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Vesicles on a hierarchical lattice: an exact renormalization group approach

M Di Stasio†, F Seno‡|| and A L Stella§

† International School for Advanced Studies-SISSA Trieste, Italy
‡ Dipartimento di Fisica, Università di Padova, and Centro Interuniversitario di Struttura della Materia, Padova, Italy
§ Dipartimento di Fisica and INFN, Università di Bologna, and Centro Interuniversitario di Struttura della Materia, Padova, Italy

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Abstract. A model of two-dimensional vesicles on a Sierpinski gasket is introduced and solved by iterative methods. The effect of osmotic pressure is obtained by associating a fugacity to each plaquette of the underlying triangular lattice enclosed by the vesicle. Several results concerning the critical behaviour and phase diagram are discussed. In particular it is shown exactly that deflated critical vesicles fall into the universality class of branched polymers.

1. Introduction

The physics of biological membranes, which can consist of lipid bilayers assuming the shape of closed vesicles [1, 2], motivates theoretical interest in two-dimensional models of these objects, both in the continuum and on the lattice [3, 4]. The goal in this case consists in understanding the scaling properties and the different shapes of geometrical ring-like objects, which fluctuate thermally under the influence of fugacities controlling, for example, the length and enclosed area. More complicated situations, in which bending rigidity effects come into play, are also of much interest [4].

A possible model is given, for example, by self-avoiding rings (SAR) on a regular lattice, with a fugacity K associated with each step, and a fugacity W associated with each elementary lattice plaquette enclosed by the ring. The fugacity W clearly mimics the effect of an osmotic pressure difference Δp ($W = e^{A\Delta p/kT}$, with A representing the area of a plaquette) between the interior and exterior of the vesicle.

This model of lattice statistics poses problems which are interesting in their own right. Recently a number of results have been either exactly established or conjectured on the basis of numerical evidence. For example, it is by now well established that, for $W = 1$, the average number of plaquettes enclosed within a ring scales like $(K_c(1) - K)^{-2\nu_{SAR}}$ for $K \to K_c(1)^-$, where $\nu_{SAR} = \frac{3}{4}$ is the SAR exponent in $d = 2$ [5] and $K_c(W)$ represents the critical step fugacity [6, 7].

|| Present address: Department of Theoretical Physics, Oxford University, UK.

In addition, a number of results could be established on the form of $K_c(W)$ for both $W \lesssim 1$ and $W \gtrsim 0$ and on the relation between enclosed area and perimeter of the rings at criticality in the $W < 1$ region [7, 8].

A relevant property, which has been conjectured [3] for the whole deflated regime ($W < 1$), is that the average radius of gyration of the ring should behave as $(K_c(W) - K)^{-\nu_{BP}}$, where ν_{BP} is the exponent of lattice animals, or branched polymers in $d = 2$ [9]. So far, however, this property has escaped all attempts to establish it in full rigour, and its validity is supported only by plausible arguments and numerical evidence [4, 7, 8].

More recently, on the basis of Monte Carlo evidence, a very rich phase diagram for a $d = 2$ off-lattice vesicle model has been conjectured when bending rigidity contrasts the deflating pressure [10]. This phase diagram includes critical points and a first-order line and implies a highly non-trivial role for fluctuations in these systems.

This situation qualifies the issue of $d = 2$ vesicles as one of those for which additional information, possibly gained from exact calculations on simplified, hierarchical lattices, could definitely be of value. Indeed, models on fractal lattices have been proposed as a new context for the study of critical phenomena [11], and exact results established for them can be important indicators of the actual situation in the regular case.

2. Model and recursions

In this work we take such an attitude and present an exact renormalization group (RG) approach to a model of deflated vesicles on a Sierpinski gasket. Both the model and the RG solution fully reflect the relative complexity of the physics we want to describe. We believe they should also be of methodological interest in their own right: indeed, with due computational effort, our approach allows exact answers to many difficult questions, often untractable in regular geometries, to be obtained.

