Effects of self-avoidance on the tubular phase of anisotropic membranes

M. Bowick*
Physics Department, Syracuse University, Syracuse, New York 13244-1130

E. Guitter†
CEA, Service de Physique Théorique de Saclay, F-91191 Gif sur Yvette Cedex, France

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We study the tubular phase of self-avoiding anisotropic membranes. We discuss the renormalizability of the model Hamiltonian describing this phase, and from a renormalization group equation derive some general scaling relations for the exponents of the model. We show how particular choices of renormalization factors reproduce the Gaussian result, the Flory theory, and the Gaussian variational treatment of the problem. We then study the perturbative renormalization to one loop in the self-avoiding parameter using dimensional regularization and an ϵ expansion about the upper critical dimension, and determine the critical exponents to first order in ϵ. [S1063-651X(97)07512-0]

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I. INTRODUCTION

The statistical mechanics of isotropic tethered membranes has been extensively studied [1,2]. In a recent paper Radzihovsky and Toner (RT) [3] showed that intrinsically anisotropic tethered membranes are surprisingly rich systems. In particular, they exhibit an intermediate tubular phase between the crumpled and flat phases typical of isotropic tethered membranes [4–9]. The tubular phase is characterized by being extended in one direction and crumpled in the other. Furthermore, any degree of anisotropy is expected to be relevant, so such systems could be widespread in nature and very important. It is not hard to imagine many situations in which the polymerization of a fluid membrane occurs anisotropically.

Recently, the existence of this tubular phase for physical anisotropic membranes has been confirmed by large-scale Monte Carlo simulations [10] and the crumpled-to-tubular and tubular-to-flat phase transitions both observed. In the case of self-avoiding tethered membranes, current numerical evidence suggests that the crumpled phase is destroyed in physical dimensions [11]. This enhances the possible significance of an ordered tubular phase for self-avoiding anisotropic physical membranes—the only transition left in this case may be the tubular-to-flat transition.

In this paper we study the effects of self-avoidance in the tubule model of a self-avoiding tubule, previously introduced and analyzed by RT [3]. This model may be considered as the analog of the Edwards model of self-avoiding membranes [12–14], appropriately adapted to the tubular geometry, with bending rigidity in the extended direction of the tubule and self-avoidance in its crumpled direction.

In Sec. II we use a renormalization group equation to reproduce some of the critical exponent scaling relations of RT, and derive some new ones. These relations hold provided that the bending energy term is not renormalized, and imply that there is only one independent exponent in the model. Special cases of this treatment reproduce the trivial Gaussian model as well as the Flory theory and the Gaussian variational approximation results of RT. In Sec. III we establish the perturbative renormalizability of the model, and prove that the bending energy term is indeed not renormalized.

In Sec. IV we calculate the critical exponents to first order in an ϵ expansion about the upper critical dimension for the relevance of self-avoidance. We use the techniques of dimensional regularization and the multilocal operator product expansion of Ref. [15]. We give the corresponding predictions of all relevant critical exponents for the case of a physical membrane in the tubular phase.

II. SCALING RELATIONS

We start by reviewing RT's model and scaling results for the tubular phase of self-avoiding anisotropic membranes [3]. We consider the generalized case of D-dimensional objects ($D=2$ corresponding to membranes) with one stiff direction y and $(D-1)$ soft directions $x_\perp$ [see Fig. 1(a)]. In the tubular phase, such an object will be extended in the y direction and crumpled in the transverse direction. Using a Monge-like representation, the point with coordinates $(x_\perp, y)$ in the membrane will occupy a position $[\mathbf{h}(x_\perp, y), y]$ in the d-dimensional embedding space, with $\mathbf{h}$ a $(d-1)$-dimensional vector field perpendicular to the y direction. Adapting the Edwards model for self-avoiding membranes to the geometry of the tubular phase, RT obtained the Hamiltonian [3]

$$\mathcal{H}=\tfrac{1}{2}\int d^{D-1}x_\perp dy\{[\partial_y^2\mathbf{h}(x_\perp,y)]^2+[\partial_\perp\mathbf{h}(x_\perp,y)]^2\}+\frac{b}{2}\int d^{D-1}x_\perp d^{D-1}x'_\perp dy\,\delta^{(d-1)}[\mathbf{h}(x_\perp,y)-\mathbf{h}(x'_\perp,y)]. \tag{2.1}$$

*Electronic address: bowick@npac.syr.edu
†Electronic address: guitter@spht.saclay.cea.fr

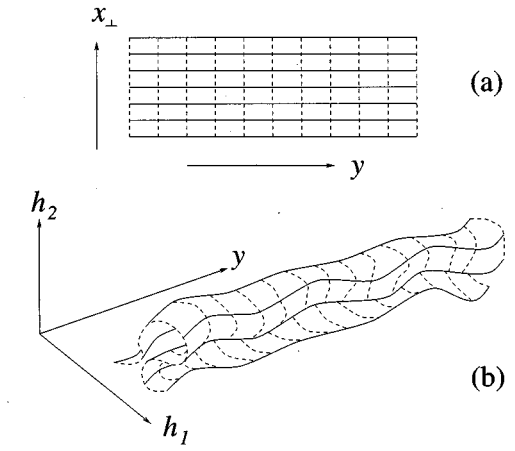

FIG. 1. (a) An anisotropic membrane with a stiff y direction and a soft $x_\perp$ direction; (b) after embedding, the membrane forms a tubule, extended in the stiff y direction and crumpled in the soft direction.

The first two terms describe the elastic properties of the membrane in the absence of self-avoidance, and represent a bending energy term in the extended stiff y direction and an effective entropically generated elastic term in the crumpled direction. The third term is a two-body contact interaction with excluded volume (or self-avoiding) parameter b. Due to the extended nature of the tubule in the y direction, the self-avoiding interaction involves only points which have the same y coordinate along the membrane [3].

The engineering dimensions of the fields and coordinates are $[y]=1$, $[x_\perp]=2$ and

$$\zeta_0 \equiv [\mathbf{h}] = \tfrac{5}{2} - D. \tag{2.2}$$

This implies $[b]=-\epsilon$ with [3]

$$\epsilon = 3D - \frac{1}{2} - \left(\frac{5}{2} - D\right) d. \tag{2.3}$$

We consider the model for $\frac{3}{2}<D<\frac{5}{2}$ only, where the bare roughness exponent ζ_0, Eq. (2.2), satisfies $0<\zeta_0<1$. Setting $\epsilon=0$ fixes the upper critical dimension for the relevance of the self-avoiding interaction to be [3]

$$d_{\rm uc}(D) = \frac{6D-1}{5-2D}, \tag{2.4}$$

with, in particular, $d_{\rm uc}(2)=11$.

