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Universality of neighbour-avoiding and self-avoiding walks on the square lattice

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Abstract. It is shown that, within position-space renormalisation group (PSRG) theory, neighbour-avoiding walks (NAWs) and self-avoiding walks (SAWs) on the square lattice obey the same 'end-to-end distance' critical exponent ν. This universality is shown by applying a recent finite lattice renormalisation transformation to ordinary and oriented NAW and SAW problems and then using an exact equivalence between SAWs on an oriented lattice and NAWs on its covering lattice. The universality class includes several oriented walk problems.

1. Introduction

The SAW problem on a lattice is of considerable importance as it takes account, in a realistic way, of the excluded volume effect of a polymer chain in dilute solutions (Domb 1963). SAWs are random walks that contain no self-intersections. This model is related to the Ising model (Domb 1970, Fisher and Sykes 1959) and it is also equivalent to the n-component spin model, in the limit $n \to 0$ (de Gennes 1972). Modern notions in the theory of critical phenomena were soon carried over to polymer models in order to establish their relation to critical phenomena and derive scaling laws for polymers (McKenzie 1976).

In particular the notion of universality implies that the 'end-to-end distance' critical exponent ν, defined by

$$\langle R_N^2 \rangle \sim N^{2\nu} \tag{1}$$

where N is the number of steps of the SAWs, would not depend on the lattice but would depend on its dimensionality. This universality hypothesis is strongly supported by most numerical studies (McKenzie 1976, Watts 1975, Domb 1963). As pointed out by Whittington (1982) the next question is whether the universality class includes other models as well as the SAW model. Such extensions have been suggested by various authors (Hioe 1967, Domb and Joyce 1972, Watson 1970, 1974, Malakis 1975). A very convincing extension concerns the NAW problem (Hioe 1967, Watson 1974, Malakis 1975). NAWs are SAWs that contain no nearest-neighbour contacts. The work of Watson (1974) when combined with the above stated universality hypothesis suggests that NAWs and SAWs are in the same universality class.

The primary aim of this paper is to provide evidence for the above long standing conjecture in a way that does not depend on the universality hypothesis. We use a finite lattice renormalisation transformation to compare oriented and ordinary walk problems on the square lattice. The method has been recently introduced by Prentis (1984) in order to compare SAWS on the Manhattan-oriented and the (ordinary non-oriented) square lattice. It is a simple generalisation of the finite lattice PSRG theory of SAWS (Stanley *et al* 1982, Redner and Reynolds 1981).

We employ two well known orientations on the square (S) lattice shown in figure 1 (Kasteleyn 1963, Malakis 1975, 1976). The oriented lattice in figure 1(*a*) is known as the Manhattan square (MS) lattice. The other oriented lattice in figure 1(*b*) has no standard name, recently Guttmann (1983) used the name 'L lattice' whereas in earlier papers the name 'underlying lattice of the Manhattan square (UMS) lattice' was used. This notation (UMS lattice) serves as a reminder of the fact that the two oriented graphs in figure 1 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 the one point to the other if the corresponding arcs of G are consecutive. The MS lattice is the covering graph of the oriented lattice in figure 1(*b*) (UMS or L lattice).

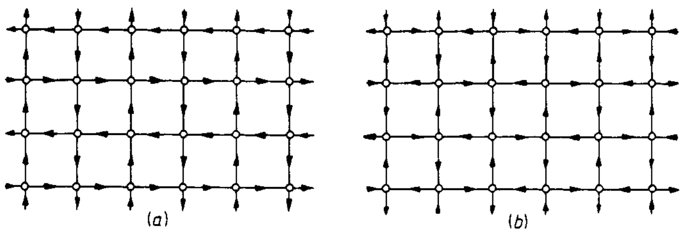

Figure 1. (*a*) The Manhattan square (MS) lattice. (b) The underlying of the Manhattan square (UMS) lattice or L lattice.