In the literature about critical phenomena on Sierpinski gaskets and similar fractal lattices, there already exist separate treatments of both SAR [12] and lattice animals [13]. The critical behaviour of flaccid, or deflated vesicles, is already expected to fall in at least the universality classes of both these geometrical problems. Thus, the first issue to face is whether the hierarchical model we choose is flexible enough to reproduce in a realistic way the effects of a deflating pressure on a ring, by allowing the correct universal features to show up in each physical situation.

It is immediately realized that the geometry of the Sierpinski gasket does not allow a strictly SAR to develop closed subloops or strips within up-pointing triangles of the structure, as a part of its global configuration (figure 1(*a*)). To get such configurations one has to allow self-intersections or multiple points of the ring. On the other hand, studies of bond lattice animals on a Sierpinski gasket show that dangling ramifications attached to a triangle vertex and vertex–vertex connections (figure 1(*b*)), with their interplay, are crucial in determining branched polymer behaviour [13]. Clearly, the vesicle drawn in figure 1(*a*), with its multiple points (which can be conceived as narrowings for the vesicle) seems to be a reasonable candidate to play a role similar to that of configuration 1(*b*) at a coarse grained level. For this to be true it is necessary, but not sufficient, that coarse graining, in an RG sense, implies a progressive deflation of the vesicle.

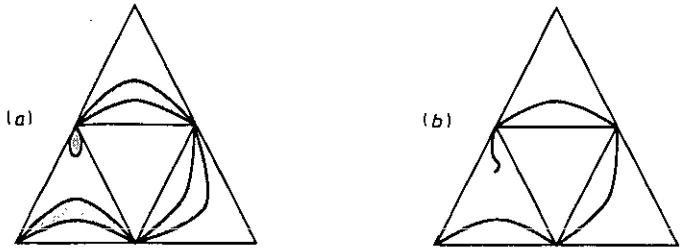

Figure 1. (*a*) Schematic representation of a vesicle limited by a ring with multiple points. Self-intersections, to be interpreted as narrowings of the shaded interior of the vesicle, occur at each junction between up-pointing triangles. Such a ring can mimic the branched polymer configuration in (*b*).

On the basis of these considerations we choose as contours of the vesicle in our model the silhouettes of closed 1-tolerant trails on the gasket. These are closed random walks, which are allowed to visit each lattice edge at most once.

In the absence of a pressure difference ($W = 1$), models of this kind have already been studied, and are known to belong to the same universality class as SAR on the gasket [14]. Thus, after introduction of the fugacity W to control the enclosed area, such silhouettes are plausible candidates to represent the physics of $d = 2$ vesicles.

In order to set up an iterative RG solution of the problem, it is helpful, although not strictly necessary, to restrict the possible topologies of our silhouettes. We thus allow only configurations in which the region enclosed by the silhouette is simply connected, taking into account that doubly visited sites can be assimilated to narrowings through which 'the interior' of the vesicle does not suffer interruptions. In other words we restrict the topology to that of the circle. This results in a sensible simplification of the RG recursions.

Due to the fractal character of the gasket, it is important to choose a sensible convention for the evaluation of the enclosed area. The only way to get physically interesting results consists in weighing the whole area enclosed by the silhouette, i.e. in counting all internal elementary plaquettes of the underlying, triangular lattice (see figure 2).

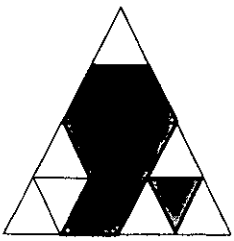

Figure 2. A vesicle of our silhouette model on the Sierpinski gasket at the third stage of construction (side equal to 2^2 in units of the lattice spacing). All internal plaquettes of the underlying lattice are weighed in order to get physical results. Edges belonging to the triangular lattice and not to the gasket are dotted.

