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LETTER TO THE EDITOR

Real space renormalisation theory of self-avoiding walks on a Manhattan lattice

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Abstract. The real space renormalisation group theory is applied to the self-avoiding walk (SAW) problem on a two-dimensional oriented lattice known as the Manhattan lattice. A finite lattice renormalisation transformation is used to calculate the connectivity constant μ and the size exponent ν. A more general SAW model is defined that contains the oriented and non-oriented lattice problems as special cases. A renormalisation group analysis of this model provides evidence that the SAW on the Manhattan lattice is in the same universality class as the ordinary non-oriented SAW problem.

A random walk that contains no self-intersections is known as a self-avoiding walk (SAW). It is used as a simple model to represent the physical problem of a long chain molecule (polymer). The SAW problem consists of calculating the total number and the average end-to-end distance of the class of SAW configurations with a given number of steps. In general, it is an unsolved mathematical problem. The SAWs are usually confined to a regular, non-oriented lattice. We consider the SAW problem on a two-dimensional oriented square lattice, known as the Manhattan lattice (see figure 1). The direction of each step of a SAW on this lattice must be oriented with the underlying bond direction.

Recently, there has been considerable interest in the effect of various types of directionality, typically characterised by a global anisotropy, when imposed on lattice statistics problems, including SAWs (Redner and Majid 1983), percolation (De'Bell and Essam 1983) and lattice animals (Herrmann *et al* 1983). The solvability of the recent directed SAW problems (Redner and Majid 1983) is attributed to the nature of the directionality which essentially removes the self-avoiding constraint by forcing the constraint to exist trivially in only a single dimension of the problem. In contrast, the Manhattan orientation preserves the self-avoiding constraint and in this sense, the Manhattan lattice problem remains non-trivial.

The SAW problem on a Manhattan lattice was first studied by Kasteleyn (1963). 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 point of the lattice. The Manhattan orientation makes the Hamilton walk problem susceptible to the powerful methods of graph theory (Kasteleyn 1967) and, as a consequence, renders this problem exactly solvable.

For the general SAW problem (not restricted to the Hamilton class) on any regular lattice, an exact solution does not exist if the dimension of space $d > 1$. Recently, however, an exact solution for $d = 2$, based on some plausible assumptions, has been

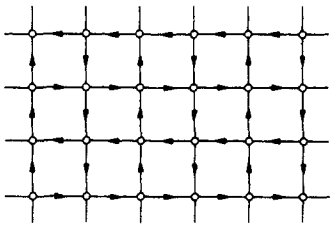

Figure 1. The Manhattan lattice.

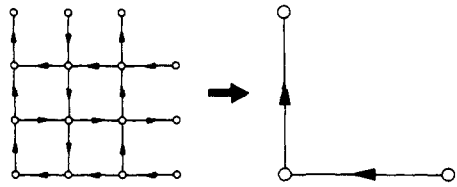

Figure 2. Finite Manhattan lattice ($b = 3$ cell) renormalisation. The lattice site rescaling and the bond orientation renormalisation are illustrated.

calculated (Nienhuis 1982) for an unphysical model which can be mapped onto the non-oriented SAW problem on a hexagonal lattice.

The statistical behaviour of a SAW is determined by the total number Z_N and the mean square end-to-end distance $\langle R^2 \rangle_N$ of the class of SAWs of N steps. The asymptotic ($N \to \infty$) behaviour of these quantities assumes the form (McKenzie 1976)

$$Z_N \sim \mu^N N^{\gamma-1}, \qquad \langle R^2 \rangle_N \sim N^{2\nu}. \tag{1}$$

This defines the 'critical' exponents γ and ν and the connectivity constant μ. For the general SAW on a regular non-oriented square lattice, the current best numerical estimates (McKenzie 1976, and references therein) are

$$\mu = 2.6385 \pm 0.0003, \qquad \gamma = 1.335 \pm 0.005\ (43/32), \qquad \nu = 0.750 \pm 0.0025\ (3/4). \tag{2}$$

The values in the parentheses are the conjectured results based on the indirect exact solution (Nienhuis 1982).

