Phases of a stack of membranes in a large number of dimensions of configuration space

M. E. S. Borelli* and H. Kleinert†
Institute for Theoretical Physics, Freie Universitäet Berlin Arnimallee 14, 14195 Berlin, Germany
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The phase diagram of a stack of tensionless membranes with nonlinear curvature energy and vertical harmonic interaction is calculated exactly in a large number of dimensions of configuration space. At low temperatures, the system forms a lamellar phase with spontaneously broken translational symmetry in the vertical direction. At a critical temperature, the stack disorders vertically in a meltinglike transition. The critical temperature is determined as a function of the interlayer separation l.

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I. INTRODUCTION

Under suitable conditions, lipid membranes in aqueous solution are known to form lamellar structures, characterized by a parallel arrangement of the membranes alternating with thin layers of water.[1] The existence of such structures is in contrast to the behavior of a single tensionless membrane subject to thermal fluctuations, which is always in a disordered, crumpled phase, filling the embedding space completely.[2] In a stack, this phase is suppressed by the steric repulsion between the membranes which prevents them from passing through each other,[1] thus constraining the amplitude of the height fluctuations of each membrane to be less than the distance to its nearest neighbors.

Recently, a model for a finite stack of tensionless membranes was studied with respect to the effects of higher-order terms of the curvature energy.[3] As in previous studies,[1] the steric repulsion between the layers was replaced with an harmonic interaction potential. The approach was perturbative, using the renormalization group to sum infinitely many terms. It was shown that thermal fluctuations induce the melting of the stack into a vertically disordered phase. By its nature, the perturbative expansion was able to give a satisfactory description only for the ordered phase.

For a description of the disordered phase and a better understanding of the entire transition, we analyze in this paper the behavior of a stack of tensionless membranes exactly for very large dimension d of the embedding space. Since the model is exactly solvable in this limit, we can calculate all its relevant properties explicitly, in particular, its complete phase diagram as a function of the interlayer separation l.

II. THE MODEL

As in Ref. 3, we consider a model in which a multilayer system is made up of $(N+1)$ fluid membranes, parallel to the xy plane of a Cartesian coordinate system, separated a distance l. If the vertical displacement of the mth membrane with respect to this reference plane is described by a function $u_m(\mathbf{x}) \equiv u(\mathbf{x}_\perp, ml)$, where $\mathbf{x}_\perp = (x,y)$, the energy of the stack reads

$$E = \sum_m \int \mathrm{d}^2 x_\perp \sqrt{g_m} \left[\frac{1}{2} \kappa_0 H_m^2 + \frac{B_0}{2l} (u_m - u_{m-1})^2 \right]. \quad (1)$$

Here, $H_m = \partial_a N_{m,i}$ is the mean curvature, where $\mathbf{N}_m \propto (-\partial_1 u_m, -\partial_2 u_m, 1)$ is the unit normal to the mth membrane, and

$$g_{m,ij} = \delta_{ij} + \partial_i u_m \partial_j u_m \quad (2)$$

the induced metric, with $i,j = 1,2$, $\partial_1 = \partial/\partial x, \partial_2 = \partial/\partial y$ and $g_m = \det[g_{m,ij}]$. The parameter κ_0 is the bending rigidity of a single membrane, and B_0 the compressibility of the stack. In Eq. (1), as in the following, the subscript 0 denotes bare quantities, whereas renormalized parameters will carry no subscript.

For slow spatial variations, the discrete variable ml may be replaced with a continuous one, and $u(\mathbf{x}_\perp, ml) \to u(\mathbf{x})$, where $\mathbf{x} = (\mathbf{x}_\perp, z)$. In this limit, the energy (1) reduces to

$$E = \int_0^{L_\parallel} \mathrm{d}z \int \mathrm{d}^2 x_\perp \sqrt{g} \left[\frac{1}{2} K_0 H^2 + \frac{1}{2} B_0 (\partial_z u)^2 \right]. \quad (3)$$

Here we have introduced the bulk version of the bending rigidity $K_0 \equiv \kappa_0 / l$, and defined $L_\parallel \equiv Nl$. The gradient energy $(\partial_z u)^2$ has the unphysical feature that it gives z-dependent reparametrizations a kinetic energy. It should therefore be replaced by the normal gradient energy $(\mathbf{N} \cdot \boldsymbol{\nabla} u)^2$. We have seen in Ref. 3 that this changes the critical exponent with which the renormalized B vanishes as the bending rigidity becomes critical. However, in the limit of large d, which we are going to investigate, the difference between the two gradient energies will be negligible.

