Self-Avoiding Random Surfaces: Monte Carlo Study using Oct-tree Data-structure

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Abstract

Self-avoiding random surfaces on a cubic lattice are studied by extensive Monte Carlo sampling. The surfaces have empty boundary and the topology of a 2-sphere. An oct-tree data-structure allows to obtain good statistics for surfaces whose plaquette number is almost an order of magnitude greater than in previous investigations. Maximum likelihood determinations of the critical plaquette fugacity, μ^{-1}, and entropic exponent, θ, can be extrapolated to the estimates: $\mu = \cdots \pm \cdots$, and $\theta = \cdots \pm \cdots$. The linear regression estimate for the radius of gyration exponent is $\nu = \cdots \pm \cdots$. The results support a location of the problem within the branched polymers universality class.

I. Introduction

Both lattice and continuum models of random surfaces (RS) have attracted much attention in the recent literature. Among the many motivations for this interest are connections with lattice gauge theories [BDI75,DI79] and possible applications to problems in condensed matter physics. RS are geometrical generalizations of random walks, which play a very fundamental role in fields like polymer physics. Indeed, from the onset of studies of RS, there has been a natural tendency to treat their statistics within the framework of schemes directly inspired by those used in polymer physics. On the other hand, RS

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models are expected to display a much richer variety of universality classes than their random walk counterparts, so that application of schemes used for random walk requires some caution.

At present, our understanding of RS models in finite dimensions relies on numerical investigations, mostly using Monte Carlo methods. As we've already mentioned, analysis of results is more delicate than for random walks. Another barrier to carrying out such investigations is the need to store a very large amount of information in order to describe the configuration of RS. This information is much greater than that normally needed in walk problems of comparable size. Thus, RS simulation is another field in which substantial progress can be made only if efficient data-structures and robust numerical methods are introduced in such a way as to allow sufficiently fast and accurate computations.

In this study we consider a model of RS on a 3-dimensional cubic lattice, i.e. the RS is constructed by gluing together elementary square plaquettes of the lattice according to the following prescription: A surface S is given by a set of $|S|$ distinct plaquettes. Each plaquette is used only once to build S, and at each of its four edges, it is connected to one and only one other plaquette. A self-avoidance constraint is understood in the sense that not only plaquettes but also their edges (which coincide with the bonds of the 3-d lattice) enter at most once in S. Corner overlaps are still allowed. We must also specify the boundary conditions and the topology. Our surfaces are closed, so that the boundary is fixed but null. It is known [Sokal] that convergence with fixed boundary conditions is much longer than with free boundaries. We assume the topology to be that of a 2-sphere (i.e. genus 0), thereby excluding handles. An excellent review of this problem is given in [Gl88].

There are two quantities of primary interest to us: $N(n)$, the number of possible surface configurations with $|S| = n$; and, $R(n)$ the radius of gyration with respect to the centroid of each configuration, averaged over all $N(n)$ configurations with $|S| = n$. In counting, we assume that each configuration is equivalent to all others obtained by lattice translations. Thus, by "surface configuration" we imply an equivalence class of configurations which coincide under such translations. On the basis of heuristic arguments, the following asymptotic behaviors are expected at large n:

$$N(n) \sim n^{-\theta} \mu^n \tag{1}$$

and

$$R(n) \sim n^{\nu} \tag{2}$$

The existence of $\lim \ln N/n$ could be established by generalizing a theorem of Hammersley [Ha61] on self-avoiding walks to self-avoiding surfaces [DFJ83]. The exponent θ has an entropic connotation, while ν can be naturally interpreted as the reciprocal of the fractal, or capacity dimension for surfaces.

Very little exact information is available about self-avoiding RS (SARS) models such as that described above. In particular, the determination of θ, μ and ν is essentially an open question. A property of self-avoiding surface modes is that they most probably collapse into non-interacting branched polymers in the limit of high dimensionality, implying $\nu = 1/4$ and $\theta = 5/2$ [DFJ84]. Early real-space renormalization-group calculations and Flory arguments, in the style of polymer statistics, suggested that the exponent ν of SARS at low dimensionality could be distinct from that of self-avoiding branched polymers, although the two problems would share the same upper critical dimension [MS84].

