Self-Consistent Theory of Polymerized Membranes

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We study D-dimensional polymerized membranes embedded in d dimensions using a self-consistent screening approximation. It is exact for large d to order $1/d$, for any d to order $\epsilon=4-D$, and for $d=D$. For flat physical membranes ($D=2$, $d=3$) it predicts a roughness exponent $\zeta=0.590$. For phantom membranes at the crumpling transition the size exponent is $\nu=0.732$. It yields identical lower critical dimension for the flat phase and crumpling transition $D_{\rm lc}(d)=2d/(d+1)$ ($D_{\rm lc}=\sqrt{2}$ for codimension 1). For physical membranes with *random* quenched curvature $\zeta=0.775$ in the new $T=0$ flat phase in good agreement with simulations.

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There are now several experimental realizations of polymerized or solidlike membranes, such as protein networks of biological membranes [1,2], polymerized lipid bilayers [3], and some inorganic surfaces [4]. Unlike linear polymers, two-dimensional sheets of molecules with fixed connectivity and nonzero shear modulus are predicted to exhibit a flat phase with broken orientational symmetry. Out-of-plane thermal undulations of solid membranes which induce a nonzero local Gaussian curvature are strongly suppressed because they are accompanied by in-plane shear deformations [5]. As a result, even "phantom" tethered membranes should be flat at low temperatures [5,6], and exhibit a quite remarkable anomalous elasticity, with wave-vector-dependent elastic moduli that vanish and a bending rigidity that diverges at long wavelength [7]. Excluded volume interactions, present in physical membranes, further stabilize the flat phase [8] but are usually assumed to be otherwise irrelevant to describe its long-distance properties. Motivated by recent experiments on partially polymerized vesicles [3], studies of models with quenched in-plane disorder have shown that the flat phase is unstable at $T=0$ to either local random stresses [9] or random spontaneous curvature [10].

Flat membranes of internal dimensionality D and linear size L are characterized by a roughness exponent ζ such that transverse displacements scale as L^{ζ}. Nelson and Peliti (NP), using a simple one-loop self-consistent theory [5] for $D=2$ which *assumes* nonvanishing elastic constants, found that phonon-mediated interactions between capillary waves lead to a renormalized bending rigidity $\kappa_R(q)\sim q^{-\eta}$ with $\eta=1$. Since $\zeta=(4-D-\eta)/2$ they predicted $\zeta=\frac{1}{2}$ for physical membranes. An $\epsilon=4-D$ expansion [7] confirmed that the flat phase was described by a nontrivial fixed point, but with *anomalous* elastic constants $\lambda(q)\sim\mu(q)\sim q^{\eta_u}$, $\eta_u>0$, with $\eta_u=4-D-2\eta$ as a consequence of rotational invariance. Thus, in general, $\zeta=(4-D+\eta_u)/4$ and the NP approximation corresponds to setting $\eta_u=0$.

There is presently some uncertainty on the precise value of the roughness exponent for physical membranes. Numerical simulations of tethered surfaces display a range of values for ζ from 0.5 [2], 0.53 [11], 0.64 [8,12], to 0.70 [13]. On the other hand, the $O(\epsilon)$ result [7] suggests a value very close to the NP value $\frac{1}{2}$ (0.52 by naively setting $\epsilon=2$). ζ should soon be measured from experiments, either directly from light scattering on diluted solutions [4] or indirectly from the scale dependence of the elasticity [14] of lamellar stacks of solid membranes presently under experimental study. The buckling transition [6], if observed, is controlled by a single exponent related to ζ. It thus seems desirable to explore further possible theoretical predictions for ζ.

In this Letter we introduce a self-consistent approximation which improves on the Nelson-Peliti theory [5] by allowing a nontrivial renormalization of the elastic moduli. It is exact in three different limits and compares well with numerical simulations. We construct two coupled self-consistent equations for the renormalized bending rigidity $\kappa_R(q)$ and elastic moduli $\mu_R(q),\lambda_R(q)$ and solve them in the long-wavelength limit. $\kappa_R(q)$ is determined by the propagator for the $d_c=d-D$ components $\mathbf{h}$ of the out-of-plane fluctuations $G(q)\sim 1/q^{4-\eta}$ while the elastic moduli are determined by the four-point correlation function of $\mathbf{h}$ fields. Physically, our calculation includes the additional effect of relaxation of in-plane stresses by out-of-plane displacements. As a result, curvature fluctuations soften elastic constants and screen the phonon-mediated interaction. A similar self-consistent screening approximation (SCSA) was introduced by Bray [15] to estimate the η exponent of the critical O(n) model (here d_c plays the role of the number of components n) and amounts to a partial resummation of the $1/d_c$ expansion. By construction, the method is exact for large codimension d_c to first order in $1/d_c$ and arbitrary D. Solving self-consistently then leads to an improved approximation of $\eta(d_c,D)$ (and thus ζ) for the small (physical) values of d_c.