The general SAW problem on a Manhattan square lattice has received considerably less attention than the non-oriented problem. Numerical studies (Barber 1970, Malakis 1975) indicate that the statistical descriptors of this problem have the values

$$\mu_{\text{Man}} = 1.733 \pm 0.003, \qquad \gamma_{\text{Man}} = 1.33 \pm 0.03, \qquad \nu_{\text{Man}} = 0.745 \pm 0.005. \tag{3}$$

The bond orientation constraint at each vertex makes it natural for the connectivity constant μ_{Man}, which is an effective coordination number and thus a non-universal property, to be significantly less than the μ characterising the non-oriented lattice. However, the values for the exponents strongly suggest that the asymptotic behaviour of the SAW on the oriented (Manhattan) and non-oriented lattices are identical.

A proof of the identity of the exponents would be significant because it would place the Manhattan lattice problem in the same universality class defined by the ordinary two-dimensional non-oriented SAW. Malakis (1975) has studied the effect of two non-trivial types of lattice orientation (Manhattan included) and provides additional numerical evidence that the exponent ν is unchanged. The technical and practical utility of the existence of a single universality class arises when the oriented lattice version of the problem, although perhaps artificial, is more tractable.

It may be argued that universality is not surprising if the only effect of the lattice orientation is to introduce short range correlations in the SAW which should not change the asymptotic behaviour. However, the main concern of this letter is to provide an example of how the renormalisation group theory can be used as an analytic tool to

understand the effect of directionality, whether relevant (crossover) or irrelevant (universality), on a given problem.

The real space realisation of the renormalisation group theory has been adapted (Stanley *et al* 1982) to the polymer problem and other 'geometrical' critical phenomena on non-oriented lattices. We now formulate the real space renormalisation theory on the oriented lattice and use it to calculate μ and ν characterising the Manhattan SAW.

The generating functions (grand canonical representation) for Z_N and $\langle R^2\rangle_N$ are defined by

$$Z(K)=\sum_{N=0}^{\infty} K^N Z_N, \tag{4}$$

$$\xi^2(K)=\sum_{N=0}^{\infty} K^N \langle R^2\rangle_N Z_N / Z(K). \tag{5}$$

In the K-space (fugacity space) representation, the asymptotic form of Z_N and $\langle R^2\rangle_N$ in (1) translates into the following critical power law behaviour for K very near and less than K_c:

$$Z(K)\sim (K_c-K)^{-\gamma}, \tag{6}$$

$$\xi^2(K)\sim (K_c-K)^{-2\nu}, \tag{7}$$

where

$$K_c=1/\mu. \tag{8}$$

It is in the K-space representation that the renormalisation theory is most easily formulated and used to calculate ν and K_c.

The construction of the real space renormalisation transformation on the Manhattan oriented lattice proceeds as follows. The original square Manhattan lattice is partitioned into cells such that the lattice of cells is also a square Manhattan lattice, but with a lattice spacing that is increased by a scale factor b. In this rescaling step of the renormalisation theory, not only must the number of lattice sites (bonds) be thinned out, but the lattice bond orientational 'degrees of freedom' must also be coarse grained. The bond orientation must be renormalised in such a way as to preserve the Manhattan structure in the renormalised lattice. 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.

The next step in the real space renormalisation program is to construct the explicit renormalisation transformation. This is a map that relates the value of K in the original (K) and the renormalised (K') systems such that the underlying physics remains invariant. One of the simplest and most successful transformations is defined by the 'connectivity rule' (Stanley *et al* 1982). According to this rule, all the SAWs that span a cell in a given direction map onto a single renormalised bond. The existence of four types of cells (due to their bond orientations) on the Manhattan lattice presents a problem not encountered in the non-oriented lattices. To ensure that the transformation is unique, we define 'spanning' the cell so that the resulting transformation is independent of the cell type. Consider the $b=3$ cell in figure 2. The set of SAWs that

begin at any of the three vertices at the bottom (left) of the cell, preserve the bond orientation at each step, and exit from the cell by way of the top (right) edge, renormalise to a single vertical (horizontal) bond. A simple average over the three initial starting points is then performed. With each N-step walk is associated the weight K^N. In the single cell finite lattice approximation, there exists a single bond in the renormalised lattice with a weight K'. We find that the $b=3$ cell Manhattan lattice renormalisation transformation is

$$K' = \tfrac{1}{3}(2K^3 + K^4 + 3K^5 + K^6 + 2K^7 + K^8 + 2K^9). \tag{9}$$

The critical fugacity K_c and exponent ν are obtained from the non-trivial fixed point K^* of $K'(K)$ and the eigenvalue λ of the linearised version of $K'(K)$ at K^*:

$$K_c = K^* \qquad \text{where } K^* = K'(K^*), \tag{10}$$

$$\nu = \ln b / \ln \lambda \qquad \text{where } \lambda = \mathrm{d}K'/\mathrm{d}K|_{K^*}. \tag{11}$$

