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LETTER TO THE EDITOR

Cell renormalisation study of biased self-avoiding walks

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Abstract. We present a cell renormalisation approach for the biased self-avoiding walks and show that a stiff-to-isotropic crossover exponent is exactly one in all dimensions and for all cell sizes. We also show, by use of renormalisation flow diagrams, a substantial difference between two and three dimensions in the crossover from stiff limit to isotropic limit as the length of walk $N \to \infty$ for fixed gauche weight p. In three dimensions, a crossover seems to occur first to random walk limit and then to self-avoiding walk limit, while, in two dimensions, it seems to occur directly to self-avoiding walk limit in agreement with recent observations based on Monte Carlo simulations.

In recent years there has been renewed interest in the conformation of semiflexible long chain polymers [1, 2] both from theoretical [3-6] and experimental [3, 4] points of view. In our recent Monte Carlo study [6] of such a chain, performed using the biased self-avoiding walk (BSAW) model [5], we pointed out a dramatic difference in the effect of excluded volume between two and three dimensions in the vicinity of the extremely stiff limit. In this model p is the probability of taking a gauche step and N is the number of steps in the chain. A crossover from its one-dimensional limit to an isotropic flexible chain limit occurs as the product $N^{\phi}p$ is increased from $N^{\phi}p \ll 1$ to $N^{\phi}p \gg 1$ where the index ϕ serves the role of a crossover exponent.

The purpose of this letter is two-fold. Firstly, by cell renormalisation we show the stiff-to-isotropic crossover exponent ϕ to be exactly one in agreement with the numerical results [5, 6]. While the previous argument [5] for this result was based on a scaling assumption, the present work is based on renormalisation rather than an explicit scaling assumption. Secondly, we show a substantial dimensional difference between two and three dimensions and that in the 'Flory' limit of $N \to \infty$ with fixed p the chain eventually crosses over to the self-avoiding walk (SAW) limit as $Np \to \infty$ by use of the renormalisation flows.

The dimensional difference referred to above results from the manner in which the isotropic limit $Np \gg 1$ is probed. If p is held fixed, however small, and $N \to \infty$, then the resulting behaviour should be that of an ordinary SAW. On the other hand, if $p \to 0$ and $N \to \infty$ with fixed $Np = C$ and then C is increased, we should obtain an isotropic random walk (RW) behaviour in three dimensions while the SAW results are still obtained in two dimensions. Such a dimensional difference was already anticipated by Petscheck [7], and can be illustrated using a simple physical picture [6].

In our previous Monte Carlo study [6], we have generally fixed p and varied N; however, a clear crossover from RW to the SAW limit was not observed in three dimensions (even for very large N in some cases). Nevertheless we concluded that such a crossover was about to take place based on the universality concept, as the

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local slope of $\log\langle R^2\rangle$ against $\log N$ was beginning to show a marked deviation from its RW value for the largest values of N and for $p = 0.2$ and 0.3.

The crossover from RW behaviour to SAW behaviour in this Flory limit was recently estimated [8] by a Flory-type approximation to occur at

$$N^* p^{d/(4-d)} \sim 1. \tag{1}$$

When $d = 2$ (1) predicts the RW-to-SAW crossover to occur in the vicinity of the stiff-to-isotropic crossover, so that there is no isotropic RW regime in two dimensions. On the other hand, in three dimensions, $N^* \sim p^{-3}$ is very large for small p, and there is a large isotropic RW region with the eventual RW-to-SAW crossover being virtually unobservable by Monte Carlo simulations unless the chain length is considerably extended for $p \ll 1$.

To illustrate our approach, let us first review the basic cell renormalisation method for the BSAW model. The statistical weight of a BSAW in each stage of Monte Carlo simulation is described by a probability p of taking a gauche step and $1-p$ of a trans step. Correspondingly, we assign the fugacity G to each gauche step and K to each trans step in the grand canonical ensemble of BSAW. If $A(N, N_G)$ is the number of N-step BSAW with N_G gauche steps, the generating function for BSAW is given by

$$W(K, G) = \sum_{N=0}^{\infty} \sum_{N_G=0}^{N} A(N, N_G) K^{N-N_G} G^{N_G}. \tag{2}$$

