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On the universality classes of growing self-avoiding walks and trails

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Abstract. It is shown that within a two-parameter 3×3 cell to bond position space renormalisation group theory, growing self-avoiding walks and growing self-avoiding trails on the square lattice are in the same universality class.

1. Introduction

The success of self-avoiding walks (SAW) as a model for linear polymers stimulated several authors [1, 2] to study kinetic versions of SAW. In the ordinary SAW on a lattice of coordination number q, the walker chooses the next site from among the nearest-neighbour sites (with the exception of the site just visited). There are thus $(q-1)$ sites to choose from and the $(q-1)$ choices are taken as equally likely. If the walker happens to step onto a site which has been visited previously, the walk terminates. In the growing version of SAW (GSAW) the walker restricts its choice to those nearest-neighbour sites which have never been visited. The growing self-avoiding walk terminates when it arrives at a site which has no unvisited nearest neighbours. In this way the walker checks its environment and tries to avoid early termination. It was also suggested that these models could describe the Θ-point behaviour of linear polymers [1], which is governed by different exponents from those of the usual SAW. A more detailed study of this model [3] shows that the different definition of the one-step probabilities does not change the critical behaviour but only shifts the asymptotic scaling regime to much larger N values, where N is the number of steps in the walk. Recently Lyklema introduced a kinetic version of the self-avoiding trail problem (SAT) [4] which he called growing self-avoiding trail (GSAT). In its usual form the SAT is constructed similarly to the SAW, except that each bond rather than each site can be occupied only once. A new bond is attached to the chain with equal probability for all bonds. If the chosen bond is occupied, the walk is terminated. From this construction one expects the same critical exponents as for the SAW, because the paths generated in this way are the same, as has been shown recently [5-7]. In the GSAT, we have the same rules as for the SAT except that we write the one-step transition probability p_i as

$$p_i = 1/(\text{number of free bonds}). \tag{1}$$

Since the GSAT can only terminate at the origin, in contrast to all other walks in the SAW universality class, Lyklema expects that it has different asymptotic behaviour from

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the usual SAW. In fact his Monte Carlo study of this model on the square lattice with N up to 700 yields an estimate for the radius of gyration exponent $\nu = 0.54$, in contrast to the usual SAW value $\nu = \frac{3}{4}$ [8]. A similar study on the simple cubic lattice yields values of ν very close to the Gaussian value $\nu = \frac{1}{2}$. He therefore conjectures that the upper critical dimension for GSAT is 3 and suggests that it models the Θ-point in linear polymers. In this paper we study the universality classes of GSAW and GSAT using a generalisation of the two-parameter renormalisation group method used by Malakis [5] to study the SAW and SAT problems. Malakis studied the SAW problem on the Manhattan square lattice using a two-parameter renormalisation group. Similarly, the SAT problem was studied on the underlying Manhattan lattice or L lattice. Using the fact that the Manhattan square lattice is the covering graph for the L lattice, he concluded that SAW and SAT are in the same universality class. Here we generalise this method to study the universality classes of GSAW and GSAT on Manhattan square and L lattices respectively. From this we conclude that GSAW and GSAT on the square lattice are in fact in the same universality class, within a two-parameter 3×3 renormalisation group.

2. GSAW on Manhattan square lattice

The SAW problem on a Manhattan square lattice was first studied by Kasteleyn [9]. In this study, the enumeration of the total number of Hamilton or compact walks on a two-dimensional square Manhattan lattice was solved exactly. A Hamilton walk is a SAW which visits every site of the lattice. The Manhattan square lattice is shown in figure 1(a). A more general SAW that contains the oriented and non-oriented lattice problem as special cases has been studied by Prentis [10] using a two-parameter renormalisation group method. To accomplish this renormalisation, we construct cells with b bonds on a side, where b must be an odd integer. The renormalised bond associated with a given cell assumes a direction that is determined by a 'majority rule'. This rule is most easily illustrated by the example in figure 2 for a $b = 3$ cell. This lattice rescaling and bond orientation renormalisation result in a renormalised lattice that preserves the square symmetry and the Manhattan orientation of the original lattice. To study the GSAW problem on this lattice, consider the $b = 3$ cell in figure 2. We enumerate the set of all GSAW that begin at any of the three vertices at the bottom of the cell and exit from the cell by way of the top edge, irrespective of the lattice orientation at each step. A simple average over the three initial starting points is then