The attractive feature of our theory is that it becomes exact in several other limits. First, because of the Ward identities associated with rotational invariance, we find that $\eta(d_c,D)$ is exact to first order in $\epsilon=4-D$ for arbitrary d_c and is thus compatible with all presently known results [6,7]. Second, for $d_c=0$ it gives $\eta=(4-D)/2$ which is the exact result since clearly $\eta_u=0$ for $d=D$, and [7] $\eta_u=4-D-2\eta$. This is at variance with the O(n) model for which the SCSA [15] is not exact for $n=0$. Thus we expect this method to give more accurate results for the present problem. Two-loop calculations are in progress [16] to estimate the deviation. An encouraging indication is the similarity of our method with the remarkably accurate self-consistent approximation of Kawasaki [17] for the critical dynamics of the binary fluid mixture, which was shown to be exact to order ϵ, again because of Ward identities, and incorrect to order ϵ^2 by a tiny amount. We also apply this method to the crumpling transition of phantom membranes, and to flat membranes with quenched disorder. Details can be found in Ref. [16].

In the flat phase, the membrane in-plane and out-of-plane displacements are parametrized respectively by a D-component phonon field $u_\alpha(x)$, $\alpha=1,\ldots,D$, and a $d_c=d-D$ component out-of-plane height fluctuations field $\mathbf{h}(x)$. A monomer of internal coordinate x is at position $\mathbf{r}(x)=[x_\alpha+u_\alpha(x)]\mathbf{e}_\alpha+\mathbf{h}(x)$, where $\mathbf{e}_\alpha$ are a set of D orthonormal vectors. The effective free energy is the sum of a bending energy and an in-plane elastic energy

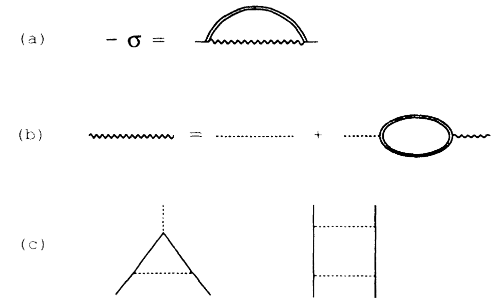

FIG. 1. Graphical representation of the SCSA: (a) self-energy and (b) interaction. (c) UV finite vertex and box diagrams.

(most relevant terms):

$$F=\int d^Dx\left[\frac{\kappa}{2}(\nabla^2\mathbf{h})^2+\mu u_{\alpha\beta}^2+\frac{\lambda}{2}u_{\alpha\alpha}^2\right], \qquad (1)$$

where the strain tensor is

$$u_{\alpha\beta}=\tfrac{1}{2}(\partial_\alpha u_\beta+\partial_\beta u_\alpha+\partial_\alpha\mathbf{h}\cdot\partial_\beta\mathbf{h}).$$

To discuss the SCSA in the flat phase it is convenient to first integrate out the phonons [1,5], and to work with the d_c-component $\mathbf{h}$ field. In terms of Fourier components the free energy takes the form of a critical theory:

$$F_{\text{eff}}=\frac{\kappa}{2}\int dk\,k^4|\mathbf{h}(k)|^2+\frac{1}{4d_c}\int dk_1dk_2dk_3R_{\alpha\beta,\gamma\delta}(q)k_{1\alpha}k_{2\beta}k_{3\gamma}k_{4\delta}\mathbf{h}(k_1)\cdot\mathbf{h}(k_2)\mathbf{h}(k_3)\cdot\mathbf{h}(k_4) \qquad (2)$$

with $q=k_1+k_2$ and $k_1+k_2+k_3+k_4=0$ and we use $\int dk$ to denote $\int d^Dk/(2\pi)^D$. The four-point-coupling fourth-order tensor $R(q)$ is transverse to q, the longitudinal part having been eliminated through phonon integration. It can be written as $R(q)=bN(q)+\mu M(q)$ with