Sterling and Greensite [SG83] performed the first Monte Carlo calculation in 3-d for a SARS. They considered the same model described here and, working in a grand canonical ensemble, estimated $\theta = 0.5 \pm 0.05$, which would seem to exclude, at least for θ, the possibility of $\theta = 3/2$ and $\nu = 1/2$, the values expected for branched polymers in 3-d [PS81]. On the other hand, in an exact enumeration up to 10 plaquettes, Redner [Re85] found values of θ and ν which seemed compatible with those of branched polymers. (He, however, did not apply restrictions on the type of boundaries nor on the topology.) Further evidence for $\theta = 3/2$ and $\nu = 1/2$ was obtained by Glaus and Einstein [GE87,Gl88] with extensive Monte Carlo simulations, which improved on the work of [SG83]. Concurrently, Karowski [Ka86] presented Monte Carlo results for our model suggesting that the exponent ν could indeed be distinct from $1/2$ and instead have a value of the type first suggested by Maritan and Stella [MS84]. Although Karowski's approach seems less systematic and accurate than Glaus's, he did test a domain of larger n, closer to the asymptotic limit. His results thus cast some doubt on the identification of the model with branched polymers.

Because of this somewhat unsettled situation, we decided to undertake a new Monte Carlo investigation of the model, based on a more efficient computational approach than previous ones. This paper presents the results of such a study, and includes a thorough discussion of the computational strategy, with particular emphasis on the implementation of an oct-tree data-structure, which is unfamiliar to most physicists. To our knowledge, oct-trees have not yet been applied to this sort of problem, and we hope that our application of them will convince readers of the utility of sparse data-structures in complex problems of computational physics.

The rest of this paper is organized as follows: In the second section we outline our Monte Carlo method and illustrate how the oct-tree data-structure works. When appropriate, we also draw comparisons with the methods used in previous work. Section 3 is devoted to the presentation and analysis of our results. In the last section, we give our conclusions.

II. Monte Carlo Algorithm and Oct-tree Data-structure

Our Monte Carlo procedure generates SARS on a cubic lattice in a grand canonical ensemble at fixed plaquette fugacity β. Thus, the statistics of the generated surfaces can be derived from a partition function of the form

$$Z(\beta) = \sum_S |S|^x \beta^{|S|} \propto \sum_n n^x N(n) \beta^n \tag{3}$$

where we have chosen $x = 2$ or 3 in this study. As in refs [GE87,Gl88], our algorithm is a refinement of the Monte Carlo procedure first introduced by Sterling and Greensite. Given a surface S, an attempt to modify it is made by searching for elementary cubes of the lattice having at least one face belonging to S. If such a cube is found, we reverse the status of each of its 6 faces, regarding whether or not each belongs to the surface S. This process leads to a new surface S', which can be accepted only if it turns out to obey the geometrical and topological constraints imposed on the model. If the constraints are satisfied, then the acceptance of the new surface is subject to satisfaction of the usual Metropolis condition consistent with the grand-canonical fugacity β in the partition function.

In [SG] the search for cubes was made by sweeping through all those contained in a $10 \times 10 \times 10$ box. In subsequent studies [G,EG], the search was restricted to the set of cubes with at least one face belonging to the surface. In this way, surfaces fitting in a $20 \times 20 \times 20$ box could be generated. This box still imposes a rather severe finite-size limitation. These approaches are inefficient in that a well-defined location in computer memory must be reserved for each cube in the box, whether or not it actually touches the surface. We can, however, store information about the surface configuration using a sparse data-structure, the oct-tree, in which memory is only used for those cubes which actually touch the surface, while all others can be ignored. This procedure allows us to escape the restriction that surfaces fit in a finite box.

