Fluctuations of incompatible elastic bilayers

Pearson W. Miller
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Fluctuating membranes make appearances throughout physics, biology and engineering. Here, we extend existing results pertaining to the behavior of thermalized membranes to consider a new class of geometrically incompatible surfaces created by the addition of a small spontaneous curvature to an otherwise flat membrane. Using perturbative renormalization group methods, we derive the behavior of key elastic constants under rescaling, and further derive the scale-dependence of the height-correlation function $\langle |h(q)|^2 \rangle = q^{-\eta}$. Using these results, the relevancy of the incompatible curvature coupling field is demonstrated and its the scaling the applied curvature $\bar{\kappa}$ with renormalization is found. Finally, there is a brief discussion of similar results for systems with quenched disorder, and for surfaces with non-flat reference configurations.

INTRODUCTION

The statistical mechanics of two-dimensional elastic surfaces has been and continues to be a rich area of research, essential to the understanding of a wide range of natural and engineered systems, ranging from graphene to the lipid membranes of red blood cells. [1] In contrast to the behavior of polymers in $d = 3$, whose configurations are largely self-avoiding random walk, shape fluctuations of fixed connectivity membranes are strongly surpressed due to the coupling of local Gaussian curvature with energetically expensive in-plane sheer deformation. As a consequence, thermalized membranes are characterized by a crumpling transition between a low-temperature flat phase, and a high temperature crumpled phase. [2, 3] An ongoing topic of research asks how the behavior of these surfaces changes when the membrane in question exhibits some geometric incompatibilities - in other words, when the surface in question does not have a stress-free equillibrium configuration. [4] Incompatibility can arise for a number of reasons in a natural surface - for instance, due to impurities in a randomly polymerized membrane.[5] Existing theory on the subject has in particular focused on models featuring preferred height profiles or spontaneous curvatures implemented as random quenched disorder on an otherwise flat membrane. [6]

In this paper, we investigate scaling behavior associated with the introduction of a different class incompatibility to a membrane. Motivated by recent experimental work in differential growth, [7] incompatibility is introduced as slowly varying field coupled linearly to the mean curvature. In the first section, we review the governing free energy for a uniform, connected membrane. Next, the system is treated via perturbative renormalization, from which the flow equations are derived, and in turn we obtain the critical exponent η which governs height fluctuations. [8] Armed with these results, the scaling behavior of an experimentally motivated class of weak, incompatibility is explored. Finally, we briefly compare our results with existing results for non-uniform, disordered incompatibility.

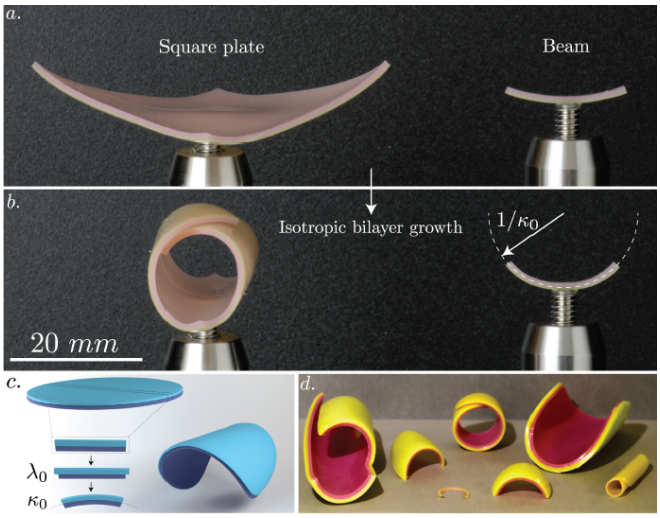

FIG. 1. (a) A bilayer disk and beam, lacking initial curvature preference. (b) Residual swelling at different rates between the two monolayers leads to change in the natural curvature of the surfaces. (c-d) Variation in the relative growth of the two monolayers leads to a variety of adopted curvatures and assumed shapes. Figure reproduced from [9].

FLUCTUATIONS OF UNIFORM MEMBRANES

To begin, we consider a membrane without any incompatibility. Consider a surface in d-dimensional space, for which we define a preferred configuration $\bar{X}(x^i) = x^i \hat{e}_i$, where x_i and $\hat{e}_i$ are the normal euclidean coordinates and orthonormal tangent vectors and i runs from $1, ..., D$. Following convention, the in-plane displacements of the surface from this reference configuration are represented as a D-component vector $u_i(\vec{x})$, $i = 1, ..., D$, and the out of plane displacement as a $d_c = d - D$ dimensional field $h_\alpha(\vec{x})$, $\alpha = D + 1, ..., d$, so that the position of the reference point $\vec{x}$ in the deformed configuration is given by