In Sec. III we will show that the Hamiltonian (2.1) renormalizes onto itself. In other words, one can find renormalization factors Z, $Z_\perp$, and Z_b such that the renormalized theory, using the renormalized Hamiltonian

$$\mathcal{H}^R = \frac{1}{2}\int d^{D-1}x_\perp^R dy \{Z[\partial_y^2 \mathbf{h}^R(x_\perp^R,y)]^2 + Z_\perp[\partial_\perp^R \mathbf{h}^R(x_\perp^R,y)]^2\}$$
$$+ \frac{Z_b b^R \mu^\epsilon}{2}\int d^{D-1}x_\perp^R d^{D-1}x_\perp'^R dy\, \delta^{(d-1)}$$
$$\times[\mathbf{h}^R(x_\perp^R,y) - \mathbf{h}^R(x_\perp'^R,y)], \tag{2.5}$$

gives finite results at $\epsilon=0$ when expressed in terms of the renormalized self-avoiding parameter b^R. We will moreover show that the bending energy term is not renormalized; that is,

$$Z = 1. \tag{2.6}$$

This assumption is crucial in the derivation of the scaling laws below. The bare [Eq. (2.1)] and renormalized [Eq. (2.5)] and renormalized [Eq. (2.5)] Hamiltonians can be made identical by appropriate rescalings of the height field $\mathbf{h}^R$, transverse coordinate $x_\perp^R$, and self-avoiding coupling b^R in the following way:

$$\mathbf{h}^R(x_\perp^R,y) = Z_\perp^{(1-D)/4}\mathbf{h}(x_\perp,y),$$
$$x_\perp^R = Z_\perp^{1/2} x_\perp, \tag{2.7}$$
$$b^R = b\mu^{-\epsilon} Z_b^{-1} Z_\perp^{(1-D)(d+3)/4}.$$

Consider now the height fluctuations in the bare model as determined by the correlation function

$$G(x_\perp,y) \equiv -\frac{1}{2(d-1)}\langle[\mathbf{h}(x_\perp,y)-\mathbf{h}(0,0)]^2\rangle. \tag{2.8}$$

From Eq. (2.7) the renormalized version of this correlation function satisfies

$$G^R(x_\perp^R,y) \equiv -\frac{1}{2(d-1)}\langle[\mathbf{h}^R(x_\perp^R,y)-\mathbf{h}^R(0,0)]^2\rangle_R$$
$$= Z_\perp^{(1-D)/2} G(x_\perp,y). \tag{2.9}$$

Writing $\mu d/d\mu|_0[Z_\perp^{(D-1)/2} G_R(x_\perp^R,y)]=0$, where the derivative is taken at fixed bare parameter b, we obtain the renormalization group equation

$$\mu\frac{\partial}{\partial\mu}G^R + \tfrac{1}{2}\delta x_\perp \frac{\partial}{\partial x_\perp}G^R + \frac{D-1}{2}\delta G^R = 0, \tag{2.10}$$

where $\delta = \mu d/d\mu|_0 \ln Z_\perp$. We suppose here that an infrared stable fixed point is reached, describing the large scale properties of the membrane. Equation (2.10) holds precisely at this fixed point. On the other hand, simple scaling gives the homogeneity equation

$$\mu\frac{\partial}{\partial\mu}G^R - y\frac{\partial}{\partial y}G^R - 2x_\perp\frac{\partial}{\partial x_\perp}G^R + (5-2D)G^R = 0. \tag{2.11}$$

We thus obtain the fixed point renormalization group equation

$$y\frac{\partial}{\partial y}G^R + \frac{1}{z}x_\perp\frac{\partial}{\partial x_\perp}G^R - 2\zeta G^R = 0, \tag{2.12}$$

where the anisotropy exponent z and the roughness exponent ζ are given by

$$z = \frac{2}{4+\delta},$$

$$\zeta=\zeta_0+\frac{1-D}{4}\,\delta, \tag{2.13}$$

with the bare roughness exponent ζ_0 given by Eq. (2.2). Equation (2.12) implies the scaling

$$G_R(x_\perp^R,y)\sim y^{2\zeta}F_1[y/(x_\perp^R)^z]\sim(x_\perp^R)^{2\nu}F_2[y/(x_\perp^R)^z], \tag{2.14}$$

where the size exponent ν and roughness exponent ζ are related by $\nu=\zeta z$. Eliminating δ in Eq. (2.13), we thus find the very general scaling relations

$$\zeta=\frac{3}{2}+\frac{1-D}{2z},\qquad \nu=\frac{3z}{2}+\frac{(1-D)}{2}. \tag{2.15}$$

Rewriting Eq. (2.14) in momentum space, and using the derived scaling relations, one finds that the inverse of the height field propagator $\tilde{G}^{-1}(q,p_\perp)$ scales as $\tilde{G}^{-1}(q,p_\perp)=q^4f(q/p_\perp^z)$. Thus the anomalous dimension η for the bending rigidity vanishes, as required by the nonrenormalization theorem $Z=1$. Similarly it is simple to show that $\tilde{G}^{-1}(q,p_\perp)=p_\perp^{2+\eta_\perp}g(q/p_\perp^z)$, with $\eta_\perp=4z-2$. Since the size exponent ν must exceed its phantom value $\zeta_0/2$, one has $z>1/2$ and therefore $\eta_\perp>0$.

From the above scaling relations, we end up with only one independent exponent in the theory, depending on the precise value of δ. This value, and the subsequent predictions for all exponents, may be fixed by imposing one more constraint on the renormalization factors of our model Hamiltonian. At this stage, this extra imposed constraint is totally arbitrary, and different constraints lead to different values of the exponents. It is interesting nevertheless to explore limiting cases where scaling is dominated by one component of the Hamiltonian only, either the elastic term or the self-avoiding interaction. The corresponding limiting values of the exponents indeed define the range of values in which the exact exponents are expected to fall. One can fix the scaling from the elastic terms only by assuming the absence of renormalization for the **h** field, i.e., by imposing $Z_\perp=1$, yielding $\delta=0$. One then recovers the bare values $\zeta=\zeta_0$, $z=\frac{1}{2}$, and $\nu=\zeta_0/2$ of the Gaussian theory without self-avoidance. On the other hand, we can consider the strong coupling limit where scaling is fixed by the self-avoiding term only. This yields the Gaussian variational result, as discussed in Sec. II B below and also treated in Ref. [3]. A third, intermediate, estimate of the exponents is the Flory result, obtained by balancing the elastic and self-avoiding contributions in the Hamiltonian, as discussed in Sec. II A and in Ref. [3]. Notice finally that these different estimates become exact and identical on the $\epsilon=0$ line, and can be used as starting points for a systematic expansion in the (D,d) plane around this line. This idea was used in Ref. [16] for the self-avoiding isotropic membrane Edwards model. In Sec. IV, we will calculate the correction to the Gaussian, Flory, and variational estimates of the roughness exponent ζ, at first order in ϵ and for fixed $D=2$.