Indeed, weighing only elementary up-pointing triangles, whose edges belong to the gasket, can be seen to lead to trivial one-dimensional self-avoiding walk exponents, if rings enclosing down triangles of any size are allowed. On the other hand, persistence of SAR behaviour results for the whole deflated regime, if the same rings are forbidden.

The generating function for the problem we want to solve can be written as

$$Z(K,W) = \lim_{n\to\infty} 3^{-n} \sum_r K^{\partial r} W^{|r|} \equiv \lim_{n\to\infty} 3^{-n} Z_n \tag{1}$$

where the sum is over all the previously specified ring silhouettes, r, on the nth generation Sierpinski gasket (side 2^n: $n = 0, 1, 2 \ldots$). ∂r and $|r|$ indicate the perimeter and number of enclosed plaquettes of ring r, respectively. The normalization factor 3^{-n} is introduced to ensure a finite Z in the thermodynamic limit.

The calculation of Z and similar generating functions can be performed recursively. One can show that, in view of the topology restrictions, twelve restricted generating functions are needed in order to have a closed set of equations, allowing iterative calculation of Z. The recursions express the restricted functions for the $(n+1)$th generation gasket in terms of those of the nth generation one. The terms occurring in the recursions are already so many and with so high multiplicities, that the calculation is most conveniently done by exact enumeration techniques on the computer.

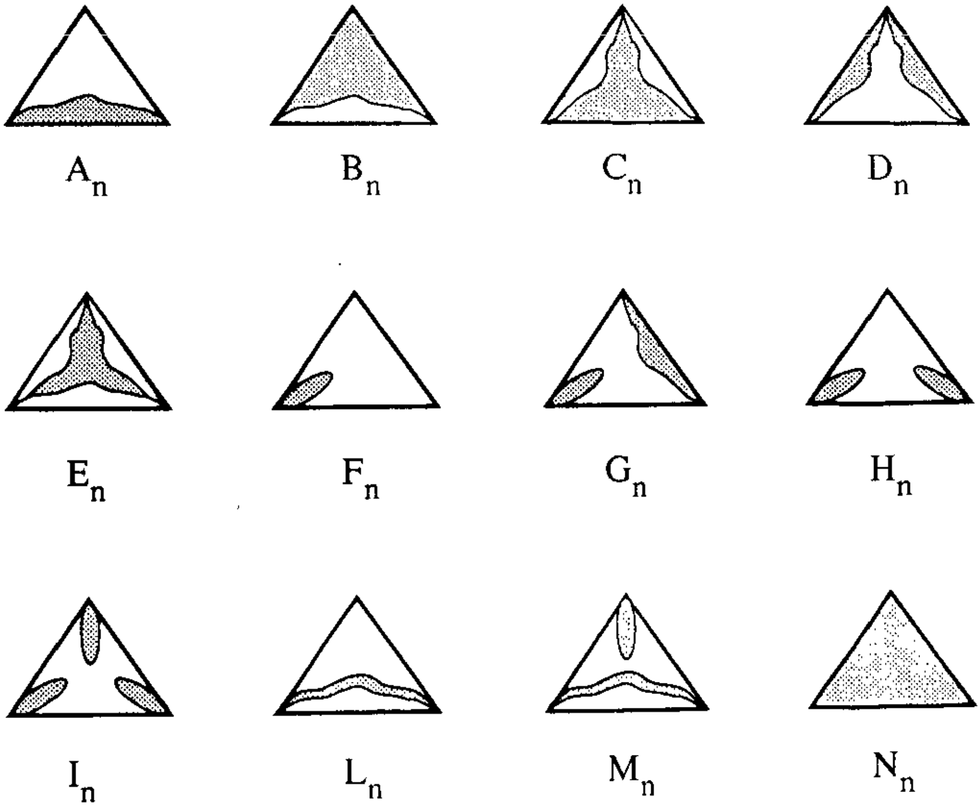

Figure 3. Diagrams representing typical contributions to the twelve generating functions. The hatched regions are supposed to belong to the interior of a vesicle.