III. LARGE-d ANALYSIS

For arbitrary d, the vertical displacement of the mth membrane in the stack becomes a $(d-2)$-vector field $\mathbf{u}_m(\mathbf{x}_\perp)$.

A. Partition function and the energy

It is useful to consider g_{ij} as an independent field,[4] and impose relation (2) with help of a Lagrange multiplier λ_{ij}. We write the partition function as a functional integral over all possible configurations $\mathbf{u}_m(\mathbf{x}_\perp)$ of the individual membranes in the stack, as well as over all possible metrics $g_{m,ij}$. After taking again the continuum limit, the partition function reads

$$Z=\int \mathcal{D}g\,\mathcal{D}\lambda\,\mathcal{D}\mathbf{u}e^{-E_0/k_BT}, \tag{4}$$

with

$$E_0=\int dz\,d^2x_\perp\sqrt{g}\left\{\sigma_0+\frac{1}{2}B_0(\partial_z\mathbf{u})^2+\frac{1}{2}K_0(\partial_k^2\mathbf{u})^2+\frac{1}{2}K_0\lambda^{ij}(\delta_{ij}+\partial_i\mathbf{u}\partial_j\mathbf{u}-g_{ij})-\frac{1}{4}\tau_0\lambda_{ii}^2\right\}, \tag{5}$$

where $\mathbf{u}$ is a $(d-2)$-dimensional vector function of $\mathbf{x}_\perp, z$. Note that the functional integral over λ in Eq. (4) has to be performed along the imaginary axis to result in a δ function. We have also introduced a term proportional to λ_{ii}^2. This term is necessary to renormalize the theory, and its coefficient τ_0 corresponds to the large-d in-plane compressibility of the membranes. Since we take the membranes to be incompressible, we shall set the renormalized τ equal to zero at the end of our calculations. We have also included a surface tension σ_0, again to absorb infinities and to be set equal to zero after renormalization.

The functional integral over $\mathbf{u}$ in Eq. (4) is Gaussian and can be carried out to yield an effective energy

$$E_{\rm eff}=\tilde{E}_0+E_1, \tag{6}$$

with

$$\tilde{E}_0=\int dz\,d^2x_\perp\sqrt{g}\left[\sigma_0+\frac{1}{2}K_0\lambda^{ij}(\delta_{ij}-g_{ij})-\frac{1}{4}\tau_0\lambda_{ii}^2\right] \tag{7}$$

and

$$E_1=\frac{d-2}{2}k_BT\,\mathrm{Tr}\ln[B_0\omega^2+K_0(q_\perp^4-q_i\lambda^{ij}q_j)], \tag{8}$$

where the functional trace Tr is here an integral over space as well as the integral over wave vectors $\mathbf{q}_\perp$ and ω, after replacing $\partial_z^2\to-\omega^2$ and $g^{ij}\partial_i\partial_i\to-\mathbf{q}^2$. Note that the discrete nature of the stack restricts the integral over the wave vectors ω to the first Brillouin zone $|\omega|<\pi/l$.

In the large-d limit, the partition function (4) is dominated by the saddle point of the effective energy (6) with respect to the metric g_{ij} and the Lagrange multiplier λ^{ij}. For very large membranes, the saddle point can be assumed to be symmetric and homogeneous:[5–7]

$$g_{ij}=\varrho_0\delta_{ij};\quad \lambda^{ij}=\lambda_0 g^{ij}=\frac{\lambda_0}{\varrho_0}\delta^{ij}, \tag{9}$$

with constant ϱ_0 and λ_0. At the saddle point the effective energy (6) becomes the free energy of the system.

In the following we shall investigate both, the case of an infinite and a finite stack of membranes. As we will see, the large-d approximation allows for the vertical melting even in an infinite stack, which is not found perturbatively.[1]

B. Infinite stack

Let us first analyze the case of an infinite stack. To simplify our calculations, we assume the number $N+1$ of membranes in the stack to be very large, making the distance l between them very small. In this regime, we may extend the limits $\pm\pi/l$ of the integral over ω to infinity. The explicit l dependence will be introduced later into our calculations.