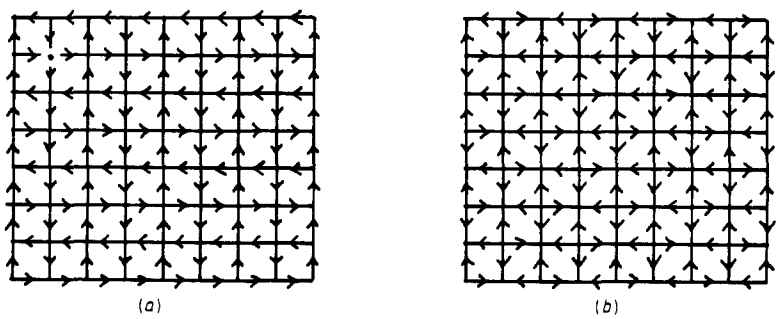

Figure 1. (a) Manhattan lattice, (b) L lattice.

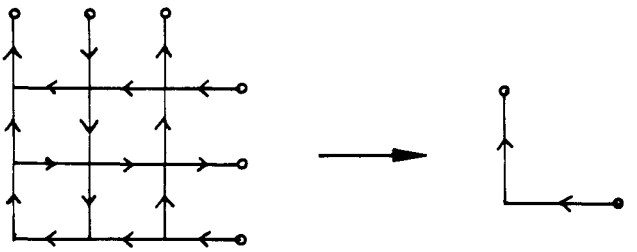

Figure 2. Finite Manhattan lattice ($b=3$ cell) renormalisation. The lattice site rescaling and the bond orientation renormalisation are shown.

performed. Each step of the walk is associated with a fugacity $k/$(number of free sites). The orientation of the lattice is taken into account by introducing an extra parameter $h \leqslant 1$. The number of free sites at each step can be either 3, 2 or 1. Suppose that at a given site there are N_e ways of leaving the site obeying the lattice orientation, N_g ways of leaving which violate the lattice orientation and $S = N_e + N_g$ free sites. In case both N_e and N_g are non-zero, we choose the weight for the next step as follows. The orientational weight for a step which obeys the lattice direction is $[1+(N_g/N_e)h] \times (k/S)$ while the weight for opposing the lattice direction is $[1-h](k/S)$. In the case when either N_g or N_e is equal to zero, then the weight for the next step is always taken as (k/S), irrespective of the lattice orientation. This choice ensures that $h=1$ is a fully oriented walk, that $h=0$ is an unoriented walk and that the sum of the fugacities to all unoccupied sites is k. A typical walk and its associated fugacities is illustrated in figure 3. This shows a seven-step walk, denoted by the bold line, which enters vertically from the bottom and exits from the top of the cell. The full circle indicates the site on which the walk in the cell begins. The fugacity for this walk is shown as a product of factors in the same sequence in which each step of the walk occurs. Notice that the sixth step has a factor $k/2$ since in this step $N_e=0$. Assuming that the walk always enters vertically from the bottom of the cell and defining $x \equiv 1+h/2$, $y \equiv 1+2h$, $w \equiv 1-h$, $z \equiv 1+h$, $p \equiv k/3$, and similarly for the renormalised quantities $p' \equiv k'/3$, and h', we obtained the recursion relation:

$$p'(1+h') = f_1(k, h) \tag{2}$$

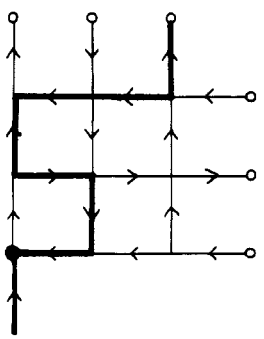

Figure 3. A seven-step GSAW on the Manhattan square lattice, shown by the bold line, which starts at the site denoted by the full circle in a 3×3 cell and exits by way of the top edge. The fugacity of the whole walk is