Before describing the data-structure explicitly, we comment on the way in which our grand-canonical weight in the partition function (3) is actually obtained. In [G,EG], each move of the surface was made by selecting randomly among the cubes having faces in common with it. If we denote by $\|S\|$ the number of such cubes for a surface S, the random choice implies a factor $1/\|S\|$ in the transition rate from S to any configuration S' accessible from S. Detailed balance then clearly implies that the grand canonical weight for a surface S should contain a factor $\|S\|$. Here we prefer to proceed in a way such that $|S|$, rather than $\|S\|$ factors appear in the grand canonical weight, as anticipated in eqn. (3). Thus, in our case the first random choice is made within the set of all $|S|$ elementary plaquettes of S. We then choose one of the two cubes sharing this plaquette and perform the usual inversion operation on it. Since this process allows the same cube to be chosen with more than one plaquette choice, we must unbias the procedure so that each distinct possible modification of S has an equal *a priori* probability. Again, calling S' the surface produced by inversion of the chosen cube, the move $S \to S'$ actually has probability $\kappa_{SS'}/|S|$ in the biased procedure, where $\kappa_{SS'}$ is the number of different plaquettes in S the choice of which can lead to the selection of the cube in question.

We can get rid of this bias if we slow down the rate by a factor of $1/\kappa_{SS'}$ by the usual Metropolis procedure of stopping the transition if a random number chosen in $[0,1]$ is greater than $1/\kappa_{SS'}$. In order to finally obtain the weight in eqn. (3), we have to apply $|S'|/(|S|+|S'|)$, one further slowing down process.

In fact, our calculation inserts two filters. The first determined by the ratio

$$\frac{|S|}{|S|+|S'|}.$$

in all cases, and the second by

$$\frac{|S'|^x}{|S|^x+|S'|^x}\beta^{|S'|-|S|}$$

in case $|S'| > |S|$ and otherwise,

$$\frac{|S'|^x}{|S|^x + |S'|^x}$$

In this way we get a transition rate for an allowed move $S \to S'$ that is of the form:

$$\omega(S \to S') = \begin{cases} A(S,S')|S'|^x \beta^{|S'|-|S|} & \text{if } |S'| > |S| \\ A(S,S')|S'|^x & \text{if } |S'| \leq |S| \end{cases} \tag{4}$$

where $A(S,S') = A(S',S)$. Detailed balance then clearly implies that the equilibrium probability of a surface $|S|$ is proportional to $|S|^x \beta^{|S|}$, consistent with eq. (3). The ability to vary x is important because by increasing x we can boost the percentage of large surfaces produced in a Monte Carlo run at any particular given subcritical $\beta < \mu^{-1} = \beta_c$.

In our runs, the probability of occurrence of a surface with $|S| = n$ is

$$P(|S| = n) = \frac{n^x \beta^n}{\sum_{l=6}^{\infty} l^x N(l) \beta^l} \tag{5}$$

Unlike the simulations reported in [DFJ84,GE87,Gl88], we do not keep one plaquette of the surface fixed. In those simulations, the fixed plaquette served to increase x effectively by one. Another increase of one compared to [SG83] was achieved in refs. [GE87,Gl88] by sweeping only over the surface rather than the whole box. (Note, however, that we do not allow the last remaining cube of a surface to vanish, so that we always have $n \geq 6$).

As has been mentioned, we have been able to perform simulations that generate very large configurations, because we use a sparse data-structure, the oct-tree. Oct-trees are a data-structure for storing information about 3-d space. Briefly stated, the oct-tree data-structure represents a cube of arbitrary size. The same amount of computer memory can represent a physically small cube as well as a large one. Part of each cube's data-structure denotes whether the cube is empty, full, or partially full. If the cube is empty or full, there is nothing else to describe. If the cube is partially full, it is divided into eight sub-cubes (figure [ ]), hence the term oct. Each of these may in turn be either empty, full, or partially full. This description is continued recursively until all partially full octs are described in terms of empty or full octs, or until some desired degree of resolution has been reached. This hierarchical representation of a volume is an oct-tree. The first oct in the tree is called the oct-root. For the purposes of our work, the term cube refers to a unit cube of the lattice (i.e. an oct of the smallest resolution). An example of a four cube volume is shown in figure [ ].

