Symmetries and Solutions of the Membrane Shape Equation

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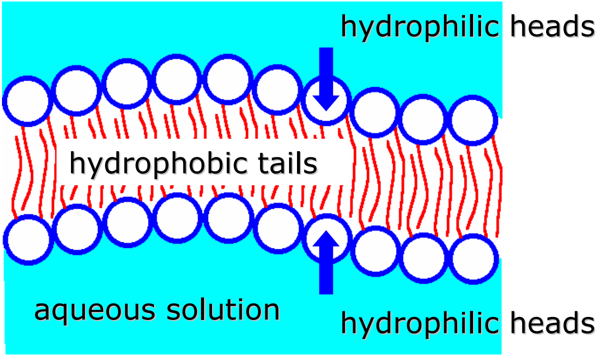
Outline

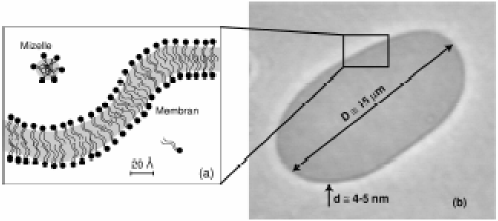
Closed Biomembranes – Vesicles

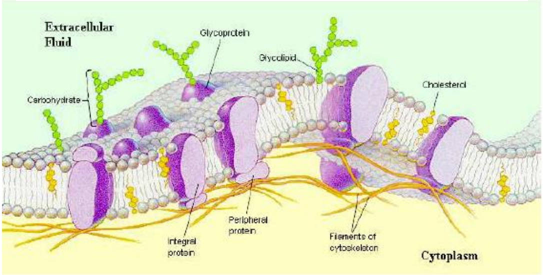
Lipid Vesicles Formation

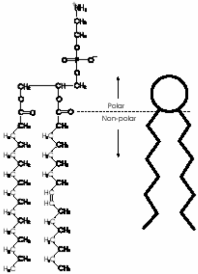
- In aqueous solution, amphiphilic molecules (e.g., phospholipids) may form bilayers, the hydrophilic heads of these molecules being located in both outer sides of the bilayer, which are in contact with the liquid, while their hydrophobic tails remain at the interior.
- A bilayer may form a closed membrane – vesicle. Vesicles constitute a well-defined and sufficiently simple model system for studying basic physical properties of the more complex cell biomembranes.

bilayer


hydrophilic heads
hydrophobic tails
aqueous solution
hydrophilic heads


Mizelle
Membran
(a)
d = 4-5 nm
(b)


Extracellular Fluid
Glycoprotein
Glycolipid
Carbohydrate
Cholesterol
Peripheral protein
Integral protein
Filaments of cytoskeleton
Cytoplasm


Polar
Non-polar

Closed Biomembranes – Vesicles

Equilibrium Shapes

Spontaneous Curvature Model (Helfrich, 1973)

The equilibrium shapes of lipid vesicles are determined by the extremals of the Helfrich's functional

$$\mathcal{F} = \mathcal{F}_c + \lambda \int_S dS + p \int dV$$

$\mathcal{F}_c = \frac{k_c}{2} \int_S (2H - \mathbb{h})^2 dS + k_G \int_S K dS$ – curvature free energy

k_c, k_G – bending and Gaussian rigidities
λ – tensile stress
p – osmotic pressure
H, K – mean and Gaussian curvatures

$\mathbb{h}$ – Helfrich's spontaneous curvature

Closed Biomembranes – Vesicles

Equilibrium Shapes

Membrane Shape Equation

$$\Delta H + (2H - \mathbb{h})(H^2 + \frac{\mathbb{h}}{2}H - K) - \frac{\lambda}{k_c}H + \frac{p}{2k_c} = 0$$

- is Euler-Lagrange equation of the Helfrich's functional $\mathcal{F}$
- derived by Ou-Yang and Helfrich (1989)
- describes the equilibrium shapes of lipid vesicles
- λ, p (stress and pressure) – Lagrangian multipliers

Δ – Laplace-Beltrami operator
$H, K, \mathbb{h}$ – mean, Gaussian and spontaneous curvatures
k_c – curvature bending rigidity

Equilibrium Vesicle Shapes I

- Spheres and Circular Cylinders
  Ou-Yang and Helfrich, 1989
- Clifford tori
  Ou-Yang, 1990, 1993; Hu and Ou-Yang, 1993
- Delaunnay Surfaces
  Naito, Okuda and Ou-Yang, 1995; Mladenov, 2002
- Circular Biconcave Discoids
  Naito, Okuda and Ou-Yang, 1993, 1996

