# Measuring bending elasticity of lipid bilayers

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The model of Milner & Safran [1987] links the mean squared amplitudes of spherical harmonics, $\langle|U_n^m(t)|^2\rangle$, to the elastic modulus, $k_c$, and the mode's number, $n$:

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

The unknown quantity $\bar{\sigma}$ (physical meaning of lateral stretching tension) could be determined if two (or more) modes are measured experimentally.

Due to the spherical symmetry, $\langle|U_n^m(t)|^2\rangle$ do not depend on $m$.

What is observed by a phase-contrast microscope is the equatorial cross-section of the vesicle membrane with the focal plane of the microscope:

$$r(\varphi, t) = R[1 + u(\frac{\pi}{2}, \varphi, t)]$$

where $u(\frac{\pi}{2}, \varphi, t)$ is the deviation from the circular shape. Writing it in series of spherical harmonics, $Y_n^m(\frac{\pi}{2}, \varphi)$, gives:

$$u(\frac{\pi}{2}, \varphi, t) = \sum_{n} \sum_{m=-n}^{n} U_n^m(t) Y_n^m(\frac{\pi}{2}, \varphi)$$

The angular autocorrelation function, $\zeta(\gamma, t)$, is defined as:

$$\zeta(\gamma, t) = \frac{1}{2\pi} \int_0^{2\pi} u(\frac{\pi}{2}, \varphi, t) \overset{*}{u}(\frac{\pi}{2}, \varphi + \gamma, t) d\varphi$$

Replacing $u(\theta, \varphi, t)$ with its series expansion:

$$\zeta(\gamma, t) = \frac{1}{2\pi} \int_0^{2\pi} \sum_k \sum_l U_k^l(t) Y_k^l(\frac{\pi}{2}, \varphi) \sum_n \sum_m \overset{*}{U}{}_n^m(t) \overset{*}{Y}{}_n^m(\frac{\pi}{2}, \varphi + \gamma) d\varphi$$

and rearranging the terms gives:

$$\zeta(\gamma, t) = \frac{1}{2\pi} \sum_k \sum_l \sum_n \sum_m U_k^l(t) \overset{*}{U}{}_n^m(t) \int_0^{2\pi} Y_k^l(\frac{\pi}{2}, \varphi) \overset{*}{Y}{}_n^m(\frac{\pi}{2}, \varphi + \gamma) d\varphi$$

Integrating the spherical harmonics leads to:

$$\zeta(\gamma, t) = \sum_k \sum_n \sum_m U_k^m(t) \overset{*}{U}{}_n^m(t) Y_k^m(\frac{\pi}{2}, 0) \overset{*}{Y}{}_n^m(\frac{\pi}{2}, \gamma)$$

The time averaged angular autocorrelation function, $\zeta(\gamma)$, is:

$$\zeta(\gamma) = \langle \zeta(\gamma, t) \rangle = \sum_k \sum_n \sum_m \langle U_k^m(t) \overset{*}{U}{}_n^m(t) \rangle Y_k^m(\frac{\pi}{2}, 0) \overset{*}{Y}{}_n^m(\frac{\pi}{2}, \gamma)$$

Due to the independence of different modes,

$$\langle U_k^m(t)\overset{*}{U}{}_n^m(t)\rangle = \langle U_n^m(t)\overset{*}{U}{}_n^m(t)\rangle\delta_{kn} = \langle |U_n^m(t)|^2\rangle\delta_{kn}$$

the sum over $k$ could be performed:

$$\zeta(\gamma) = \sum_n \sum_m \langle |U_n^m(t)|^2\rangle Y_n^m(\frac{\pi}{2},0)\overset{*}{Y}{}_n^m(\frac{\pi}{2},\gamma)$$

According to model of Milner & Safran [1987], $\langle |U_n^m(t)|^2\rangle$ does not depend on $m$, so:

$$\zeta(\gamma) = \sum_n \langle |U_n^m(t)|^2\rangle \sum_m Y_n^m(\frac{\pi}{2},0)\overset{*}{Y}{}_n^m(\frac{\pi}{2},\gamma)$$