In figure 3 we sketch typical contributions to each of the 12 restricted generating functions, which are labelled in progressive alphabetic order. The exact enumeration gives RG recursions for the generating functions which are reported below:

$$
\begin{aligned}
A_{n+1} = {} & A_n^2 + A_n B_n^2 N_n + 2A_n B_n D_n N_n + 2A_n C_n F_n \\
& + 2A_n C_n L_n + 2A_n C_n + A_n D_n^2 N_n + 2C_n^2 F_n + C_n^2 H_n \\
& + C_n^2 + 2C_n G_n L_n
\end{aligned}
$$

$$
\begin{aligned}
B_{n+1} = {} & A_n^2 B_n + 2A_n B_n C_n + B_n^2 N_n^2 + 2B_n C_n G_n \\
& + 2B_n D_n N_n^2 + D_n^2 N_n^2
\end{aligned}
$$

$$
\begin{aligned}
C_{n+1} = {} & 2A_n C_n E_n + 2A_n C_n L_n + B_n^2 C_n N_n + 2B_n C_n D_n N_n \\
& + 2C_n^2 L_n + 2C_n^2 M_n + C_n D_n^2 N_n + 2C_n E_n G_n
\end{aligned}
$$

$$
D_{n+1} = A_n^2 D_n + 2A_n C_n D_n + 2C_n D_n G_n
$$

$$
E_{n+1} = C_n^3 N_n + 6E_n^2 L_n + 6E_n^2 M_n + 3E_n L_n^2
$$

$$
\begin{aligned}
F_{n+1} = {} & A_n^2 C_n N_n + E_n F_n^2 + 4E_n F_n L_n + 2E_n F_n \\
& + 2E_n H_n L_n + 2E_n L_n + E_n + 2F_n L_n^2 \\
& + 2F_n L_n + F_n + 2L_n^3 + 2L_n^2 M_n + 2L_n^2 + 2L_n
\end{aligned}
$$

$$
\begin{aligned}
G_{n+1} = {} & A_n^2 E_n + A_n^2 F_n + 2A_n^2 L_n + 2A_n C_n F_n \\
& + 2A_n C_n H_n + 2A_n C_n L_n + 4A_n C_n M_n + 2A_n E_n G_n \\
& + 2A_n G_n L_n + B_n^2 G_n N_n + 2B_n D_n G_n N_n + C_n^2 F_n \\
& + 2C_n^2 H_n + C_n^2 I_n + 2C_n G_n L_n + 4C_n G_n M_n \\
& + D_n^2 G_n N_n + E_n G_n^2
\end{aligned}
$$

$$
\begin{aligned}
H_{n+1} = {} & 2A_n C_n G_n N_n + 2E_n F_n^2 + 2E_n F_n H_n + 6E_n F_n L_n \\
& + 8E_n F_n M_n + 2E_n F_n + 6E_n H_n L_n + 4E_n H_n M_n \\
& + 2E_n H_n + 2E_n I_n L_n + 2E_n L_n + 4E_n M_n \\
& + 2F_n^2 L_n + F_n^2 + 6F_n L_n^2 + 4F_n L_n M_n \\
& + 4F_n L_n + 3H_n L_n^2 + 2H_n L_n + 2L_n^3 \\
& + 8L_n^2 M_n + 3L_n^2 + 6L_n M_n^2 + 4L_n M_n
\end{aligned}
$$