$$[(1-h)k/3]^3[(1+h)k/2][(1-h)k/3](1/2)[(1+h/2)k/3].$$

where the function $f_1(k, h)$ is given by

$$\begin{aligned}f_1(k,h) = {} & p^3(2x^3+w^3)+p^4(2x^2w^2+w^4+2xw^3+x^3w+2xyw^2+2x^2yw+x^3y+yw^3)\\ & +p^5[10x^2yw^2+yw^4+2xyw^3+3(x^5+x^2yw^2+yw^3+xw^3z+x^2yw)]\\ & +p^6[x^4yw+3xy^2w^2+3xyw^3+\tfrac{3}{2}(yw^4+x^5w+x^3ywz+y^2w^3+x^4yz)\\ & +\tfrac{5}{2}(x^2yw^3+x^2y^2w^2+x^4w^2)+\tfrac{9}{4}(w^3z+yw^3z+x^2yw^2+x^2y^2w)]\\ & +p^7[2x^4yw^2+3xy^2w^3+\tfrac{3}{2}(x^3yw^2z+x^4yw^2)\\ & +\tfrac{9}{4}(2yw^4z+2xyw^3z+2x^5z+3x^4yw+3x^3ywz+y^2w^3+x^4ywz)]\\ & +p^8[\tfrac{9}{2}(x^3y^2wz+x^3y^2w)+\tfrac{27}{8}(yw^4z+x^4yw^2+y^2w^3z\\ & +x^4yz^2+x^5wz+x^2yw^2z)]\\ & +p^9[\tfrac{81}{16}(yw^4z^2+x^2y^2w^2z+x^4ywz+2x^5z^2+x^2yw^2z^2)\\ & +\tfrac{27}{4}(x^3yw^2z+x^4ywz)]. \end{aligned} \tag{3}$$

The renormalised quantities on the left-hand side of (2) are obtained by averaging over the possibilities shown in figure 4, where the full circle denotes the renormalised site and the bold vertical line represents the renormalised step which could have come from the bottom, left or right of the renormalised site. Similarly, by reversing all directions in the cell we obtain another recursion relation:

$$p'(1-h') = f_2(k, h) \tag{4}$$

where the function $f_2(k, h)$ is given by

$$\begin{aligned}f_2(k,h) = {} & p^3(2xw^2+x^2w)+p^4[2(xyw^2+x^2yw+x^2w^2+xw^3)+xy^3+yw^3+w^4+x^3w]\\ & +p^5[10xyw^3+x^3yw+2x^2yw^2+3(w^5+x^2w^3+x^2yw+x^2ywz+yw^3)]\\ & +p^6[xy^2w^3+3x^2w^4+2xyw^4+3xy^2w^2+\tfrac{9}{4}(x^2y^2z+x^2ywz+xw^4)\\ & +\tfrac{3}{2}(x^2y^2w+x^2yw^3+xw^4z+w^5z+x^2yw^2)+\tfrac{5}{2}xw^5+\tfrac{21}{4}xyw^3]\\ & +p^7[2xyw^5+3xy^2w^3+\tfrac{9}{2}(x^2y^2wz+xy^2w^2z+w^5z+yw^4z)\\ & +\tfrac{3}{2}(xyw^4z+x^2w^5)+\tfrac{9}{4}(xy^2w^2+xw^5z+yw^4z+3xw^5)]\\ & +p^8[\tfrac{27}{8}(xy^3wz+x^2w^5+xy^2w^2z+w^5z^2+xw^5z+y^2w^3z)+\tfrac{9}{2}(yw^5z+xw^5)]\\ & +p^9[\tfrac{81}{16}(xy^3wz^2+xyw^4z+xw^5z+2w^5z^2+y^2w^3z^2)\\ & +\tfrac{27}{4}(xyw^4z+yw^5z)]. \end{aligned} \tag{5}$$

Equations (2)–(5) may be solved to yield the two-dimensional map $k'(k, h)$ and $h'(k, h)$. The global structure characterising this renormalisation mapping is displayed in the phase diagram of figure 5. The diagram illustrates the global flow pattern, the fixed points and the critical surface that are obtained from iterating the map. There exists one non-trivial fixed point at $(k, h) = (1.257, 0.0)$ corresponding to the GSAW problem

Figure 4. Three possibilities for the renormalised quantities k' and h' for GSAW on the Manhattan square lattice. The full circles denote the renormalised sites and the bold lines denote the renormalised steps, whose fugacities are also shown.