The present use of oct-trees is quite different from the typical one. The ordinary implementation starts with a single oct that represents the total working volume. The oct is divided as objects of importance are discovered in the workspace. This is carried out recursively down to whatever resolution is required. Our representation task is similar, but instead of splitting octs to get more resolution, we double the linear dimension of octs when our volume grows. The finest level of resolution is fixed at the unit cube throughout the calculation, but the working volume is not fixed. When a cube appears outside of the oct-tree, we create a new root for the tree that is large enough for the new object. The old root oct becomes one of the children of the new root oct. When an oct's eighth child is filled, the oct is marked as full and all storage previously used to store the children is released. Each parent notices when its last child has become full and executes the same procedure. This recursive process keeps the actual amount of storage in the oct-tree to a minimum. An inverse process occurs when an oct's only child is deleted. The oct is marked empty and space reserved for children is released. This is also executed recursively, as each parent notices when its last child has become empty and releases space no longer used.

Functionally, all an oct consists of is pointers to children. For application to SARS, we have augmented this with a parent pointer, a single coordinate to identify one corner of the oct in space, and a count of the number of children in the current oct. We have also augmented the oct structure so that it stores any faces that lie on the surface. This is easily done with a six-element bit map for the six possible faces on each cube.

One procedure is of special interest because it is the most heavily used and illustrates a particularly nice feature of the oct-tree in physical simulations. **oct-find** is used to find the oct at a given coordinate. Since the height of the oct tree is logarithmic with the size of the lattice, searching is very efficient. Starting at the root, the procedure compares the coordinate to the midpoint in each direction. With three comparisons, the appropriate sub-oct is located within which the x, y, z coordinate is guaranteed to lay. This process is recursively repeated until we arrive at the correct cube. As we step down through the oct tree, the linear dimension of the working volume is halved in each direction. Thus, the search time is

$$O(3\log_8(n)) = O(\log_2(n)) \tag{6}$$

- a binary search. Thus, if it takes k steps to execute **oct-find** in a $2 \times 2 \times 2$ lattice, it takes $5k$ steps to do so in a $32 \times 32 \times 32$ lattice, and only $20k$ steps in a $1,048,576 \times 1,048,576 \times 1,048,576$ lattice.

III. Monte Carlo Results and Their Analysis

We performed extensive Monte Carlo runs on a Convex C120 computer, generating surfaces consistent with the equilibrium partition function (3) with $x = 2$ and $x = 3$. Following [GE87], we chose the value $\beta = 0.56$. This is expected to be slightly below the actual critical value of the model, μ^{-1}, which for [GE87] was 0.577. It is crucial that we have $\beta < \beta_c$ to prevent the surface from growing without bound. In earlier work [SG83], a smaller value of β (0.531) was needed because of the stringent finite-size limitation. Karowski[Ka86] examined many values of β between 0.53 and 0.54.

According to eqn. (2.3), at fixed value of β the Monte Carlo-generated distribution of surface areas should peak at larger values of n as x increases. This behavior is clear from the plots of distributions from our runs of 10^9 Monte Carlo steps (MCS) for $x = 2$ and 3. Thus, runs with $x = 3$ have the advantage of sampling a relatively higher percentage of surfaces with high $|S|$. Interestingly, this is also the disadvantage of using larger x: since the mean configuration size is larger, autocorrelation is a more serious problem. We found that 20,000 MC steps between samples were needed. It is also apparent from Figs. 1 that for relatively small n (less than about 50), there are actually two distributions: there are far more surfaces with areas n that are odd multiples of 2 than even multiples (and in fact none with $|S| = 8$ or 12). This observation is related to the fact that not every value of $|S|$ is possible (e.g. only 6, 10, and 14 can occur for small configurations). This is reflected in the bimodal values in the plots of effective exponents vs. $1/n_{\min}$ discussed below.