$$N_{\alpha\beta,\gamma\delta}=\frac{1}{D-1}P_{\alpha\beta}^TP_{\gamma\delta}^T,$$
$$M_{\alpha\beta,\gamma\delta}=\tfrac{1}{2}(P_{\alpha\gamma}^TP_{\beta\delta}^T+P_{\alpha\delta}^TP_{\beta\gamma}^T)-N_{\alpha\beta,\gamma\delta}, \qquad (3)$$

where $P_{\alpha\beta}^T=\delta_{\alpha\beta}-q_\alpha q_\beta/q^2$ is the transverse projector. μ is the shear modulus and $b=\mu(2\mu+D\lambda)/(2\mu+\lambda)$ is proportional to both shear and bulk moduli. The convenience of this decomposition is that M and N are mutually orthogonal projectors under tensor multiplication (e.g., $M_{\alpha\beta,\gamma\delta}M_{\gamma\delta,\mu\nu}=M_{\alpha\beta,\mu\nu}$, etc.).

We set up two coupled integral equations for the propagator of the $\mathbf{h}$ field and for the renormalized four-point interaction. We want to evaluate $\langle h_i(-k)h_j(k)\rangle=\delta_{ij}G(k)$ with $G^{-1}(k)=\kappa_R(k)k^4=\kappa k^4+\sigma(k)$, where $\sigma(k)$ is the self-energy. The SCSA is defined in diagrammatic form by the graphs of Figs. 1(a) and 1(b), where the double solid line denotes the dressed propagator $G(q)$, the dotted line the bare interaction $R(q)$, and the wiggly line the "screened" interaction $\tilde{R}(q)$ dressed by the vacuum polarization bubbles. We thus obtain two equations, one for $\sigma(k)$ which determines η, and the other for R which determines η_u:

$$\sigma(k)=\frac{2}{d_c}k_\alpha k_\beta k_\gamma k_\delta\int dq\,\tilde{R}_{\alpha\beta,\gamma\delta}(q)G(k-q), \qquad (4a)$$

$$\tilde{R}(q)=R(q)-R(q)\Pi(q)\tilde{R}(q), \qquad (4b)$$

where $\Pi_{\alpha\beta,\gamma\delta}(q)=\int dp\,p_\alpha p_\beta p_\gamma p_\delta G(p)G(q-p)$ is the vacuum polarization and tensor multiplication is defined above. Because of the transverse projectors, only the component $\Pi(q)_{\text{sym}}$ of $\Pi(q)$ proportional to the fully symmetric tensor $S_{\alpha\beta,\gamma\delta}=\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}$ contributes in (4b). Defining $\Pi(q)_{\text{sym}}=I(q)S$, simple algebra gives $\tilde{R}(q)=\tilde{\mu}(q)M+\tilde{b}(q)N$ with renormalized shear and shear-bulk moduli, and the new equations

$$\tilde{\mu}(q)=\frac{\mu}{1+2I(q)\mu},\quad \tilde{b}(q)=\frac{b}{1+(D+1)I(q)b}, \qquad (5a)$$

$$\sigma(k)=\frac{2}{d_c}\int dq\,\frac{\tilde{b}(q)+(D-2)\tilde{\mu}(q)}{D-1}[kP^T(q)k]^2G(k-q). \qquad (5b)$$

We now solve these equations in the long-wavelength limit. Substituting $G(k)\sim\sigma(k)\sim Z/k^{4-\eta}$ in (5a) and (5b), with Z a nonuniversal amplitude, we find that the vacuum polarization integral diverges as

$$I(q)\sim Z^2A(D,\eta)q^{-\eta_u}, \qquad (6)$$

where $\eta_u=4-D-2\eta$ is the anomalous exponent of phonons. Substituting in (5a) and (5b), and defining the amplitude,

$$\int dq\, q^{\eta_u}(k-q)^{-(4-\eta)}[kP^T(q)k]^2=B(D,\eta)k^{4-\eta},$$

one finds (for $\mu,b>0$) that the Z and $k^{4-\eta}$ factors cancel and that η is determined self-consistently by the equation for the *amplitude*:

$$d_c=D/(D+1)[B(D,\eta)/A(D,\eta)],$$

which after calculation of the integrals defining A,B gives

$$d_c=\frac{2}{\eta}D(D-1)\frac{\Gamma[1+\frac{1}{2}\eta]\Gamma[2-\eta]\Gamma[\eta+D]\Gamma[2-\frac{1}{2}\eta]}{\Gamma[\frac{1}{2}D+\frac{1}{2}\eta]\Gamma[2-\eta-\frac{1}{2}D]\Gamma[\eta+\frac{1}{2}D]\Gamma[\frac{1}{2}D+2-\frac{1}{2}\eta]}. \tag{7}$$