This observation was the basis of Kasteleyn's treatment of the Hamiltonian walk problem on the MS lattice. The importance of the covering operation is that one can relate apparently different walk problems. In Kasteleyn's study Hamiltonian walks (circuits) on the MS lattice are related to Eulerian walks (circuits) on the UMS lattice, and this latter problem is solvable. As it has been pointed out (Malakis 1975), the equivalence can be carried over to other walk problems on these two oriented lattices. It is again one of these equivalences, stated in § 6 as theorem 1, that, when combined with PSRG theory, provides the main conclusion of this paper.

The renormalisation approach has already been applied to the SAW problem in 1972 by de Gennes. He appealed to the ε-expansion of critical exponents by using a spin field for the isomorphic $(n \to 0)$-component spin model. Shapiro (1978) was the first to apply a direct decimation transformation to the problem. Since, several direct renormalisation procedures have been suggested including a Niemeijer–van Leeuwen approach (Napiorkowski *et al* 1979, Malakis 1980), a Monte Carlo renormalisation (Kremer *et al* 1981), a phenomenological approach (Derrida 1981), and a cell-to-bond PSRG transformation (de Queiroz and Chaves 1980, Family 1981, Redner and Reynolds 1981, Stanley *et al* 1982).

This last method is simple and systematic. Furthermore, the analysis of the method by Redner and Reynolds (1981) suggests that the approximations converge to the correct behaviour as the cell size is increasing. The recent generalisation of the method, introduced by Prentis (1984), provides a powerful tool to compare critical behaviour of oriented and non-oriented walk problems. For our purposes it is necessary to describe the Prentis approach in a slightly more general way and we shall do so in § 2.

The renormalisation scheme in § 2 may be applied to a wide class of oriented walk problems and not only to the SAW problem on the MS lattice. However, it is the combination of the PSRG theory with the covering property of the MS lattice that permits comparison of SAWs and NAWs on the square lattice, something that cannot be done by the PSRG transformation alone. In the remainder we shall apply the method to compare SAWs on the UMS and square lattices (§ 3) and NAWs on the MS and square lattices (§ 4). In § 5 we consider two oriented walk problems for which the critical behaviour is expected to be different from that of the ordinary problems. Our conclusions are summarised in §§ 6 and 7.

2. Renormalisation of oriented and non-oriented walk problems

We assume that the orientations of interest on the square lattice have the following two properties: (i) If all bond orientations are reversed, then the resulting 'anti-oriented' lattice is by symmetry identical to the original oriented lattice. Both lattices in figure 1 have this property. (ii) If b is an odd integer we can divide the oriented lattice into $b \times b$ bond cells, such as shown in figure 2(a) for the UMS lattice. 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 bonds obeys the same orientation as the original lattice.

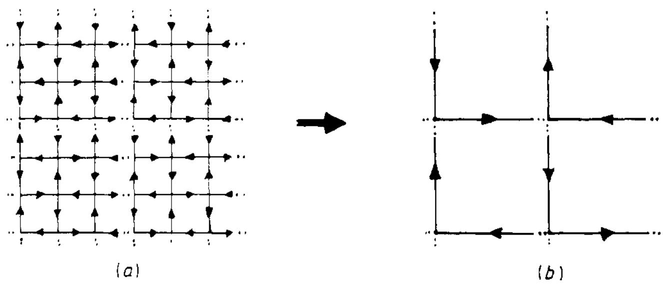

Figure 2. (a) Division of the UMS lattice into 3×3 bond cells. (b) The lattice after renormalisation.

Now, consider a non-oriented walk C entering the cell via any bottom (left)-point and leaving via any top (right)-point; we say that C spans the cell in the vertical (horizontal) direction. Let n be the number of steps of C within the cell and n_0 the number of steps that preserve the bond orientation. Then $n_v = n - n_0$ is the number of steps that violate the bond orientation. The cell weight of C is

$$W_{\text{cell}}(C) = K^n p^{n_0} (1-p)^{n_v} \tag{2}$$

where p has the meaning of the probability that a step preserves the bond orientation. The fugacity K is as usual introduced as a measure of the step weights (Kp or $K(1-p)$) and the rate of divergence at its critical value yields physical quantities of interest.