Equilibrium Vesicle Shapes II

- Nodoidlike and Unduloidlike Shapes
  Naito, Okuda and Ou-Yang, 1995
- Willmore and Constant Squared Mean Curvature Surfaces
  Willmore, 1993; Konopelchenko, 1997;
  Vassilev and Mladenov, 2004
- Generalized Cylindrical Surfaces
  Ou-Yang, Liu and Xie, 1999;
  Vassilev, Djondjorov and Mladenov, 2008

- $\mathcal{S} : x^3 = w(x^1, x^2)$ – Mongé representation of $\mathcal{S}$
- (x^1, x^2, x^3) – Cartesian coordinates of $\mathbb{R}^3$
- $w(x^1, x^2)$ – Mongé gauge of $\mathcal{S}$ immersed in $\mathbb{R}^3$

- $w_{\alpha_1\alpha_2\ldots\alpha_k} = \frac{\partial^k w}{\partial x^{\alpha_1}\ldots\partial x^{\alpha_k}}, \quad k = 1, 2, \ldots$
- $(g^{\alpha\beta})$ – first fundamental tensor (contravariant components)
- $g = \det(g^{\alpha\beta})$

Fourth-Order PDE

$$\frac{1}{2}g^{-1/2}g^{\alpha\beta}g^{\mu\nu}w_{\alpha\beta\mu\nu} + \Phi(x^1, x^2, w, w_1, \ldots, w_{222}) = 0$$

$\Phi(x_1, x_2, w, w_1, \ldots, w_{222})$ – third-order differential equation

Membrane Shape Equation

Conformal Metric Representation

Conformal Metric (Konopelchenko, 1997)

- $ds^2 = 4q^2\varphi^2(dx^2 + dy^2)$ – conformal metric
- $(b_{\alpha\beta}) = \begin{pmatrix} \vartheta & \omega \\ \omega & 8q^2\varphi(1 + \mathbb{I}\mathrm{h}\varphi) - \vartheta \end{pmatrix}$ – second fundamental tensor
- $q(x, y)$, $\varphi(x, y)$, $\vartheta(x, y)$, $\omega(x, y)$ – unknown functions

Gauss-Codazzi-Mainardi Equations

$$(\Gamma^2_{12})_x - (\Gamma^2_{11})_y + \Gamma^1_{12}\Gamma^2_{11} + \Gamma^2_{12}\Gamma^2_{12} - \Gamma^2_{11}\Gamma^2_{22} - \Gamma^1_{11}\Gamma^2_{12} = -g_{11}K$$
$$(b_{11})_y - (b_{12})_x - b_{11}\Gamma^1_{12} - b_{12}(\Gamma^1_{12} - \Gamma^1_{11}) + b_{22}\Gamma^2_{11} = 0$$
$$(b_{12})_y - (b_{22})_x - b_{11}\Gamma^1_{22} - b_{12}(\Gamma^2_{22} - \Gamma^1_{12}) + b_{22}\Gamma^2_{12} = 0$$

- $\Gamma^{\sigma}_{\alpha\beta}$ – Christoffel symbols (depend on $q, q_x, q_y, \varphi, \varphi_x, \varphi_y$)

System of Second-Order PDEs (De Matteis, 2002)

$$q^2(\varphi_{xx}+\varphi_{yy})+2q\varphi(q_{xx}+q_{yy})-2\varphi(q_x^2+q_y^2)+ \\ +q^4(8\varphi+\alpha_2\varphi^2+\alpha_3\varphi^3+\alpha_4\varphi^4)=0$$

$$\vartheta_y-\omega_x-(8+\tfrac{\alpha_2}{3}\varphi)(\varphi q_y+q\varphi_y)=0$$

$$\omega_y+\vartheta_x-\tfrac{\alpha_2}{3}q\varphi(\varphi q_x+q\varphi_y)+8q\varphi q_x=0$$

$$4q\varphi^2(q_{xx}+q_{yy})+4\varphi q^2(\varphi_{xx}+\varphi_{yy})-4\varphi^2(q_x^2+q_y^2)-4q^2(\varphi_x^2+\varphi_y^2)- \\ -\omega^2-\vartheta^2+(8+\tfrac{\alpha_2}{3}\varphi)q^2\varphi\theta=0$$

- four equations
- four unknown functions: $q(x,y),\varphi(x,y),\vartheta(x,y),\omega(x,y)$
- conformal coordinates: (x,y)

Symmetry Algebra
(De Matteis, 2002)

- Case I: $(\alpha_2, \alpha_3, \alpha_4) \neq (0, 0, 0)$
  Special Conformal Transformations ($\hat{L}_I = \hat{L}_c$)

$$V_c(\xi) = \xi\partial_z + \xi_z \left[-(\vartheta - i\omega)\partial_\vartheta - \right.$$
$$\left. -(\omega + i\vartheta - 4iq^2\varphi - i\tfrac{\alpha_2}{6}q^2\varphi^2)\partial_\omega - \tfrac{q}{2}\partial_q \right] + \text{c.c.}$$

