Crossover Between Weakly and Strongly Self-avoiding Random Surfaces

C.F. Baillie
Physics Dept.
University of Colorado
Boulder, CO 80309
USA

and

D.A. Johnston
Dept. of Mathematics
Heriot-Watt University
Riccarton
Edinburgh, EH14 4AS
Scotland

October 29, 2021

Abstract

We investigate the crossover between weak and strong self-avoidance in a simulation of random surfaces with extrinsic curvature. We consider both dynamically triangulated and rigid surfaces with the two possible discretizations of the extrinsic curvature term.

Submitted to Phys Lett B.
In recent papers we have investigated the limits of weak \(^1\) and strong \(^2\) self-avoidance in both fixed and dynamically triangulated random surfaces. We examined the behaviour of a gaussian plus extrinsic curvature action of the form

\[
\sum_{T} \int \prod_{i=1}^{N-1} dX_i^\mu \exp\left(-\left(S_g + \lambda S_{a,e}\right)\right),
\]

(1)

where the gaussian action \(S_g\) is a straightforward discretization of the Polyakov string action \(^3\)

\[
S_g = \frac{1}{2} \sum_{<ij>} (X_i^\mu - X_j^\mu)^2.
\]

(2)

and the alternative discretizations of the extrinsic curvature term, usually subscripted “area” and “edge” respectively can be written as

\[
S_a = \sum_i \frac{1}{\Omega_i} \left( \sum_{j(i)} (X_i^\mu - X_j^\mu) \right)^2
\]

(3)

for the area term and

\[
S_e = \sum_{\Delta, \hat{\Delta}} \left( 1 - \hat{n}_{\Delta} \cdot \hat{n}_{\Delta} \right)
\]

(4)

for the edge term. The sum over triangulations, which in effect makes the surfaces dynamical, is omitted in the fixed mesh simulations. At low \(\lambda\) surfaces are in a crumpled phase and at large \(\lambda\) in a smooth phase, with a crumpling transition occurring at some finite \(\lambda\).

An action of the form equ.1 was originally suggested both in the context of QCD strings and as a potential action for real surfaces such as cell membranes \(^4\). It has been the subject of considerable interest as a candidate discretized string action \(^5\), because it appears that \(S_g + S_e\) may have a crumpling transition at which the string tension scales so as to give a non-trivial continuum theory \(^6\). This work has been done without self-avoidance as it is not relevant from the string theory point of view, at least for purely bosonic models. There has been parallel work in solid state physics on realistic surface models which are strongly self-avoiding \(^7\), to date mostly of fixed (termed “polymerized”) mesh surfaces. Self-avoidance can be incorporated into such simulations by surrounding each point on the discretized mesh with spheres of diameter \(\sigma\) and linking them with tethers that cannot extend beyond some given length \(l\). If \(l < \sqrt{3} \sigma\) a sphere, and hence the surface itself, cannot be threaded through three other spheres and the surface is said to be strongly self-avoiding - even distant portions of the surface in the intrinsic metric cannot intersect. If \(l \geq \sqrt{3} \sigma\) intersections are possible, but there is still a local excluded volume effect due to the spheres, and the surface is said to be weakly self-avoiding. It is usually more convenient from the computational point of view to divide the embedding space into boxes and ensure single occupancy, rather than putting in the spheres explicitly. The current state of opinion in the solid state physics community, after some initial confusion, is that fixed mesh surfaces with strong self-avoidance do not display crumpling \(^8\). Our work in \(^2\) is in agreement with this, finding that the peak in the specific heat that signals the crumpling transition is suppressed on fixed meshes by strong self-avoidance. There has been less work on dynamical surfaces with strong self-avoidance, but \(^9\) and the independent work of Kroll and Gompper in \(^8\) are in broad agreement, finding a branched-polymere phase at low \(\lambda\) rather than a crumpled phase and a smoother phase at large \(\lambda\). It is currently unclear whether there is a bona fide crumpling transition here or whether the smooth phase is simply a finite size effect. In addition \(^9\) claimed to find a crumpled phase for a strongly self-avoiding dynamical surface at zero \(\lambda\), but their numerical results are, in fact, compatible with those for a branched polymer. The only work on weak self-avoidance has been that in \(^8\), where we found that weak self-avoidance had little effect on the crumpling transition.