A. Flory theory

In Flory theory one assumes that elastic energies are comparable to self-avoiding energies. If this is to remain true under renormalization, one should require that both terms renormalize in the same way, viz., $Z_\perp=Z_b$. Given this assumption, one finds from Eq. (2.7) that

$$b^R=b\mu^{-\epsilon}Z_\perp^{(1-D)(d+3)/4-1}. \tag{2.16}$$

In this case the fixed point condition directly determines δ in terms of ϵ to be

$$\delta_F=\frac{-4\epsilon}{\{4+(D-1)(d+3)\}}, \tag{2.17}$$

with ϵ as in Eq. (2.3). Using Eqs. (2.13) and (2.15), the size exponent ν is then found to be

$$\nu_F=\frac{(D+1)}{(d+1)}, \tag{2.18}$$

which coincides with the Flory prediction found in Ref. [3]. This is nothing but the usual Flory result for a $(D-1)$-dimensional self-avoiding object in a $(d-1)$-dimensional embedding space, and corresponds to treating the different transverse slices of the tubule as independent [3]. The other exponents are likewise determined in this approximation to be

$$z_F=\frac{4+(D-1)(d+3)}{3(d+1)},\qquad \zeta_F=\frac{3(D+1)}{4+(D-1)(d+3)}. \tag{2.19}$$

The corresponding values for the physical tubule ($D=2$ and $d=3$) are $\delta_F=-\frac{8}{5}$, $\nu_F=\frac{3}{4}$, $z_F=\frac{5}{6}$, and $\zeta_F=\frac{9}{10}$.

B. Gaussian variational approximation

A different approximation one can make is to assume that the self-avoiding term is not renormalized viz. $Z_b=1$. This is exactly the approximation which is made in a Gaussian variational treatment of the problem, where the exact density functional is approximated by the best possible Gaussian weight for the field **h**, using a variational principle [3]. In this case the field **h** is renormalized, but the self-avoiding interaction term is not. Repeating the above analysis in the case $Z_b=1$, one finds easily from the fixed point condition that

$$\delta_{\rm var}=\frac{-4\epsilon}{(D-1)(d+3)}. \tag{2.20}$$

The size exponent ν in this approximation, first obtained by RT, is

$$\nu_{\rm var}=\frac{7(D-1)}{(3d-5)}, \tag{2.21}$$

and the other exponents are likewise determined to be

$$z_{\rm var}=\frac{(D-1)(d+3)}{(3d-5)},$$
$$\zeta_{\rm var}=\frac{7}{(d+3)}. \tag{2.22}$$

The corresponding values for the physical tubule are $\delta_{\rm var}=-\frac{2}{3}$, $\nu_{\rm var}=\frac{7}{4}$, $z_{\rm var}=\frac{3}{2}$, and $\zeta_{\rm var}=\frac{7}{6}$. The unphysical nature of these values (ν and ζ cannot exceed 1) indicates that, in this approximation, the tubular phase is unstable. For $D=2$, in fact, one sees from Eq. (2.21) that the tubular phase is unstable below $d=4$. It is known, however, that the Gaussian variational method is a strong coupling method which usually overestimates the size exponent.

III. RENORMALIZABILITY

We now turn to the issue of the perturbative renormalizability of the theory for $\epsilon \geqslant 0$. We rely on the general formalism introduced in Ref. [15] for the treatment of nonlocal interactions. In the diagrams of the perturbative expansion in b, we first identify the singular configurations of interacting points which contain possible divergences. We then use a short distance multilocal operator product expansion (MOPE) to analyze these singularities, and show that they are proportional to the insertion of multilocal operators. A simple power counting argument allows us to extract from all singular configurations those which give rise to actual divergences. This, together with some symmetry arguments, singles out all the operators which require renormalization. From this analysis, we deduce that the Hamiltonian (2.1) renormalizes onto itself, according to Eq. (2.5) and moreover, $Z=1$, i.e., there is no renormalization of the bending energy term. Our analysis will be presented for $D=2$, but it could be extended easily to the range $\frac{3}{2}<D<\frac{5}{2}$, where the roughness exponent $\zeta_0=(5-2D)/2$ satisfies $0<\zeta_0<1$.

Let us concentrate on the partition function $\mathcal{Z}$ associated with the Hamiltonian (2.1) at $D=2$:

$$\mathcal{Z}_b=\int \mathcal{D}[\mathbf{h}(x,y)]\exp(-\mathcal{H}[\mathbf{h}]). \tag{3.1}$$

It can be expanded in powers of b according to

$$\mathcal{Z}_b=\mathcal{Z}_0\sum_{N=0}^{\infty}\frac{(-b/2)^N}{N!}\int\prod_{i=1}^{N}dx_i dx_i' dy_i \times\left\langle\prod_{i=1}^{N}\delta^{(d-1)}[\mathbf{h}(x_i,y_i)-\mathbf{h}(x_i',y_i)]\right\rangle_0, \tag{3.2}$$

where $\mathcal{Z}_0$ is the partition function of the non-self-avoiding ($b=0$) theory and $\langle(\ )\rangle_0$ denotes the corresponding Gaussian average

$$\langle(\cdots)\rangle_0=\frac{1}{\mathcal{Z}_0}\int\mathcal{D}[\mathbf{h}(x,y)]\exp\left(-\tfrac{1}{2}\int dx\,dy\{[\partial_y^2\mathbf{h}(x,y)]^2+[\partial_x\mathbf{h}(x,y)]^2\}\right)(\cdots). \tag{3.3}$$

Each δ function in Eq. (3.2) can be written as

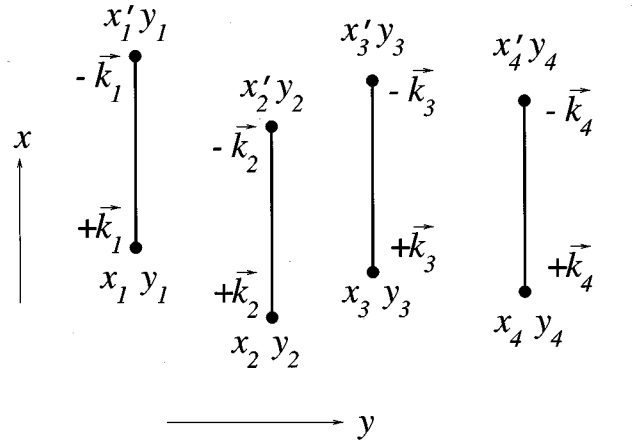

FIG. 2. The diagram of order N in Eq. (3.2) is made of N dipoles. The two end points of a given dipole are located at the same position y_i in the y direction but at different positions x_i and x_i' in the x direction.

