Determining the membrane bending modulus from the measured R(φ) of a giant vesicle

Raghuveer Parthasarathy
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<u>Supercedes earlier (Nov. 2010) notes, which are wrong.</u>

Theory

Vesicle contour $r(\theta,\phi,t)=\bar{R}(1+u(\theta,\phi,t))$. Note that u is dimensionless. See Meleard 1997, Eq. 4, or Faucon 1989, Eq. 4. $\bar{R}$ is the radius as determined by the volume – I'd guess that this is extremely close to the average of r.

u can be decomposed into spherical harmonics – Meleard 1997 Eq. 11, where the angle-dependent part is given by the harmonics for $n\geq 2$, with coefficients U_n^m.

The spherical harmonic coefficients are simply related to the bending modulus (κ_c) and reduced tension ($\bar{\sigma}=\sigma R^2/\kappa_c$) by Faucon eq. 34 (or Meleard Eq. 17-18).
Faucon Eq. 34:

$$\left\langle \left|U_n^m(t)\right|^2 \right\rangle = \frac{k_B T}{\kappa}\frac{1}{(n-1)(n+2)\left[\bar{\sigma}+n(n+1)\right]}$$

(Note that the above expression for reduced tension is correct for $c_0=0$. More generally (Faucon Eq. 15): $\bar{\sigma}=\dfrac{\sigma R^2}{\kappa_c}+2c_0R+\dfrac{1}{2}c_0^2R^2$. This may be useful if we can extract the radius dependence of $\bar{\sigma}$.

We cannot measure U_n^m, since we observe the equatorial cross-section of the vesicle, $\rho(\phi,t)=r(\theta=\pi/2,\phi,t)$ and not its entire surface. The autocorrelation function of ρ can provide useful information:

$$\xi(\gamma,t)=\frac{1}{R^2}\left[\frac{1}{2\pi}\int_0^{2\pi}\rho(\phi+\gamma,t)\rho^*(\phi,t)d\phi\ -\rho^2(t)\right]$$

Why is there a complex conjugate, since ρ is necessarily real?

Faucon 1989 defines the contour angle average as $\rho(t)=\dfrac{1}{2\pi}\oint\rho(\phi,t)d\phi$, which makes sense. (Also in Bouvrais 2008.) Meleard 1997 provide a strange definition that, for a constant radius, gives a value of 4*R*.

This autocorrelation function can be decomposed into Legendre polynomials, with coefficients B_n. Faucon Eq. 46 (or Meleard 18):

$$B_n(\bar{\sigma}, \kappa_c) = \frac{k_B T}{4\pi\kappa_c} \frac{2n+1}{(n-1)(n+2)\left[\bar{\sigma} + n(n+1)\right]} \text{ for } n \geq 2 .$$

(With this notation, n=1 is the constant term and n=2 is the cosine term; in MATLAB's notation, the constant term is ignored and the indexing starts at 1 with the cosine term.) Do we have to worry that B_n could be negative? Probably not, since this is an autocorrelation.

To use this, we can't simply solve for κ_c, since $\bar{\sigma}$ is unknown. Could do a 2-parameter non-linear fit. Or: Can we linearize anything as a function of *n*?

$$\frac{k_B T}{4\pi B_n} \frac{2n+1}{(n-1)(n+2)} = \kappa_c \left[\bar{\sigma} + n(n+1)\right]$$

A bit awkward, but plotting the left side vs. n(n+1) should give a line with slope κ_c (and intercept $\kappa_c\bar{\sigma} = \sigma R^2$ for zero spontaneous curvature).

Implementation

Determining the vesicle edge: see "GUV FLUCTUATION ANALYSIS FUNCTIONS.DOC" Functions trackedge_kn.m, slopeEdge_kn.m (& others called).

Calculating the edge autocorrelation function, $\xi(\gamma)$, of the vesicle edge ($R(\phi)$). Function: autocorrguv.m .

Decompose $\xi(\gamma)$ into Legendre polynomials, coefficients B_n. Function: legendre_kn.m

Analyze the B_n to give the bending modulus and tension: Function: **`calc_kappa.m`** (noting the above difference in indexing of Legendre polynomials).

References

1. Meleard, P., Gerbeaud, C., Pott, T., Fernandez-Puente, L., Bivas, I., Mitov, M. D., Dufourcq, J., and Bothorel, P. Bending elasticities of model membranes: influences of temperature and sterol content. *Biophys J* **72**, 2616-29 (1997).

2. Faucon, J. F. , Mitov, M. D., Meleard, P., Bivas, I., and Bothorel, P. Bending elasticity and thermal fluctuations of lipid membranes. Theoretical and experimental requirements. *J. Phys. France* **50**, 2389-2414 (1989).

See also
Henriksen and Ipsen 2004

Niggeman and Helfrich 1995
pecreaux bassereau vesicle fluctuation 2004