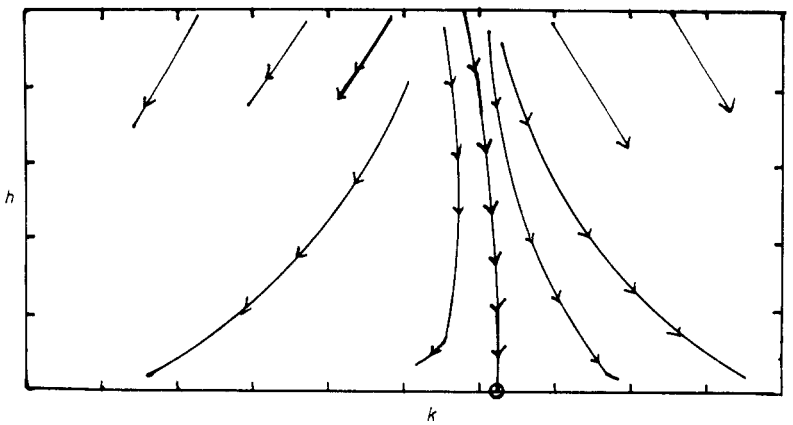

Figure 5. Phase diagram generated from the finite lattice renormalisation transformation for GSAW on the Manhattan square lattice. The non-trivial fixed point is denoted by the circle. The set of GSAW that flow into this fixed point constitutes the critical surface. The intersection of the critical surface with the $h = 1$ axis is a statement of the universality of these problems.

on the non-oriented lattice. The set of GSAW which flow into the non-trivial fixed point defines the critical surface and forms a universality class. In particular, the intersection of the critical surface with the $h = 1$ axis is a statement of the universality of the Manhattan oriented walk and the non-oriented walk. The intersection point determines the non-universal critical fugacity k_c characterising the Manhattan lattice problem. We find this intersection point at $k_c = 1.167$. This shows that within a two-parameter 3×3 cell to bond renormalisation transformation, GSAW on Manhattan square and GSAW on square lattices are in the same universality class.

3. GSAT on L lattice

The L lattice is shown in figure 1(b). If b is an odd integer, we can divide the oriented lattice into $b \times b$ cells, such as shown in figure 6(a) for $b = 3$. Furthermore, if for each cell we substitute a vertical and a horizontal renormalised bond of length b with an orientation determined by a majority rule, then the resulting lattice of the renormalised bond obeys the same orientation as the original lattice. This is shown in figure 6(b). For a 3×3 cell we enumerate all GSAT that start at any of the three vertices at the bottom of the cell, assuming that they all enter the cell vertically from below, irrespectively of the orientation of the bonds and exit by way of the top edge. A simple average over the three initial starting points is then performed. The orientation of the lattice can be taken into account by introducing an extra parameter $H \leqslant 1$, just as in the last section for GSAW. A typical GSAT with eight steps and its associated fugacity is shown in figure 7. The fugacity is shown as a product of factors appearing in the same sequence as the steps in the trail, which is denoted by the bold line. It enters the cell vertically from the bottom, starts at the site shown as a full circle in the cell and leaves it by way of the top edge. Assuming that the trail always enters the cell vertically from the bottom and defining $X \equiv 1 + H/2$, $Y \equiv 1 + 2H$, $W \equiv 1 - H$, $P \equiv K/3$ we obtain the following recursion relation:

$$P'(1 + H') = F_1(K, H) \tag{6}$$

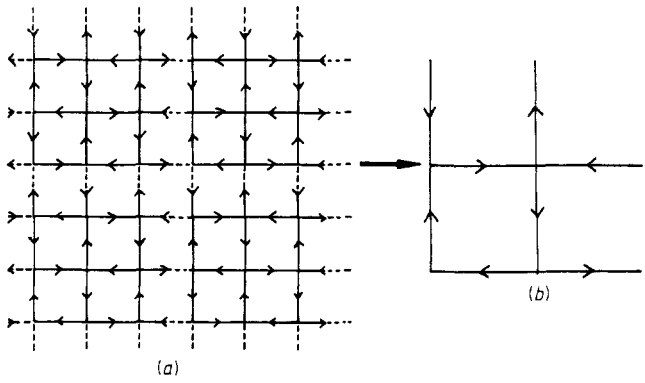

Figure 6. (*a*) Division of the L lattice into 3×3 cells. (*b*) The lattice after renormalisation.