$$\delta^{(d-1)}[\mathbf{h}(x_i,y_i)-\mathbf{h}(x_i',y_i)]=\int\frac{d^{d-1}\mathbf{k}_i}{(2\pi)^{d-1}}e^{i\mathbf{k}_i\cdot[\mathbf{h}(x_i,y_i)-\mathbf{h}(x_i',y_i)]}, \tag{3.4}$$

and one is led to evaluate the Gaussian average

$$\left\langle\prod_{i=1}^{N}e^{i\mathbf{k}_i\cdot[\mathbf{h}(x_i,y_i)-\mathbf{h}(x_i',y_i)]}\right\rangle_0 =\exp\Bigg(-\tfrac{1}{2}\sum_{i,j=1}^{N}\mathbf{k}_i\cdot\mathbf{k}_j\{G_0(x_i-x_j,y_i-y_j) -G_0(x_i'-x_j,y_i-y_j)-G_0(x_i-x_j',y_i-y_j) +G_0(x_i'-x_j',y_i-y_j)\}\Bigg), \tag{3.5}$$

where G_0 is the two-point function

$$G_0(x,y)\equiv-\frac{1}{2(d-1)}\langle[\mathbf{h}(x,y)-\mathbf{h}(0,0)]^2\rangle_0 =-\frac{1}{2\sqrt{\pi}}|x|^{1/2}\exp\left(-\frac{y^2}{4|x|}\right)-\tfrac{1}{4}y\ \mathrm{erf}\left(\frac{y}{2|x|^{1/2}}\right). \tag{3.6}$$

Here $\mathrm{erf}(u)$ denotes the usual error function $\mathrm{erf}(u)\equiv(2/\sqrt{\pi})\int_0^u dt\ \exp(-t^2)$.

The term of order N in the perturbative expansion (3.2) is therefore naturally represented by a diagram of N ''dipoles'' of interacting points located at $(x_i,y_i;x_i',y_i)$ with ''charge'' $\pm\mathbf{k}_i$, as depicted in Fig. 2. Note that the two end points of a given dipole i are located at the same position y_i in the y direction, but at different positions x_i and x_i' in the x direction. A singular configuration of interacting points is found when the quadratic form

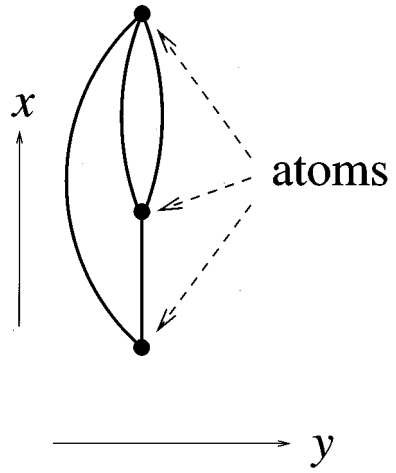

FIG. 3. A molecule with two loops made of a connected assembly of four dipoles. This molecule has three atoms located at different values of x but at the same value of y.

$$Q(\{\mathbf{k}_i\})=\sum_{i,j}\mathbf{k}_i\cdot\mathbf{k}_j\{G_0(x_i-x_j,y_i-y_j)-G_0(x_i'-x_j,y_i-y_j)-G_0(x_i-x_j',y_i-y_j)+G_0(x_i'-x_j',y_i-y_j)\} \quad (3.7)$$

appearing in Eq. (3.5) is not positive definite. Using the integral representation of the two-point function

$$G_0(x,y)=\int\frac{dp}{2\pi}\frac{dq}{2\pi}\frac{e^{i(px+qy)}-1}{q^4+p^2}, \quad (3.8)$$

we obtain

$$Q(\{\mathbf{k}_i\})=\int\frac{dp}{2\pi}\frac{dq}{2\pi}\frac{\left|\sum_i\mathbf{k}_i e^{iqy_i}(e^{ipx_i}-e^{ipx_i'})\right|^2}{q^4+p^2}. \quad (3.9)$$

The quadratic form Q is thus positive definite except for those configurations of end points $\{x_i,x_i',y_i\}$ for which one can find a set of charges $\{\mathbf{k}_i\}$, not all zero, satisfying

$$\sum_i\mathbf{k}_i e^{iqy_i}(e^{ipx_i}-e^{ipx_i'})=\mathbf{0},\quad\forall(p,q)$$

$$\Leftrightarrow\boldsymbol{\rho}(x,y)\equiv\sum_i\mathbf{k}_i\delta(y-y_i)[\delta(x-x_i)-\delta(x-x_i')]=\mathbf{0},\quad\forall(x,y). \quad (3.10)$$

This latter condition is the requirement that the charge density $\boldsymbol{\rho}(x,y)$ vanishes identically, while some of the charges $\mathbf{k}_i$ remain nonzero. This is possible if some of the N dipoles arrange to form a so-called ''molecule,'' i.e., attach their end points and assemble into a connected diagram with at least one loop, such as in Fig. 3. A set of end points in contact form what is called an ''atom,'' and their common position is the position of the atom. A zero of Q is obtained by an appropriate choice of nonzero charges, keeping all the atoms neutral, which is possible in the presence of a loop. Note that all the atoms of a molecule have the same position in the y direction. Note also that singularities coming from disconnected molecules can be treated separately, and that dipoles in the molecule which do not belong to a loop (dead branches) do not contribute to the singularity and can be ignored.

The construction above identifies the singular configurations of end points which give rise to possible divergences. Such a configuration is characterized by a set of M atoms labeled by p, and with position (x_p,y), with the same y coordinate for all the atoms. For each atom p, we denote by I_p the set of dipoles i which attach their first end point at the atom p [i.e., $(x_i,y_i)=(x_p,y)$], and by J_p the set of dipoles j which attach their second end point at the atom p [i.e., $(x_j',y_j)=(x_p,y)$]. The singularity can be analyzed by use of the general short distance MOPE introduced in Ref. [15]. In practice, one can return to the operator level [the left hand side of Eq. (3.5)] and write the contribution of the atom p in Eq. (3.5)