After evaluating the functional trace in Eq. (8), we obtain

$$E_1=\frac{dk_BT}{2}\int dz d^2x_\perp\varrho_0\sqrt{\frac{K_0}{B_0}}\left\{\frac{\Lambda^4}{8\pi}+\frac{\lambda_0}{8\pi}\Lambda^2+\frac{\lambda_0^2}{64\pi}\left[1-2\ln\left(\frac{4\Lambda^2}{\lambda_0}\right)\right]\right\}, \tag{10}$$

where ultraviolet divergences are regularized by introducing a sharp transverse wave vector cutoff Λ and $d-2$ has been replaced by d for large d.

We may now absorb the first term in Eq. (10) by renormalizing σ_0, so that

$$\sigma=\sigma_0+\frac{dk_BT}{16\pi}\sqrt{\frac{K_0}{B_0}}\Lambda^4 \tag{11}$$

is the physical surface tension, which is set equal to zero. The second, quadratically divergent term in Eq. (10) is used to define the critical temperature as

$$\frac{1}{T_c}\equiv\frac{dk_B}{16\pi}\frac{\Lambda^2}{\sqrt{BK}}. \tag{12}$$

The next divergent term, proportional to λ_0^2, is regularized by introducing a renormalization scale μ and modifying the in-plane compressibility to

$$\tau=\tau_0+\frac{dk_BT}{32\pi}\sqrt{\frac{K_0}{B_0}}\ln\left(4e^{-1/2}\frac{\Lambda^2}{\mu^2}\right). \tag{13}$$

The physical in-plane compressibility τ is now set equal to zero, as explained in the previous section.

The effective energy thus becomes

$$E_{\rm eff}=\int dz\,d^2x_\perp K\lambda\varrho\left\{\left(\frac{1}{\varrho}-1\right)+\frac{T}{T_c}+\frac{aT}{\sqrt{K}}\lambda\left[\ln\left(\frac{\lambda}{\bar{\lambda}}\right)-\frac{1}{2}\right]\right\}, \tag{14}$$

with the constants $a\equiv dk_B/64\pi\sqrt{B}$, $\bar{\lambda}\equiv\mu^2e^{-1/2}$.

From the second derivative matrix of $E_{\rm eff}$ with respect to ϱ and λ we find that the stability of the saddle point is guaranteed only for $\lambda<\bar{\lambda}$.

Extremizing the above expression with respect to ϱ, we find two solutions for λ, namely, $\lambda=0$ and $\lambda=\lambda_\infty$, with

$$\lambda_\infty\left[\ln\left(\frac{\lambda_\infty}{\bar{\lambda}}\right)-\frac{1}{2}\right]=\frac{\sqrt{K}}{a}\left(\frac{1}{T}-\frac{1}{T_c}\right). \tag{15}$$

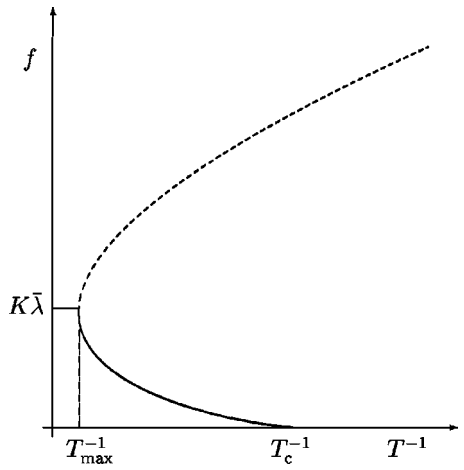

FIG. 1. Free-energy density of an infinite stack of membranes. The dashed curve indicates the unphysical branch of the solution of Eq. (15).

For $T<T_c$, this equation has no solution for λ_∞. In this case, the only possible solution is $\lambda=0$, which corresponds to the ordered phase as we shall verify later. For $T>T_c$, the saddle point lies at $\lambda=\lambda_\infty$, which is now well defined. This is the vertically disordered phase.

The free-energy density at the extremum is given by

$$f=K\lambda_\infty \tag{16}$$

and its behavior is similar to the one found perturbatively in Ref. 3 (see Fig. 1).

Extremizing the effective energy (14) with respect to λ, we find ϱ as a function of temperature. For $T<T_c$ it is given by

$$\varrho_-^{-1}=1-\frac{T}{T_c}. \tag{17}$$

This as T approaches T_c from below, indicating the vertical melting at T_c. In the disordered phase, ϱ is found to be

$$\varrho_+^{-1}=\frac{T}{T_c}-1-\frac{a\lambda_\infty T}{\sqrt{K}}. \tag{18}$$

As T approaches T_c from above, λ_∞ tends to zero, and ϱ goes again to infinity.