The theorem of summation of spherical harmonics reads:

$$\sum_m Y_n^m(\frac{\pi}{2},0)\overset{*}{Y}{}_n^m(\frac{\pi}{2},\gamma) = \frac{2n+1}{4\pi}P_n(\cos\gamma)$$

where, $P_n(\cos\gamma)$ is the Legendre polynomial.
Thus, the time averaged angular autocorrelation function finally is:

$$\zeta(\gamma) = \sum_n \frac{2n+1}{4\pi}\langle|U_n^m(t)|^2\rangle P_n(\cos\gamma) = \sum_n B_n P_n(\cos\gamma)$$

with:

$$B_n = \frac{2n+1}{4\pi}\langle|U_n^m(t)|^2\rangle = \frac{k_B T}{4\pi k_c}\frac{2n+1}{(n-1)(n+2)[\bar{\sigma}+n(n+1)]}$$

When one measure the vesicle radius, $\rho(\varphi)$ in a given direction, $\varphi$, the result has two components: the radius itself, $r(\varphi)$, and a measurement error, $\varepsilon(\varphi)$, having the property, $\langle\varepsilon(\varphi)\rangle = 0$:

$$\rho(\varphi) = r(\varphi) + \varepsilon(\varphi)$$

The experimentally measured time averaged angular autocorrelation function is:

$$\zeta(\gamma) = \frac{1}{2\pi}\int_0^{2\pi}\langle\rho(\varphi)\rho(\varphi+\gamma)\rangle d\varphi$$

$$\frac{1}{2\pi}\int_0^{2\pi}\langle(r(\varphi)+\varepsilon(\varphi))(r(\varphi+\gamma)+\varepsilon(\varphi+\gamma))\rangle d\varphi$$

Taking into account that the radius, $r(\varphi)$, and the error of its measurements, $\varepsilon(\varphi)$, are non correlated one can write:

$$\zeta(\gamma) =$$
$$\frac{1}{2\pi}\int_0^{2\pi}\langle(r(\varphi)+\varepsilon(\varphi))(r(\varphi+\gamma)+\varepsilon(\varphi+\gamma))\rangle d\varphi =$$
$$\frac{1}{2\pi}\int_0^{2\pi}\langle r(\varphi)r(\varphi+\gamma)\rangle d\varphi + \frac{1}{2\pi}\int_0^{2\pi}\langle r(\varphi)\rangle\langle\varepsilon(\varphi+\gamma)\rangle d\varphi +$$
$$\frac{1}{2\pi}\int_0^{2\pi}\langle\varepsilon(\varphi)\rangle\langle r(\varphi+\gamma)\rangle d\varphi + \frac{1}{2\pi}\int_0^{2\pi}\langle\varepsilon(\varphi)\varepsilon(\varphi+\gamma)\rangle d\varphi$$

The second and third terms are zero, because $\langle\varepsilon(\varphi)\rangle = 0$, so:

$$\zeta(\gamma) = \frac{1}{2\pi}\int_0^{2\pi}\langle r(\varphi)r(\varphi+\gamma)\rangle d\varphi + \frac{1}{2\pi}\int_0^{2\pi}\langle\varepsilon(\varphi)\varepsilon(\varphi+\gamma)\rangle d\varphi$$

Let us consider the last term. One can suppose that the measurement errors, $\varepsilon(\varphi)$, for different directions, $\varphi$, are non correlated, so:

$$\frac{1}{2\pi}\int_0^{2\pi}\langle\varepsilon(\varphi)\varepsilon(\varphi+\gamma)\rangle d\varphi = C^2\delta(\gamma)$$

where: $C^2$ is the dispersion of $\varepsilon(\varphi)$ and $\delta(\gamma)$ is the Dirac's delta function. Finally the experimentally measured time averaged angular autocorrelation function is:

$$\zeta(\gamma) = \frac{1}{2\pi}\int_0^{2\pi}\langle r(\varphi)r(\varphi+\gamma)\rangle d\varphi + C^2\delta(\gamma)$$