$$
\begin{aligned}
I_{n+1} = {} & 3C_n G_n^2 N_n + 3E_n F_n^2 + 6E_n F_n H_n + 6E_n F_n L_n \\
& + 12E_n F_n M_n + 3E_n H_n^2 + 12E_n H_n L_n + 24E_n H_n M_n \\
& + 6E_n I_n L_n + 12E_n I_n M_n + F_n^3 + 6F_n^2 L_n \\
& + 6F_n H_n L_n + 9F_n L_n^2 + 12F_n L_n M_n + 12H_n L_n^2 \\
& + 12H_n L_n M_n + 3I_n L_n^2 + 2L_n^3 + 12L_n^2 M_n \\
& + 24L_n M_n^2 + 14M_n^3
\end{aligned}
$$

$$
L_{n+1} = A_n C_n^2 N_n + 2E_n^2 F_n + E_n^2 H_n + E_n^2
$$

$$+2E_nF_nL_n+4E_nL_n^2+4E_nL_nM_n+2E_nL_n+L_n^3+L_n^2$$

$$M_{n+1}=C_n^2G_nN_n+E_n^2F_n+2E_n^2H_n+E_n^2I_n$$
$$+2E_nF_nL_n+2E_nH_nL_n+3E_nL_n^2+10E_nL_nM_n$$
$$+7E_nM_n^2+F_nL_n^2+2L_n^3+3L_n^2M_n$$

$$N_{n+1}=N_n^4. \tag{2}$$

For Z_n the recursion takes the usual form of inhomogeneous RG equation of free energy like quantities:

$$Z_{n+1}=3Z_n+A_n^3N_n+3F_n^2L_n+3F_n^2+6F_nL_n+6F_n+3H_nL_n^2+3L_n^2+3L_n. \tag{3}$$

Of course the analysis of these nonlinear recursions can be performed in general only with the use of the computer.

3. Analysis of the recursions

For given K and W the thermodynamics of the model is determined by the fixed point to which the RG recursions take the set of generating functions as $n\to\infty$. This clearly depends on the initial conditions. In our case we have

$$\begin{array}{lll} A_0=K & B_0=KW & C_0=K^2W \\ D_0=K^2 & E_0=K^3W & F_0=0 \\ G_0=0 & H_0=0 & I_0=0 \\ L_0=0 & M_0=0 & N_0=W \end{array} \tag{4}$$

since for $n=0$ the gasket reduces to an elementary up triangle.

The structure of the RG recursions has features which immediately allow interesting conclusions to be drawn about the critical behaviour of the system. First of all, looking at the transformation of $N_n(N_n=N_{n-1}^4, N_0=W)$, we conclude that $N_n=W=1$ is an invariant subspace of the transformation. In this subspace a non-trivial fixed point describing SAR critical behaviour can be found ($A^*=0.6108$, $B^*=0.6108$, $C^*=0$, $D^*=0$, $E^*=0$, $F^*=0.2310$, $G^*=0.1427$, $H^*=0.0533$, $I^*=0.0123$, $L^*=0$, $M^*=0$, $N^*=1$). Indeed, within the $W=1$ invariant space, the relevant exponent associated to this fixed point is $y_1=1.2521\ldots$, which implies $\nu=1/y_1=0.7986\ldots$, the same ν_{SAW} obtained for other models of SAW on our Sierpinski gasket [12]. This result is rather natural, because on the gasket, as on a Euclidean lattice, for a trail model like ours, only excluded volume effects can influence the asymptotic behaviour, if $W=1$. The previously described fixed point is reached, after an infinite number of iterations, when $K=K_c(1)=0.4316\ldots, W=1$. By allowing $W\neq1$ we obtain extra exponents at this SAR fixed point: the relevant one, determining crossover, is $y_2=2$, as follows clearly from the recursion for N_n. If, for example, we have $N_0=W<1$, which is the most interesting region for the model [8], the recursions can only lead to fixed points at $N = 0$. The crossover exponent at $W = 1$ is $\phi = y_2/y_1 = 1.5973\ldots$.