Using the maximum likelihood method, we analyzed the distributions depicted in Figs. 1 to extract estimates for θ and μ. Application of this method to self-avoiding walks is discussed extensively by [BS85]. It was used by [GE87,Gl88] for our SARS problem. In the simplest mode, one assumes the relation (1) is strictly satisfied for $n > n_{\rm min}$. Pursuant to this assumption, one observes the "experimental" expectation values of the two quantities

$$O_1(S) = |S|\Theta(|S| - n_{\rm min}) \tag{7}$$

and

$$O_2(S) = \ln(|S|)\Theta(|S| - n_{\rm min}), \tag{8}$$

where Θ is the Heaviside unit step function. The maximum likelihood estimates of ν and θ are then obtained as solutions of the pair of equations

$$< O_1 >_{\rm obs} = < O_1 >_{\rm th} \tag{9}$$

$$< O_2 >_{\rm obs} = < O_2 >_{\rm th} \tag{10}$$

where the left-hand sides are the computed Monte Carlo expectation values, while on the right-hand sides we insert the theoretical expectation values based on eqn. (1), assumed valid for $n > n_{\rm min}$

$$< O_1 >_{th} = \frac{\sum_{n \geq n_{\rm min}}^{\infty} O_1(n) n^{-\theta} \mu^n \beta^n}{\sum_{n \geq n_{\rm min}}^{\infty} n^{-\theta} \mu^n \beta^n} \tag{11}$$

The numerical solution of this nonlinear system requires great care. For one thing, the computed Monte Carlo expectation values require summing over many terms of widely differing magnitudes. We found that to avoid roundoff and truncation difficulties, it was necessary to use all terms on the left-hand side of the equations for which simulation data were taken, and on the right-hand side, use 1000 terms and sort the terms before summing, and compute the sums in double precision. A more serious difficulty is presented by the nonlinear equations themselves. Let $F(\mu, \theta)$ be the difference between the right and left-hand sides of Equations (9) and (10). Figure xx is a plot of $\|F\|$ as a function of μ and θ. The flat "trough" running roughly north-east to south-west contains the minimum of $\|F\|$. Along this trough, large changes in (μ, θ) cause only small changes in $\|F\|$ so that the minimum is difficult to locate. (This behavior is typical of the systems of equations arising form the use of maximum likelihood for exponential families.) We carried out this calculation in double precision, using the NAG routine SNSQSE.

We obtained estimates of θ and μ for both $x = 2$ and $x = 3$, for many different values of $n_{\rm min}$. In principle, the higher $n_{\rm min}$, the closer the result should be to the correct asymptotic value. Indeed, corrections of the order of $1/n_{\min}$ can be expected, as well as possibly more dominant corrections to scaling arising from deviations from the asymptotic behavior of relation (1).

In Table 1, we report our θ and μ determinations. We see that for values of $n_{\min}$ up to 70, the determinations are reasonably consistent. For higher values of $n_{\min}$, poor statistics leads to more erratic behavior. Moreover, we see that the exponents for $n_{\min}$ an odd multiple of two may differ from those with $n_{\min}$ an even multiple. We did a weighted least squares fit of $\ln(data)$ linearized with weights $data/\sigma$, where the Fisher information matrix gives the statistical σ of each maximum likelihood data entry. Extrapolating over the range of good statistics, as a function of $1/n_{\min} = 1/18$ to $1/n_{\min} = 0$ we find, consistent with our assumptions,

$$(\mu, \theta) = (1.73, 1.495)$$

There is, of course, additional systematic uncertainty due to the unknown strength of corrections to scaling. We did not attempt to estimate these corrections, but note from [GE87] that they should not change the general behavior in terms of $1/n_{\min}$. Since we have been able to go to much larger $n_{\min}$ than previous workers, our values are presumably more nearly asymptotic.

The exponent ν was more simply estimated by a linear regression method. Figs. 4 show our Monte Carlo results for the mean square radius of gyration, $R(n)$, of surfaces with $|S| = n$. Both for $x = 2$ and $x = 3$, the log-log plots become linear rapidly, indicating that a high degree of asymptoticity has already been reached in both cases. The estimate of the asymptotic slope was also done disregarding values for $n \leq n_{\min}$ A least-squares fit gives estimates of ν of $0.504 \pm xx$ and $0.512 \pm xx$ respectively. A final extrapolation for ν in the limit $n_{\min} \to \infty$ gave: $\nu = xx$ again an average of the results for the two values of x.