$z = x + iy, \quad \xi = \xi^1 + i\xi^2$ – complex notation

ξ^1, ξ^2 – arbitrary real harmonic functions of z

$\xi^1_y = -\xi^2_x, \;\; \xi^1_x = \xi^2_y$ – Cauchy-Riemann conditions

Symmetry Algebra
(De Matteis, 2002)

- Case II: $(\alpha_2, \alpha_3, \alpha_4) = (0, 0, 0)$
  Conformal Transformations and Dilatations ($\hat{L}_{II} = \hat{L}_c \oplus \hat{L}_d$)

$$V_c(\xi) = \xi \partial_z + \xi_z \left[-(\vartheta - i\omega)\partial_\vartheta - (\omega + i\vartheta - 4iq^2\varphi)\partial_\omega - \tfrac{q}{2}\partial_q \right] + \text{c.c.}$$

$$V_d = \vartheta \partial_\vartheta + \omega \partial_\omega + \varphi \partial_\varphi$$

$z = x + iy, \quad \xi = \xi^1 + i\xi^2$ – complex notation

ξ^1, ξ^2 – arbitrary real harmonic functions of z

$\xi^1_y = -\xi^2_x, \;\; \xi^1_x = \xi^2_y$ – Cauchy-Riemann conditions

Reduced System of Second-Order ODEs for Solutions Invariant under the Subgroup Generated by $V_c(1/2) = \partial_x$

$$q^2 \frac{d^2\varphi}{dy^2} + 2q\varphi \frac{d^2 q}{dy^2} - 2\varphi \left(\frac{dq}{dy}\right)^2 + q^4(8\varphi + \alpha_2\varphi^2 + \alpha_3\varphi^3 + \alpha_4\varphi^4) = 0$$

$$\frac{d\vartheta}{dy} - (8 + \frac{\alpha_2}{3}\varphi)q(\varphi\frac{dq}{dy} + q\frac{d\varphi}{dy}) = 0$$

$$4q\varphi^2 \frac{d^2 q}{dy^2} + 4\varphi q^2 \frac{d^2\varphi}{dy^2} - 4\varphi^2 \left(\frac{dq}{dy}\right)^2 - 4q^2 \left(\frac{d\varphi}{dy}\right)^2 - \alpha_5^2 - \vartheta^2 + \\ + (8 + \frac{\alpha_2}{3}\varphi)q^2\varphi\vartheta = 0$$

- three equations
- three unknown functions: $q(y), \varphi(y), \vartheta(y)$; $\omega(y) \equiv \text{const}$
- three phenomenological constants: $\alpha_2, \alpha_3, \alpha_4$; $\alpha_5 = \omega$

Classification of the Group-Invariant Solutions of the Membrane Shape Equation (De Matteis, 2002)

- All one-parameter subgroups of the general symmetry group of the membrane shape equation (in the above conformal metric presentation) are equivalent through the adjoint representation of the symmetry group on its Lie algebra.
- Any solution invariant under one-parameter subgroup of the general symmetry group of the membrane shape equation can be obtained by applying a symmetry group transformation to some solution invariant under the one-parameter symmetry subgroup generated by $V_c(1/2) = \partial_x$.

Vesicle Shapes Derived from Solutions Invariant Under the Translation Symmetry Subgroup

$$(x, y, q, \varphi, \vartheta, \omega) \mapsto (x + \varepsilon, y, q, \varphi, \vartheta, \omega), \quad \varepsilon \in \mathbb{R}$$

(De Matteis, 2002)

- Sphere (for $H = \text{const}$)
- Delaunay's Surfaces (for $H = \mathbb{I}\mathrm{h}$)
- Toroidal Surfaces (for $q = \text{const}$)
- Circular Biconcave Discoid (for $q = \frac{\rho(\varphi)}{2\varphi}, \;\; \rho\varphi_\rho = -c\varphi^2$)

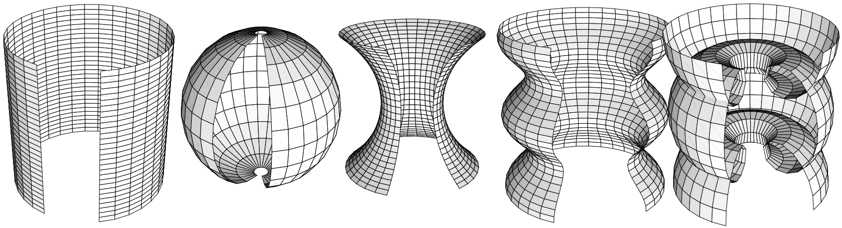


Figure : The open parts of the Delaunay surfaces - cylinder, sphere, catenoid, unduloid and nodoid.