The positivity of ϱ and the stability of the saddle point imply that there is a maximum temperature given by

$$\frac{1}{T_{\max}}=\frac{1}{T_c}-\frac{a\bar{\lambda}}{\sqrt{K}}, \tag{19}$$

below which our assumption that the membranes in the stack are in-plane incompressible does not lead to a stable system.

C. Finite stack of many membranes

Let us now analyze the case of a finite stack of size $L_\parallel$. Now the functional trace in Eq. (8) involves a sum over the discrete wave vectors ω_n, given by

$$\omega_n=\frac{2\pi}{L_\parallel}n, \quad n=0,\pm1,\pm2,\ldots. \tag{20}$$

For small λ_0, a series expansion leads to

$$E_1=\int dz\, d^2\sigma \frac{dk_BT}{2}\varrho_0 e_1, \tag{21}$$

with

$$\begin{aligned} e_1=&\frac{\Lambda^4}{8\pi}\sqrt{\frac{K_0}{B_0}}-\frac{\pi}{12}\sqrt{\frac{B_0}{K_0}}\frac{1}{L_\parallel^2}+\frac{\lambda_0}{8\pi}\sqrt{\frac{K_0}{B_0}}\Lambda^2\\ &+\frac{\lambda_0}{4\pi L_\parallel}\ln\left(\frac{L_\perp^2}{L_\parallel}\sqrt{\frac{B_0}{K_0}}\right)\\ &+\frac{\lambda_0^2}{64\pi}\sqrt{\frac{K_0}{B_0}}\left[3-2\gamma+2\ln\left(\frac{\lambda_0}{8\pi\Lambda^2}\frac{L_\perp^2}{L_\parallel}\sqrt{\frac{B_0}{K_0}}\right)\right]\\ &+\sqrt{\pi}\sum_{m=3}^{\infty}\frac{(-1)^{m+1}\lambda_0^m}{m\,2^{2m}\pi^m}L_\parallel^{m-2}\left(\frac{K_0}{B_0}\right)^{(m-1)/2}\\ &\times\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\zeta(m-1). \end{aligned} \tag{22}$$

As in the case of the infinite stack, we absorb the logarithmic divergence by renormalizing the in-plane compressibility via Eq. (13), setting τ equal to zero for incompressible membranes. The surface tension receives now an $L_\parallel$-dependent renormalization

$$\sigma=\sigma_0+\frac{dk_BT}{16\pi}\sqrt{\frac{K_0}{B_0}}\Lambda^4-dk_BT\frac{\pi}{24}\sqrt{\frac{B_0}{K_0}}\frac{1}{L_\parallel^2}, \tag{23}$$

and σ is again set equal to zero to describe a stack of tensionless membranes.

Extremization of the renormalized combined effective actions (7) and (21) with respect to ϱ leads again to two possible solutions for the saddle point, namely, $\lambda=0$ or $\lambda=\lambda_{L_\parallel}$, with

$$\begin{aligned} &\lambda_{L_\parallel}\left[\ln\left(\frac{\lambda_{L_\parallel}}{\bar{\lambda}}\right)-\frac{1}{2}\right]+\lambda_{L_\parallel}\left[1-\gamma+\ln\left(\frac{L_\perp^2}{L_\parallel}\frac{1}{8\pi}\sqrt{\frac{B}{K}}\right)\right]\\ &+32\pi^{3/2}\sum_{m=3}^{\infty}\frac{(-1)^{m+1}\lambda_{L_\parallel}^{m-1}}{m\,2^{2m}\pi^m}L_\parallel^{m-2}\left(\frac{K}{B}\right)^{(m-2)/2}\\ &\times\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\zeta(m-1)=\frac{\sqrt{K}}{a}\left(\frac{1}{T}-\frac{1}{T_{L_\parallel}}\right), \end{aligned} \tag{24}$$

where

$$\frac{1}{T_{L_\parallel}}=\frac{1}{T_c}+\frac{dk_B}{8\pi}\frac{1}{KL_\parallel}\ln\left(\frac{L_\perp^2}{L_\parallel}\sqrt{\frac{B}{K}}\right) \tag{25}$$

is the inverse critical temperature for a stack of size $L_\parallel$.

