First order phase transitions in polymerized phantom membranes

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The crumpled-to-flat phase transition that occurs in $D$-dimensional polymerized phantom membranes embedded in a $d$-dimensional space is investigated nonperturbatively using a field expansion up to order eight in powers of the order parameter. We get the critical dimension $d_c(D)$ that separates a second order region from a first order one everywhere between $D = 4$ and $D = 2$. Our approach strongly suggests that the phase transitions that take place in physical membranes are of first order in agreement with most recent numerical simulations.

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Fluctuating or random surfaces are a recurrent concept in physics [1, 2]. They occur in soft matter physics or in biology as assemblies of amphiphilic molecules that can form plane or closed structures (vesicles) according to the chemical composition of the membrane itself and its surroundings. Random surfaces also appear in high-energy physics, especially in string theory, as the world-sheet swept out by a string during its spacetime evolution. More recently membranes have received a renewed interest in condensed matter physics where it has been realized that, from the point of view of their mechanical properties, novel materials, like graphene [3], identify with polymerized membranes, providing the first and unique example of genuinely two-dimensional membrane [4, 5]. The coexistence of two-dimensional geometry and thermal fluctuations is at the origin of a variety of behaviours depending on the nature of the internal structure of the membrane. Fluid membranes are made of molecules that freely diffuse and rearrange rapidly when a shear or a stress is performed. This implies that, in absence of an external tension, the dominant energy is the bending energy. It has been shown that, in this case, the height fluctuations are sufficiently strong to prevent the appearance of long-range order; fluid membranes are thus always crumpled [6, 7]. Polymerized – or tethered – membranes display a drastically different behaviour. Indeed the existence of an underlying network of linked molecules induces elastic (shearing and stretching) energy contributions that lead to a coupling between height and transverse – phonons – modes. It results from this situation a frustration of the height fluctuations [8] that are strongly reduced at low temperatures giving rise to the appearance of a flat phase with long-range order between the normals [9, 10]. The existence of a low-temperature phase accompanied with spontaneous symmetry breaking of rotational invariance is a prior in contradiction with the Mermin-Wagner theorem. However it appears that the effective phonon-mediated interaction between the height fields (more precisely between the Gaussian curvatures) is of long-range kind, allowing to evade the conditions of application of the Mermin-Wagner theorem [9]. Correlatively the low-temperature phase of membranes is characterized by non trivial scaling behaviour in the infrared [11-13]:

$$
\begin{align*}
G_{hh}(q) & \sim q^{-(4-\eta)} \\
G_{uu}(q) & \sim q^{-(6-D-2\eta)}
\end{align*}
$$

where $G_{hh}(q)$ and $G_{uu}(q)$ are the correlation functions of the out-of-plane and in-plane excitations respectively. The exponent $\eta$ characterizes stable membranes including, for instance, sheets of graphene. The determination of this exponent has been the object of an intense activity. Early perturbative approaches performed below the upper critical dimension $D = 4$ at first order in $\epsilon = 4 - D$ have led – with $\epsilon = 2$ – to the questionable value $\eta \approx 0.96$ [11]. On the other hand large-$d$ expansion performed at lowest order and extrapolated to the finite value $d = 3$ has produced another doubtful value: $\eta = 2/3$ [10, 13]. More sophisticated computations performed in the aftermath have revealed a remarkable stability of the results with the order of the approximations. For instance self-consistent screening approximations (SCSA) at leading and next-to-leading order have led to close values: $\eta \approx 0.821$ [14-17] and $\eta = 0.789$ [15] respectively. Non-perturbative renormalization group (NPRG) approaches have also been used, first within a double field and field-derivative expansion leading to the value $\eta \approx 0.849$ [18]. This computation has been extended by including the momentum dependence of the vertices that were considered in Ref.[18]. Very surprisingly an almost unchanged value of $\eta$ has been obtained: $\eta \approx 0.85$ [19, 20]. This exponent has also been computed by means of Monte Carlo simulations of membranes leading to the values $\eta = 0.813(3)$ [21] and $\eta = 0.750(5)$ [22], and recently using a Fourier Monte Carlo simulation the value $\eta = 0.795(10)$ [23]. Finally Monte Carlo simulations of graphene using a realistic potential have concluded in favor of the value $\eta \approx 0.85$ [24] in agreement with the SCSA and even bet-
ter with NPRG approaches. This agreement between the field theoretical approaches and the Monte Carlo computations of membranes or materials like graphene has proven the relevance of the continuum models to describe the long-distance behaviour of these systems in the flat phase. It has also shown the adequacy of the approximations used within these field theoretical approaches – see below for considerations about the NPRG computations.