Sphere

Obtained from Group-Invariant Solution for $H = H_0 = \text{const} \neq \mathbb{h}$

Cartesian Coordinates

$$x^1 = -\frac{R \sin x'}{\cosh y'}, \quad x^2 = -\frac{R \cos x'}{\cosh y'}, \quad x^3 = -R \tanh y'$$

Metric

$$ds^2 = \frac{1}{H_0^2 \cosh^2 y'}(dx'^2 + dy'^2)$$

Second Fundamental Form

$$\Omega = \frac{1}{H_0 \cosh^2 y'}(dx'^2 + dy'^2)$$

$(x', y') = \delta_0(x, y)$ – coordinate scaling
$R = 1/H_0$ – radius of the sphere
$\delta_0 = \text{const}$; $\mathbb{h}$ – spontaneous curvature

Delaunay Surfaces

Obtained from Group-Invariant Solution for $H = \mathbb{h}$
Nodoids obtained for $\mathbb{h}^3\vartheta_0 < 0$
Unduloids obtained for $0 < \mathbb{h}^3\vartheta_0 < 1$

Metric
$$ds^2 = p^2 d\Phi^2 - \frac{4p^2}{4\mathbb{h}^2 p^4 + 2\vartheta_0 \mathbb{h}^3 - \mathbb{h}^2 - 4} dp^2$$

Second Fundamental Form
$$\Omega = (\mathbb{h} p^2 + \frac{1}{4}\vartheta_0 \mathbb{h}^2) d\Phi^2 - \frac{4\mathbb{h} p^2 - \vartheta_0 \mathbb{h}^2}{4\mathbb{h}^2 p^4 + 2\vartheta_0 \mathbb{h}^3 + \mathbb{h}^2 - 4} dp^2$$

$$p = \sqrt{r\left(1 - \sigma^2 \mathrm{sn}(2\sqrt{2}y, \sigma)\right)}, \quad \Phi = 2x/\mathbb{h}$$
$$r = C(\mathbb{h})/4, \;\; \sigma = \sqrt{2C(\mathbb{h})/r}$$
$$C(\mathbb{h}) = \sqrt{\mathbb{h}^6 - \mathbb{h}^4/4 - 4\mathbb{h}^3 + 4}$$

– $(x, y) \to (\Phi, p)$ coordinate change

$\mathbb{h}$ – spontaneous curvature

Clifford Torus

Obtained from Group-Invariant Solution for $q = q_0 = \text{const}$
Detected Experimentally by Mutz and Bensimon (1991)

Cartesian Coordinates

$$\left[(x^1)^2 + (x^2)^2 + (x^3)^2 + \frac{1}{\mathbb{h}^2}\right]^2 = \frac{8}{\mathbb{h}^2}\left[(x^1)^2 + (x^2)^2\right]$$

Metric

$$ds^2 = \rho^2 d\theta^2 - \frac{d\rho^2}{1+2\sqrt{2}\mathbb{h}\rho+\mathbb{h}^2\rho^2}$$

Second Fundamental Form

$$\Omega = (\mathbb{h}\rho^2 + \sqrt{2}\rho)d\theta^2 - \frac{\mathbb{h}d\rho^2}{1+2\sqrt{2}\mathbb{h}\rho+\mathbb{h}^2\rho^2}$$

θ – rotation angle through the x^3 axis
ρ – radius; $\mathbb{h}$ – spontaneous curvature

Circular Biconcave Discoid

Obtained from Group-Invariant Solution for $q = q(\varphi) = \rho(\varphi)/2\varphi$
Shape of the Red Blood Cells

Cartesian Coordinates
$x^1 = \cos x, \quad x^2 = \sin x, \quad x^3 = \int \tan\psi(\rho) d\rho + z_0$

Metric
$ds^2 = \rho^2 dx^2 + \frac{\rho^2}{f(\rho)} d\rho^2$

Second Fundamental Form
$\Omega = 2\mathbb{h}\rho^2 \ln\left(\frac{\rho}{\rho_0}\right) dx^2 + 2\mathbb{h}\rho^2 \left(\ln\left(\frac{\rho}{\rho_0}\right) + 1\right) \frac{1}{f(\rho)} d\rho^2$

> x – angular variable; $\quad \rho$ – radius; $\rho_0, f_0, z_0 = \mathrm{const}$
> $(1/\varphi^2)(d\varphi/d\rho) = -2\mathbb{h}/\rho$ – definition of $\rho(\varphi)$
> ψ – angle between the tangent to the contour and the radius
> $f(\rho) = \rho^2 \left(f_0 - 4\mathbb{h}^2\rho^2 \ln^2\left(\frac{\rho}{\rho_0}\right)\right); \quad \sec^2\psi(\rho) = \rho^2/f(\rho)$

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