$$\prod_{i\in I_p}e^{i\mathbf{k}_i\cdot\mathbf{h}(x_i,y_i)}\prod_{j\in J_p}e^{-i\mathbf{k}_j\cdot\mathbf{h}(x_j',y_j)}=\left\langle\prod_{i\in I_p}e^{i\mathbf{k}_i\cdot\mathbf{h}(x_i,y_i)}\prod_{j\in J_p}e^{-i\mathbf{k}_j\cdot\mathbf{h}(x_j'y_j)}\right\rangle_0:\prod_{i\in I_p}e^{i\mathbf{k}_i\cdot\mathbf{h}(x_i,y_i)}\times\prod_{j\in J_p}e^{-i\mathbf{k}_j\cdot\mathbf{h}(x_j',y_j)}:, \quad (3.11)$$

i.e., separate in the right hand side of Eq. (3.5) the propagators G_0 which involve only points inside the atom p, and which reconstruct precisely the Gaussian average above, from those involving at least one end point not in the atom p, corresponding to a normal product prescription. This separation allows us to isolate the singularity in the factorized Gaussian average, while the normal product has a regular expansion in x_i-x_p $(i\in I_p)$, $x_j'-x_p$ $(j\in J_p)$ and $y_k-y(k\in I_p\cup J_p)$

$$:e^{i\mathbf{k}_p\cdot\mathbf{h}(x_p,y)}\left(1+i\sum_{i\in I_p}[(x_i-x_p)\mathbf{k}_i\cdot\partial_x\mathbf{h}(x_p,y)+(y_i-y)\mathbf{k}_i\cdot\partial_y\mathbf{h}(x_p,y)]-i\sum_{j\in J_p}[(x_j'-x_p)\mathbf{k}_j\cdot\partial_x\mathbf{h}(x_p,y)+(y_j-y)\mathbf{k}_j\cdot\partial_y\mathbf{h}(x_p,y)]+\cdots\right):, \quad (3.12)$$

with $\mathbf{k}_p=(\Sigma_{i\in I_p}\mathbf{k}_i-\Sigma_{j\in J_p}\mathbf{k}_j)$ being the total charge of the atom p. The same treatment can be applied to all the atoms of the molecule, creating for each atom p an exponential factor $e^{i\mathbf{k}_p\cdot\mathbf{h}(x_p,y)}$, together with insertions of various ∂_x and/or ∂_y derivatives of the field $\mathbf{h}$ at the point (x_p,y). As in Ref. [15], the MOPE is obtained by performing the integration over the charges $\mathbf{k}_i$ for the dipoles i forming the molecule. This expands the corresponding product of bilocal operators $\Pi_i\delta^{(d-1)}[\mathbf{h}(x_i,y_i)-\mathbf{h}(x_i',y_i)]$ around the chosen singular configuration in terms of general M-body operators of the form

$$\Phi(x_1,\ldots,x_M)=\int d^{d-1}\mathbf{h}\prod_{p=1}^{M} A_p(x_p,y) \times\nabla_{\mathbf{h}}^{\mathbf{m}_p}\delta^{(d-1)}[\mathbf{h}-\mathbf{h}(x_p,y)], \quad (3.13)$$

multiplied by singular coefficients (see Ref. [15] for details). Here $A_p(x_p,y)$ denotes either the unity operator 1 or a local operator in the derivatives of the field $\mathbf{h}$ at point (x_p,y) and $\nabla_{\mathbf{h}}^{\mathbf{m}}$ is a shorthand notation for $\Pi_{\alpha=1}^{d-1}\partial_{h_\alpha}^{m_\alpha}$. The above operators are multilocal in the x direction, but local in the y direction. This is because all the atoms in the molecule have the same y position. We will see two explicit examples of the MOPE in Sec. IV, where explicit one-loop calculations are presented.

At this stage, let us mention the following important result concerning the case where one inserted operator involves ∂_y derivatives only [such as $(\partial_y^2\mathbf{h})^2$]. Indeed, such a term comes from the expansion of some operator $e^{i\mathbf{k}_i\cdot\mathbf{h}(x_i,y_i)}$ taken at $x_i=x_p$ exactly (we suppose here that $i\in I_p$ rather than $i\in J_p$). However, in contrast with the coordinate x_i (x_i'), which appears only in the atom p, the coordinate y_i appears in a second atom p' (such that $i\in J_{p'}$), which is in general distinct from p. The expansion in y_i-y can be done simultaneously on the operator $e^{i\mathbf{k}_i\cdot\mathbf{h}(x_i,y_i)}$ above for $x_i=x_p$, and for the operator $e^{-i\mathbf{k}_i\cdot\mathbf{h}(x_i',y_i)}$ for $x_i'=x_{p'}$, in which case the operator to be expanded in y_i-y is $e^{i\mathbf{k}_i\cdot[\mathbf{h}(x_p,y_i)-\mathbf{h}(x_{p'},y_i)]}$. We thus obtain the important result that those operators with only partial derivatives in the y direction can be regrouped so that they involve the difference of the $\mathbf{h}$ field at two (in general different) points of the molecule. An example of such operator is the two-body operator

$$\{\partial_y[\mathbf{h}(x_1,y)-\mathbf{h}(x_2,y)]\}^2\delta^{(d-1)}[\mathbf{h}(x_1,y)-\mathbf{h}(x_2,y)]. \quad (3.14)$$

If the two end points of the dipole i happen to belong to the same atom p, then the operator to be expanded is 1, which means that this dipole cannot give rise to insertions of local operators with only ∂_y derivatives.

This latter remark has an important implication for the renormalization of local operators, coming from the particular case of singular configurations where the molecule has only one atom. In this case, each dipole in the molecule falls automatically in the class just described of dipoles with their two end points in the same, unique, atom. We thus obtain the important result that local operators with only ∂_y derivatives are not created by renormalization. Such terms, when absent from the original Hamiltonian (2.1), never appear, and the only such operator present in Eq. (2.1) [namely, $(\partial_y^2\mathbf{h})^2$] is *not* renormalized, that is

$$Z=1. \quad (3.15)$$

Having identified the singular configurations and the corresponding general multilocal operators to which their singularities are proportional, it remains to identify those singularities which are not integrable and give rise to actual divergences. If the molecule is made of K dipoles, the operator which is expanded via the MOPE is the product of $K\delta^{(d-1)}$ factors, with canonical dimension $-K\zeta_0(d-1)$ in units of y. The dimension of the multilocal operator Φ in Eq. (3.13) is

$$(d-1)\zeta_0+\sum_{p=1}^{M}\{\dim[A_p]-[|\mathbf{m}_p|+(d-1)]\zeta_0\}, \quad (3.16)$$

with the notation $|\mathbf{m}|=\Sigma_{\alpha=1}^{d-1}m_\alpha$. The corresponding singular coefficient in the MOPE has thus the dimension

$$-(K+1)(d-1)\zeta_0-\sum_{p=1}^{M}\{\dim[A_p]-[|\mathbf{m}_p|+(d-1)]\zeta_0\}. \quad (3.17)$$

