The influence of thermal fluctuations on the bending rigidity of fluid membranes

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Thermal fluctuations soften the response of fluid membranes to bending deformations. These notes provide a short “semi-heuristic” derivation of this result.

I. INTRODUCTION

The classical description of fluid membranes on the level of continuum elasticity goes back to the seminal papers by Canham [1] and Helfrich [2]. Given some shape $\mathscr{S}$ of a membrane, the curvature-elastic energy is obtained as the following a functional surface integral:

$$E[\mathscr{S}] = \int \mathrm{d}A \, \frac{1}{2}\kappa K^2[\mathscr{S}] \; , \tag{1}$$

where $K = K[\mathscr{S}]$ is the total curvature of the membrane and κ is the (bare) bending modulus. A second quadratic term proportional to the Gaussian curvature has been neglected, since by virtue of the Gauss-Bonnet theorem [3] it only depends on the boundary and topology of the membrane and is thus usually irrelevant. A term proportional to the mean curvature has also been omitted, since we will only consider up-down symmetric membranes. Notice finally that Eqn. (1) corresponds to membranes with vanishing (bare) tension, as there is no term proportional to the area.

Equation (1) determines the *energy* of a membrane, not the *free energy*. It is thus a ground state description. However, suppose we bend a membrane such as to give it some *average shape* $\overline{\mathscr{S}}$ that extends over a characteristic length scale λ. At nonzero temperature this membrane will display thermal fluctuations on all length scales smaller than λ, while length scales *bigger* than λ are supposed to be under our control and therefore not determined by the heat bath. The work required to obtain this average shape $\overline{\mathscr{S}}$ is not necessarily given by its energy $E[\overline{\mathscr{S}}]$ as calculated via Eqn. (1), but is modified by these fluctuations. Indeed, for such problems there is no guarantee that the coarse grained free energy, obtained by integrating out some small-scale fluctuations, can be calculated by a functional which displays some resemblance to Eqn. (1). In fact, it generally doesn't. In this case, however, the influence of fluctuations, among other things, is to create new terms that formally look like the already existing curvature contribution. It then appears as if the bending rigidity κ has a different value which depends on the temperature as well as on the length scale λ up to which we would like to coarsen our description. The standard lingo for this situation is that the bending rigidity is thermally renormalized in a length scale dependent way. The first predictions of this effect have been due to Helfrich [4], Peliti and Leibler [5], and Förster [6] – all producing different prefactors. Kleinert [7] gave a careful analysis of the origin of the discrepancy.

II. SETTING UP THE CALCULATION

A. Flat surfaces

A rigorous treatment of bending renormalization is very difficult and not intended here. We will restrict to the classical situation of essentially flat surfaces and perform a perturbation analysis up to quadratic order in the fluctuations, following essentially the presentation given by Kleinert [7]. Moreover, the measure to be used for tracing out the fluctuations will be determined heuristically. We will nevertheless get the correct result, even though somewhat fortuitously. Below we will provide a brief discussion of these difficulties.

B. Monge parametrization and quartic expansion

For essentially flat surfaces the most convenient description of the membrane is in terms of a so-called *Monge parametrization* (or “gauge”), *i.e.*, by specifying the height h of the surface as a function of the Euclidean coordinates x and y of the flat base plane. This parametrization can of course not describe overhangs, but then, essentially flat surfaces do not have overhangs.

The total curvature K in Monge gauge is

$$K = \boldsymbol{\nabla} \cdot \left(\frac{\boldsymbol{\nabla} h}{\sqrt{1 + (\boldsymbol{\nabla} h)^2}} \right) \; , \tag{2}$$

where $\boldsymbol{\nabla} = (\partial_x, \partial_y)^\top$ is the two-dimensional nabla operator in the base plane. Notice that this expression is nonlinear in the shape $h(x, y)$ due to the occurrence of the square root in the denominator. One hence usually expands this term up to lowest nontrivial order and obtains $K = \nabla^2 h + \mathscr{O}(3)$. But as it turns out, to see the influence of thermal fluctuations on the bending rigidity we need to go to higher than linear order. The simple reason is this: if K is linear in h, the Hamiltonian is quadratic in h and thus harmonic; but then all modes fluctuate independently. Let us, therefore, expand Eqn. (2) up to *cubic* order in the derivatives:

$$\begin{aligned} K &= \partial_i \big[h_i (1 - \tfrac{1}{2} h_j h_j + \mathscr{O}(4)) \big] \\ &= h_{ii} (1 - \tfrac{1}{2} h_j h_j + \mathscr{O}(4)) + h_i (-h_{ij} h_j + \mathscr{O}(4)) \\ &= h_{ii} - \tfrac{1}{2} h_{ii} h_j h_j - h_i h_{ij} h_j + \mathscr{O}(5) \; , \end{aligned} \tag{3}$$

where $h_i = \partial_i h$ denotes a partial derivative. We thus get

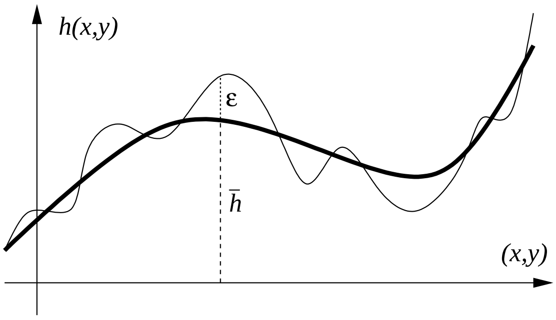

FIG. 1: The shape of a fluctuating membrane is decomposed into a large scale average shape $\bar{h}$ and small fluctuations on shorter wavelengths, ε.

the square of the total curvature up to quartic order as:

$$\begin{aligned} K^2 &= \left[h_{ii} - \tfrac{1}{2}h_{ii}h_jh_j - h_ih_{ij}h_j + \mathscr{O}(5)\right]^2 \\ &= (h_{ii})^2 - (h_{ii})^2h_jh_j - 2h_{ii}h_jh_{jk}h_k + \mathscr{O}(6)\ . \end{aligned} \quad (4)$$

Finally, we must consider that we don't really want to perform the surface integral in Eqn. (1) over curved membrane but rather over the base plane (x, y). The relation between these two measures involves the square root of the metric determinant: $\mathrm{d}A = \sqrt{g}\,\mathrm{d}x\,\mathrm{d}y = \sqrt{1 + (\boldsymbol{\nabla}h)^2}\,\mathrm{d}x\,\mathrm{d}y$. This nonlinearity needs to be expanded as well. If we do so up to quadratic order, we get the integrand within Monge parametrization up to quartic order:

$$\begin{aligned} \sqrt{g}K^2 &= \left[1 + \tfrac{1}{2}h_lh_l + \mathscr{O}(4)\right] \times \left[(h_{ii})^2 - (h_{ii})^2h_jh_j - 2h_{ii}h_jh_{jk}h_k + \mathscr{O}(6)\right] \\ &= (h_{ii})^2 - \tfrac{1}{2}(h_{ii})^2h_jh_j - 2h_{ii}h_jh_{jk}h_k + \mathscr{O}(6)\ . \end{aligned} \quad (5)$$

C. Fluctuations around mean shape

Equation (5) is the approximate integrand we need to work with. It is quartic in h, since we argued that going only up to quadratic order would not get us anywhere. Unfortunately, quartic Hamiltonians are nowhere near as easy to handle as quadratic ones! Hence, we will now introduce a *second* approximation, which is inspired by the original problem we wanted to solve: We will write our shape h as the sum of an *average shape* $\bar{h}$ plus some *small fluctuations* ε: $h = \bar{h} + \varepsilon$, see Fig. 1. The idea is now to insert this into the expression (5) for the integrand and expand *simultaneously* up to quadratic order in $\bar{h}$ *and* ε. The reason for this is that (*i*) we shall be perfectly content with obtaining a renormalized bending rigidity on the level of a linearized Monge Hamiltonian; and (*ii*) higher than quadratic order in ε will be impossible to integrate out and, hopefully, small anyways. Inserting this decomposition into Eqn. (5) and expanding gives us

$$\begin{aligned} \sqrt{g}K^2 &= (\bar{h}_{ii} + \varepsilon_{ii})^2 - \tfrac{1}{2}(\bar{h}_{ii} + \varepsilon_{ii})^2(\bar{h}_j + \varepsilon_j)(\bar{h}_j + \varepsilon_j) - 2(\bar{h}_{ii} + \varepsilon_{ii})(\bar{h}_j + \varepsilon_j)(\bar{h}_{jk} + \varepsilon_{jk})(\bar{h}_k + \varepsilon_k) + \mathscr{O}(6) \\ &= (\bar{h}_{ii})^2 + 2\bar{h}_{ii}\varepsilon_{jj} + (\varepsilon_{ii})^2 \\ &\quad -\tfrac{1}{2}\left[(\bar{h}_{ii})^2\varepsilon_k\varepsilon_k + 4\bar{h}_{ii}\bar{h}_k\varepsilon_{jj}\varepsilon_k - \bar{h}_k\bar{h}_k(\varepsilon_{jj})^2\right] \\ &\quad -2\left[2\bar{h}_{ii}\bar{h}_j\varepsilon_{jk}\varepsilon_k + 2\bar{h}_j\bar{h}_{jk}\varepsilon_{ii}\varepsilon_k + \bar{h}_{ii}\bar{h}_{jk}\varepsilon_j\varepsilon_k - 2\bar{h}_j\bar{h}_k\varepsilon_{ii}\varepsilon_{jk}\right] + \mathscr{O}(\bar{h}^3, \varepsilon^3)\ . \end{aligned} \quad (6)$$

