\partial^2 \underline{f}}{\partial \underline{X}^2} \frac{\partial \underline{X}}{\partial \Theta^\alpha} \frac{\partial \underline{X}}{\partial \Theta^\beta} \lambda^\beta + \frac{\partial \underline{f}}{\partial \underline{X}} \frac{\partial^2 \underline{X}}{\partial \Theta^\alpha \partial \Theta^\beta} \lambda^\beta$$

$$\underline{a}_{\alpha,\beta} = \nabla\nabla \underline{f}\,[\underline{A}_\alpha \otimes \underline{A}_\beta] + \nabla \underline{f}\, \underline{A}_{\alpha,\beta}$$

$$\underline{\underline{b}} = (\underset{\sim}{n} \cdot \underline{a}_{\alpha,\beta})\, \underline{a}^\alpha \otimes \underline{a}^\beta \quad \text{- curvature tensor}$$

$$\underline{\underline{b}} = b_{\alpha\beta}\, \underline{a}^\alpha \otimes \underline{a}^\beta \qquad \underline{\underline{b}} \in \mathrm{Sym}(\mathbb{E}^2)$$

(continuity of mixed 2nd partials)

$$\boxed{b_{\alpha\beta} \equiv \underset{\sim}{n} \cdot \underline{a}_{\alpha,\beta} = -\underset{\sim}{n}_{,\alpha} \cdot \underline{a}_\beta}$$

p.f.

$$\underset{\sim}{n} \cdot \underline{a}_\beta \equiv 0$$

$$\underset{\sim}{n}_{,\alpha} \cdot \underline{a}_\beta + \underset{\sim}{n} \cdot \underline{a}_{\beta,\alpha} = 0$$

$$\underline{n} \cdot \underline{a}_{\alpha,\beta} = -\underset{\sim}{n}_{,\alpha} \cdot \underline{a}_\beta$$

Hyperelasticity

$$W = W(\underline{\underline{F}}, \underline{\underline{b}}) \qquad \text{Free Energy fn Deformation}$$

(MO)

$$W(\underline{\underline{F}}, \underline{\underline{b}}) = W(\underline{\underline{Q}}\,\underline{\underline{F}}, \underline{\underline{Q}}\,\underline{\underline{b}}\,\underline{\underline{Q}}^T) \quad \forall\, \underline{\underline{Q}} \in SO(3)$$

Define deformation in ref config.

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} \quad - \text{ Right Cauchy-Green surface strain tensor}$$

$$= (\underline{A}^\alpha \otimes \underline{a}_\alpha)\cdot(\underline{a}_\beta \otimes \underline{A}^\beta) \qquad \mathbf{C} : T_X \longrightarrow T_X^D$$

(Dual space)

$$= a_{\alpha\beta}\, \underline{A}^\alpha \otimes \underline{A}^\beta \qquad a_{\alpha\beta} \text{ - metric tensor}$$

(1st Fund. Form)

$$\mathbf{K} = \mathbf{F}^T \mathbf{b}\, \mathbf{F} \quad - \text{ relative curvature tensor}$$

$$= b_{\gamma\lambda}\, (\underline{A}^\alpha \otimes \underline{a}_\alpha)\, \underline{a}^\gamma \otimes \underline{a}^\lambda (\underline{a}_\beta \otimes \underline{A}^\beta)$$

$$= b_{\gamma\lambda}\, \underline{A}^\alpha \otimes \underline{A}^\beta\, \delta^\lambda_\beta\, \delta^\gamma_\alpha$$

$$= b_{\alpha\beta}\, \underline{A}^\alpha \otimes \underline{A}^\beta$$

Objective ?

$$\mathbf{F} \rightarrow \mathbf{Q}\mathbf{F}$$

$$\mathbf{b} \rightarrow \mathbf{Q}\,\mathbf{b}\,\mathbf{Q}^T$$

$$\mathbf{C} \rightarrow \mathbf{F}^T \overset{\mathbf{I}}{\cancel{\mathbf{Q}^T\mathbf{Q}}}\, \mathbf{F} = \mathbf{F}^T\mathbf{F} = \mathbf{C}$$

$$\mathbf{K} \rightarrow \mathbf{F}^T \overset{\mathbf{I}}{\cancel{\mathbf{Q}^T\mathbf{Q}}}\, \mathbf{b}\, \overset{\mathbf{I}}{\cancel{\mathbf{Q}^T\mathbf{Q}}}\, \mathbf{F} = \mathbf{F}^T\mathbf{b}\,\mathbf{F} = \mathbf{K}$$

$$\Rightarrow \boxed{W(\mathbf{F}, \mathbf{b}) = W(\mathbf{C}, \mathbf{K})}$$

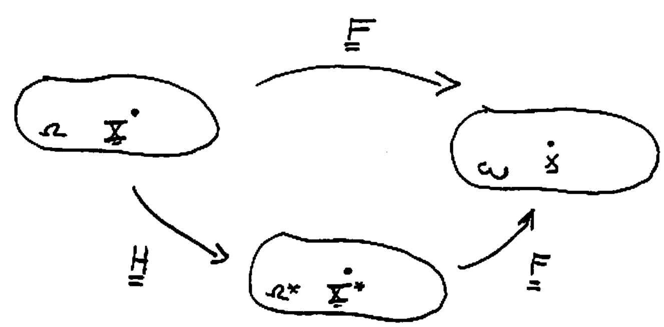
Material Symmetry

"Arm-chair Experiment"