This coefficient has to be integrated over the $2K-M$ relative x coordinates and the $K-1$ relative y coordinates of the $2K$ end points of the dipoles approaching the positions of the M atoms. This gives a superficial degree of convergence for the corresponding integral

$$\omega=2(2K-M)+(K-1)+[M-(K+1)](d-1)\zeta_0 +\sum_{p=1}^{M}(|\mathbf{m}_p|\zeta_0-\dim[A_p])=3(M-2)+\epsilon(K-M+1) +\sum_{p=1}^{M}(|\mathbf{m}_p|\zeta_0-\dim[A_p]), \quad (3.18)$$

with $\epsilon=5-(d-1)\zeta_0$. Note that $K-M+1$ is nothing but the number of loops in the molecule. A divergence is found whenever $\omega\leqslant 0$. It is easy to check that all the local operators A but the unit operator have a strictly negative dimension in units of y, as a consequence of the relation $\zeta_0<1$. At $\epsilon=0$, $\omega\leqslant 0$ requires either $M=2$, $\mathbf{m}_1=\mathbf{m}_2=\mathbf{0}$, and $A_1=A_2=1$, which is nothing but the original contact interaction in Eq. (2.1), or $M=1$, in which case Φ is either the unity operator 1 or a local operator $A(x,y)$ which moreover must satisfy $\dim[A]\geqslant -3$. We already know from the previous discussion that A must contain at least one ∂_x derivative since terms with only ∂_y derivatives are not created. Due to the $x\to -x$ symmetry, the coefficient of a term with only one ∂_x vanishes, and one thus needs at least two ∂_x derivatives. The term with largest dimension satisfying this criterion is the original elastic term in Eq. (2.1) $(\partial_x\mathbf{h})^2$ which already has dimension -3. It is thus, together with the unity operator, the only renormalized local operator in the theory. The renormalization of the unity operator is simply a shift in the free energy of the system. In particular, it disappears in the computation of average values of physical observables, and can simply be ignored.

In conclusion, we have shown that the Hamiltonian (2.1) renormalizes onto itself, with $Z=1$, as announced. For $\epsilon>0$, the theory is super-renormalizable, since ω in Eq. (3.18) increases with the number of loops of the molecule.

IV. ONE-LOOP CALCULATIONS

Let us now present one-loop calculations, which give corrections at first order in ϵ for the critical exponents ζ, ν, and

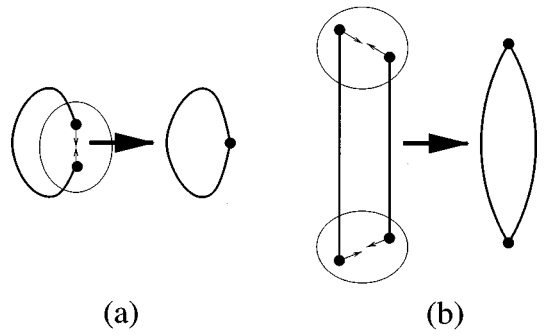

FIG. 4. The two singular configurations leading to (a) a one-loop renormalization of $(\partial_x \mathbf{h})^2$ and (b) a one-loop renormalization of $\delta^{(d-1)}[\mathbf{h}(x,y)-\mathbf{h}(x',y)]$.

z. Here we use dimensional regularization by considering the theory at $\epsilon>0$, and by calculating the renormalization factors $Z_\perp$ and Z_b needed to make the theory finite for $\epsilon=0$ at one-loop order in b_R. We use a minimal subtraction scheme where we keep for the first order correction in $Z_\perp$ and Z_b only the corresponding pole in ϵ.

We obtain our results in the framework of the MOPE described above, which we use here in two simple cases: the one-atom molecule made of a single dipole with its two end points approaching each other [see Fig. 4(a)] and the two-atom molecule made of two dipoles approaching each other [see Fig. 4(b)]. The first situation will give us a renormalization of the local operator $(\partial_x \mathbf{h})^2$, and hence a first order correction to $Z_\perp$. The second situation will give us a renormalization of the bilocal operator $\delta^{(d-1)}[\mathbf{h}(x,y)-\mathbf{h}(x',y)]$, and hence a first order correction to Z_b.

To analyze the divergence for Fig. 4(a), we use the operator product expansion (OPE):

$$e^{i\mathbf{k}\cdot[\mathbf{h}(x,y)-\mathbf{h}(x',y)]}=e^{\mathbf{k}^2 G_0(x-x',0)}\{1+i(x-x')\mathbf{k}\cdot:\partial_x\mathbf{h}(x_0,y):-\tfrac{1}{2}(x-x')^2 k_\alpha k_\beta :\partial_x h_\alpha(x_0,y)\partial_x \times h_\beta(x_0,y):+\cdots\}, \tag{4.1}$$

where $x_0=(x+x')/2$, and

$$G_0(x-x',0)=-\frac{1}{2\sqrt{\pi}}|x-x'|^{1/2}. \tag{4.2}$$

When integrated over $\mathbf{k}$ this gives the MOPE:

$$\delta^{(d-1)}[h(x,y)-\mathbf{h}(x',y)] = \frac{1}{(4\pi)^{(d-1)/2}}\left\{\frac{1}{[-G_0(x-x',0)]^{(d-1)/2}} \times 1-\frac{1}{4}\frac{(x-x')^2}{(-G_0(x-x',0))^{(d+1)/2}}\times:[\partial_x\mathbf{h}(x_0,y)]^2: +\cdots\right\}. \tag{4.3}$$

We use the above formula for the renormalized theory (2.5), expanded to first order in b^R. As in Eq. (3.2), the bilocal δ interaction comes with a factor $-b^R\mu^\epsilon/2$, and the singularity in (4.3) proportional to $(\partial_x\mathbf{h}^R)^2$ will be canceled by the corresponding counterterm, appearing with a factor $-(Z_\perp-1)/2$, provided we choose

$$\frac{(Z_\perp-1)}{2}=b^R\frac{\mu^\epsilon}{2}\int_{|X|\leqslant\mu^{-2}}dX\,\frac{1}{4}\frac{(2\sqrt{\pi})^6}{(4\pi)^5}\frac{X^2}{(|X|^{1/2})^{6-\epsilon}} \tag{4.4}$$

where $X=x^R-x'^R$, and where we used Eq. (4.2) and $d=11-2\epsilon$. This leads to

$$Z_\perp=1+\frac{b^R}{16\pi^2}\frac{1}{\epsilon}. \tag{4.5}$$

Let us now analyze the divergence for Fig. 4(b). We now use the OPE for the first atom,