On the opposite the question of the nature of the crumpled-to-flat transition is still largely open. In this context several perturbative approaches have also been used to investigate the critical physics of $D$-dimensional polymerized membranes embedded in a $d$-dimensional space. A weak-coupling perturbative approach performed in the vicinity of the upper critical dimension $D = 4$ [25] has led to predict a second order phase transition for $d > d_{cr}$ and first order phase transitions for $d < d_{cr}$ with $d_{cr} \approx 219$ just below $D = 4$. However, again, these results are not directly relevant for two-dimensional membranes. Alternatively 1/d expansion [10, 13] or SCSA [14] have been employed to investigate this transition. However a main problem with these approaches is their inability to identify the existence – and thus to get the value – of the critical dimension $d_{cr}(D)$ separating the first from the second order region. Finally the crumpled-to-flat transition has been investigated by means of Monte Carlo and cluster variation method (CVM) computations for membranes or related models. While early computations favored a second order phase transition (see [2, 26, 27] for reviews) more recent computations exhibit clear first order behaviours [28–31], see also [32–34].

Recently NPRG approaches have been used to investigate both the flat phase and the nature of the crumpled-to-flat transition [18–20]. These approaches are based on the concept of running effective action [35] (see [36–40] for reviews), $\Gamma_k[\phi]$, a functional of the order parameter field $\phi$, that describes the effective physics at a coarse-grained scale $k$. Technically the index $k$ stands for a running scale that separates the high-momentum modes, with $q > k$, from the low-momentum ones, with $q < k$ and $\Gamma_k[\phi]$ represents a coarse grained free energy where only fluctuations with momenta $q > k$ have been integrated out. The running of $k$ towards $k = 0$ thus corresponds to gradually integrating over all fluctuations. The $k$-dependence, RG flow, of $\Gamma_k$ is provided by an exact – albeit one-loop – evolution equation now known as the Wetterich equation [35]. Solving this equation allows to get the RG flows and thus the critical properties. However although exact the Wetterich equation cannot be solved exactly and approximations must be performed in order to make the computations tractable. Several kinds of approximations are possible and some of them have already been used in the context of membranes: i) a double expansion of the effective action in powers of the field and derivatives of the field [18] ii) a field expansion of the effective action where the full momentum dependence of the vertices is kept [19, 20]. On the basis of these approaches, that have been performed up to order four in powers of the field, a second order phase transition has been predicted for polymerized membranes, allowing nevertheless the possibility of first order transitions. A crucial point within the NPRG context is to guess the suitable approximation of the effective action $\Gamma_k[\phi]$ and to check the convergence of the results when enriching its content. We address here the question of the relevance of the high-order vertices that have been discarded in both [18] and in [19, 20]. To do this we consider an expansion up to order eight in powers of the field, keeping only their local – zero momentum – part, extending thus the computation performed in [18]. Our motivation is threefold: i) to probe the importance of terms that, from the point of view of standard power-counting, are the most relevant – and in particular more relevant than the non-local ones considered in [19, 20] ii) to optimize our results using different kinds of cut-off families iii) to test the convergence of our results with respect to the field content. We show that the terms considered here drastically affect the critical behaviour since they very likely turn the second order phase transition into first order ones.

We consider a $D$-dimensional membrane embedded in a $d$-dimensional Euclidean space. The location of a point on the membrane is realized by the use of $D$-dimensional internal coordinates $x \equiv x_\mu, \mu = 1 \ldots D$ while a configuration of the membranes in the Euclidean space is realized through the embedding: $x \rightarrow R(x)$ with $R \equiv (R^i), i = 1 \ldots d$. The energy of a polymerized membrane is made of a bending energy part and a stretching energy part. In the spirit of a Landau-Ginzburg-Wilson approach this energy can be expressed as an expansion in powers of the microscopic field $R$ and its derivatives. Here translational invariance in the embedding space and rotational invariance – in the embedding as well as in the internal space – of the energy lead to an expansion in terms of the tangent vectors $\partial_\mu R$, $\mu = 1 \ldots D$. The energy is given by:

$$H[R] = \int d^Dx \frac{k}{2} (\partial_\mu \partial_\nu R)^2 + \frac{t}{2} (\partial_\mu R)^2 + \ldots$$

$$+ u (\partial_\mu R, \partial_\nu R)^2 + v (\partial_\mu R, \partial_\nu R, \partial_\rho R)^2 + \ldots$$

with $\partial_\mu = \partial/\partial x_\mu$, $\mu = 1 \ldots D$. In (1) the first term represents the bending energy with $k$ the rigidity constant, the second one a tension while the other terms correspond to stretching energy with $u$ and $v$ being the Lamé coefficients. Finally note that the temperature $T$ has been absorbed in the bare coupling constants. Let us consider a mean-field approach of the crumpled-to-flat phase transition, with the assumptions $u > 0$ and $u + vD > 0$. For $t > 0$ the minimum of (1) is given by a crumpled phase with a vanishing average value of the order parameter: $\langle \partial_\mu R \rangle = 0$ expressing the absence
of long-range orientational order. For $t < 0$ the minimum of (1) is given by non-vanishing values of:

$$\partial_\mu r = \langle \partial_\mu R \rangle = \zeta e_\mu$$  \hspace{1cm} (2)

where $\mu = 1 \ldots D$ where $\zeta = \sqrt{-t/4(\mu + vD)}$ and where the $e_\mu$ form an orthonormal set of $D$ vectors with $e_\mu e_\nu = \delta_{\mu\nu}$ that span the flat phase. This occurrence of long-range orientational order with non-vanishing values of the mean tangent vectors $\partial_\mu r$ at low-temperature is analogous to the occurrence of ferromagnetism in spin systems, the tangent vectors playing the role of order parameters with magnitude given by $\zeta$. Thus at $t = 0$, in the mean-field approximation, there is a phase transition between a high-temperature, crumpled phase and a low-temperature, flat phase displaying long-range orientational order.

From now on we employ the effective action, obtained through a Legendre transform of the free energy [37], in terms of which the Wetterich equation is written. We consider a derivative expansion of the effective action:

$$\Gamma_k[r] = \int d^D x \frac{Z_k}{2} (\partial_\mu \partial_\nu r)^2 + U_k[\partial_\mu r] + O(\partial_\mu^2)$$

In this expression $Z_k$ is a field-independent field renormalization, $U_k[\partial_\mu r]$ is the potential part of the effective action that we expand in powers of the field $\partial_\mu r$ around the flat phase configuration (2):

$$U_k[\partial_\mu r] = \sum_{n_1, \ldots, n_D \geq 0} a_{n_1, \ldots, n_D} \langle \text{Tr}[g]^{n_1} \ldots \text{Tr}[g^D] \rangle^{n_D}$$  \hspace{1cm} (3)

where $g$ stands for the -- metric -- tensor with elements: $g_{\mu\nu} = \partial_\mu r \partial_\nu r - \zeta^2 \delta_{\mu\nu}$. We have considered the expansion (3) up to order eight in the field, which means to follow the flow of 10 coupling constants. Note that the engineering dimension of the order parameter $\partial_\mu r$ is given by: $[\partial_\mu r] = (D - 2)/2$. The dimension of a generic coupling constant entering in (3) is thus given by $[a_{n_1, \ldots, n_D}] = D - (D - 2)(n_1 + 2n_2 + \cdots + Dn_D)$. Therefore the coupling constants of (3) are all relevant with dimension 2 in $D = 2$. This is in contrast with the terms considered in [20] which involves at least two additional derivatives and are thus at best marginal. One can thus anticipate from this power counting that the terms considered here play a more significant role than those treated in [20].