$$\vec{r} = [x_i + u_i(\vec{x})]\,\hat{e}_i + h^\alpha(\vec{x})\hat{n}_\alpha$$

where $\hat{n}_\alpha$ are a basis of normals to our surface. We choose to focus on the small strain limit, and so the linearized strain tensor is defined via

$$u_{ij} = \frac{1}{2}\left(\partial_i u_j + \partial_j u_i + \partial_i \vec{h}\cdot\partial_j\vec{h}\right)$$

and subsequently the unmodified energy functional takes the form

$$F_0 = \int d^D\vec{x}\left[\mu\bar{u}_{ij}^2 + \frac{1}{2}\lambda\bar{u}_{ii}^2 + \kappa(\nabla^2\vec{h})^2\right] \qquad (1)$$

where κ is the bending rigidity and μ and λ are the Lamé coefficients.[1] In this functional, the in-plane deformation u_i is coupled to the out of plane deformation $\vec{h}$ via the first and second terms, and need to be eliminated. Fortunately, the in plane modes appear only up to the second order, and can be integrated out to give an effective free energy strictly in terms of out of plane fluctuations:

$$\begin{aligned}F_{eff} = &\frac{\kappa}{2}\int d^D\vec{x}(\partial^2\vec{h})^2\\ &+\frac{\mu}{4(d-D)}\int d^D\vec{x}(P^T_{\alpha\delta}\partial_\alpha\vec{h}\cdot\partial_\beta\vec{h})(P^T_{\beta\gamma}\partial_\gamma\vec{h}\cdot\partial_\delta\vec{h})\\ &+\frac{\mu\lambda}{4(d-D)(2\mu+\lambda)}\int d^D\vec{x}(P^T_{\alpha\beta}\partial_\alpha\vec{h}\cdot\partial_\beta\vec{h})^2\end{aligned}$$

where $P^T_{\alpha\beta} = \delta_{\alpha\beta} - \frac{\partial_\alpha\partial_\beta}{\nabla^2}$ is the standard projection operator onto the traverse modes. The general D-dimensional form of this integral can be treated in full via renormalization group methods,[6] but as the particular case of interest for membranes is $D = 2$, we forgo the general treatment. For $D = 2$, the simplification $P^T_{\alpha\beta} = (\hat{z}\times\partial)_\alpha(\hat{z}\times\partial)_\beta$ reduces the effective energy to a much more approachable form:

$$\begin{aligned}F_{eff} = &\frac{\kappa}{2}\int d^2\vec{x}(\partial^2\vec{h})^2\\ &+\frac{Y}{8(d-2)}\int d^2\vec{x}(P^T_{\alpha\beta}\partial_\alpha\vec{h}\cdot\partial_\beta\vec{h})^2\end{aligned}$$

where $Y = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}$ is the Young's modulus. Thus, in the absence of intrinsic geometric incompatibility, only two material parameters are at play: Y_0 and κ. To the quadratic order, this free energy gives correlation functions

$$\langle h_i(\mathbf{q})h_j(\mathbf{q'})\rangle_0 = \frac{k_BT(2\pi)^2\delta_{ij}\delta(\mathbf{q}-\mathbf{q'})}{\kappa q^4}$$

PERTURBATIVE RENORMALIZATION

Addressing the effect of higher order terms cannot be done exactly, and is generally approached via either an $\epsilon = 4-D$ expansion [3] or the self-consistent screening approximation (SCSA). [6] In this paper, we will follow the perturbative method implemented in [10], which works as follows. First, the free energy is re-expressed in Fourier modes:

$$\begin{aligned}F_{eff} &= \frac{\kappa}{2}\int\frac{d^2\mathbf{q}}{(2\pi)^2}q^4|\vec{h}(\mathbf{k})|^2\\ &= \frac{Y}{8(d-2)}\int\frac{d^2\mathbf{q}_1d^2\mathbf{q}_2d^3\mathbf{q}_3}{(2\pi)^{3d}}[N_{\alpha\beta,\gamma\delta}(\mathbf{q}_1+\mathbf{q}_2)\\ &\times q_{1\alpha}q_{2\beta}q_{3\gamma}q_{4\delta}\vec{h}(\mathbf{q}_1)\cdot\vec{h}(\mathbf{q}_2)\vec{h}(\mathbf{q}_3)\cdot\vec{h}(\mathbf{q}_4)]\end{aligned}$$

where $\mathbf{q}_4 = -\mathbf{q}_1 - \mathbf{q}_2 - \mathbf{q}_3$, and $N_{\alpha\beta,\gamma\delta}(\mathbf{q}) = P^T_{\alpha\beta}(\mathbf{q})P^T_{\delta\gamma}(\mathbf{q})$. Note that in Fourier space, $P^T_{\alpha\beta} = \delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2}$. Following the usual procedure, we integrate over a momentum shell $\Lambda/b < q < \Lambda$, while rescaling as

$$\begin{aligned}\vec{x} &= b\vec{x}'\\ \vec{h} &= b^{\zeta_h}\vec{h}'(\vec{x}')\end{aligned}$$