The amplitudes, $B_n$, of Legendre polynomials are:

$$B_n \int_0^\pi [P_n(\cos(\gamma))]^2 \sin(\gamma) d\gamma = \int_0^\pi \zeta(\gamma) P_n(\cos(\gamma)) \sin(\gamma) d\gamma$$

The last term in the equation for the experimental autocorrelation function, $\zeta(\gamma)$, thus reads:

$$C^2 \int_0^\pi \delta(\gamma) P_n(\cos(\gamma)) \sin(\gamma) d\gamma = C^2 P_n(\cos(0)) \sin(0) = 0$$

Due to the properties of the Dirac's $\delta(\gamma)$ function and Legendre polynomials, the integral evaluates to zero. So the experimental error in determination of $\rho(\varphi)$ do not influence the mean values of $B_n$ *(in condition all the hypotheses made are true)*.

Some authors prefer to consider the time averaged angular autocorrelation function, $\zeta(\gamma)$, as a Fourier series:

$$\zeta(\gamma) = \sum_m A_m e^{\imath m\gamma}$$

where the coefficients $A_m$ are:

$$A_m = \frac{1}{2\pi} \int_0^{2\pi} \zeta(\gamma) e^{-\imath m\gamma} d\gamma$$

We already know that:

$$\zeta(\gamma) = \sum_n \sum_m \langle |U_n^m(t)|^2 \rangle Y_n^m(\frac{\pi}{2}, 0) \overset{*}{Y}{}_n^m(\frac{\pi}{2}, \gamma) + C^2 \delta(\gamma)$$

After rearrangement and change of order of summation:

$$\zeta(\gamma) = \sum_m \sum_{n>=m} \langle |U_n^m(t)|^2 \rangle \overset{*}{Y}{}_n^m(\frac{\pi}{2}, 0) Y_n^m(\frac{\pi}{2}, \gamma) + C^2 \delta(\gamma)$$

The Fourier amplitudes are:

$$A_m = \sum_{n>=m} \langle |U_n^m(t)|^2 \rangle \overset{*}{Y}{}_n^m(\frac{\pi}{2}, 0) \left( Y_n^m(\frac{\pi}{2}, \gamma) e^{-\imath m \gamma} \right) + \frac{C^2}{2\pi}$$

where the product $\left( Y_n^m(\frac{\pi}{2}, \gamma) e^{-\imath m \gamma} \right)$ does not depend on $\gamma$ (the term $e^{-\imath m \gamma}$ exactly cancels out the $\gamma$ dependency in $Y_n^m(\frac{\pi}{2}, \gamma)$).

The Legendre polynomial amplitudes (for comparison) are:

$$B_n = \frac{2n+1}{4\pi} \langle |U_n^m(t)|^2 \rangle = \frac{k_B T}{4\pi k_c} \frac{2n+1}{(n-1)(n+2)[\bar{\sigma} + n(n+1)]}$$

Comparison between Legendre polynomial amplitudes, $B_n$, and Fourier amplitudes, $A_m$:

- $A_m$ are complicated sums over $n$; $B_n$ are simple rational expressions
- $A_m$ are influenced (biased) by a constant value due to the errors in determination of the equatorial radius; $B_n$ are not. (This bias must be subtracted from experimentally measured Fourier amplitudes *but not all authors really do it*).
- $A_m$ must be fitted using 3 parameters: $k_c$, $\bar{\sigma}$ and the bias $C^2$; $B_n$ are fitted with 2: $k_c$ and $\bar{\sigma}$.

References:

1. S.T. Milner, S.A. Safran [1987]: Dynamical fluctuations of droplet microemulsions and vesicles, Phys. Rev. A **36**, 4371–4379.