The RG flow of $\Gamma_k$ is provided by the Wetterich equation [35]:

$$\frac{\partial \Gamma_k}{\partial t} = \frac{1}{2} \text{Tr} \left\{ \frac{\partial R_k}{\partial t} (\Gamma_k^{(2)} + R_k)^{-1} \right\}$$  \hspace{1cm} (4)

where $t = \ln k/\Lambda$, $\Lambda$ being some ultraviolet scale. The trace has to be understood as a $D$-dimensional momentum integral as well as a summation over internal indices. In Eq.(4), $\Gamma_k^{(2)}$ is the inverse propagator, the second derivative of $\Gamma_k$ with respect to the field $r$, taken in a generic, nonvanishing field configuration. $R_k(q)$ is a cut-off function that suppresses the propagation of modes with momenta $q < k$ and makes that $\Gamma_k$ encodes only modes with momenta $q > k$. It also regulates the ultraviolet behaviour. For our study we have used three cut-off families parametrized by a real number $\lambda$: $R_k^{(\lambda)}(q) = Z_k \lambda (k^4 - q^4)^{\theta(2k^2 - q^2)}$, $R_k^{(2)}(q) = Z_k \lambda q^4/\exp(q^2/k^4) - 1$ and $R_k^{(3)}(q) = Z_k \lambda \exp(-q^4/k^4)$. The RG equations for the different coupling constants entering in (3) are obtained by expressing them as functional derivatives of $\Gamma_k[r]$, taking their t-derivatives and using (4). We have successively considered the order four, six and eight of the expansion in powers of $\partial_\mu r$, with the eight order appearing as the last order manageable within the current abilities and a reasonable period of time [47].

Flat phase. Within our formalism the RG equations in this phase are obtained by taking the limit where the dimensionless magnitude $\zeta$ goes to infinity (see [18]) corresponding to the decoupling of the phonon modes and to a spectrum of excitations dominated by the height fluctuations. Our analysis shows that the RG equations obtained in the flat phase at order four in [18] are not modified by any higher power of the field (see [41] for technical details). Thus the results derived in [18], and in particular the value of $\eta \simeq 0.849$, are correct at all orders within an expansion in powers of $\partial_\mu r$. This fact explains in a great extent the agreement between our prediction for $\eta$ and that obtained with the Monte Carlo simulation. It remains however to understand also why the derivative terms considered in [20] do almost not modify the value of $\eta$.

Crumpled-to-flat transition. The situation is very different for the crumpled-to-flat transition. At each order, four, six and eight in powers of the field we have determined the value of $d_{cr}(D)$. We have used the three families of cut-off functions $R_{k,1}$, $R_{k,2}$ and $R_{k,3}$ and optimized the result by applying the principle of minimal sensitivity, see [42, 43]. For almost each family of cut-off we have found a marked minimum of $d_{cr}(D)$ as a function of the parameter $\lambda$. This is illustrated at order six in powers of the field and for $D = 2$ in Fig.1. Then, at each order, we have averaged over the different values obtained from different cut-off families. The results are displayed in Fig.2, the bar corresponding to the dispersion of values of $d_{cr}(D = 2)$. As can be seen from Fig.2, $d_{cr}$ displays an oscillating behaviour with amplitudes decreasing with the order of the expansion. This damped oscillating behaviour is typically observed for critical exponents or other physical quantities in various systems within the field expansion [42–46]. This strongly suggests a convergence toward a value located between 4.5 and 6.5, excluding in particular the value $d = 3$ and thus a second order phase transition. This conclusion is
strengthened by the fact that the dispersion of results when varying the cut-off functions decreases with the order of the expansion. Finally Fig. 3 displays the shape of the curve $d_{cr}(D)$ everywhere between the upper critical dimension $D = 4$ and $D = 2$ computed for the cut-off $R_{k,1}$.

**FIG. 1:** Optimization of $d_{cr}(D = 2)$ as function of the parameter $\lambda$ for the approximation of order six for the cut-off functions $R_{k,2}$ and $R_{k,3}$.

**FIG. 2:** Critical dimension $d_{cr}(D = 2)$ as a function of the order of the expansion.

**Conclusion.** Taking into account orders beyond the power four of the field within a field expansion deeply modifies the critical behaviour of polymerized membranes at the crumpled-to-flat transition, contrary to what happens for the flat phase that displays a strong stability. Our study favours the existence of first order phase transitions for phantom polymerized membranes in agreement with most recent numerical computations [31]. Note that since the order eight appears as the last manageable order of the field expansion a definite conclusion would certainly require a full treatment of the potential part of the effective action as well as managing (a part of) derivative terms [41]. However, the behaviour of the critical dimension $d_{cr}$ with the order of the field expansion, combined with knowledge acquired from other systems, makes highly unlikely a change of the nature of the transition compared with the present results.

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