For $T<T_{L_\parallel}$, Eq. (24) has no solution. In this case, the stack is in the ordered phase, the only available solution for the saddle point being $\lambda=0$. For $T>T_{L_\parallel}$, there exists a nonzero solution $\lambda_{L_\parallel}$, where the system is in the vertically disordered phase.

Let us now examine the saddle point solutions for ϱ. In the vertically disordered phase where $\lambda=\lambda_{L_\parallel}$ is nonzero, we may expand the effective energy in a small-$L_\parallel$ series. Extremization with respect to $\lambda_{L_\parallel}$ leads to

$$\varrho_+^{-1}=\frac{T}{T_{L_\parallel}}-1-\frac{a\lambda_{L_\parallel}T}{\sqrt{K}}-\frac{dk_BT}{2K}\sqrt{\pi}\sum_{m=3}^{\infty}\frac{(-1)^{m+1}\lambda_{L_\parallel}^{m-1}}{2^{2m}\pi^m}$$
$$\times\left(1-\frac{2}{m}\right)L_\parallel^{m-2}\left(\frac{K}{B}\right)^{(m-1)/2}\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\zeta(m-1). \tag{26}$$

The positivity of ϱ and the stability of the saddle point again define a maximal temperature, given by

$$\frac{1}{T_{\max}^{L_\parallel}}=\frac{1}{T_{\max}}-\frac{dk_BT}{16\pi KL_\parallel}\ln\left(\frac{16\pi}{dk_BT_c}\frac{\sqrt{BK}}{\lambda}\right), \tag{27}$$

above which our assumption that the membranes in the stack are in-plane incompressible cannot be maintained.

In the ordered phase, the situation is more delicate. For $\lambda=0$, ϱ can be calculated exactly, and we obtain

$$\varrho_-^{-1}=1-\frac{dk_BT}{8\pi KL_\parallel}\ln\left[\frac{\sinh\left(\frac{8\pi KL_\parallel}{dk_BT_c}\right)}{\frac{L_\parallel}{2L_\perp^2}\sqrt{\frac{K}{B}}}\right], \tag{28}$$

with an infrared regulator $L_\perp$ equal to the inverse lateral size of the membranes in the stack. If the size $L_\parallel$ of the stack is large, Eq. (28) may be approximated by

$$\varrho_-^{-1}\approx 1-\frac{T}{T_{L_\parallel}}. \tag{29}$$

For smaller stacks, however, the positivity of ϱ is not guaranteed. For a fixed, but small stack size $L_\parallel$, and for fixed lateral size $L_\perp$ of the membranes in the stack, there is a characteristic temperature defined by

$$T^*=\frac{8\pi KL_\parallel}{dk_B\ln(16\pi\sqrt{BK}L_\perp^2/dk_BT_c)}, \tag{30}$$

above which ϱ_- changes sign, and Eq. (28) is no longer applicable. Interestingly, for all $L_\perp$ and for all finite sizes $L_\parallel$ of the stack, the critical temperature $T_{L_\parallel}$ is lower than T^*, so that the vertical melting still occurs. The behavior of ϱ is depicted in Fig. 2.

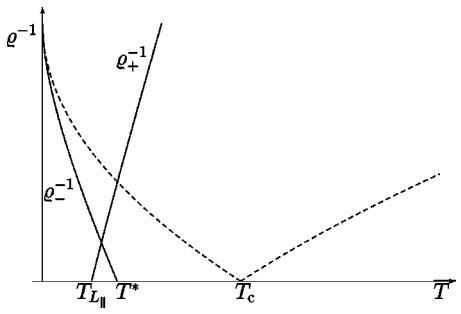

FIG. 2. Behavior of ϱ^{-1} as a function of T. The solid lines indicate the solutions of the saddle point for ϱ^{-1} for a finite stack. Above $T_{L_\parallel}$, ϱ^{-1} is given by Eq. (26), and below $T_{L_\parallel}$ by Eq. (28). The dashed lines indicate the behavior of ϱ^{-1} for an infinite stack.

Note that Eq. (30) reflects the existence of a characteristic horizontal length scale. At fixed temperature $T_{L_\parallel}<T<T^*$, and for membranes of lateral size $L_\perp$ smaller than

$$L_p=\Lambda^{-1}\exp\left(\frac{4\pi KL_\parallel}{dk_BT}\right), \tag{31}$$

the height fluctuations of the individual membranes are not strong enough to destroy the ordered phase. The characteristic length L_p corresponds to the de Gennes–Taupin persistence length ξ_p (Ref. 8) of the individual membranes, below which crumpled membranes appear flat.

