On the universality class of planar self-avoiding surfaces with fixed boundary

1987 J. Phys. A: Math. Gen. 20 L105

(http://iopscience.iop.org/0305-4470/20/2/011)

J. Phys. A: Math. Gen. 20 (1987) L105-L111. Printed in the UK

LETTER TO THE EDITOR

On the universality class of planar self-avoiding surfaces with fixed boundary

U Glaus† and T L Einstein

Department of Physics and Astronomy, University of Maryland, College Park, MD 20742, USA and Surface Science Division, National Bureau of Standards, Gaithersburg, MD 20899, USA

Received 20 October 1986

Abstract. Using a modified version of a Monte Carlo algorithm proposed by Sterling and Greensite, we obtain the exponents $\theta = 1.51 \pm 0.25$ and $\nu = 0.502 \pm 0.024$ for planar self-avoiding surfaces with fixed boundary in three dimensions, consistent with the conjectured exact values for branched polymers. We show how the modifications are needed to obtain a viable distribution of surfaces.

The present letter is intended to settle a recent controversy concerning the statistical properties of self-avoiding random surfaces (SARS) with a fixed boundary in low dimensions. Such objects appear naturally in the high-temperature expansion of lattice gauge theories (Balian *et al* 1975). In three dimensions they may also elucidate some pathological interface problems where the common idealisation of neglecting overhangs is not invoked. For a comprehensive review and many further applications of random surfaces, see Froehlich (1985).

In the following, we consider self-avoiding surfaces with empty boundary on the cubic lattice Z^3. Each surface S consists of a set of pairwise different elementary plaquettes in Z^3, each of which is connected by each of its four edges to exactly one other plaquette of S. S is anchored at a fixed plaquette p_0. Self-avoiding means that each elementary bond in Z^3 occurs at most once in S. S is, however, allowed to touch at 'corners'; a site in Z^3 may be the boundary of six elementary bonds of S.

Furthermore, we require S to be planar, i.e. topologically equivalent to a sphere. We are interested in the number $N(n)$ of configurations of such surfaces that can be made out of n plaquettes and in the dependence of the radius of gyration $R(n)$ on n. Asymptotically, for large n, these are expected to behave, respectively, as

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

$$R(n) \sim n^{\nu}. \tag{1b}$$

Durhuus *et al* (1983) have actually proven that $N(n)$ is exponentially bounded and have given the estimate

$$[3(d-2)]^{1/4} \leqslant \mu \leqslant (2d-3) \qquad d \geqslant 3 \tag{2}$$

for μ, where d is the dimension of the embedding space. They also showed that μ is independent of the shape and size of the fixed boundary ∂S of S.

† Present address: Department of Physics, Clarkson University, Potsdam, NY 13676, USA.

0305-4470/87/020105+07$02.50

The controversy centres around the values of the 'critical exponents' θ and ν. In the absence of a self-avoiding constraint on the surfaces, Durhuus *et al* (1984) have given strong arguments that the corresponding model (PRS model) collapses into non-interacting branched polymers in all dimensions, implying $\theta = \frac{5}{2}$ and $\nu = \frac{1}{4}$. These values were also obtained by Drouffe *et al* (1980) from a mean-field theory for SARS, expected to become exact as the dimensionality d goes to infinity. By a real space renormalisation group calculation, Maritan and Stella (1984) obtained values for ν in $3 \leq d \leq 8$ for a SARS model that were considerably lower than the ones expected for branched polymers. A Flory argument for ν agreed roughly with their RG calculation. By a Monte Carlo calculation to be described below, Sterling and Greensite (1983) obtained $\theta = 0.5 \pm 0.05$ for SARS with fixed boundary in three dimensions, very different from the conjectured exact values $\theta = \frac{3}{2}$, $\nu = \frac{1}{2}$ for branched polymers (Parisi and Sourlas 1981). Estimates close to $\theta = \frac{3}{2}$, $\nu = \frac{1}{2}$ were obtained by Glaus (1986) with Monte Carlo and Redner (1985, 1986) with exact enumeration for a SARS model with free boundary in three dimensions. Baumann and Berg (1985), using the Monte Carlo method, found $\nu = \frac{1}{4}$, $\theta = \frac{11}{4}$ for a PRS model without spikes in $d = 4$. They concluded that this model does not collapse into non-interacting branched polymers.

