# Elastic Properties and Line Tension of Bilayer Membranes

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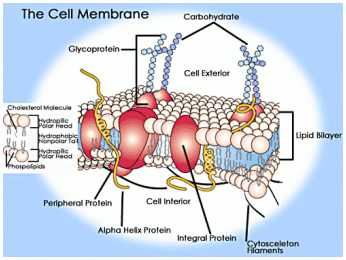
**Abstract:** The elastic properties of a self-assembled bilayer membrane are studied using the self-consistent field theory, applied to a model system composed of flexible amphiphilic chains dissolved in hydrophilic polymeric solvents. Examining the free energy of bilayer membranes with different geometries allows us to calculate their bending modulus, Gaussian modulus, two fourth-order membrane moduli, and the line tension. The dependence of these parameters on the microscopic characteristics of the amphiphilic chain, characterized by the volume fraction of the hydrophilic component, is systematically studied. The theoretical predictions are compared with the results from a simple monolayer model, which approximates a bilayer membrane by two monolayers.

## Introduction




http://www.sparknotes.com/biology/cellstructure/cellmembranes/section2.rhtml

Amphiphilic molecules, such as lipids, surfactants and block copolymers, are composed of hydrophilic and hydrophobic components. When dispersed in water, the amphiphilic molecules spontaneously self-assemble into a variety of structures, e.g., spherical and cylindrical micelles or bilayer membranes. The self-assembly is driven by the competing interactions between water and different parts of the amphiphilic molecules. Specifically, in the case of bilayers the hydrophilic parts stay on the outside of the bilayer, while the hydrophobic blocks are hidden in the interior. At the mesoscopic scale, the membranes can be modeled as two-dimensional surfaces. The properties of the membrane within this surface model are then described by a set of elastic parameters including the spontaneous curvature, the bending modulus, the Gaussian modulus, and the line tension of an open membrane edge.

In the elastic model, the bilayer membrane is represented by a two-dimensional surface whose energy is described in terms of its elastic energy. If this tensionless bilayer is not highly curved, its free energy can be well represented by a linear elastic model (the Helfrich model)

$$F_2 = \int \left[2\kappa_M (M - c_0)^2 + \kappa_G G\right] \mathrm{d}A + \int \sigma \mathrm{d}L$$

where $M = (c_1 + c_2)/2$ and $G = c_1 c_2$ are the local mean and Gaussian curvatures of the deformed bilayer ($c_{1,2}$are the two principal curvatures). The last term represents the edge energy of an open membrane, and it vanishes for closed membranes. The elastic constants of interest, $c_0, \kappa_M, \kappa_G, \sigma$ are the spontaneous curvature, the bending modulus, the Gaussian modulus and the edge line tension, respectively. In the current work, we derive the elastic parameters from the free energy calculated by self-consistent field theory (SCFT). The high accuracy of SCFT allows us to also determine the high-order elastic constants

$$F_4 = F_2 + \int \left[\kappa_1 M^4 + \kappa_2 M^2 G + \kappa_3 G^2\right] \mathrm{d}A.$$

## Model and Method

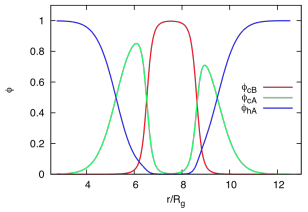
In order to extract information on the various elastic properties, we calculate the excess free energy of a bilayer membrane in the following five geometries: (i) an infinite planar bilayer membrane, (ii) a cylindrical bilayer membrane with a radius *r*, which is extended to infinity in the axial direction, (iii) a spherical bilayer with a radius *r*, (iv) an axially symmetric disk-like membrane patch with a radius *R*, and (v) a planar membrane with a circular pore of radius *R*. The first three geometries, which can be reduced to a one-dimensional problem by an appropriate coordinate transformation, are employed to extract the bending modulus and the Gaussian modulus as well as higher-order curvature moduli.