1. Apply deformation s.t. at $\underline{\underline{X}} \in \Omega$, we have "strains" $\underline{\underline{C}}$ & $\underline{\underline{K}}$ "Measure" $W(\underline{\underline{C}}, \underline{\underline{K}})$

2. a) Perform a unimodular (density preserving) deformation at $\underline{\underline{X}}$

   b) apply deformation of 1



$$\underline{x} = \underline{f}\left(\underline{\underline{H}}\left(\underline{\underline{X}}(\theta^\alpha)\right)\right) \qquad \det \underline{\underline{H}} = 1$$

$$\underline{\underline{H}}\Big|_{T_X} : T_X \rightarrow T_X \qquad \Rightarrow \underset{\sim}{N} = \underset{\sim}{N}^*$$

$$\Rightarrow \quad \underline{A}^*_\alpha = \underline{\underline{H}}\,\underline{A}_\alpha \qquad A^*_\alpha, A_\alpha \in T_X$$

Note: Treating Ω & Ω^* as locally flat ref. configs. Intrinsic curvature of arbitrary ref. would introduce discrepancy btw $\underline{\underline{K}}$ & $\underline{\underline{K}}^*$ since $\underline{\underline{B}} \neq \underline{\underline{B}}^*$
($\underline{\underline{B}} = B_{\alpha\beta}\,\underline{A}^\alpha \otimes \underline{A}^\beta \quad \underline{\underline{B}}^* = B^*_{\alpha\beta}\,\underline{A}^{*\alpha} \otimes \underline{A}^{*\beta}$ curvature tensors in Ω & Ω^*)

$$\underline{\underline{F}} \rightarrow \underline{\underline{F}}\,\underline{\underline{H}}$$

$$\underline{\underline{C}} \rightarrow \underline{\underline{H}}^T \underline{\underline{F}}^T \underline{\underline{F}}\,\underline{\underline{H}} = \underline{\underline{H}}^T \underline{\underline{C}}\,\underline{\underline{H}} \qquad \Rightarrow \text{If } W(\underline{\underline{H}}^T\underline{\underline{C}}\,\underline{\underline{H}}, \underline{\underline{H}}^T\underline{\underline{K}}\,\underline{\underline{H}}) = W(\underline{\underline{C}}, \underline{\underline{K}})$$

$$\underline{\underline{K}} \rightarrow \underline{\underline{H}}^T \underline{\underline{F}}^T \underline{\underline{b}}\,\underline{\underline{F}}\,\underline{\underline{H}} = \underline{\underline{H}}^T \underline{\underline{K}}\,\underline{\underline{H}} \qquad \text{then } \underline{\underline{H}} \text{ forms symmetry group}$$

Couch in terms of unimodular isotropic invariants

Isotropy: $\quad W(\mathbf{C}, \mathbf{K}) = W(\mathbf{Q}\mathbf{C}\mathbf{Q}^T, \mathbf{Q}\mathbf{K}\mathbf{Q}) \qquad \forall\ \mathbf{Q} \in O(2)$

$$\Rightarrow \quad W = \Phi(\operatorname{tr}\mathbf{C}, \det\mathbf{C}, \operatorname{tr}\mathbf{K}, \det\mathbf{K}, \mathbf{C}\cdot\mathbf{K})$$

Representation Theory:

Zheng, Q. S. Two-dimensional tensor fn for all kinds of material symmetry. Proc. Roy. Soc. Lond. A443 127-138 1993

Limit ourselves to unimodular invariants

$$\det\mathbf{C} \qquad \det\mathbf{K} \qquad \sigma = \operatorname{tr}\mathbf{C} + \operatorname{tr}\mathbf{K} - \mathbf{C}\cdot\mathbf{K}$$

$$\begin{aligned}\det\mathbf{C} &= \det \mathbf{H}^T\mathbf{C}\mathbf{H} \\ &= \cancel{\det\mathbf{H}^T}^{\,1} \det\mathbf{C}\ \cancel{\det\mathbf{H}}^{\,1} \\ &= \det\mathbf{C}\end{aligned}$$