$$e^{i[\mathbf{k}_1\cdot\mathbf{h}(x_1,y_1)+\mathbf{k}_2\cdot\mathbf{h}(x_2,y_2)]} =e^{-\mathbf{k}_1\cdot\mathbf{k}_2 G_0(x_1-x_2,y_1-y_2)}:e^{i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{h}(x_0,y_0)}\{1+\cdots\}:, \tag{4.6}$$

where $x_0=(x_1+x_2)/2$ and $y_0=(y_1+y_2)/2$, and the similar OPE for the second atom,

$$e^{-i[\mathbf{k}_1\cdot\mathbf{h}(x_1',y_1)+\mathbf{k}_2\cdot\mathbf{h}(x_2',y_2)]} =e^{-\mathbf{k}_1\cdot\mathbf{k}_2 G_0(x_1'-x_2',y_1-y_2)}:e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{h}(x_0',y_0)}\{1+\cdots\}:, \tag{4.7}$$

where $x_0'=(x_1'+x_2')/2$. The MOPE is obtained by integrating over $\mathbf{k}_1$ and $\mathbf{k}_2$. More precisely, we define $\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2$ and $\mathbf{q}=(\mathbf{k}_1-\mathbf{k}_2)/2$, so that $\mathbf{k}_1\cdot\mathbf{k}_2=-q^2+O(\mathbf{k}^2)$. This latter $O(\mathbf{k}^2)$ term can be set to zero if we are interested in the leading singularity, which is responsible for the divergence. Integrating over $\mathbf{k}$ reconstructs a bilocal δ operator, and we obtain the following MOPE:

$$\delta^{(d-1)}[\mathbf{h}(x_1,y_1)-\mathbf{h}(x_1',y_1)]\delta^{(d-1)}[\mathbf{h}(x_2,y_2)-\mathbf{h}(x_2',y_2)] =\frac{1}{(4\pi)^{(d-1)/2}}\frac{1}{[-G_0(x_1-x_2,y_1-y_2)-G_0(x_1'-x_2',y_1-y_2)]^{(d-1)/2}}\,\delta^{(d-1)}[\mathbf{h}(x_0,y_0)-\mathbf{h}(x_0',y_0)]+\cdots. \tag{4.8}$$

We are interested in the pole in ϵ obtained when integrating the coefficient of the δ term on the right hand side of Eq. (4.8) over the relative coordinates x_1-x_2, $x_1'-x_2'$ and y_1-y_2. Defining $Y=|y_1-y_2|+|x_1-x_2|^{1/2}+|x_1'-x_2'|^{1/2}$, $u=|x_1-x_2|^{1/2}/|y_1-y_2|$, and $v=|x_1'-x_2'|^{1/2}/|y_1-y_2|$, and using again the explicit formula (3.6) for G_0 and $d=11-2\epsilon$, we obtain a pole in ϵ equal to

$$32\,\frac{(2\sqrt{\pi})^5}{(4\pi)^5}\int_0^{\mu^{-1}} dY\,\frac{Y^4}{Y^{5-\epsilon}}\times\int_0^\infty du\int_0^\infty dv\,\frac{uv}{[f(u)+f(v)]^5}, \tag{4.9}$$

where $f(u)=u\,\exp(-1/4u^2)+(\sqrt{\pi}/2)\mathrm{erf}(1/2u)$. The integral over Y gives a pole $\mu^{-\epsilon}/\epsilon$. The integral over u and v is convergent, and will be denoted by

$$I\equiv\int_0^\infty du\int_0^\infty dv\,\frac{uv}{[f(u)+f(v)]^5}=\tfrac{1}{24}\int_0^\infty da[F(a)]^2, \tag{4.10}$$

where $F(a)\equiv a^2\int_0^\infty du\;ue^{-af(u)}$. The function $F(a)$ satisfies $F(a)\underset{a\to 0}{\to}1$ and $F(a)\underset{a\to\infty}{\sim}\exp(-a\sqrt{\pi}/2)$. The integral I can be estimated numerically to $I=0.068\,373\,636(1)$.

Applying, as before, the MOPE of Eq. (4.8) to the *renormalized* theory, now expanded as in Eq. (3.2) to second order in b^R, the $N=2$ diagram gives two δ interactions with a factor $(b^R\mu^\epsilon)^2/8$, leading to a divergence equal to

$$2\times\frac{(b^R\mu^\epsilon)^2}{8}\,\frac{1}{\pi^{5/2}}\,\frac{\mu^{-\epsilon}I}{\epsilon} \tag{4.11}$$

with a factor of 2 coming from the two ways of assembling the two dipoles of the diagram into a one-loop molecule. This divergence will be canceled by the δ interaction counterterm in the renormalized Hamiltonian, which comes in the expansion with a factor $-(Z_b-1)b^R\mu^\epsilon/2$, provided

$$Z_b=1+\frac{b^R}{2\pi^{5/2}}\,\frac{I}{\epsilon}. \tag{4.12}$$

Using Eqs. (4.5) and (4.12), we relate the bare and renormalized coupling constants as in Eq. (2.7) for $D=2$ and $d=11-2\epsilon$:

$$b=\mu^\epsilon b^R\left(1+\frac{I}{2\pi^{5/2}}\,\frac{b^R}{\epsilon}\right)\left(1+\frac{1}{16\pi^2}\,\frac{b^R}{\epsilon}\right)^{(7-\epsilon)/2}+O((b^R)^3), \tag{4.13}$$

leading, after differentiation with respect to μ at fixed b, to the one-loop Wilson function

$$\beta(b^R)\equiv\mu\frac{d}{d\mu}\bigg|_0 b^R=-\epsilon b^R+\left(\frac{I}{2\pi^{5/2}}+\frac{7-\epsilon}{2}\,\frac{1}{16\pi^2}\right)(b^R)^2+O((b^R)^3). \tag{4.14}$$

We thus obtain an infrared stable fixed point at

$$b^{R\star}=\frac{\epsilon}{\dfrac{I}{2\pi^{5/2}}+\dfrac{7}{2}\,\dfrac{1}{16\pi^2}}+O(\epsilon^2). \tag{4.15}$$

This fixes the value of the anomalous dimension δ through

$$\begin{aligned}\delta(b^R)\equiv\mu\frac{d}{d\mu}\bigg|_0\ln Z_\perp&=\beta(b^R)\,\frac{d}{db^R}\ln Z_\perp\\&=[-\epsilon b^R+O((b^R)^2)]\left(\frac{1}{16\pi^2}\,\frac{1}{\epsilon}+O(b^R)\right)\\&=-\frac{b^R}{16\pi^2}+O((b^R)^2)\end{aligned} \tag{4.16}$$

and

$$\delta\equiv\delta(b^{R\star})=-\frac{\epsilon}{\dfrac{8I}{\sqrt{\pi}}+\dfrac{7}{2}}+O(\epsilon^2). \tag{4.17}$$

