Toroid G_{bend} 3

11 October, 2019 1:08 PM

Changes from Toroid G_{bend} 2: renamed coordinates/variables

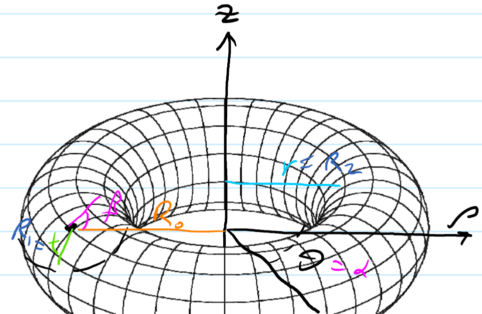
$r \to t$	$t \to R_0$	$t \to r$

Note: Per MB Jackson (2010), a toroidal pore would be the maximum energy conformation. The membrane would less stressed if folded into a hemi-elipse rather than a hemicircle around the pore rim

Setup

$$G_{bend} = \frac{K_b}{2}\int dS\left(\frac{1}{R_1}+\frac{1}{R_2}-H_0\right)^2$$

spontaneous curvature



Note: R_1 is const but R_2 will dep on z

Assume: • Torroidal pore in flat membrane

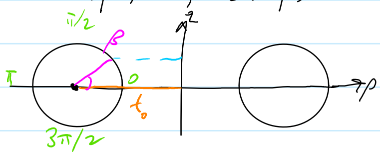
↳ symmetry

no bending except the pore

• $H_0 = 0$

Parametrization:

$$(\rho, \theta, z) \longrightarrow (R_0 - t\cos\beta,\ \alpha,\ t\sin\beta) \equiv \vec{v}$$



From torus SA calc, know: $\|\vec{v}_\alpha \times \vec{v}_\beta\| = r$

$R_1 \equiv$ (membr sep dist) $\frac{1}{2}$

1 nm for fusion

6 nm ~ hydration equilib

$R_2 \equiv r = R_0 - t\cos\beta$

Calculation

use symmetry ($z=0$ reflection)

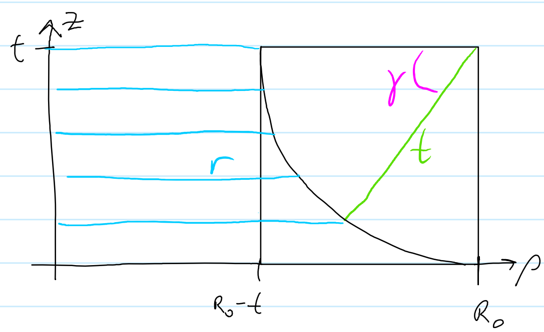
calc'd in torus SA page

$$\frac{K_b}{2}\int dS\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2 = \frac{K_b}{2}\, 2\int_0^{\pi/2}\int_0^{2\pi}\left(\frac{1}{t}+\frac{1}{R_0 - t\cos\beta}\right)^2 \|\vec{v}_\alpha \times \vec{v}_\beta\|\, d\alpha\, d\beta$$

$$= K_b \int_0^{\pi/2}\int_0^{2\pi}\left(\frac{1}{t}+\frac{1}{R_0-t\cos\beta}\right)^2 r\, d\alpha\, d\beta$$

$$G_b = 2\pi K_b \int_0^{\pi/2}\left(\frac{1}{t}+\frac{1}{R_0-t\cos\beta}\right)^2 r\, d\beta$$

Comparison to solution from modeling a protrusion base as a torus



$$r = R_0 - t\cos\gamma$$

$$\downarrow$$

$$r = R_0 - t\cos\left[\arcsin\left(\frac{t-z}{t}\right)\right]$$

$$\gamma = \arcsin\left(\frac{t-z}{t}\right)$$

$\therefore$ $R_1 = t$

$R_2 = R_0 - t\cos\left[\arcsin\left(\frac{t-z}{t}\right)\right]$

$$G_b = \frac{K_b}{2}\int dS\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2$$

$$= K_b\int_0^t\int_0^{2\pi}\left(\frac{1}{R_1}+\frac{1}{R_2}\right)^2 d\theta\, dz$$

use symmetry: $\int_0^{2t} f(\rho,\theta,z)\,dz = 2\int_0^t f(\rho,\theta,z)\,dz$

$$= 2\pi K_b\int_0^t\left(\frac{1}{t}+\left[R_0 - t\cos\left[\arcsin\left(\frac{t-z}{t}\right)\right]\right]^{-1}\right)^2 dz$$