D. Integrating out the fluctuations

We now need to integrate out the small fluctuations ε, *i.e.*, perform a partial partition function over small length scale fluctuations. However, what is the correct "measure" to be used in the partition function when summing up this continuous field degrees of freedom?

We will not attempt a rigorous treatment here (see [7, 8]. Rather, we use a heuristic approach based on our "experience" from the quadratic level. If in Eqn. (6) we set $\bar{h} \equiv 0$, we obtain the Hamiltonian

$$E = \int \mathrm{d}^2r\ \frac{1}{2}\kappa(\varepsilon_{ii})^2\ . \quad (7)$$

Let us expand ε in a Fourier series,

$$\varepsilon = \sum_{\boldsymbol{q}} \hat{\varepsilon}_{\boldsymbol{q}}\,\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \quad , \quad \boldsymbol{q} = \frac{2\pi}{L}\begin{pmatrix} n_x \\ n_y \end{pmatrix} \quad , \quad n_i \in \mathbb{Z}\ , \quad (8)$$

where L is the total side length of the membrane in x and y direction, and where the complex Fourier components satisfy $\hat{\varepsilon}_{\boldsymbol{q}} = \hat{\varepsilon}^*_{-\boldsymbol{q}}$. Inserting this expansion into the quadratic Hamiltonian (7), we immediately get

$$E = \sum_{\boldsymbol{q}} \tfrac{1}{2}(\kappa L^2 q^4)|\hat{\varepsilon}_{\boldsymbol{q}}|^2 \ . \tag{9}$$

This is not only quadratic, the different Fourier components are even nicely decoupled. The Hamiltonian is a sum of harmonic oscillators, *provided* we consider the $\hat{\varepsilon}_{\boldsymbol{q}}$ as our fundamental degrees of freedom, which hence amounts to making an assumption about our measure of integration for the partition function. We now do not even need to perform this integration, since the equipartition theorem ($\frac{1}{2}k_{\rm B}T$ energy on average per quadratic degree of freedom) gives us all we need:

$$\langle \hat{\varepsilon}_{\boldsymbol{q}} \hat{\varepsilon}_{\boldsymbol{q}'} \rangle = \frac{k_{\rm B}T}{L^2 \kappa q^4} \delta_{\boldsymbol{q},-\boldsymbol{q}'} \ . \tag{10}$$

We finally transform this back into real space by multiplying on both sides with $\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}'\cdot\boldsymbol{r}'}$, summing over $\boldsymbol{q}$ and $\boldsymbol{q}'$, and using Eqn. (8). The result is

$$\langle \varepsilon(\boldsymbol{r})\varepsilon(\boldsymbol{r}')\rangle = \frac{k_{\rm B}T}{L^2\kappa} \sum_{\boldsymbol{q}} q^{-4}\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \ . \tag{11}$$

If we want to know the average of particular derivatives, and all evaluated at a single $\boldsymbol{r} = \boldsymbol{r}'$, this gives

$$\begin{aligned} \langle \varepsilon_{i\cdots}(\boldsymbol{r})\varepsilon_{k\cdots}(\boldsymbol{r})\rangle &= \langle \varepsilon_{i\cdots}(\boldsymbol{r})\varepsilon_{k\cdots}(\boldsymbol{r}')\rangle\big|_{\boldsymbol{r}=\boldsymbol{r}'} \\ &= \frac{k_{\rm B}T}{L^2\kappa} \sum_{\boldsymbol{q}} q^{-4}(\mathrm{i}q_i)\cdots(-\mathrm{i}q_k)\cdots \ , \end{aligned} \tag{12}$$

where the index appearing on q now refer to the *component* of the vector $\boldsymbol{q}$. Notice that an term containing a total *odd* number of derivative indices vanishes identically, because these will give rise to at least one $\boldsymbol{q}$-component which occurs linearly and therefore sums to zero.