For $D=2$ this equation can be simplified, and one finds (Fig. 2)

$$\eta(D=2,d_c)=\frac{4}{d_c+(16-2d_c+d_c^2)^{1/2}}. \tag{8}$$

Thus for physical membranes we obtain $\eta=0.821$, $\eta_u=0.358$, and

$$\zeta=1-\frac{\eta}{2}=\frac{\sqrt{15}-1}{\sqrt{15}+1}=0.590\ldots \tag{9}$$

roughly at midvalue of the present numerical simulations. From (5) we also obtain $\lim_{q\to 0}\tilde{\lambda}(q)/\tilde{\mu}(q)=-2/(D+2)$ (i.e., a negative Poisson ratio).

Expanding result (7) in $1/d_c$ one obtains

$$\eta=\frac{8}{d_c}\frac{D-1}{D+2}\frac{\Gamma[D]}{\Gamma[D/2]^3\Gamma[2-D/2]}+O\left(\frac{1}{d_c^2}\right)$$
$$=\frac{2}{d_c}+O\left(\frac{1}{d_c^2}\right)\quad(\text{for } D=2) \tag{10}$$

which coincides with the exact result [6,7], as expected by construction of the SCSA. Similarly, expanding (7) to first order in $\epsilon=4-D$ one finds

$$\eta=\frac{\epsilon}{2+d_c/12} \tag{11}$$

also in agreement with the exact result [6,7]. This is not a general property of SCSA. Here it can be traced to the vertex and box diagrams of Fig. 1(c) being *convergent.* Indeed, because of the transverse projectors in (2) and (3) one can always extract one power of external momentum from each external **h** leg, which lowers the degree of divergence from naive power counting. As a result, if one decouples the four-point vertex $\underset{\sim}{R}$ via a mediating field, the only counterterms needed are for two-point functions.

We have analyzed the crumpling transition of phantom membranes by the same method, applied to the isotropic theory of Ref. [18]. The exponent $\eta=\eta_{\rm cr}$ at the transition is determined by [16]

$$d=\frac{D(D+1)(D-4+\eta)(D-4+2\eta)(2D-3+2\eta)\Gamma[\frac{1}{2}\eta]\Gamma[2-\eta]\Gamma[\eta+D]\Gamma[2-\frac{1}{2}\eta]}{2(2-\eta)(5-D-2\eta)(D+\eta-1)\Gamma[\frac{1}{2}D+\frac{1}{2}\eta]\Gamma[2-\eta-\frac{1}{2}D]\Gamma[\eta+\frac{1}{2}D]\Gamma[\frac{1}{2}D+2-\frac{1}{2}\eta]}. \tag{12}$$

At the transition the radius of gyration scales as $R_G\sim L^{\nu}$ with $\nu=(4-D-\eta_{\rm cr})/2$. For $d=3$ and $D=2$ we find $\eta_{\rm cr}=0.535$ and $\nu=0.732$ (Haussdorf dimension $d_H=2.73$). The embedding dimension $d_u(D)$ above which self-avoidance is *irrelevant* for the membrane *at* the crumpling transition is determined by the condition $d_u=4D/[4-D-\eta_{\rm cr}(d_u)]$. Using (12) we find that $d_u(2)=4.98$.

The present method gives interesting predictions for lower critical dimensions. In the flat phase, orientational order (i.e., in $\nabla\mathbf{h}$) disappears for $D<D_{\rm lc}$, where $2-\eta(D_{\rm lc},d_c)=D_{\rm lc}$. From (7) this is equivalent to $d_c=D_{\rm lc}(D_{\rm lc}-1)/(2-D_{\rm lc})$. On the other hand, the lower critical dimension $D'_{\rm lc}(d)$ for the crumpling transition is defined by $2-\eta_{\rm cr}(D'_{\rm lc},d)=D'_{\rm lc}$, or equivalently from (12), $d=D'_{\rm lc}/(2-D'_{\rm lc})$. Since $d=D/(2-D)$ is clearly equivalent to $d_c=D(D-1)/(2-D)$ we find that the lower critical dimensions of the crumpling transition and of the flat phase, as predicted by SCSA, are identical, and given by $D_{\rm lc}(d)=2d/(1+d)$. Since they originate from very different calculations, this indicates that the SCSA is quite consistent. For codimension 1 manifolds $D_{\rm lc}=\sqrt{2}$ and for fixed embedding space $d=3$, $D_{\rm lc}=\frac{3}{2}$. $D_{\rm lc}$ increases from $D_{\rm lc}=1$ for $d_c=0$ to $D_{\rm lc}=2$ when