There exist trivial fixed points, $K^*=0$ and $K^*=\infty$, which represent the 'empty' and 'full' lattice limits, respectively. From (9), we find the non-trivial fixed point $K^*=0.7244$ and eigenvalue $\lambda = 4.74$. Thus, this simple finite lattice renormalisation theory of the SAW problem on a square Manhattan lattice yields the estimates

$$\mu_{\mathrm{Man}} = 1.38, \qquad \nu_{\mathrm{Man}} = 0.706. \tag{12}$$

These renormalisation group estimates are to be compared with the numerical results in (3). The uncontrolled nature of the approximation, inherent in all real space renormalisation calculations, makes it difficult to ascertain the reliability of these estimates. However, experience with SAWs on non-oriented lattices (Stanley *et al* 1982) suggests that the small cell results are qualitatively reliable and extrapolate (rather slowly) to 'correct' values for increasing cell size.

In order to address the question of universality, the model and renormalisation theory above must be modified. A single, more general SAW problem must be formulated such that it encompasses both the oriented and the non-oriented lattice problems. This unified problem is defined as follows. It is always assumed that the underlying lattice structure has the Manhattan orientation. All possible SAWs, whether they violate or obey the underlying lattice orientation, are allowed to coexist on the lattice. The set of Manhattan walks defines a small subset of all possible walks. We introduce a variable p, $0 \leqslant p \leqslant 1$, which is defined as a probability weight to be associated with each step direction that obeys ($1-p$ if it violates) the underlying orientation of the bond associated with the step.

The generating function for the total number $Z(N, N_o, N_v)$ of SAWs with N steps, N_o of which obey (o) the orientation and N_v which violate (v) the orientation ($N_o + N_v = N$), is defined by the following 'grand partition function':

$$Z(K,p) = \sum_{N=0}^{\infty} \sum_{N_o=0}^{\infty} \sum_{N_v=0}^{\infty} K^N p^{N_o} (1-p)^{N_v} Z(N, N_o, N_v). \tag{13}$$

Similarly, corresponding to the mean square end-to-end distance, we define the 'correlation length function':

$$\xi^2(K,p) = \sum_{N=0}^{\infty} \sum_{N_o=0}^{\infty} \sum_{N_v=0}^{\infty} K^N p^{N_o} (1-p)^{N_v} \langle R^2 \rangle_N Z(N, N_o, N_v) / Z(K,p). \tag{14}$$

The introduction of the variable p essentially provides a mechanism to classify the

various walks among the set of all possible SAWs according to their degree of orientation. In particular, the following relations are satisfied:

$$Z(K, p=1) = \sum_{N=0}^{\infty} K^N Z(N = N_o, N_v = 0), \tag{15}$$

$$Z(K, p=0) = \sum_{N=0}^{\infty} K^N Z(N = N_v, N_o = 0), \tag{16}$$

$$Z(K, p=\tfrac{1}{2}) = \sum_{N=0}^{\infty} (K/2)^N Z_N. \tag{17}$$

Similar relations exist for the correlation length function $\xi^2(K, p)$. Thus the points $(K, p=1)$ and $(K, p=0)$ represent the SAWs on a Manhattan lattice which completely obey (Manhattan walk) and completely violate ('anti-Manhattan' walk) all the underlying bond orientations, respectively. By symmetry, these problems are identical. The point $(K, p=\frac{1}{2})$ corresponds to the ordinary SAW problem on the non-oriented lattice but with a transformed fugacity $K/2$.