The renormalization flow equations, in terms of $l = \log b$, can be written as

$$\begin{aligned}\frac{d\kappa}{dl} &= 2(\zeta_h-1)\kappa + Z_\kappa\\ \frac{d\tilde{Y}}{dl} &= 2(2\zeta_h-1)Y + Z_Y\end{aligned}$$

where the first term in each equation immediately follows from the quadratic order scaling. The terms Z_κ and Z_Y represent the correction due to the quartic terms, which we determine to one loop order (Fig. 2)to be:

$$\begin{aligned}Z_\kappa &= \frac{d}{dl}\left[Y\int_{\Lambda/b}^{\Lambda}\frac{d^2\mathbf{p}}{(2\pi)^2}(1-(\hat{q}\cdot\hat{p})^2)^2\langle\vec{h}(\mathbf{p})\vec{h}(-\mathbf{p})\rangle\right]\\ Z_Y &= -\frac{d}{dl}\left[\frac{Y^2A}{2k_BT}\int_{\Lambda/b}^{\Lambda}\frac{d^2\mathbf{p}}{(2\pi)^2}(1-(\hat{q}\cdot\hat{p})^2)^2p^4\langle\vec{h}(\mathbf{p})\vec{h}(-\mathbf{p})\rangle^2\right]\end{aligned}$$

Expanding these results for $\langle\vec{h}(q)\vec{h}(-q)\rangle \approx \frac{k_BT}{A\kappa q^4}$ yields

$$\begin{aligned}\frac{d\kappa}{dl} &= 2(\zeta_h-1)\kappa + \frac{3k_BTY}{16\pi\kappa\Lambda^2}\\ \frac{dY}{dl} &= (4\zeta_h-2)Y - \frac{3k_BTY^2}{32\pi\kappa^2\Lambda^2}\end{aligned}$$

To ensure that $\kappa' = \kappa$, we must set the renormalization factor to

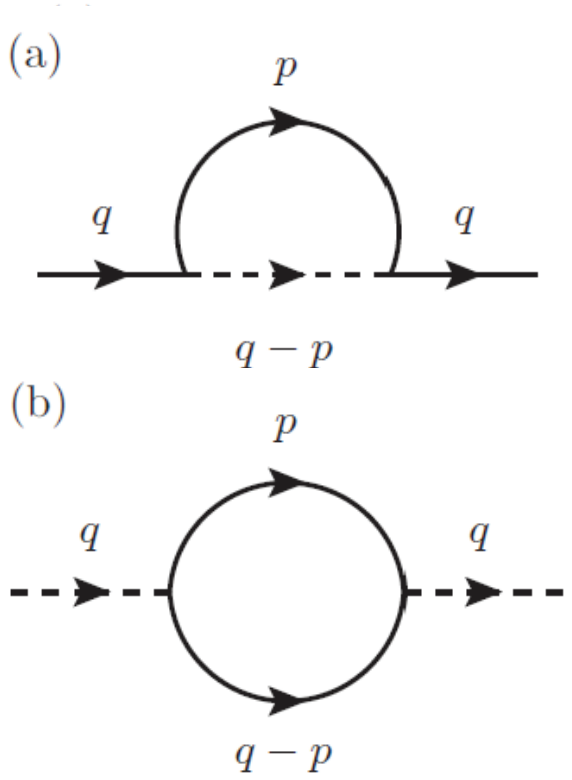

FIG. 2. Diagrammatic representation of one loop corrections to the renormalization of the material constants κ (a) and Y (b). Solid lines represent the propagator $G(q) = \frac{T}{\kappa q^4}$, and dashed lines are the momentum carried by the vertex Y. Figure reproduced from [10]

$$\zeta_h(l) = 1 - \frac{3k_BTY'(l)}{32\pi\kappa_0^2\Lambda^2}$$

which leads the renormalized Young's modulus to take the form

$$Y'(l) \sim \begin{cases} Y_0(l/a)^2 & l \ll l_{th} \\ \frac{64\pi\kappa_0^2\Lambda^2}{15k_BT} & l \gg l_{th} \end{cases}$$

where the thermal lengthscale $l_{th} \sim \frac{\kappa_0}{\sqrt{k_BTY_0}}$. The consequence of this is that the stiffness grows as we integrate out the smallest scales, but once renormalization passes the characteristic lengthscale l_{th}, Y approaches a fixed point value on the order of $Y_0(l_{th}\Lambda)^2$. The critical exponent η can be determined from the relations $\zeta_h = 1-\eta/2$, so in the Gaussian approximation we have $\eta = 0$, but for one loop, $\eta = 4/5$. The self-consistent screen approximation mentioned above, by contrast, calculates $\eta = 0.82$. [6], while $\epsilon = 4 - D$ expansion yields the substantially different result $\eta = 12\epsilon/25$.[3]