IV. Concluding Remarks

The results discussed in Section III are obtained from statistics involving surfaces with areas nearly an order of magnitude larger than those considered in refs. [GE87,Gl88]. We could achieve this higher degree of asymptoticity by removing the box constraint and by considering, in particular, the distribution (2.1) with $x = 3$. Higher values of x, or β's closer to the estimated β_c would have enriched the sampling of high n, but at the price of inconveniences, such as longer correlation times. Our choice of β and of x seemed a reasonable compromise in view of our computational capabilities. Only one set of calculations have been reported that involve larger surfaces than ours[Ka86], and we seriously question the statistical significance of those results (cf. [Gl88]). In [Ka86] determination of ν was accomplished by using very large surfaces generated with β close to the β_c of 0.531 previously determined by [SG83], which is considerably lower than our estimate of 0.577 for β_c. Especially with such a small β, the sampling of very large surfaces (n near 5000) appears to us to be quite problematical.

Our estimates of ν are clearly quite consistent with the value of Glaus [GE87,Gl88] and strongly corroborate the conjecture that our self-avoiding surfaces indeed have the same exponent, $\nu = 1/2$, expected for branched polymers in 3-d. The determination of θ was subject to greater uncertainty; the value is less decisively in the universality class of branched polymers, and we feel that a definitive conclusion on this issue has unfortunately not yet been reached, even by our extensive analysis. Nonetheless, we believe our determination of θ represents an advance over [GE87,Gl88] in that we have been able to include a substantially larger range of $n_{\min}$ and, hence, could explore separate extrapolations of values that are odd and even multiples of 2. The latter series was neglected in [GE87,Gl88].

As already stressed by Glaus, an additional important indicator of the nature of SARS in the critical limit is the surface-to-volume ratio $< |S|/V >$. Our data for this ratio seem to extrapolate, as $n_{\min} \to \infty$, to a value close to 3.8. The fact that this ratio remains different from zero indicates that our surfaces enclose a region with fractal dimension not higher than $1/\nu$. The fact that the ratio is close to 4 is an indication that ramified tubular configurations with tubes of minimal size presumably dominate in the RS statistics. If each elementary cube on average gets about four plaquettes, the critical activity for each cube is a number close to 10. It is interesting to notice that the estimated critical bond fugacity for branching trees (without loops) on a hypercubic lattice is about 9.53 [GS82]. Even if a strict coincidence of the two numbers is not to be expected, it seems to us that agreement in the order of magnitude also supports the possible identification.

Previous studies based on exact enumeration [R85] and Monte Carlo [Gl86,Gl88] gave evidence for exponents (at least ν) very close to those we found in our model. In particular, Redner found ν close to 1/2 in the case of surfaces with unrestricted boundaries and topologies. We believe that this apparent, and somewhat unexpected, independence of critical behavior on the genus of the surfaces favors the idea that these surfaces are all in the universality class of branched polymers. It is indeed known [GS82] that branching trees without loops have the same critical behavior as lattice animals, for which loops are allowed. In view of the above picture of our surfaces as thinly ramified objects, the loops of lattice animals could correspond to the possibility of forming handles, and thus of changing the genus of our surfaces.

The results of this paper, particularly the strong indication that SARS realize the critical behavior of branched polymers in the scaling limit, leads to an obvious question: What are the requirements of a SARS model in order that it represents a genuine fractal surface in the scaling limit rather than a linear, even if highly ramified, object? We think that one way to achieve different critical behavior is to enrich the model by allowing a local interaction with an effect analogous to an extrinsic curvature dependence in the continuum. For example, an appropriate fugacity could be introduced to control the number of links joining plaquettes not lying in the same plane. If coplanar adjoining plaquettes are sufficiently favored over plaquettes joining at right angles, it seems likely that a more compact structure than branched polymers should appear in the simulations. Thus, one could possibly observe interesting multicritical phenomena in this generalized model near the transition between SARS behavior as the fugacity is varied. The study of such multicritical phenomena might well reveal new universality classes for the generalized model.

A model, in which an effect similar to that of the above local interaction is provided by the inclusion of Ising vacancies, has been recently discussed in ref. [MSS90].

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