Numerical values for the exponents at $D=2$ and $d=3$ are obtained by setting $\epsilon=4$ in the above formula, giving

$$\delta=-1.050, \tag{4.18}$$

and thus the estimates

$$\begin{aligned}z&=0.678,\\\nu&=0.517,\\\zeta&=0.762.\end{aligned} \tag{4.19}$$

To understand the values we obtain for these exponents more clearly, notice that the factor $\frac{7}{2}$ in the denominator of Eq. (4.17) is actually the factor $(d+3)/4=(\frac{7}{2})-(\epsilon/2)$, appearing in the exponent of $Z_\perp$ in Eq. (2.7), to first order in ϵ. It is therefore legitimate, at first order, to replace this factor $\frac{7}{2}$ by the factor $\frac{3}{2}$ obtained by setting $d=3$ directly. This in practice amounts to making a partial two-loop correction. This leads to new estimates $\delta=-2.212$ and $\zeta=1.053$, well above the original estimate (4.19), and actually even unphysical since larger than 1. We see here that, due to the large value of $\epsilon=4$ at the physical dimension $d=3$, the first order estimates (4.19) are not robust with respect to second order corrections and cannot be reliable.

It is also interesting to develop alternative expressions for the roughness exponent ζ, as was done for the isotropic membrane Edwards model in Ref. [16]. Indeed, the above estimate of ζ relies on expression (2.13), expressing the deviation of ζ from its Gaussian value ζ_0 at $\epsilon=0$, in terms of the anomalous exponent $\delta=\mu(d/d\mu)|_0\ln Z_\perp$, which we estimated to first order in ϵ in Eq. (4.17). Using relation (2.7) between the bare and renormalized coupling constants, however, we can write, at the fixed point, the two following equivalent definitions of δ:

$$\begin{aligned}\delta&=\delta_F-\frac{4}{\{4+(D-1)(d+3)\}}\,\mu\,\frac{d}{d\mu}\bigg|_0\ln\frac{Z_b}{Z_\perp}\\&=\delta_{\mathrm{var}}-\frac{4}{(D-1)(d+3)}\,\mu\,\frac{d}{d\mu}\bigg|_0\ln Z_b,\end{aligned} \tag{4.20}$$

leading directly to the two identities

$$\zeta=\zeta_F+\frac{D-1}{\{4+(D-1)(d+3)\}}\,\mu\,\frac{d}{d\mu}\bigg|_0\ln\frac{Z_b}{Z_\perp}$$
$$=\zeta_{\rm var}+\frac{1}{d+3}\,\mu\,\frac{d}{d\mu}\bigg|_0\ln Z_b\,. \tag{4.21}$$

These relations express the deviation of ζ from its Flory value and its variational value, respectively. As we did for δ in Eqs. (4.16) and (4.17), we can obtain for $D=2$ and $d=11-2\epsilon$ the estimates to first order in ϵ:

$$\mu\frac{d}{d\mu}\bigg|_0\ln\frac{Z_b}{Z_\perp}=\frac{1-\dfrac{8I}{\sqrt{\pi}}}{\dfrac{8I}{\sqrt{\pi}}+\dfrac{7}{2}}\,\epsilon+O(\epsilon^2),$$
$$\mu\frac{d}{d\mu}\bigg|_0\ln Z_b=-\frac{\dfrac{8I}{\sqrt{\pi}}}{\dfrac{8I}{\sqrt{\pi}}+\dfrac{7}{2}}\,\epsilon+O(\epsilon^2). \tag{4.22}$$

One can easily check that the two Eqs. (4.21) give exactly the same estimate as before for ζ at first order in ϵ, provided that the quantities ζ_F and $\zeta_{\rm var}$, and the different factors appearing in Eq. (4.21), which involve d, are themselves expanded to first order in ϵ.

On the other hand, one could also decide not to expand any of these factors and impose $d=3$ directly. If one moreover restores the factor $(d+3)/4$ instead of $\frac{7}{2}$, as discussed above, all the various expressions reproduce the unphysical estimate $\zeta=1.053$. If only some of the terms are expanded in ϵ, we obtain lower values of ζ. We thus expect that the original estimate $\zeta=0.762$, obtained by expanding all terms at first order in ϵ, is actually a lower bound on the exact value of ζ.

V. CONCLUSIONS

In this paper we studied, within the ϵ expansion, the effects of self-avoidance in the tubule model introduced by RT, going beyond their variational and Flory theory treatments of self-avoidance. We first show that the model is renormalizable and, furthermore, that the bending energy term is not renormalized. We then derive very general scaling relations for the critical exponents of the model at an infrared stable fixed point. These relations imply there is only one independent exponent. For special choices of the renormalization factors we are able to reproduce three different limits of the model, viz. the trivial Gaussian model, the Flory approximation and the Gaussian variational approximation [3]. This shows the power of this approach. We then treat the fluctuations of the model to one loop in the self-avoiding parameter in an ϵ expansion about the upper critical dimension. This yields predictions for all the critical exponents to first order in ϵ.

One should notice that our results have been obtained for an infinitely large membrane. For a finite membrane with extension L_y in the y direction and $L_\perp$ in the transverse direction, finite size scaling laws can be derived in the above renormalization group framework [3]. Due to the anisotropic nature of the tubular phase, however, there are many different scaling regimes, depending in particular on the relative scaling of L_y and $L_\perp$.

Finally, let us stress that the above analysis of renormalizability does not depend on the precise form of the Gaussian elastic term in the y direction. One could imagine replacing the bending energy term by a tension term $(\partial_y\mathbf{h})^2$, describing for instance a tubule under longitudinal tension. The theory would then also be renormalizable in an $\epsilon=2D-1-(d-1)(2-D)/2$ expansion, with again no renormalization of this tension term and only one independent exponent in the theory. In this case, however, the calculation cannot be performed at $D=2$ directly, where the upper critical dimension is infinite. As for self-avoiding isotropic membranes, a complete study of the problem for $D<2$ is required.

After this paper was completed we were informed by RT that the Hamiltonian equation (2.1) is not sufficient for a complete description of polymerized tubules in $d=3$. RT argued that a more involved Hamiltonian, including the anharmonic elastic terms of RT, Eq. (5), in addition to the self-avoiding interaction, is needed. Since the present paper is rigorous and self-consistent, we feel that it nevertheless makes a vital contribution to our present understanding of tubules. The analysis of the fuller model suggested by the remarks above presents a very definite challenge—to our knowledge there does not exist in the literature any proper renormalization group treatment of a theory with both nonlinear elasticity and two-body self-avoidance.

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