D. Finite number of membranes

Until now we have performed our calculations in the somewhat unphysical continuum approximation, by letting the interlayer separation l be very small making the number of membranes in the stack very large. Let us now investigate the properties of the stack for a fixed number $N+1$ of membranes at a finite interlayer distance l.

For this purpose, we replace the continuum derivative ∂_z^2 in the z direction with the discrete gradient operator ∇^2, whose eigenvalues are given by

$$\nabla^2 g=\frac{2(1-\cos\omega_n l)}{l^2}g, \tag{32}$$

where g is some test function. The discrete wave vectors ω_n are now given by

$$\omega_n=\frac{n\pi}{Nl},\quad n=1,2,\ldots,N. \tag{33}$$

For small-interlayer separation l, the free energy is given by Eq. (21) with

$$e_1=\frac{\Lambda^4}{8\pi}\sqrt{\frac{K_0}{B_0}}+\frac{1}{Nl^2}\sqrt{\frac{B_0}{K_0}}+\frac{\lambda_0}{8\pi}\sqrt{\frac{K_0}{B_0}}\Lambda^2$$
$$+\frac{\lambda_0}{4\pi Nl}\left[-\ln N+2N\ln\left(l\sqrt{\frac{K_0}{B_0}}\Lambda^2\right)\right]$$
$$+\frac{\lambda_0^2}{64\pi}\sqrt{\frac{K_0}{B_0}}\left[1-2\ln\left(\frac{4\Lambda^2}{\lambda_0}\right)\right]$$
$$+\frac{1}{N\sqrt{\pi}}\sum_{m=2}^{\infty}\frac{(-1)^{m+1}\lambda_0^m}{m\,2^{(3m+1)/2}}l^{m-2}$$
$$\times\left(\frac{K_0}{B_0}\right)^{(m-1)/2}\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\bar{\zeta}_N(m-1), \tag{34}$$

where we have defined the modified zeta function

$$\bar{\zeta}_N(m)=\sum_{n=1}^{N}\frac{1}{\left[1-\cos\left(\frac{n\pi}{N}\right)\right]^{m/2}}. \tag{35}$$

We proceed by renormalizing the in-plane compressibility via Eq. (13), setting τ equal to zero for incompressible membranes as before. The surface tension receives an l-dependent renormalization

$$\sigma=\sigma_0+\frac{dk_BT}{16\pi}\sqrt{\frac{K_0}{B_0}}\Lambda^4-\frac{dk_BT}{2Nl^2}\sqrt{\frac{B_0}{K_0}} \tag{36}$$

and σ is set equal to zero to describe a stack of tensionless membranes, as before. But now the bulk bending rigidity is also modified to

$$K=K_0-\frac{dk_BT}{4\pi l}\ln\frac{\Lambda^2}{\mu^2}. \tag{37}$$

Note that this renormalization agrees with the known result for a single membrane.[9]

The saddle point for λ is now given by $\lambda=0$ or $\lambda=\lambda_l$, with

$$\lambda_l\left[\ln\left(\frac{\lambda_l}{\bar{\lambda}}\right)-\frac{1}{2}\right]+32\sqrt{\pi}\sum_{m=2}^{\infty}\frac{(-1)^{m+1}\lambda_l^{m-1}}{m\,2^{(3m+1)/2}}l^{m-2}$$
$$\times\left(\frac{K}{B}\right)^{(m-2)/2}\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\bar{\zeta}_N(m-1)=\frac{\sqrt{K}}{a}\left(\frac{1}{T}-\frac{1}{T_l}\right) \tag{38}$$

where

$$\frac{1}{T_l}=\frac{1}{T_c}+\frac{dk_B}{8\pi N\kappa}\left\{-\ln N+2N\left[\ln\left(l\sqrt{\frac{K}{B}}\bar{\lambda}\right)+\frac{1}{2}\right]\right\} \tag{39}$$

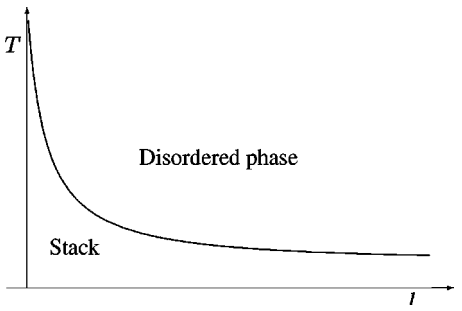

FIG. 3. Qualitative phase diagram in the $l\times T$ plane. The critical line is plotted for $l>l_{\min}$, for a fixed number $N+1$ of membranes in the stack. As l increases, the critical temperature T_l goes asymptotically to zero.