The total weight of a walk C is the product of (2) over all cells spanned by C

$$W(C)=\prod_{C\text{-cells}} W_{\text{cell}}(C). \tag{3}$$

Assuming a mapping in which every renormalised walk C' is the image of a set $\{C\}_{C'}$ of walks C on the original lattice, the weight of C' is

$$W'(C')=\sum_{C\in\{C\}_{C'}} W(C)=\prod_{C\text{-cells}}\left\{\sum_{C\in\{C\}_{C'}} W_{\text{cell}}(C)\right\}. \tag{4}$$

We can write $W'(C')$ as product of its step weights and since the steps of C' correspond to cells spanned by C, we have

$$W'_{\text{step}}(C')=\sum_{C\in\{C\}_{C'}} W_{\text{cell}}(C). \tag{5}$$

To achieve 'connectivity' for C its entry point in the cell must be fixed and in order to avoid arbitrariness, with fixing the entry point, a simple average over the b entry points is then performed. Thus, the step weight of a renormalised step that preserves the orientation of the transformed lattice is

$$K'p'=F(K,p,1-p)/b \tag{6}$$

where F is the sum of the weights (2) for all walks starting from any bottom (left)-point in the cell and ending at any top (right)-point. It should be noted that the above averaging ensures also that the various types of cell (four for the MS and two for the UMS lattice) renormalise in the same way. By the symmetry property (i) the weight for a renormalised step that violates the bond orientation is

$$K'(1-p')=F(K,1-p,p)/b. \tag{7}$$

The transformation equations (6) and (7) describe both oriented and non-oriented walk problems. For $p=1$ (or $p=0$) only oriented (or anti-oriented) walks renormalise and property (ii), for the cell division of the oriented lattice, ensures that the resulting renormalised walks obey the same orientation rules as the original walks. For $p=\frac{1}{2}$ the transformation is identical to the cell-to-bond PSRG for the non-oriented walks with a transformed fugacity $\frac{1}{2}K$ (Prentis 1984).

In order to discuss critical behaviour we note that

$$\sum_{C'} W'(C')=\sum_{C'}\left\{\sum_{C\in\{C\}_{C'}} W(C)\right\}=\sum_{C} W(C) \tag{8}$$

so that the correlation lengths, defined by

$$\xi^2=\sum_{C} R^2(C)W(C)\Big/\sum_{C} W(C) \tag{9}$$

are related by

$$\xi(K',p')=\xi(K,p)/b. \tag{10}$$

For any orientation it is expected that there exist a non-trivial fixed point at $K^*\neq 0$, ∞ and $p^*=\frac{1}{2}$ corresponding to the ordinary (non-oriented) walk problem, whose connective constant μ and critical exponent ν are given by:

$$\mu=1/(K^*/2) \tag{11}$$

and

$$\nu = \ln b / \ln \lambda \tag{12}$$

where λ is the relevant eigenvalue of the transformation at the fixed point. The connective constant μ describes the asymptotic behaviour ($N \to \infty$) of the number C_N of N-step walks

$$C_N \simeq N^g \mu^N. \tag{13}$$

The global structure of the renormalisation mapping and the existence of additional non-trivial fixed points may depend on the orientation. The situation will be elucidated in the following sections.

3. SAWS on the UMS and S lattices

In order to compare the critical behaviour of SAWS on the UMS and S lattices, we shall use the 3×3 cell-to-bond PSRG transformation. The function $F(K, p, 1-p)$ in equation (6) can be found by enumeration of SAWS which span the $b = 3$ cell:

$$\begin{aligned} F(K, X, Y) = {} & K^3(2X^2Y + XY^2) + K^4(6X^3Y + 6XY^3) \\ & + K^5(4X^5 + 2X^4Y + 10X^3Y^2 + 2X^2Y^3 + 4XY^4 + 2Y^5) \\ & + K^6(4X^6 + 6X^4Y^2 + 6X^2Y^4 + 4Y^6) \\ & + K^7(6X^6Y + 6X^4Y^3 + 2X^3Y^4 + 6X^2Y^5) \\ & + K^8(4X^5Y^3 + 4X^3Y^5) + K^9(2X^7Y^2 + 4X^5Y^4 + 2X^3Y^6). \end{aligned} \tag{14}$$