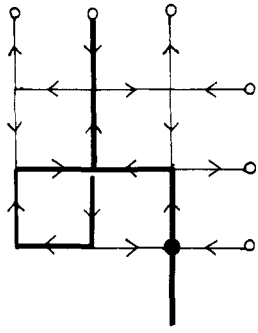

Figure 7. An eight-step GSAT on the L lattice, shown by the bold line, which starts at the site denoted by the full circle in a 3×3 cell and exits by way of the top edge. The fugacity of the whole trail is

$$[(1+2H)K/3][(1+H/2)K/3][(1-H)K/3]^4[K][(1-H)K/3].$$

where

$$\begin{aligned}F_1(K,H) = {} & P^3(2Y^2W+YW^2)+6P^4(X^2YW+YW^3)\\ & +2P^5[W^5+X^2W^3+X^4W+2(X^4Y+YW^4+X^2YW^2)+3XY^2W^2]\\ & +P^6(4W^6+4X^6+6XYW^4+6X^3YW^2)\\ & +2P^7[X^4Y^2W+Y^2W^5+X^3W^4+2(XYW^5+X^5YW)+3X^2Y^2W^3]\\ & +4P^8[X^2YW^5+X^4YW^3+3(XYW^5+X^5YW+YW^6+X^3Y^2W^2)]\\ & +2P^9[XY^2W^6+X^3Y^2W^4+X^2Y^3W^4+X^5Y^2W^2\\ & +3(X^5W^3+XW^7+X^5YW^2+X^2W^6)\\ & +6(YW^7+X^3Y^2W^3+X^3YW^4+X^7Y)\\ & +9(X^2W^5+X^3W^4+X^6W+X^3YW^3+W^7+X^2YW^4)]\\ & +6P^{10}[X^6YW^2+X^2YW^6+XY^3W^5+X^4Y^2W^3+X^2Y^2W^5\\ & +XYW^7+2X^3Y^2W^4\\ & +6(W^8+X^3YW^4+X^4W^4+X^5W^3+X^8+X^2YW^5)]\\ & +18P^{11}(X^3Y^2W^4+2X^3YW^5). \end{aligned} \tag{7}$$

The renormalised quantities on the left-hand side of (6) are obtained by averaging over the three possibilities shown in figure 8, where the full circle represents the renormalised site and the renormalised step is denoted by the bold vertical line. It could have come from the bottom, left or right of the renormalised site. Similarly, by reversing all the directions in the cell, we obtain another recursion relation:

$$P'(1-H') = F_2(K, H) \tag{8}$$

where

$$\begin{aligned} F_2(K,H) = {} & P^3(2YW^2 + Y^2W) + 6P^4(YW^3 + X^2YW) \\ & + 2P^5[X^4Y + X^2YW^2 + YW^4 + 2(X^4W + X^2W^3 + W^5) + 3XYW^3] \\ & + P^6[4(X^6 + W^6) + 6(X^3YW^2 + XYW^4)] \\ & + 2P^7[YW^6 + X^4YW^2 + X^3YW^3 + 2(XW^6 + X^5W^2) + 3X^2YW^4] \\ & + 4P^8[X^4YW^3 + X^2YW^5 + 3(XYW^5 + X^5YW + X^3Y^2W^2 + YW^6)] \\ & + 2P^9[X^5YW^3 + X^3YW^5 + X^2Y^2W^5 + XYW^7 \\ & + 3(X^2YW^5 + X^5Y^2W + XYW^6 + X^5YW^2) \\ & + 6(X^7W + X^3W^5 + X^3YW^4 + W^8) \\ & + 9(X^3Y^2W^2 + X^2Y^2W^3 + YW^6 + X^2YW^4 + X^6Y + X^3YW^3)] \\ & + 6P^{10}[XYW^7 + X^4Y^2W^3 + 2X^3Y^2W^4 + X^2YW^6 + X^6YW^2 + XY^3W^5 \\ & + X^2Y^2W^5 + 6(X^8 + X^4W^4 + X^3YW^4 + X^2YW^5 + W^8 + X^5W^3)] \\ & + 18P^{11}(X^2Y^2W^5 + X^2Y^3W^4 + X^3Y^2W^4). \end{aligned} \tag{9}$$