$$F^C = -2\kappa_M c_0 c + \frac{\kappa_M}{2} c^2 + \frac{\kappa_1}{16} c^4,$$

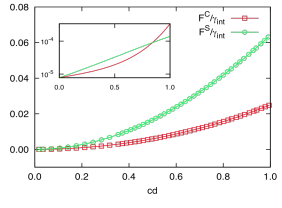
$$F^S = -4\kappa_M c_0 c + (2\kappa_M + \kappa_G) c^2 + (\kappa_1 + \kappa_2 + \kappa_3) c^4,$$

The last two geometries, which are two-dimensional systems due to their axial symmetry, are used to extract the line tension of the membrane edge.

$$F^D A = 2\pi\sigma R, \quad F^P A = 2\pi\sigma R.$$

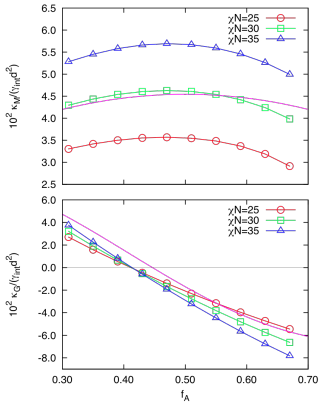



The concentration profile for a bilayer membrane in the spherical geometry with parameters $r = 7.7R_g$ and $f_A = 0.5$




The excess free energy as a function of dimensionless curvature $cd$ for membranes with $f_A = 0.5$

## Bending and Gaussian Moduli




We first investigate the bending and Gaussian moduli as a function of diblock asymmetry and the degree of segregation.

The bending modulus is a convex function of $f_A$ and increase as $\chi N$ increases.

The Gaussian modulus is a decreasing function of $f_A$ and not sensitive to $\chi N$.

The pink lines are results from two-monolayer approximation:

$$\kappa_M = 2\bar{\kappa}_M,$$
$$\kappa_G = 2\left[\bar{\kappa}_G - 4\bar{\kappa}_M \bar{c}_0 \delta\right].$$

## Fourth-order Moduli

Two higher order moduli are plotted as a function of $f_A$.

$$B_C = \kappa_1/16,$$
$$B_S = \kappa_1 + \kappa_2 + \kappa_3.$$

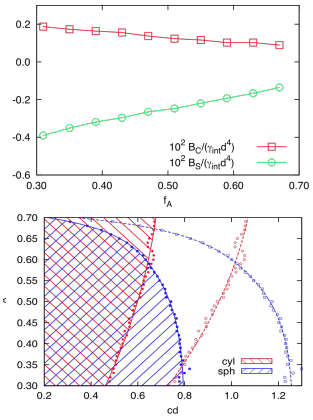
With our results for the second and fourth-order moduli, we can now determine a boundary separating the region where the fourth-order corrections are negligible from that where the fourth-order terms start to play an important role.

We require that the relative energy difference,

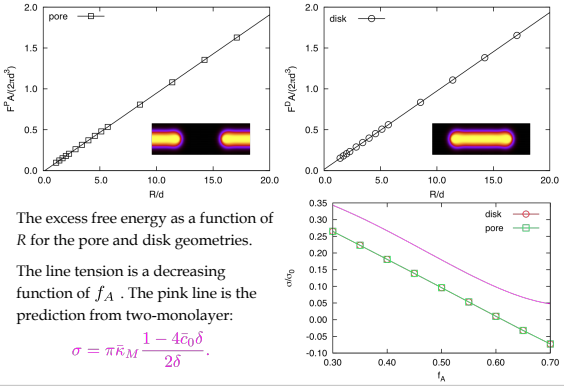
$$\Delta E = \frac{|F_4 - F_2|}{F_2},$$

does not exceed a given threshold

$$\Delta E^* = \%2, \%5.$$




## Line Tension




The excess free energy as a function of *R* for the pore and disk geometries.

The line tension is a decreasing function of $f_A$ . The pink line is the prediction from two-monolayer:

$$\sigma = \pi\bar{\kappa}_M \frac{1 - 4\bar{c}_0\delta}{2\delta}.$$

[1] Helfrich, Z. Naturforsch. C **28**, 693 (1973).
[2] Li, Pastor, Shi, Schmid, & Zhou, Phys. Rev. E, **88**, 012718 (2013)

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