The diagram in figure 3 illustrates the flow pattern of the renormalisation mapping and is similar to the one found by Prentis—using the orientation of the MS lattice in order to determine the bond orientation of a step. The location of the non-trivial fixed point ($K^* = 0.8788$, $p^* = \frac{1}{2}$) and the relevant eigenvalue (K-direction) $\lambda_K = 4.52$ are the same as those found by Prentis. There are some insignificant differences between the diagrams obtained for the two orientations. In the present case there exist no trivial fixed points at $K^* = \infty$, $p^* = 1$ or $= 0$ and the flow is different for large K. The values of the irrelevant p-eigenvalue are $\lambda_p = 0.26$ for the UMS lattice and $\lambda_p = 0.61$ for the MS lattice.

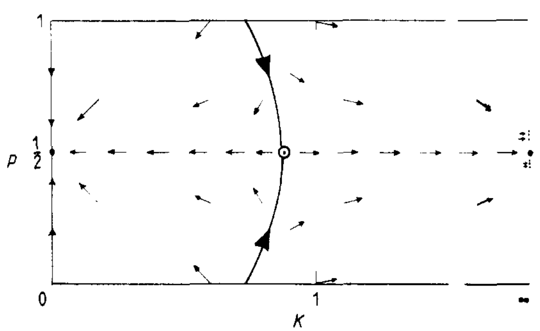

Figure 3. Flow diagram from the 3×3 transformation as applied to SAWS on UMS and square lattices. The points on the critical surface (full curve) flow into the non-trivial fixed point (⊙) at $p = \frac{1}{2}$. Trivial fixed points (●) are also shown.

However, the critical behaviour is the same. There exists a critical surface which intersects the $p=1$ and $p=0$ lines at $K_c=0.7383$. The points of this surface (line), including the points (K_c, $p=1$ or 0), flow into the non-trivial fixed point at $p=\frac{1}{2}$ and form a universality class. For each value of p we have a 'partially' oriented SAW problem and all these obey the same critical exponent. The estimate of the 3×3 cell-to-bond transformation is

$$\nu=\ln 3/\ln 4.52=0.7283, \tag{15}$$

about 3% lower than the best numerical estimates or the conjectured value 0.75.

Among these equivalent problems are the SAW problem on the UMS lattice ($p=1$ or 0) and the ordinary SAW problem on the square lattice ($p=\frac{1}{2}$). With regard to the connective constant, the approximation yields for the ordinary SAW problem on the square lattice

$$\mu_{\mathrm{S}}^{\mathrm{SAW}}=2.28 \tag{16}$$

a value that is 13% lower than the best known estimate (=2.6385, for numerical results see McKenzie 1976 and references therein). For the SAW problem on the UMS lattice the connective constant is determined by the intersection of the critical surface with the $p=1$ or $p=0$ axis

$$\mu_{\mathrm{UMS}}^{\mathrm{SAW}}=1/K_c=1.355. \tag{17}$$

This is to be compared with the numerical result 1.56 ... (Guttmann 1983).

4. NAWs on the MS and S lattices

We can use the same method to compare NAWs on the MS and S lattices. Again we have to find by enumeration of NAWs the function $F(K, p, 1-p)$ for the $b=3$ cell

$$\begin{aligned}F(K, X, Y)=&K^3(2X^3+Y^3)+K^4(X^4+3X^3Y+4X^2Y^2+3XY^3+Y^4)\\&+K^5(3X^5+10X^3Y^2+2X^2Y^3+XY^4)\\&+K^6(X^5Y+2X^4Y^2+X^3Y^3)+K^7(2X^5Y^2).\end{aligned} \tag{18}$$

The resulting flow diagram is shown in figure 4. It has the same features as that of Prentis for the SAW problem on the MS lattice. There exist trivial fixed points at $K^*=\infty$,

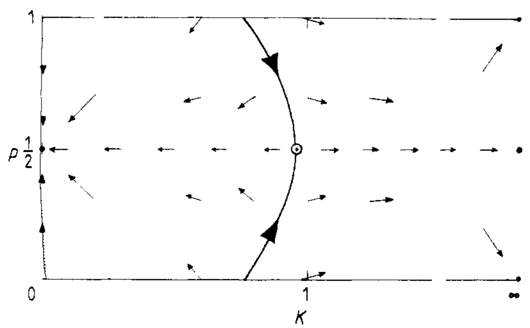

Figure 4. Flow diagram for NAWs on MS and square lattices.