Sterling and Greensite (1983, hereafter denoted by SG) have proposed an efficient Monte Carlo procedure to generate self-avoiding surfaces with a fixed boundary. Their algorithm produces SARS with an empty boundary in a grand canonical ensemble at a fixed plaquette activity β. Each n-plaquette SARS has the probability $\beta^n/\Xi(\beta)$ of occurring in the ensemble, where

$$\Xi(\beta) = \sum_S \beta^{|S|} = M \sum_{n=6}^{\infty} N(n)\beta^n \tag{3}$$

is the grand partition function. Here, $|S|$ denotes the number of plaquettes in S and the proportionality constant M is equal to the number of sites stored in the computer, because $N(n)$ counts only the number of different configurations modulo lattice translations. The SG algorithm has been used extensively for various surface models (Schrader 1985, Karowski and Thun 1985). Berg and Billoire (1983) and Glaus (1986) use a data structure, which only stores the surface in the computer and is therefore especially useful in high dimensions. Recently, a MC simulation was performed on a triangulated version of self-avoiding surface model (Kantor *et al* 1986).

Given a surface S, the SG method consists of sweeping sequentially through the sites dual to the cubes of Z^3. Each site is checked to see whether the original lattice cube C has one or more of its faces belonging to S. If this is the case, an attempt is made to produce a new surface S' obtained from S by simultaneously reversing the occupied/empty status of all six plaquettes bounding C. S' is accepted if it is self-avoiding and planar and passes the standard Metropolis test that produces surfaces according to the equilibrium distribution of equation (3).

We have simulated the fixed-boundary SARS model in three dimensions using a modified version of the SG algorithm. The modifications, the motivations for which will be discussed shortly, are as follows.

(i) One plaquette p_0 is kept fixed; the two cubes having p_0 as one of their faces are never visited during the simulation.

(ii) Instead of sweeping sequentially through all the cubes of the lattice, the cubes that have faces belonging to S are accessed at random.

(iii) The simulation is actually not performed in Z^3 but in a large cube L of size $(20 \times 20 \times 20)$. In order to eliminate any finite-size effect we used 'pseudoperiodic'

boundary conditions. If the surface S leaves L, it is periodically continued into L. At each step, we keep track of the maximal extension of S in all three coordinate directions. The activity β is then chosen such that all surfaces created by the simulation fit into the cube L. In this way, all finite-size effects are eliminated.

With these modifications, it follows that the transition probabilities for our Monte Carlo algorithm are

$$W(S\to S')=\begin{cases}\dfrac{1}{C(S)}\,p(\beta, S\to S')\chi_{\mathrm{SA}}(S') & S'\sim S\\ \dfrac{N(S)}{C(S)}\,(1-p(\beta, S\to S')) & S'=S.\end{cases} \tag{4}$$

Here, $C(S)$ denotes the number of cubes in L that have faces belonging to S and do not contain p_0, $\chi_{\mathrm{SA}}(S')$ is the characteristic function for S' to be self-avoiding and planar, and $S'\sim S$ means that S' can be obtained from S by reversing the occupied/empty status of all plaquettes forming the boundary of a single elementary cube. Furthermore,

$$N(S)=\sum_{S':S'\sim S}(1-\chi_{\mathrm{SA}}(S')) \tag{5}$$

and $p(\beta, S\to S')$ is determined by the equations of detailed balance for the modified grand canonical ensemble:

$$\tilde{\Xi}(\beta)=\sum_{S:p_0\in S}C(S)\beta^{|S|}. \tag{6}$$

The probability $P(S)$ for a surface S to occur in the ensemble now satisfies the equation

$$P(S)=\frac{C(S)\beta^{|S|}}{\Xi(\beta)}. \tag{7}$$

From equations (4) and (7) and the detailed balance condition

$$W(S\to S')P(S)=W(S'\to S)P(S') \tag{8}$$

we obtain

$$p(\beta, S\to S')=\begin{cases}1 & \text{for } |S'|\leqslant|S|\\ \beta^{|S'|-|S|} & \text{otherwise.}\end{cases} \tag{9}$$