This crossover exponent implies that the average area enclosed by our ring, for $W = 1$, grows like $(K_c(1) - K)^{-2\nu_{\text{SAW}}}$, for $K \to K_c(1)^-$. This follows from standard scaling arguments and from the fact the average area is

$$\frac{W}{Z}\frac{\partial Z}{\partial W}(K, W) = \langle |r| \rangle (K, W).$$

If we take into account that one of the relevant scaling fields has dimension $y_1 = 1/\nu_{\text{SAW}}$, and the other one, to leading order, is proportional to $1 - W$, and has dimension $y_2 = 2$, the result clearly follows. In view of the fact that the radius of gyration of the rings should diverge as $(K_c(1) - K)^{-\nu_{\text{SAW}}}$, we conclude that the rings are 'fat', i.e. enclose an average area equal to the square of their linear dimension, at $W = 1$. This last result also holds in the case of SAR on $d = 2$ regular lattice as first conjectured [3] and later derived on the basis of Coulomb gas [6] and other scaling arguments [7]. It is interesting to notice that the key ingredient for our conclusion here is the transformation law for $W = N_0$, which implies $y_2 = d = 2$. The same law and its consequences are established in [7] for the area fugacity of a vesicle model based on SAR on a regular lattice.

The search for the critical fixed point, or points controlling the criticality of vesicles in the deflated regime, can be made by iterating the recursions with different initial conditions. For each $W < 1$, one finds a $K_c(W)$ separating initial Ks flowing to trivial high- and low-temperature fixed points.

This crossover exponent also determines the shape of the critical line $K_c(W)$ for $W \leqslant 1$. Indeed, standard scaling arguments lead to

$$K_c(W) - K_c(1) \underset{W \to 1^-}{\sim} = (1 - W)^{1/\phi}. \tag{5}$$

For each W the initial generating functions specified by W and $K_c(W)$ converge towards a critical fixed point where the parameters A_n, B_n, C_n, D_n, F_n, G_n, H_n, I_n, M_n are going to infinity when $n \to \infty$, while the other parameters approach finite values. In order to study the asymptotic behaviour, it is profitable to introduce a new set of variables, which remain finite at the fixed point. Such new variables can be defined as follows:

$$\begin{array}{llll} a = A\sqrt{N} & b = B\sqrt{N} & c = C\sqrt{N} & \\ d = D\sqrt{N} & e = E & f = FE & g = G\sqrt{N} \\ h = HE^2 & i = IE^3 & l = L & m = ME \\ n = N. & & & \end{array} \tag{6}$$

For each $W < 1$ and $K = K_c(W)$, the variables defined in (6) turn out to approach the same critical fixed point ($a^* = 0$, $b^* = 0$, $c^* = 0$, $d^* = 0$, $e^* = 0$, $f^* = 0.2009$, $g^* = 0$, $h^* = 0.0232$, $i^* = 0.0022$, $l^* = 0.3276$, $m^* = 0.0231$, $n^* = 0$). Remarkably, the non-zero components of this last fixed point exactly coincide with those already found, in a much smaller parameter space, for a branched polymer model on the gasket [13].

In the new variables defined in equation (6) the Jacobian at this fixed point has a particularly simple structure: all its elements are identically zero, except for those of a diagonal block corresponding to the non-zero components. Within this block the Jacobian coincides with the one which is obtained for the branched polymer model recursions of [13]. This guarantees that, apart from the presence of 'infinitely irrelevant' fields, the scaling dimensions at our fixed point are those of branched polymers. In particular we conclude that the ν exponent is equal to $\nu_{BP} = 0.7165\ldots$, in the whole deflated regime ($W < 1$).

This result is non-trivial, if we think that in the model of [13] the building blocks of the polymer are simply edges of the gasket.

From this we learn that the asymptotic scaling properties of our deflated vesicles are exactly the same as those of lattice animals on the gasket, a property which is also expected to apply more generally to models on regular lattices [3, 7, 8].

The behaviour of $K_c(W)$ is reported in figure 4. The crossover exponent ϕ is consistent with an infinite derivative at $W = 1$. For $W \to 0$ the function describing K_c behaves as $K_c(W) \simeq W^{-1/3}$.