III. BENDING RENORMALIZATION

The final calculation is now easy. We will *assume* that Eqn. (12) also holds when $\bar{h}$ does not identically vanish (this is wrong, see Sec. V A). We will therefore perform the canonical average over the small wavelength fluctuation by inserting this equation into the Hamiltonian belonging to the integrand (6):

$$\begin{aligned} \langle E\rangle = \frac{1}{2}\kappa \int \mathrm{d}^2 r \, \Big\{ & (\bar{h}_{ii})^2 + \langle(\varepsilon_{ii})^2\rangle \\ & -\frac{1}{2}\Big[(\bar{h}_{ii})^2\langle\varepsilon_k\varepsilon_k\rangle - \bar{h}_k\bar{h}_k\langle(\varepsilon_{ii})^2\rangle\Big] \\ & -2\Big[\bar{h}_{ii}\bar{h}_{jk}\langle\varepsilon_j\varepsilon_k\rangle - 2\bar{h}_j\bar{h}_k\langle\varepsilon_{ii}\varepsilon_{jk}\rangle\Big]\Big\} \ . \end{aligned} \tag{13}$$

The remaining task is to evaluate the angular brackets, *i. e.*, to evaluate the corresponding $\boldsymbol{q}$-sum in Eqn. (12). We will make life simple, once more, by transforming from a sum to an integral:

$$\begin{aligned} \langle\varepsilon_i\varepsilon_i\rangle &= \frac{k_{\rm B}T}{\kappa L^2}\sum_{\boldsymbol{q}}\frac{1}{q^2} \simeq \frac{k_{\rm B}T}{\kappa L^2}\left(\frac{L}{2\pi}\right)^2\int \mathrm{d}^2q\,\frac{1}{q^2} \\ &= \frac{k_{\rm B}T}{2\pi\kappa}\int_{q_{\min}}^{q_{\max}}\mathrm{d}q\,\frac{1}{q} = \frac{k_{\rm B}T}{2\pi\kappa}\ln\frac{q_{\max}}{q_{\min}} \ , \end{aligned} \tag{14}$$

$$\langle\varepsilon_i\varepsilon_j\rangle = \frac{k_{\rm B}T}{\kappa L^2}\sum_{\boldsymbol{q}}\frac{q_iq_j}{q^4} = \frac{1}{2}\delta_{ij}\langle\varepsilon_k\varepsilon_k\rangle \ , \tag{15}$$

$$\begin{aligned} \langle(\varepsilon_{ii})^2\rangle &= \frac{k_{\rm B}T}{\kappa L^2}\sum_{\boldsymbol{q}}1 \simeq \frac{k_{\rm B}T}{\kappa L^2}\left(\frac{L}{2\pi}\right)^2\int\mathrm{d}^2q\;1 \\ &= \frac{k_{\rm B}T}{2\pi\kappa}\int_{q_{\min}}^{q_{\max}}\mathrm{d}q\;q = \frac{k_{\rm B}T}{4\pi\kappa}(q_{\max}^2 - q_{\min}^2) \ , \end{aligned} \tag{16}$$

$$\langle\varepsilon_{ii}\varepsilon_{jk}\rangle = \frac{k_{\rm B}T}{\kappa L^2}\sum_{\boldsymbol{q}}\frac{q_jq_k}{q^2} = \frac{1}{2}\delta_{jk}\langle(\varepsilon_{ii})^2\rangle \ . \tag{17}$$

Inserting these expressions into Eqn. (13) and neglecting constants, we obtain the result

$$\begin{aligned} \langle E\rangle = \frac{1}{2}\int\mathrm{d}^2r\,\Big\{&\Big[\kappa - \frac{3k_{\rm B}T}{4\pi}\ln\frac{q_{\max}}{q_{\min}}\Big](\nabla^2\bar{h})^2 \\ &+\Big[-\frac{3k_{\rm B}T}{8\pi}(q_{\max}^2 - q_{\min}^2)\Big](\boldsymbol{\nabla}\bar{h})^2\Big\} \ . \end{aligned} \tag{18}$$

Notice that we have finally obtained a Hamiltonian which looks like the linearized Monge version of (1) – with two important differences: First, the bending constant is different from κ. And second, there appears an *additional* term (second line in Eqn. (18) that has the form of a surface tension.