is the inverse l-dependent critical temperature, and κ is the bending rigidity of a single membrane in the stack. The two solutions for λ again imply the existence of two different phases, with a phase transition at the critical temperature T_l, which, as in the perturbative case, depends only weakly on the number of membranes in the stack. The corresponding solutions for ϱ, obtained by extremizing the effective energy with respect to λ, are given by

$$\varrho_-^{-1}=1-\frac{T}{T_l}, \tag{40}$$

for $T<T_l$, that is, in the ordered phase, and

$$\varrho_+^{-1}=\frac{T}{T_l}-1-\frac{a\lambda_lT}{\sqrt{K}}-\frac{dk_BT}{2\sqrt{\pi}NK}$$
$$\times\sum_{m=2}^{\infty}\frac{(-1)^{m+1}\lambda_l^{m-1}}{2^{(3m+1)/2}}\left(1-\frac{2}{m}\right)$$
$$\times l^{m-2}\left(\frac{K}{B}\right)^{(m-1)/2}\frac{\Gamma\left(\frac{m-1}{2}\right)}{\Gamma\left(\frac{m}{2}\right)}\bar{\zeta}_N(m-1), \tag{41}$$

in the vertically molten phase, where $T>T_l$.

The stability of the saddle point requires a minimum interlayer separation

$$l_{\min}=\mu^{-2}\sqrt{\frac{B}{K}}N^{1/2N}\exp\left(\frac{4\pi\kappa}{dk_BT_c}\right) \tag{42}$$

below which the stack becomes unstable. $l_{\min}$ is inversely proportional to de Genne's penetration depth $\sqrt{K/B}$,[10] which is of the order of the interlayer separation in smectic liquid crystals.

The phase diagram of the stack is depicted in Fig. 3.

E. Properties of the phases

Let us now characterize both phases in more detail. For temperatures lower than T_l, the solution of the saddle point is $\lambda=0$. This corresponds to the ordered phase. Here, the structure factor

$$S_n(\mathbf{x}) = \langle \exp\{inq_0[u(\mathbf{x}) - u(0)]\}\rangle, \tag{43}$$

for coherent scattering on the plane surfaces with momentum transfer $nq_0 = 2\pi n/l$, behaves like

$$S_n(\mathbf{x}_\perp, z) = \begin{cases} z^{-n^2\eta} & \text{for } \mathbf{x}_\perp = 0 \\ |x_\perp|^{-2n^2\eta} & \text{for } z = 0. \end{cases} \tag{44}$$

This correlation function can be directly observed in x-ray scattering experiments, as half-widths at half-maximum of the anomalous Bragg peaks. As in smectic-*A* liquid crystals,[11,12] the exponent η is given by

$$\eta = \frac{k_B T}{8\pi} \frac{q_0^2}{\sqrt{BK}}. \tag{45}$$

The algebraic singularities in Eq. (44) reflect the quasi-long-range periodic order along the stack axis. This order manifests itself also in the orientational correlation function of the membranes. In the limit $N \to \infty, l \to 0$, with constant $Nl = L_\parallel$, we find

$$\langle \partial_i u(\mathbf{x}_\perp, z) \partial_j u(\mathbf{x}'_\perp, z)\rangle \sim \frac{\delta_{ij}}{|\mathbf{x}_\perp - \mathbf{x}'_\perp|^3}. \tag{46}$$

This slow, algebraic fall-off of the correlation function implies that, at large distances, the normal vectors to the membranes remain roughly parallel, so that the surfaces remain flat on the average. The effect of thermal fluctuations is suppressed, and they do not disorder the stack.