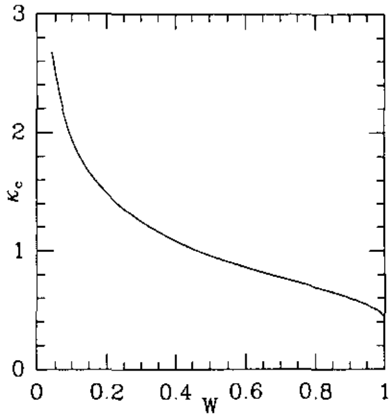

Figure 4. Sketch of K_c as a function of W.

This asymptotic dependence is determined by the fact that, asymptotically, rings with $3|r| \simeq \partial r$ are dominating the sum in equation (1), and can be derived on the basis of topological considerations and exact inequalities, by generalizing to our model, the methods discussed in [7] for the case of regular lattices. For example, in the case of a regular triangular lattice and SAR, one can show that $K_c(W) \simeq 1/W$, for $W \to 0^+$ [7].

4. Conclusions

In this work we studied, by an exact RG analysis, the statistics of vesicles, with both step and plaquette fugacity, on a deterministic fractal lattice.

In spite of the simplifications due to the fractal nature of the lattice and the topology restrictions, in order to solve a model which is adequate to mimic the physics of real vesicles, we had to work with RG recursions in a twelve-dimensional parameter space.

This high dimensionality required considerable effort in the numerical study of the RG flow and its fixed points. The numerical search was also complicated by the fact of the critical fixed points had infinite components.

Some remarks are in order concerning the specific choices made here. We imposed to our closed trails the topology of the circle, once assumed to interpret doubly visited points as narrowings of a self-avoiding contour.

This implies that, at coarse grained level, for example, in the deflated regime, our vesicles reduce to lattice animals without loops. In order to allow loops, we should release the constraint of simple connectedness, at the cost of a sensibly more complicated recursion structure (19 parameters). On the other hand, for lattice animals on a Sierpinski gasket it is by now exactly established that the presence or absence of loops does not influence the critical exponents [13].

Thus, in particular as far as the exponents of the deflated regime are concerned, we should not expect different results, when dealing with more general topologies for the trails.

Another feature of our model is that it globally counts the area enclosed by the trails. Thus the fractal lattice only imposes restrictions on the possible configurations of the trails, which are otherwise seen as embedded in a regular, triangular lattice. This leads to the transformation law $N_{n+1} = N_n^4$ of equation (2). This transformation is very important because it only allows fixed points for $W = 1$ and $W = 0$, i.e. in the flacid and infinitely deflated regime, respectively.

The results obtained in our analysis are physical and fully justify, in our opinion, the choice to work with a model on a fractal lattice. Indeed, this choice appears as the only way to get exact insight into crucial issues concerning more realistic models of vesicles on regular lattices. In this respect the most relevant result of the present analysis seems to us to be the exact identification of the universality class of deflated vesicles to be that of branched polymers. Our conclusion constitutes a strong indication of the general validity of this result, which is consistent with recent conjectures and heuristic arguments [3, 7, 8].

We are convinced that the achievements of the present work should open the way to further advances in the field.

Indeed, as mentioned in the introduction, interesting aspects of the physics of vesicles are expected to be reproduced by models also embodying, besides the area fugacity, bending rigidity effects. Monte Carlo evidence led recently to the conjecture of the possibility of a very rich behaviour of vesicles of fixed perimeter in the presence of both deflation and rigidity [10]. The methods of the present work can be generalized to embody bending rigidity in the model at the cost of a considerable, but not prohibitive, enlargement of the parameter space (22 parameters). Work is already in progress along these lines in order to make contact, in an exact context, with the physics revealed by Monte Carlo simulations of models in the continuum.

Acknowledgments

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