$p^* = 1, 0, \frac{1}{2}$ and at $K^* = 0$, $p^* = \frac{1}{2}$. The non-trivial fixed point corresponding to non-oriented NAWs is at $K^* = 0.9606$, $p^* = \frac{1}{2}$. Thus the approximation yields for the connective constant of the ordinary NAW problem on the square lattice:

$$\mu_S^{NAW} = 2.08 \tag{19}$$

(numerical result ~2.3, Hioe 1967). The relevant eigenvalue is $\lambda_K = 4.1458$ and the irrelevant $\lambda_p = 0.324$. The estimate of the 3×3 transformation for the critical exponent is

$$\nu = 0.7725 \tag{20}$$

which is 3% higher than the value 0.75. The connective constant of the NAW problem on the MS lattice is equal to the connective constant of the SAW problem on the UMS lattice (see § 6 and Malakis 1975). However, the approximation yields a slightly lower value than that previously found (1.355):

$$\mu_{MS}^{NAW} = 1.317. \tag{21}$$

The important point is that the 3×3 cell-to-bond PSRG transformation predicts a universality class including the ordinary NAW problem on the square lattice and the NAW problem on the MS lattice.

5. Other oriented problems

We now use the method to compare walk problems which obey different critical exponents. This may be considered as a test of the method.

The first example is known as the fully directed SAW problem (de Queiroz 1983). The orientation on the square lattice is shown in figure 5. A fully directed SAW is alllowed to proceed either upwards or to the right only. For this problem ($p = 1$) it is known (Malakis 1975) that $\nu_D = 1$ and de Queiroz (1983) has shown that the $b \times b$ cell-to-bond PSRG transformation produces asymptotically the exact result on the $p = 1$ axis:

$$\nu_b = 1 - \ln 2/\ln b \to 1 \qquad (b \to \infty). \tag{22}$$

In order to find the behaviour for $p \neq 1$ we may proceed as before. The F-function is now

$$\begin{aligned} F(K, X, Y) = {} & K^3(3X^3) + K^4(6X^4 + 6X^3 Y) + K^5(6X^5 + 12X^4 Y + 6X^3 Y^2) \\ & + K^6(10X^5 Y + 10X^4 Y^2) + K^7(4X^6 Y + 12X^5 Y^2 + 4X^4 Y^3) \\ & + K^8(4X^6 Y^2 + 4X^5 Y^3) + K^9(2X^7 Y^2 + 4X^6 Y^3 + 2X^5 Y^4). \end{aligned} \tag{23}$$

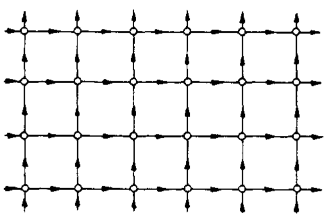

Figure 5. The orientation of the fully directed square lattice, that corresponds to the fully directed SAW problem.

The diagram in figure 6 illustrates the flow pattern of the renormalisation mapping. The behaviour is now different. The nontrivial fixed point corresponding to ordinary SAWs ($K^* = 0.8788$, $p^* = \frac{1}{2}$) has in both directions relevant eigenvalues $\lambda_K = 4.52$ and $\lambda_p = 3$. The points of the critical surface now flow into the fixed points at $K^* = 0.589$, $p^* = 1$, 0 which correspond to the fully directed SAW problem. There is a different universality class (not including the ordinary SAW problem) characterised by the critical behaviour of the fully directed SAW problem with an exponent $\nu_D = 1$ which within the 3×3 approximation is estimated:

$$\nu_D = 0.808. \tag{24}$$

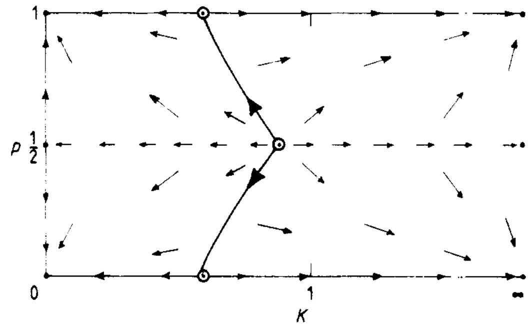

Figure 6. Flow diagram of the renormalisation mapping in the case where we compare fully directed and non-oriented SAWs on the square lattice. Points on the critical surface flow into fixed points on the $p = 1$ and $p = 0$ lines and not into the fixed point at $p = \frac{1}{2}$.

The transformation predicts a correct qualitative distinction between fully directed and ordinary SAWs, as it should. For any $p \neq \frac{1}{2}$ the problem is anisotropic and obeys the critical exponent of the fully directed SAW problem. A conclusion that could be deduced on probabilistic grounds.

The second example is the NAW problem on the UMS lattice. In this case ($p = 1, 0$) it is easily seen that, due to the restrictions imposed on the problem, there exists only one NAW for any number of steps and

$$\nu_{\text{UMS}}^{\text{NAW}} = 1. \tag{25}$$

To find the $p \neq 1$, 0 behaviour we proceed as before. The F-function is now:

$$\begin{aligned} F(K, X, Y) = {} & K^3(2X^2Y + XY^2) + K^4(6X^3Y + 6XY^3) \\ & + K^5(2X^5 + 10X^3Y^2 + 2X^2Y^3 + 2XY^4) \\ & + K^6(2X^4Y^2 + 2X^2Y^4) + K^7(2X^4Y^3). \end{aligned} \tag{26}$$

The flow pattern (figure 7) is different from all previous ones. There exists a non-trivial fixed point ($K^* = 0.9609$, $p^* = \frac{1}{2}$) corresponding to non-oriented NAWs with eigenvalues $\lambda_K = 4.1458$, $\lambda_p = 0.298$ and two more non-trivial fixed points at $K^* = 1.1$, $p^* = 1, 0$ corresponding to the NAW problem on the UMS lattice. The points of the critical surface flow into the fixed point at $p = \frac{1}{2}$ and not into the fixed points on the $p = 1$, 0 lines. The universality class includes the ordinary NAW problem as well as all 'partially' ($0 < p < 1$) oriented NAW problems. This is an interesting prediction that may be rationalised. The restrictions of the orientation plus the restrictions on the walks

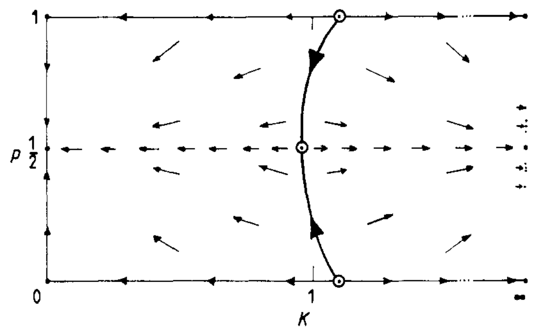

Figure 7. Flow diagram from the renormalisation; comparison between NAWs on UMS and square lattices. Points on the ciritical surface ($0<p<1$) flow into the fixed point at $p=\frac{1}{2}$. The fixed points (⊙) at $p=1$ and $p=0$ correspond to NAWs on the UMS lattice. Note the difference between this diagram and the diagrams in figures 3 and 4. In this case there exist non-trivial fixed points on the $p=1$ and $p=0$ lines.

produce an anisotropic problem only when $p=1$ or $p=0$. For any other value of p, no such anisotropy exists since the walk can proceed in all four directions on the lattice with equal probabilities.