For temperatures higher than T_l, there is a nonzero solution of the saddle point, $\lambda = \lambda_l$. This corresponds to the disordered phase. In this phase, the structure factor $S_n(\mathbf{x})$ behaves, for $z = 0$, like

$$S_n(\mathbf{x}_\perp, 0) = \exp(-2n^2 \eta \lambda |x_\perp|^2), \tag{47}$$

revealing the absence of periodic order along the z axis. In this phase, the normals to the membranes are uncorrelated beyond a length scale $\lambda_l^{-1/2}$, as can be derived from the expression for the orientational correlation function, which in the limit $N \to \infty, l \to 0$ with constant $Nl = L_\parallel$ reads

$$\langle \partial_i u(\mathbf{x}_\perp, z) \partial_j u(\mathbf{x}'_\perp, z)\rangle \sim \delta_{ij} \exp(-\sqrt{\lambda_l}|\mathbf{x}_\perp - \mathbf{x}'_\perp|). \tag{48}$$

The length scale $\lambda_l^{-1/2}$ may thus be identified with the persistence length ξ_p.[13] We note that our model allows the membranes to interpenetrate in the disordered phase, as a consequence of their harmonic interaction potential in the vertical direction, which underestimates the effect of the steric repulsion between them.

Our system is very similar to a smectic-*A* liquid crystal, which consists of vertically oriented rodlike molecules layered along the z axis. Experimentally, the spontaneously broken translational symmetry along this axis and the spontaneously broken rotational symmetry in the layers are restored in a two-step melting process. In the first transition, which can be of first or second order, the smectic melts via dislocation loop unbinding into a translationally disordered nematic. In the second, which is always first order, the orientations of the molecules in the nematic become disordered to yield a fully isotropic liquid. If we try to interpret our model as a smectic-*A* liquid crystal, we see that our vertical melting transition is analogous to the smectic-to-nematic one. The physical mechanism by which our transition takes place, however, is quite different from the dislocation loop unbinding of the defect model. Our membranes cannot split to form dislocations. Instead, they become rough (see Fig. 4). This is similar to the two possible ways of representing the superfluid transition in helium: in a defect model, it is explained by a proliferation of vortex lines, whereas in the complex ϕ^4 theory by a roughening of the order field.

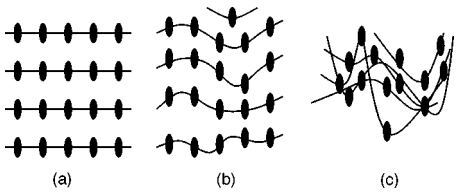

FIG. 4. Interpretation of the vertical melting of the stack as a smectic-to-nematic phase transition. (a) Smectic-*A* layers at $T = 0$, (b) layers at $0 < T < T_l$: still smectic, (c) interpenetrating rough layers at $T > T_l$: nematic.

Our model does not contain any information about the orientation of the molecules, and is thus unable to describe the second transition. The molecules may be imagined as being attached to the surface in the vertical direction. The normal vectors to the layered membranes have no relation to the molecule orientation — they are purely a geometrical property of the surfaces. A nematic phase similar to the one predicted by us was found in Ref. 14. There, the authors consider not a stack of membranes, but an open-membrane system where the topology is allowed to vary.

Let us now calculate the entropy loss in the ordered phase. By a simple scaling argument,[1] this quantity is inversely proportional to the quadratic interlayer spacing

$$-T\Delta S = \frac{a}{l^2}, \tag{49}$$

where a is a temperature-dependent proportionality constant. Explicitly, it is given by the difference between the free-energy density of a single, isolated membrane, and the free-energy density of the stack. For small values of λ, it is given by

$$-T\Delta S = \frac{1}{2}\sqrt{\frac{B}{K}}\left(1 + \cot\frac{\pi}{4N}\right)\frac{1}{Nl^2} - \frac{\lambda}{2\pi l}\left(1 - \ln\frac{\lambda l}{2}\sqrt{\frac{K}{B}}\right) + \frac{\lambda}{2\pi Nl}\sum_{n=1}^{N} \ln\sin\frac{n\pi}{2N}. \tag{50}$$

The ordered phase corresponds to $\lambda = 0$. In that case, Eq. (50) agrees with Eq. (49), and we see no correction to the entropy loss. If the size of the membranes in the stack is smaller than the characteristic length L_p, an ordered phase

still exists for small values of λ [see discussion after Eq. (31)], in which case the corrections to the first term in Eq. (50) will appear.

IV. CONCLUSIONS

In the limit of large-embedding dimension d, we have shown that a stack of tensionless and incompressible membranes melts vertically upon approaching a critical temperature, where the lamellar phase goes over into a disordered phase. In contrast to the low-temperature ordered phase, where the decay of orientational correlations is powerlike, the high-temperature disordered phase is characterized by an exponential decay of orientational correlations, with different length scales in the transversal and longitudinal directions.

*Email address: borelli@physik.fu-berlin.de
†Email address: kleinert@physik.fu-berlin.de

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