We next explain the reason for introducing these modifications to the original SG algorithm. We first note that, since $C(S)$ denotes the number minus two of cubes that have plaquettes belonging to S, it follows that

$$C(S)\sim|S|. \tag{10}$$

Therefore, the probability for a surface with n plaquettes to occur during the Monte Carlo simulation is

$$P(|S|=n)\sim n^2N(n)\beta^n\left(\sum_{m=6}^{\infty}m^2N(m)\beta^m\right)^{-1} \tag{11}$$

where one factor of n in (11) comes from $C(S)$ and the other results from keeping p_0 fixed, because $N(n)$ counts different configurations modulo lattice translations. Using (1*a*), we see that

$$P(|S|=n)\sim n^{-\theta+2}(\beta\mu)^n \tag{12}$$

which, as a function of n, has a maximum at

$$n(\beta) \sim (\theta - 2)/(\ln(\mu\beta)) \tag{13}$$

provided that

$$\theta - 2 < 0. \tag{14}$$

In other words, if inequality (14) holds, the algorithm will generate mainly surfaces of size given by equation (13). Moreover, as $\beta \to \mu^{-1}$ this typical size diverges and the scaling region becomes accessible.

We tested the validity of (14) by measuring the distribution of surface sizes during the simulation. It did peak at $n(\beta) > 0$, consistent with (13).

We performed a main run at $\beta = 0.56$ with a total of 10^8 MC steps requiring 75 minutes of CPU time on the National Bureau of Standards Cyber 205. After every 2×10^3 such MC steps, the number of plaquettes $|S|$, the radius of gyration R_S and the volume V_S enclosed by S were measured. R_S is defined to be the root-mean-square displacement of the midpoints of all plaquettes belonging to S. The analysis of the statistical and systematic errors is based on the methods described in detail in the Monte Carlo study of the self-avoiding walk in two dimensions by Berretti and Sokal (1985). The autocorrelation time τ for the observable $|S|$ is estimated to be

$$\tau = (5.6 \pm 0.8) \times 10^3 \text{ MC steps} \tag{15}$$

and the mean number of plaquettes

$$\langle |S| \rangle = 50.26 \pm 0.40. \tag{16}$$

In order to determine θ and μ, we assume that for all $n \geqslant n_{\min}$ we have

$$N(n) = a_0 \mu^n n^{-\theta}(1 + a_1/n) \tag{17}$$

i.e. that the correction-to-scaling exponent is equal to unity. Here, $n_{\min}$ is an adjustable parameter that can be raised to diminish corrections to scaling. For an observable A that depends only on the number of plaquettes, we can then define the 'theoretical average'

$$\langle A \rangle_{\text{th}} = \left(\sum_{n=6}^{\infty} A(n) n N(n) \beta^n \right) \left(\sum_{n=6}^{\infty} n N(n) \beta^n \right)^{-1}. \tag{18}$$

On the other hand, using the Monte Carlo data, we obtain the observed average

$$\langle A \rangle_{\text{obs}} = \left(\sum_{t=1}^{T} A(|S_t|) \chi(|S_t| - n_{\min})/C(S_t) \right) \left(\sum_{t=1}^{T} \chi(|S_t| - n_{\min})/C(S_t) \right)^{-1}. \tag{19}$$

Here t labels the sampled surfaces and T denotes the sample size, which is $T = 5 \times 10^4$. $\chi(m)$ is the characteristic function for m to be $\geqslant 0$. θ and μ are obtained by the maximum likelihood method which is equivalent to solving $\langle A \rangle_{\text{th}} = \langle A \rangle_{\text{obs}}$ for $A = |S|$ and $A = \ln |S|$. In figure 1, θ is plotted against $(n_{\min})^{-1}$ for $a_1 = 0.0$, 0.5, 1.0, 1.5, 2.0, where for decreasing a_1 the curves are moving towards the top of the figure. We obtain

$$\theta = 1.51 \pm 0.1 \pm 0.15 \tag{20}$$

$$\mu = 1.733 \pm 0.005 \pm 0.006. \tag{21}$$

The leftmost numbers on the right-hand sides of (20) and (21) denote our estimates, obtained by extrapolating $\theta(n_{\min}, a_1)$ and $\mu(n_{\min}, a_1)$, respectively, to $(n_{\min})^{-1} = 0$ as