INCOMPATIBLE SURFACES

One of the simplest non-trivial incompatible systems is the elastic bilayer in which each layer is subjected to isotropic growth of a different magnitude. It was recently shown that for small growth, such a bilayer has energy given by [7]

$$\mathcal{U} = \mathcal{U}_s^K + \frac{h^2}{3}\mathcal{U}_b^K - \frac{2(1+\nu)h^2}{3}\int H\mathrm{Tr}(\mathbf{b})d\omega \quad (2)$$

where the first two terms are the standard Koiter shell stretching and bending energies for an unstressed elastic shell, h is shell thickness (assumed small relative to system size), $\mathbf{b}$ is the local curvature tensor, and H is the induced local curvature (which can be derived from the relative growth of the two monolayers). In other words, the elastic incompatibility can be approximated as a potential acting linearly on the curvature. Growing bilayers are quite common in biological systems in highly thermalized environments, such as during gastrulation in Drosophila [11]. Rather than the disordered curvature coupling studied in [12], the coupled field is not disordered - instead, it is generally uniform or varies on a tunable wavelength. We can make use of the results above to examine how this coupled field under renormalization. In the shallow-shell approximation, the quantity $\mathrm{Tr}(\mathbf{b}) \approx \nabla^2 h$, and so our modified free energy can be written as

$$F_0 = \int d^D\vec{x}\left[\mu\bar{u}_{ij}^2 + \frac{1}{2}\lambda\bar{u}_{ii}^2 + \kappa(\nabla^2 h)^2 - \bar{\kappa}\cos(\vec{q_0}\cdot\vec{x})\nabla^2 h\right] \quad (3)$$

where we have introduced $\bar{\kappa} = \frac{2(1+\nu)h^2H}{3}$ as the effective applied curvature coupling, while the term $\cos(\vec{q_0}\cdot\vec{x})$ represents the spatial modulation of the field along a chosen mode q_0. Creating a bilayer with periodic differential growth is well-within the ability of modern experimentalists: this may be thought of as the simplest case of the wide-range of realizable patterned curvature profiles.[13] In the Fourier representation, this coupled field takes the form $\int \bar{\kappa}d^D\vec{x}\nabla^2 h = q_0^2(h(q_0) + h(-q))$. Notably, for $\vec{q_0} = 0$, representing a uniform field, this term vanishes, and the system behaves identically to the non-modified case. As this term is purely linear in $\vec{h}$, we expect that there will be no direct modification of the renormalization procedure discussed above. As a result, the scaling of $\bar{\kappa}$ is given as

$$\tilde{\bar{\kappa}} = b^{d-2+\zeta_h}\bar{\kappa} \quad (4)$$

and ergo $y_{\bar{\kappa}} = d - 1 - \zeta_h$. This scaling as two notable regimes:

$$y_{\bar{\kappa}} = \begin{cases} d-1 & l \ll l_{th} \\ d-\frac{7}{5} & l \gg l_{th} \end{cases}$$

In either case, in the $d = 3$ realm of real membranes, we find that $y_{\bar{\kappa}} > 0$, and thus our curvature coupling field represents a relevant operator. This result can be compared to an established one for disordered membranes. In [12], a long wavelength incompatibility was introduced to a flat metric via modification of the strain tensor:

$$u_{ij} \to u_{ij} - h_\alpha \partial_i \partial_j f_\alpha$$

with the coupled field a power-law weighted Gaussian variable: $\overline{|\vec{f}(\vec{q})|^2} = \frac{\Delta^2}{Aq^{d_h}}$ for a given exponent d_h and amplitude Δ. Under these circumstance, this external metric only became relevant under the condition $d_h > 4-\eta$, where η is the scaling for the unmodified flat metric calculated above. [12]

CONCLUSION

In this paper, we have reviewed the statistical physics of thermally fluctuating in thin elastic membranes. Using renormalization group methods, we calculated the elastic properties and determined the scaling exponent $\eta = 4/5$ which governs the height fluctuations' scale dependence. Further, we explored the behavior of an externally coupled field under this renormalization procedure. It is interesting to note, but well beyond the scope of this paper, that the implementation of a uniform curvature-coupled field becomes far less trivial in non-flat reference geometries. For example, on a spherical membrane, additional couplings between the in-plane and out-of-plane terms in the energy mean terms linear in h in the energy functional still contribute to the quadratic order to the effective free energy obtained after integrating out in-plane modes. [12] This very well could introduce a need for additional correction in the renormalization process, dependent on external field.

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