We might expect that shortening the lengths of the tethers would allow us to see the change from this weak behaviour to the qualitatively different strong behaviour as \(l\) passed through \(\sqrt{3} \sigma\). In this paper we report on the crossover, simulating sphere diameter \(\sigma = 0.25\) and tether lengths of \(0.4, 0.433, 0.5, 0.75, 1.0, 1.5\) and \(2.0\) \((l \leq 0.433\) is strong\) with both the area and edge extrinsic curvature terms and on fixed and

\(^1\)The action \(S_g + S_a\) appears to be afflicted with lattice artifacts \(^8\).
dynamical surfaces. As our aim is to see the qualitative features rather than obtaining high numerical accuracy the bulk of the simulations are carried out on modestly sized surfaces of 72 nodes, but we also simulate surfaces of 314 nodes for the case of the edge action, which is most interesting from the point of view of continuum string theory, with strong self-avoidance in order to compare the results with earlier extensive simulations without self-avoidance \[{1}\]. Again for comparison with earlier work we simulate surfaces of spherical topology. We discuss firstly the edge action on both fixed and dynamical meshes in some detail, followed by a more cursory examination of the area action results which are less interesting from the continuum theory point of view. For further details on the computational aspects of this work, see \[{2}\].

If the simulations of the solid state physicists are to be believed there should be no crumpling transition observable for strongly self-avoiding surfaces with the edge action on fixed meshes. As the tether length is relaxed to give weak self-avoidance we would expect to see the re-emergence of the crumpling transition between a low lambda crumpled phase and a large lambda smooth phase. The crossover between the two types of behaviour might be expected to occur in the region of the maximum tether length for strong self-avoidance, \(l = 0.433\). These expectations are confirmed by the results displayed in Fig. 1 for the specific heat, which is defined as

\[
C_{a,e} = \frac{\lambda^2}{N}\left( <S_{a,e}^2> - <S_{a,e}>^2 \right),
\]

(5)

for the area and edge discretizations respectively, and in Fig. 2 for the gyration radius

\[
X^2 = \frac{1}{9N(N-1)} \sum_{ij} (X_i - X_j)^2 q_i q_j.
\]

(6)

We can see from Fig. 1 that the peak in the specific heat that signals the crumpling transition is gradually suppressed as we shorten the tethers. There is no sign of a sharp change in behaviour (the results for \(l = 0.5\) are very similar to those for \(l = 0.433\), for instance) though it is possible that the changeover might be sharper on large meshes. The suppression is also evident in Fig. 2 where we see that the increase in the gyration radius that signals the transition gradually vanishes as the tether lengths are shortened. We can get some idea of asymmetries in the configuration of the surface by looking at the individual components of the moment of inertia tensor

\[
M_{\mu\nu} = \frac{1}{N^2} \sum_i \sum_j (X_i^\mu - X_j^\mu) (X_i^\nu - X_j^\nu)
\]

and in this case we find that they remain essentially equal in all the phases, indicating rough spherical symmetry. Perhaps the best way to get a qualitative idea of the surfaces’ behaviour is to look at representative “snapshots” of the surfaces rendered in three dimensional space. Previous work has shown that without self-avoidance the surfaces look genuinely crumpled at low lambda and smooth at large lambda. The behaviour of the weakly self-avoiding surfaces is similar to this: in Fig. 3 we render a 72 node weakly self-avoiding surface with \(\lambda = 0\) which is obviously crumpled, and in Fig. 4 a weakly self-avoiding surface with \(\lambda = 3\) (well into the smooth phase). As we pass over to strong self-avoidance the typical surface configurations become similar to Fig. 5 for both large and small \(\lambda\). The surfaces now appear to stay in a “knobbly” or crinkled phase, whatever the value of \(\lambda\), and the transition is lost.

The behaviour of the edge action with strong self-avoidance on a dynamical mesh is radically different. As the self-avoidance becomes stronger the peak in the specific heat, while suppressed, does not vanish entirely as can be seen in Fig. 6. The results for the gyration radius are at first sight rather bizarre, as it crosses over from an increase signaling uncrumpling for weak self-avoidance, to a decrease at the phase transition for strong self-avoidance, even though the large \(\lambda\) phase is still smooth. We have plotted this in Fig. 7. Examining the eigenvalues of the moment of inertia tensor and snapshots of 72 node surfaces \[{2}\] suggested this was the result of a low \(\lambda\) branched polymer phase. A surface in this phase has two small and one larger eigenvalues of the moment of inertia tensor, giving a larger \(X^2\) than for a crumpled phase, thus explaining the apparently anomalous results of Fig. 7. The crossover between weak and strong behaviour is, as for the rigid surfaces, rather smooth with no obvious signs of a sudden change at \(l = 0.433\). We can obtain further confirmation of the branched polymer like nature of the low \(\lambda\) phase by looking at snapshots of the larger 314 node surfaces we simulated. In Fig. 8 we show a strongly
self-avoiding surface with $\lambda = 0.5$ which clearly displays the branching tendency of the surface. This persists up to the transition point, signaled by the peak in the specific heat, above which the surfaces appear largely smooth.

The area discretization would appear to be of less interest as a potential candidate for a continuum theory because of the problems with lattice artifacts alluded to earlier [6]. We have, however, simulated this too for completeness, finding that the specific heat, which displays a bump rather than a sharp peak, is largely unchanged by increasing the strength of the self-avoidance and that the increase in $X_2$ with $\lambda$ is suppressed as the self-avoidance becomes stronger on both fixed and dynamical meshes.