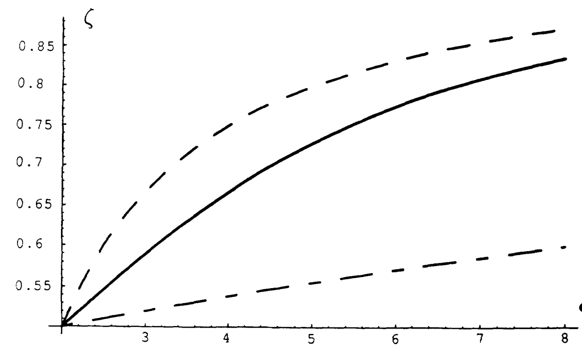

FIG. 2. ζ as a function of d for two-dimensional membranes $D=2$. The solid curve is the SCSA result (8). The long-dashed–short-dashed curve is the $O(\epsilon)$ result, setting $\epsilon=2$. The dashed curve corresponds to $\eta=2/d$ chosen (somewhat arbitrarily) in Ref. [6] as a possible interpolation to finite d (asymptotic to the solid curve for $d\to\infty$).

$d_c \to \infty$ as expected. Note that for $d > 3$ self-avoidance cannot modify the above results for D_{lc}, while for $d < 3$ it is an open question.

We can compare (8) and (12) with recent simulations [19] of $D=2$ membranes with self-avoidance in higher d_c. The membranes are found flat in $d=3,4$ with $\zeta(d=3)=0.64\pm0.04$, $\zeta(d=4)=0.77\pm0.04$, whereas we obtain 0.59,0.67, respectively. The membrane is crumpled in $d=5$ with $\nu=0.8\pm0.06$, although $d=5$ seems almost marginal, whereas we find $\nu=0.8$ *at* the crumpling transition where self-avoidance is irrelevant, although almost marginally so.

Flat membranes with random spontaneous curvature are described by adding the term $-\int d^Dx\, \mathbf{c}(x)\cdot\nabla^2\mathbf{h}(x)$ in the energy (1), where $\mathbf{c}(x)$ are Gaussian quenched random variables [10]. Within a replica symmetric SCSA, we find a marginally unstable $T=0$ fixed point, i.e., a long-wavelength solution only if $T\to 0$ first. Defining the replica connected and off-diagonal exponents η,η', by

$$\overline{\langle \mathbf{h}(-q)\mathbf{h}(q)\rangle_c} \sim q^{-(4-\eta)}, \quad \overline{\langle \mathbf{h}(-q)\mathbf{h}(q)\rangle} \sim q^{-(4-\eta')}$$

we find [16] at this fixed point $\eta'=\eta$, $\eta(d_c,D)=\eta_{\text{pure}}(4d_c,D)$. Thus one can simply replace d_c in the pure result by $4d_c$. Again this agrees with the $1/d_c$ and ϵ expansions [10]. For physical membranes $D=2$, $d_c=1$, we find from (8)

$$\eta=2/(2+\sqrt{6})=0.449, \quad \zeta=0.775,$$

comparing well with the numerical simulation [10] result $\zeta=0.81\pm0.03$. By analogy with the random-field problem [20], it is quite possible that the equality $\eta=\eta'$, conjectured in Ref. [10] to all orders, can be corrected when replica symmetry breaking is included.

In conclusion, we have presented a self-consistent theory of polymerized membranes which becomes exact in three limits (large d_c, small $\epsilon=4-D$, and $d_c=0$). By construction, it satisfies the exponent relations $\eta_u=4-D-2\eta$ and [16] $1/\nu'=D-2+\eta$. These relations are exact in the true theory because of rotational invariance [6,7]. It thus predicts $\nu'=1.218$ and $\delta'=1.436$ for the buckling transition exponents [6]. It contradicts the conjecture [2] $\zeta=\frac{1}{2}$.

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