What is the meaning of the wave vectors $q_{\max}$ and $q_{\min}$? The bigger one corresponds to a small distance cut-off, $a = 2\pi/q_{\max}$, which we expect to be on the order of the *thickness* of the membrane. The small one corresponds to the large length scale up to which we have indeed coarse grained our Hamiltonian, $\lambda = 2\pi/q_{\min}$. We then see that thermal fluctuations *soften* the membrane and create a negative surface energy:

$$\kappa(T,\lambda,a) = \kappa - \frac{3}{4\pi}\,k_{\rm B}T\,\ln\frac{\lambda}{a} \ , \tag{19a}$$

$$\sigma(T,a) \simeq -\frac{3\pi}{2}\,\frac{k_{\rm B}T}{a^2} \ . \tag{19b}$$

Equation (19a) is confirmed by numerical simulations [9]

IV. A SIMPLE APPLICATION: PERSISTENCE LENGTH

Since the bending modulus κ gets smaller on larger length scales due to thermal fluctuations, there will be one length scale, $\lambda_{\rm p}$, at which it vanishes. This scale is called the *persistence length*, since membranes beyond this scale will be crumpled (there is no bending energy left to keep them straight), while on shorter length scales membranes maintain their average orientation. Using Eqn. (19a), we find

$$\lambda_{\rm p} = a\, {\rm e}^{4\pi\kappa/3k_{\rm B}T} \, . \qquad (20)$$

How big is this? For very soft surfaces, having a bare bending resistance of $\kappa = k_{\rm B}T$, we get $\lambda_{\rm p} \simeq 1\,{\rm nm} \times {\rm e}^{4\pi/3} \simeq 70\,{\rm nm}$. Hence, these objects are crumpled on optical length scales. With only *slightly* stiffer membranes, $\kappa = 2\,k_{\rm B}T$, we already get $\lambda \simeq 4\,\mu{\rm m}$. The exponential dependence on κ is not to be underestimated! In fact, using a value $\kappa = 20\,k_{\rm B}T$, which is a typical number for phospholipid bilayers, we get $\lambda(\kappa = 20\,k_{\rm B}T) \simeq 5\,{\rm nm} \times {\rm e}^{83.4} \simeq 1.2 \times 10^{28}{\rm m}$. This is whopping – ten times the size of the universe (150 billion lightyears). It also tells us that we should not misinterpret a membrane's persistence length. In particular, it does *not* mean that membranes on much shorter length scales are basically completely flat. Membranes *do* have very pronounced thermal fluctuations – even stiff ones, even on the micron scale.

V. SKELETONS IN THE CLOSET

The above calculation is evidently not exact, and was not intended to be. But it suffers from two conceptually different kinds of error: On the obvious side, we did not work on the full nonlinear level; rather, we employed a Monge parametrization and expanded up to quartic order. Furthermore, the corresponding Hamiltonian was only expanded up to quadratic order in perturbations ε around some large scale mean shape. These are intentional simplifications. However, there are two issues we dealt with in an "approximate" way that are more dangerous, and at first sight not easy to identify as potential pitfalls.

A. Improper normal gauge

The decomposition $h = \bar{h} + \varepsilon$ is always permissible, but we incorrectly assumed that the calculation of the total curvature via Eqn. (2) remains valid with ε replacing h. Eqn. (2) applies for height functions which describe *perpendicular* deviations from a *flat* base plane, but in our case ε describes deviations which are measured from a *curved* manifold (namely, $\bar{h}$), and which moreover are not even perpendicular to it (they are perpendicular to the base plane, not to $\bar{h}$!). As has been explained in Ref. [7], this has no influence on the renormalization of κ, but it yields a new term which can be read as a renormalization of the bending rigidity corresponding to the *Gaussian* curvature. However, it *does* modify the result for the generated surface energy.

B. Improper measure

Performing partition functions over fields is a tricky business, and one has to be quite careful concerning the measure of integration one uses [8]. Here we basically assumed that the mode-counting procedure can be extended to the (improper...) modes living on the curved manifold. Treating this issue more properly, we again find that Eqn. (19a) remains unaffected, but further changes occur in the surface energy, which combined with the issue raised in Sec. V A yield $\sigma(T,a) \simeq -\pi\,\frac{k_{\rm B}T}{a^2}$, see [7]. In fact, if the original Hamiltonian had some initial nonzero tension, the renormalization of it would involve also a logarithmic term similar to the one in Eqn. (19a), but positive [8].

Using a completely different measure, Helfrich has recently even predicted that thermal fluctuations should *stiffen* a membrane [10].

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