We can summarize our results for the edge discretization as follows:

- The crossover from weakly to strongly self-avoiding behaviour appears to be rather smooth.
- On strongly self-avoiding fixed meshes snapshots suggest that only a uniform “knobbly” phase remains.
- On strongly self-avoiding dynamical meshes there is a low $\lambda$ branched polymer phase and a large $\lambda$ smooth phase.

It would thus appear that strong self-avoidance has a radically different effect on fixed meshes, which might be considered models of polymerized surfaces, and dynamical meshes, which might be considered models of fluid surfaces. It would be interesting to conduct simulations of larger surfaces at higher statistics to see if the qualitative picture for the various phases on both fixed and dynamical meshes suggested by the current work is supported by firmer numerical evidence and to compare more closely with the solid state physics simulations which have largely been with surfaces of planar topology.

This work was supported in part by NATO collaborative research grant CRG910091. CFB is supported by DOE under contract DE-AC02-86ER40253 and by AFOSR Grant AFOSR-89-0422. The computations were performed on the TC2000 Butterfly and the Sequent Symmetry at Argonne National Laboratory, the GP1000 Butterfly at Michigan State University, and the Myrias SPS-2 at the University of Colorado. We would like to thank R.D. Williams for help in developing initial versions of the dynamical mesh code.
References

[1] C. F. Baillie and D. A. Johnston, Phys. Lett. B273 (1991) 380.

[2] C. F. Baillie and D. A. Johnston, Phys. Lett. B283 (1992) 55.

[3] A. M. Polyakov, Phys. Lett. B103 (1981) 207.

[4] A. Polyakov, Nucl. Phys. B268 (1986) 406;
   H. Kleinert, Phys. Lett. B174 (1986) 335;
   W. Helfrich, J. Phys. 46 (1985) 1263.

[5] S. Catterall, Phys. Lett. B220 (1989) 207;
   C. F. Baillie, D. A. Johnston and R. D. Williams, Nucl. Phys. B335 (1990) 469;
   R. Renken and J. Kogut, Nucl. Phys. B354 (1991) 328;
   S. Catterall, Phys. Lett. B243 (1990) 121;
   C. F. Baillie, D. A. Johnston, S. M. Catterall and R. D. Williams, Nucl. Phys. B348 (1991) 543;
   J. Ambjorn, J. Jurkiewicz, S. Varsted, A. Irback and B. Petersson, Phys. Lett. B275 (1992) 295;
   J. Ambjorn, J. Jurkiewicz, S. Varsted, A. Irback and B. Petersson, Nucl. Phys. B (Proc. Suppl.) 25A 182.

[6] R. G. Harnish and J. F. Wheater, Nucl. Phys. B350 (1991) 861.

[7] Y. Kantor, M. Kardar and D. R. Nelson, Phys. Rev. Lett. 57 (1986) 791, Phys. Rev. A35 (1987) 3056;
   F. F. Abraham, W. E. Rudge and M. Plischke, Phys. Rev. Lett. 62 (1989) 1757;
   F. F. Abraham and D. R. Nelson, J. Phys. France 51 (1990) 2653;
   Y. Kantor and D. R. Nelson, Phys. Rev. Lett. 58 (1987) 2774, Phys. Rev. A36 (1987) 4020;
   M. Plischke and D. Boal, Phys. Rev. A38 (1988) 4943;
   D. Boal, E. Levinson, D. Liu and M. Plischke, Phys. Rev. A40 (1989) 3292;
   J-S. Ho and A. Baumgartner, Phys. Rev. Lett. 63 (1989) 1324.

[8] D. M. Kroll and G. Gompper, “The Conformation of Fluid Membranes: Monte Carlo Simulations”,
   Minneapolis preprint 1992.

[9] J-S. Ho and A. Baumgartner, Europhys. Lett. 12 (1990) 295.

Figure Captions

Fig. 1. The specific heat $C_e$ versus $\lambda$ on a fixed mesh.

Fig. 2. The gyration radius $X_2$ versus $\lambda$ for the edge curvature on a fixed mesh.

Fig. 3. Weakly ($l = 2$) self-avoiding 72-node fixed surface with $\lambda = 0$.

Fig. 4. Weakly ($l = 2$) self-avoiding 72-node fixed surface with $\lambda = 3$.

Fig. 5. Strongly ($l = 0.433$) self-avoiding 72-node fixed surface with $\lambda = 3$.

Fig. 6. The specific heat $C_e$ versus $\lambda$ on a dynamical mesh.

Fig. 7. The gyration radius $X_2$ versus $\lambda$ for the edge curvature on a dynamical mesh.

Fig. 8. Strongly ($l = 0.433$) self-avoiding 314-node dynamical surface with $\lambda = 0.5$. 