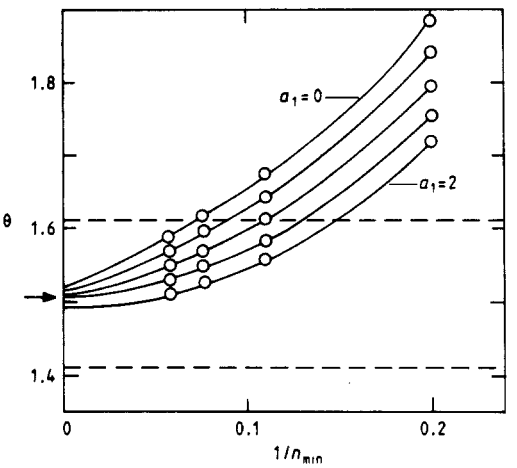

Figure 1. θ for various values of a_1 against $(n_{min})^{-1}$. Circles denote values obtained as explained in the text. Lines are guides to the eye. The arrow denotes the central estimate and broken lines indicate the estimate for systematic error. The top and bottom curves are labelled by their value of a_1.

depicted in figure 1 for θ. Our first error bar accounts for the corrections to scaling. The second error bar denotes the statistical error and is twice the variance for $n_{min} = 13$ obtained from the explicitly known covariance matrix for μ and θ, multiplied by $(2\tau)^{1/2}$ (Berretti and Sokal 1985).

The estimate for ν was obtained by minimising

$$\sum_{t=1}^{T} \left(\ln R_{S_t} - \nu \ln(|S_t| + b_1) + b_0 \right)^2 \chi(|S_t| - n_{min}) \tag{22}$$

with respect to ν and b_0 for various b_1 and n_{min}. We obtain

$$\nu = 0.502 \pm 0.012 \pm 0.012 \tag{23}$$

where the statistical error here is twice the variance for $n_{min} = 25$ obtained from least-squares theory times $(2\tau)^{1/2}$. In table 1, we list the averages of $|S|$, V_S and $|S|/V_S$, along with the statistical error bars for $|S|/V_S$ for various n_{min}, where surfaces with $|S| < n_{min}$ were discarded in calculating the averages.

Our values for θ and ν are consistent with the exact values $\theta = \frac{3}{2}$, $\nu = \frac{1}{2}$ conjectured by Parisi and Sourlas (1981) for branched polymers in three dimensions. Moreover,

Table 1. Some observed expectation values for various n_{min} together with the statistical error for $\langle |S|/V_S \rangle$. N_S denotes the number of surfaces with $|S| \geq n_{min}$.

n_{min}	N_S	$\langle |S| \rangle$	$\langle V_S \rangle$	$\langle |S|/V_S \rangle$
5	50 000	50.06	13.50	4.097 ± 0.008
9	47 188	52.68	14.25	3.984 ± 0.005
13	44 298	55.47	15.04	3.917 ± 0.005
17	41 150	58.62	15.96	3.864 ± 0.005
21	37 844	62.14	16.99	3.818 ± 0.004

from the small error for $|S|/V_S$ in table 1, it follows that the volume enclosed by S is typically proportional to $|S|$, indicating that typical surfaces have a treelike structure.

Our estimate for μ is consistent with the known crude but rigorous bounds (2). It is barely consistent with the estimate $\mu = 1.701 \pm 0.005$ of SG. More crucially, the result

$$\theta = 0.5 \pm 0.05 \tag{24}$$

obtained by SG is distinctly different from our estimate (20). From (3), it can be seen that the probability in the SG algorithm to produce an n-plaquette surface is

$$P(|S| = n) = \frac{N(n)\beta^n}{\Xi(\beta)} \sim \frac{n^{-\theta}(\mu\beta)^n}{\Xi(\beta)}. \tag{25}$$

Since we found $\theta > 0$, it follows that in this algorithm small surfaces are most probable for $\beta < \mu^{-1}$. Moreover, once $\beta > \mu^{-1}$, $P(|S| = n)$ will have a minimum as a function of n at

$$n^*(\beta) = \theta/\ln(\mu\beta). \tag{26}$$

Since $\Xi(\beta) = \infty$ for $\beta > \mu^{-1}$ in the thermodynamic limit, we would have $P(|S| = n^*) = 0$; for finite system size, $P(|S| = n^*)$ will instead be a very small number. Starting with a single cube, there is very little chance of producing a surface with $|S| > n^*$, i.e. to enter the regime where $|S|$ diverges. Due to this 'lack of ergodicity' one is therefore led to believe that even for $\beta > \mu^{-1}$, $\langle |S| \rangle$ is still finite because only surfaces with $|S| < n^*$ are produced. This accounts for the β dependence of $\langle |S| \rangle^{-1}$ shown in figure 2 of SG, because our estimate for μ^{-1} is well within the region in which their $\langle |S| \rangle$ is still finite. Moreover, SG run their MC algorithm at various temperatures β and extract their estimates for θ and μ from the β dependence of $\langle |S| \rangle$, which according to (1a) should be

$$\langle |S| \rangle = \left(\sum_{n=6}^{\infty} n^{-\theta+1}(\mu\beta)^n \right) \left(\sum_{n=6}^{\infty} n^{-\theta}(\mu\beta)^n \right)^{-1}. \tag{27}$$