On the $p=1$ line, one can carry out the transformation for any value of $b(=3, 5, \ldots)$. We find that

$$\nu_b = \ln b/\ln(2b) \to 1 \qquad (b\to\infty). \tag{27}$$

This describes the critical behaviour for the isolated fixed point on the $p=1$ (or $p=0$) line. Furthermore, the transformation on the $p=1$ line yields for the connective constant

$$\mu_b = (\tfrac{2}{3})^{1/(2b-2)} \to 1 \qquad (b\to\infty) \tag{28}$$

These results become exact as $b\to\infty$ and correspond to NAWs on the UMS lattice.

6. The universality class of ordinary SAWs

We found that within the 3×3 cell-to-bond PSRG transformation several oriented walk problems obey the same critical exponent ν as the ordinary SAW problem on the square lattice. These equivalences will be expressed below as 'statements', but before we do so we shall recall an exact equivalence.

Theorem 1. There is a one-to-one correspondence between SAWs (with N steps) on the UMS lattice and NAWs (with $N-1$ steps) on the MS lattice. The two problems are in the same universality class, i.e., they obey the same critical exponent (Malakis 1975).

It may be noted that the corresponding relationship between SAWs on a non-oriented lattice and (ordinary) NAWs on its covering lattice was demonstrated by Watson (1974) and if combined with the conjecture that ν depends only on dimensionality (universality hypothesis) suggests that SAWs and NAWs are in the same universality class. We can now reach this conclusion without the aid of the universality hypothesis. First we give a statement due to Prentis (1984).

Statement 1. SAWS on the MS lattice and SAWS on the square lattice are in the same universality class.

The following two statements are based on the flow-diagrams of §§ 3 and 4 respectively.

Statement 2. SAWS on the UMS lattice and SAWS on the square lattice are in the same universality class.

Statement 3. NAWS on the MS lattice and NAWS on the square lattice are in the same universality class.

Prentis' statement 1 is not necessary for including SAWS and NAWS on the square lattice in the same universality class. Statement 3, combined with theorem 1, implies that NAWS on the MS lattice, NAWS on the square lattice and SAWS on the UMS lattice are all in the same universality class. Then, statement 2 can be used to include in this class SAWS on the square lattice. Thus, we may summarise.

General statement. The universality class includes two ordinary walk problems on the square lattice, the SAW and the NAW problem, as well as, the following oriented walk problems: SAWS on MS and on UMS lattices and NAWS on MS lattice. Furthermore, partially ($0<p<1$) oriented SAWS and NAWS on both MS and UMS lattices are in the same universality class.

7. Discussion

Walk problems on oriented lattices may now become popular. As Guttmann (1983) points out, the MS and the UMS (or L) lattices are of particular interest for several reasons. It is also clear from this paper how the study of oriented walk problems may help in an understanding of the behaviour of ordinary walk problems. These orientations and the corresponding walk problems may be called 'isotropic', where the term implies that there is no preference for any lattice direction. This property appears to be very important.

In the past few years a considerable amount of work has been done in the study of anisotropic lattice problems. An example may be referred to here. Several recent papers considered the so-called directed SAW problem in which the walker is not allowed to proceed in one direction of the lattice. The problem is characterised by a 'direction of flow'. It was stated a long time ago (see Malakis 1975, § 2) that this problem obeys a critical behaviour similar to that of fully directed SAWS. Yet, Chakrabarti and Manna (1983) studied by computer enumeration the problem and suggested a different value for the critical exponent ν. Of course, their prediction is not correct. Cardy (1983) and Redner and Majid (1983) described correctly the critical behaviour for this problem. The direction of flow produces an anisotropy in the problem and this is reflected on the critical exponent ν which is determined by the behaviour of the average radius of the walk parallel to the anisotropy axis. A second exponent may be used to describe the transverse width in directions perpendicular to the anisotropy axis.

A final comment for the 3×3 PSRG transformation used in this paper. The scheme is only approximate and there no proof exists that the qualitative predictions of the transformation are correct. Yet, the examples considered in § 5 provide very convincing evidence in favour of the view that the transformation gives correct qualitative predictions. A study of the 5×5 transformation for the problems considered in this paper will also strengthen this view.

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