Iterating the map (6)-(9) one finds one non-trivial fixed point at $(K, H) = (1.264, 0.0)$ corresponding to the GSAT problem on the non-oriented lattice. The global structure characterising this renormalisation mapping is displayed in the phase diagram of figure 9. The set of GSAT which flow into the non-trivial fixed point defines the critical surface and forms a universality class. In particular, the intersection of the critical surface with the $H = 1$ axis is a statement of the universality of the L lattice oriented trail and non-oriented trail. The intersection point determines the non-universal critical fugacity K_c characterising the L lattice problem. We find this intersection point at $K_c = 1.260$.

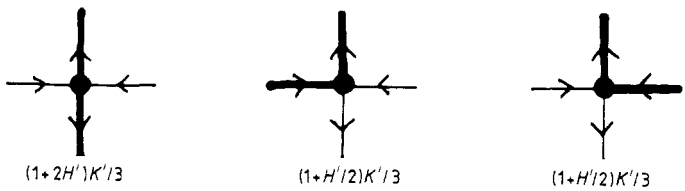

Figure 8. Three possibilities for the renormalised quantities K' and H' for GSAT on the L lattice. The full circles denote the renormalised site and the vertical lines denote the renormalised steps whose fugacities are also shown.

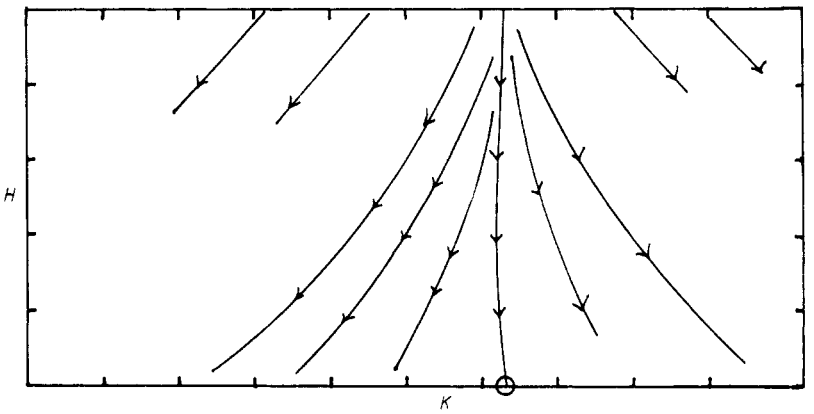

Figure 9. Phase diagram generated from finite lattice renormalisation transformation for GSAT on the L lattice. The non-trivial fixed point is denoted by the circle. The set of GSAT that flow into this fixed point constitutes the critical surface. The intersection of the critical surface with the $H = 1$ axis is a statement of the universality of these two problems.

This shows that within a two-parameter 3×3 cell to bond renormalisation transformation, GSAT on the L lattice and GSAT on the square lattice are in the same universality class.

4. Conclusion

The Manhattan square lattice and the L lattice are related by the covering operation. The covering graph G^c of an oriented graph G is defined as follows: (i) to every arc (oriented line) of G, there corresponds a point in G^c and (ii) two points of G^c are connected by an arc from one point to the other if the corresponding arcs of G are consecutive. One easily verifies that the Manhattan square lattice is the covering graph of the L lattice. By construction, GSAT on the L lattice is equivalent to GSAW on the Manhattan square lattice. Since we have shown above that within a 3×3 two-parameter renormalisation group transformation, both the GSAW on the Manhattan and the GSAT on the L lattices, besides being equivalent themselves, are also separately in the same universality class as their corresponding problems on the square lattice, we conclude that GSAT and GSAW are in the same universality class.

Acknowledgments

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