Replacing these sums by integrals and extending the lower limit of the integrals to zero, one finds

$$\langle |S| \rangle \sim (1-\theta)/(1-\mu\beta) \tag{28}$$

which is, of course, only valid for $\theta < 1$. Our modified SG algorithm avoids the two problems of 'lack of ergodicity' for $\beta > \mu^{-1}$ and implicit assumptions of the value of θ. In obtaining $\theta = 1.51$, we clearly find that the assumption $\theta < 1$ is not valid, which accounts for the dramatic difference between our estimate (20) and that of SG given by equation (24).

Baumann and Berg (1985) noted the problems encountered in the SG method of extracting θ from their Monte Carlo data. Their way should, in principle, yield correct values for the exponent θ. However, they obtained θ by using a previously determined value for μ. It is obvious that θ depends very sensitively on μ, and these two quantities should in fact be estimated simultaneously. Our results indicate that, by eliminating the spikes from the PRS model, one cannot prevent the resulting surfaces from collapsing into non-interacting branched polymers in the continuum limit and are therefore contradictory to Baumann and Berg (1985). Regarding Maritan and Stella (1984), it is well known that RG calculations are ill controlled and should not be taken at face value and the Flory theory for branched polymers (Lubensky and Isaacson 1979) is actually more appropriate to describe SARS models such as those we have considered.

The important point then is that one has to be careful in devising a Monte Carlo algorithm for a grand canonical ensemble of a lattice geometrical problem. For bond problems, one is usually guided by the $n \to 0$ limit of ferromagnetic lattice spin systems (de Gennes 1972, Lubensky and Isaacson 1979) that provide a direct link to critical phenomena. In problems involving elementary plaquettes, the relation to lattice gauge theories is much less clear, and the correct field theories for these surface models have yet to be found. Our results, especially when combined with Glaus (1986), indicate that presumably all lattice surface models with short-range self-avoiding interactions will in the continuum limit collapse into branched polymers, for which a field theoretic description has been proposed by Lubensky and Isaacson (1979).

We thank Jacques Amar for assistance in using the NBS Cyber 205. This work was supported by the Department of Energy under Grant No DE-FG 05-84ER45071.

References

Balian R, Drouffe J M and Itzykson C 1975 *Phys. Rev.* D **11** 2104
Baumann B and Berg B 1985 *Phys. Lett.* **164B** 131
Berg B and Billoire A 1983 *Phys. Lett.* **130B** 415
Berretti A and Sokal A D 1985 *J. Stat. Phys.* **40** 483
de Gennes P G 1972 *Phys. Lett.* **38A** 339
Drouffe J M, Parisi G and Sourlas N 1980 *Nucl. Phys.* B **161** 397
Durhuus B, Froehlich J and Jonsson T 1983 *Nucl. Phys.* B **225** 185
—— 1984 *Nucl. Phys.* B **240** 453
Froehlich J 1985 *Applications of Field Theory to Statistical Mechanics* (*Lectures Notes in Physics* **216**) ed L Garrido (Berlin: Springer)
Glaus U 1986 *Phys. Rev. Lett.* **56** 1996
Kantor Y, Kardar M and Nelson D R 1986 *Phys. Rev. Lett.* **57** 791
Karowski M and Thun H J 1985 *Phys. Rev. Lett.* **54** 2556
Lubensky T C and Isaacson J979 *Phys. Rev.* A **20** 2130
Maritan A and Stella A 1984 *Phys. Rev. Lett.* **53** 123
Parisi G and Sourlas N 1981 *Phys. Rev. Lett.* **46** 871
Redner S 1985 *J. Phys. A: Math. Gen.* **18** L723
—— 1986 Private communication
Schrader R 1985 *J. Stat. Phys.* **40** 533
Sterling T and Greensite J 1983 *Phys. Lett.* **121B** 345