The two-dimensional (K and p) renormalisation transformation is constructed from the same rules given above. In addition to the fugacity weight K associated with each step, there now exists the probability weight $p(1-p)$ associated with a step direction that obeys (violates) the underlying bond orientation. Enumeration of the SAWs which span the $b=3$ cell in figure 2 result in the following renormalisation transformation:

$$K'p' = F(K, p, 1-p), \tag{18}$$

$$K'(1-p') = F(K, 1-p, p), \tag{19}$$

where

$$\begin{aligned} F(K, x, y) = \tfrac{1}{3}[&K^3(2x^3+y^3)+K^4(x^4+3x^3y+4x^2y^2+3xy^3+y^4) \\ &+K^5(3x^5+2x^4y+12x^3y^2+4x^2y^3+3xy^4) \\ &+K^6(x^6+4x^5y+5x^4y^2+4x^3y^3+4x^2y^4+2xy^5) \\ &+K^7(2x^7+7x^6y+4x^5y^2+4x^3y^4+3x^2y^5) \\ &+K^8(x^8+2x^7y+2x^6y^2+x^5y^3+2x^3y^5) \\ &+K^9(2x^9+2x^8y+x^7y^2+2x^6y^3+x^3y^6)]. \end{aligned} \tag{20}$$

Note that as in the pure Manhattan case, the transformation is invariant to the cell type and in addition preserves the symmetry between the Manhattan and anti-Manhattan oriented walks. Equations (18) and (19) may be solved to yield the two-dimensional map $K'(K, p)$ and $p'(K, p)$.

The global structure characterising this renormalisation mapping is displayed in the phase diagram of figure 3. This 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 $(K/2, p) = (0.4394, \frac{1}{2})$ corresponding to the ordinary SAW problem on the non-oriented lattice. The transformation near this fixed point has a relevant (K-direction) eigenvalue $\lambda_1 = 4.52$ and an irrelevant (p-direction) eigenvalue $\lambda_2 = 0.61$. Thus the critical descriptors characterising this SAW are

$$\mu = 2.28, \qquad \nu = 0.7283. \tag{21}$$

These estimates are to be compared with the numerical results in (2).

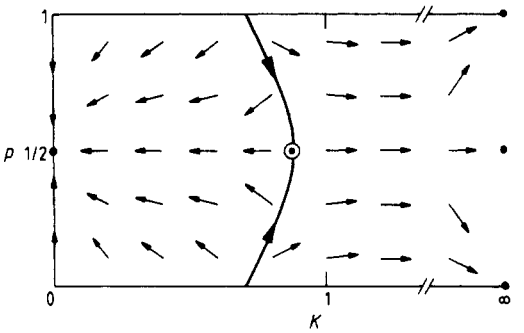

Figure 3. Phase diagram generated from the finite lattice renormalisation transformation. The intersection of the critical surface (full curve) of the ordinary non-oriented SAW fixed point (⊙) with the $p=1$ (Manhattan lattice SAW) axis is a statement of the universality of these two problems. The diagram also illustrates the local direction of the renormalisation group flow (arrows) and the trivial ($K=0$ empty lattice walk and $K=\infty$ full lattice Hamilton walk) fixed points (●).

The set of SAWs which flow into the non-trivial fixed point define the critical surface and form a universality class. Each walk in this class exhibits identical asymptotic behaviour characterised by the single exponent ν. In particular, the intersection of the critical surface with the $p=1$ ($p=0$) axis is a statement of the universality of the Manhattan (anti-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 $K_c=0.7005$. Note that this estimate for K_c is better than that obtained via the one-dimensional renormalisation transformation. The main results of the finite lattice renormalisation theory describing the SAW problem on a Manhattan lattice can be summarised as follows:

$$\mu_{\text{Man}}=1.428, \qquad \nu_{\text{Man}}=\nu=0.7283. \tag{22}$$

If greater quantitative accuracy is desired, then it is merely a technical exercise to implement the renormalisation program on larger cells.

The real space renormalisation group theory has been applied to the problem of the SAW on a Manhattan oriented lattice. The renormalisation of the bond orientational 'degree of freedom' represents a new feature that has been incorporated into the conventional real space renormalisation program. This formulation can be extended to various other oriented lattice problems and directed phenomena.

A more general SAW model has been defined by introducing a variable p, $0\leqslant p\leqslant 1$, which represents the probability that the direction of a walk step is parallel ($1-p$ if antiparallel) to the underlying bond orientation of the step. Hence, in this model, the class of all SAWs is partitioned into subclasses according to their degree of orientation. The incorporation of the p variable into the renormalisation group formalism results in a theory capable of understanding the connection between the oriented and the non-oriented lattice problems. In particular, the universality of the Manhattan and the non-oriented SAW problems (in the sense that $\nu_{\text{Man}}=\nu$) emerges naturally within the framework of this renormalisation theory. A complete proof of universality would also need to establish the identity of the exponent γ.

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