Similiarly $\det\mathbf{K}$

p.f. of 3rd invariant — Use Caley – Hamilton

$$\left[\mathbf{C}^2 - \operatorname{tr}\mathbf{C}\,\mathbf{C} + \det\mathbf{C}\,\mathbf{I} = 0\right]\mathbf{C}^{-1}$$

$$\mathbf{C} - \operatorname{tr}\mathbf{C}\,\mathbf{I} + \det\mathbf{C}\,\mathbf{C}^{-1} = 0$$

$$\det\mathbf{C}\,\mathbf{C}^{-1}\cdot\mathbf{K} = \operatorname{tr}\mathbf{C}\,\mathbf{I}\cdot\mathbf{K} - \mathbf{C}\cdot\mathbf{K}$$

$$\sigma = \det\mathbf{C}\,\mathbf{C}^{-1}\cdot\mathbf{K} = \operatorname{tr}\mathbf{C} + \operatorname{tr}\mathbf{K} - \mathbf{C}\cdot\mathbf{K}$$

$$\begin{aligned}\Rightarrow \quad \mathbf{C}^{-1}\cdot\mathbf{K} &\overset{?}{=} \operatorname{tr}\left(\mathbf{H}^{-1}\mathbf{C}^{-1}\,\overset{\mathbf{I}}{\cancel{\mathbf{H}^{-T}\mathbf{H}^{T}}}\,\mathbf{K}\,\mathbf{H}\right) \\ &= \operatorname{tr}\left(\overset{\mathbf{I}}{\cancel{\mathbf{H}\mathbf{H}^{-1}}}\,\mathbf{C}^{-1}\mathbf{K}\right) \\ &= \mathbf{C}^{-1}\cdot\mathbf{K}\end{aligned}$$

$$\Rightarrow \quad \boxed{W(\mathbf{C}, \mathbf{K}) = \Psi(\det\mathbf{C}, \sigma(\mathbf{C}, \mathbf{K}), \det\mathbf{K})}$$

Relate invariants to H (mean curvature) & K (Gaussian)

<u>Def</u>: $J = \sqrt{\frac{a}{A}} = \sqrt{\frac{\det a_{\alpha\beta}}{\det A_{\alpha\beta}}}$ – area ratio

$$\det \underline{\underline{C}} = \det\left(a_{\alpha\beta}\, \underline{A}^{\alpha} \otimes \underline{A}^{\beta}\right)$$
$$= \det\left(a_{\alpha\beta}\, A^{\alpha\gamma}\, \underline{A}_{\gamma} \otimes \underline{A}^{\beta}\right)$$
$$= \det(a_{\alpha\beta})\, \det(A^{\alpha\gamma})$$
$$= \frac{\det(a_{\alpha\beta})}{\det(A_{\alpha\gamma})}$$

$$\boxed{\det \underline{\underline{C}} = J^2}$$

<u>Note:</u>
need consistent basis to represent in matrix form

$$\begin{bmatrix} & \end{bmatrix} \underbrace{\begin{Bmatrix} \\ \end{Bmatrix}}_{\underline{A}_{\gamma}} = \underbrace{\begin{Bmatrix} \\ \end{Bmatrix}}_{\underline{A}_{\gamma}}$$

otherwise determinant does not make sense, gives incorrect value (volume for 3-vectors)

$$\det \underline{\underline{K}} = \det\left(b_{\alpha\beta}\, \underline{A}^{\alpha} \otimes \underline{A}^{\beta}\right)$$
$$= \det\left(b_{\alpha\beta}\, A^{\alpha\gamma}\, \underline{A}_{\gamma} \otimes \underline{A}^{\beta}\right)$$
$$= \det\left(a_{\alpha\delta}\, b^{\delta}_{\beta}\, A^{\alpha\gamma}\, \underline{A}_{\gamma} \otimes \underline{A}^{\beta}\right)$$
$$= \frac{\det(a_{\alpha\delta})}{\det(A_{\alpha\gamma})} \det(b^{\delta}_{\beta})$$

$$\boxed{\det \underline{\underline{K}} = J^2 K}$$

<u>Note:</u>
$$\underline{\underline{C}}\, \underline{\underline{C}}^{-1} = a_{\alpha\beta}\, \underline{A}^{\alpha} \otimes \underline{A}^{\beta} \cdot a^{\gamma\lambda}\, \underline{A}_{\gamma} \otimes \underline{A}_{\lambda}$$
$$= a_{\alpha\beta}\, a^{\beta\lambda}\, \underline{A}^{\alpha} \otimes \underline{A}_{\lambda}$$
$$= a_{\alpha\lambda}\, \underline{A}^{\alpha} \otimes \underline{A}_{\lambda}$$
$$= \underline{A}_{\lambda} \otimes \underline{A}_{\lambda}$$
$$= \underline{\underline{I}}$$

$$\sigma = \det \underline{\underline{C}}\; \underline{\underline{C}}^{-1} \cdot \underline{\underline{K}}$$
$$= J^2\, a^{\alpha\beta}\, \underline{A}_{\alpha} \otimes \underline{A}_{\beta} \cdot b_{\gamma\lambda}\, \underline{A}^{\gamma} \otimes \underline{A}^{\lambda}$$
$$= J^2\, a^{\alpha\beta}\, b_{\gamma\lambda}\, \delta^{\gamma}_{\alpha}\, \delta^{\lambda}_{\beta}$$
$$= J^2\, a^{\gamma\beta}\, b_{\gamma\beta}$$
$$= J^2\, b^{\beta}_{\beta}$$

$$\boxed{\det \underline{\underline{K}} = J^2\, 2H}$$

$$\Rightarrow \boxed{W(\underline{\underline{C}}, \underline{\underline{K}}) = \Upsilon(J, H, K)}$$