This can be rewritten as

$$W(K, G) = \sum_{N=0}^{\infty} K^N B\left(N, \frac{G}{K}\right) \tag{3}$$

where

$$B(N, x) = \sum_{N_G=0}^{N} A(N, N_G) x^{N_G}. \tag{4}$$

Since the asymptotic behaviour of $B(N, x)$ satisfies (see, e.g., [9])

$$B(N, 1) \propto \mu^N N^{\gamma-1} \tag{5a}$$

$$B(N, 0) \propto 1 \tag{5b}$$

we expect a scaling form to result

$$W(K, G) = \sum_{N=0}^{\infty} K^N f\left(N^{\phi} \frac{G}{K}\right) \tag{6}$$

with

$$f(x) \simeq \begin{cases} \text{constant} & \text{for } x \to 0 \\ x^{(\gamma-1)/\phi} \exp(x^{1/\phi}) & \text{for } x \to \infty. \end{cases} \tag{7}$$

As the partition function is to be conserved under the renormalisation in usual critical phenomena (see, e.g., [10] for a review of renormalisation group theory), we aim to conserve the generalised form of this generating function, which will in principle depend on a large number of parameters taking into account all the correlations that will be introduced upon renormalisation while rescaling all lengths by a factor of, say, b. In the framework of our cell renormalisation, we try to approximate renormalisation

by equating only spanning contributions to $W(K, G)$ within a cell of b^d, which is the statistical weight carried over to the generating function after coarse graining, with renormalised fugacity K' or G' depending on the renormalised step. The critical indices are then calculated from the eigenvalues of the recursion relations linearised about the critical fixed point in the same way as in usual critical phenomena.

For the purpose of calculating the crossover exponent ϕ, we use a two-parameter renormalisation with the so-called corner rule [11] and renormalise all outgoing walks into a single step walk. To identify the first step in the cell, we must fix the incoming step, say, going into the cell through the lower-left corner along the horizontal direction. Walks that leave the cell by way of the right edge rescale to a single horizontal step which is a rescaled trans step, while walks leaving by the top edge rescale to a single gauche step (see figure 1). The recursion relations are obtained from these two different spanning contributions to $W(K, G)$

$$K' = \sum_{m,n} a_{m,n} K^m G^n \tag{8a}$$

$$G' = \sum_{m,n} b_{m,n} K^m G^n \tag{8b}$$

where $a_{m,n}(b_{m,n})$ is the number of SAW leaving the cell along the horizontal (vertical) direction with m trans steps and n gauche steps.

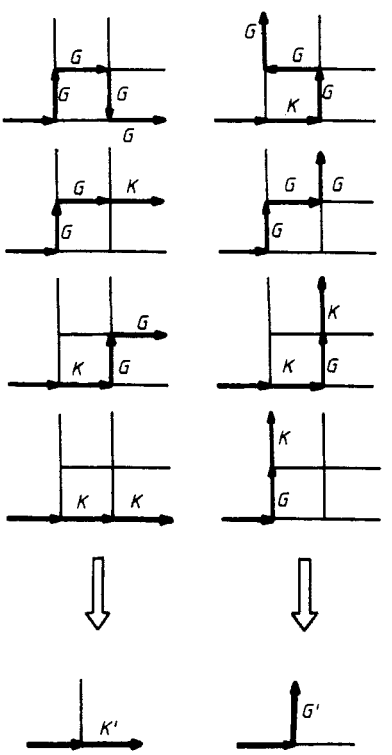

Figure 1. Two-parameter cell renormalisation of the biased self-avoiding walk is illustrated for a 2×2 cell on the square lattice. Walk configurations shown at top renormalise to the steps shown at bottom. The step coming into the cell is constrained to be horizontal.

For example, by counting all possible walks spanning the 2×2 square cell as shown in figure 2 we get the recursion relations

$$K' = K^2 + 2KG^2 + G^4 \tag{9a}$$

$$G' = GK + K^2G + G^3 + G^3K. \tag{9b}$$

We see that there exist two non-trivial fixed points at $(K^*, G^*) = (1.0, 0.0)$, (0.466, 0.466), the former being a one-dimensional fixed point and the latter being an isotropic SAW fixed point. Since we are interested in a crossover from a one-dimensional fixed point, we can linearise (9) near that point. Thus we obtain

$$\begin{bmatrix} \Delta K' \\ \Delta G' \end{bmatrix} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \Delta K \\ \Delta G \end{bmatrix}. \tag{10}$$

The eigenvalues of transformation matrix are $\lambda_{1,2} = 2$, which carry the crossover exponent of exactly one. By a similar method, critical index ν near the isotropic SAW fixed point can also be obtained resulting in the recovery of the result of earlier calculation [12] for isotropic SAW. The generalisation to a simple cubic or any hypercubic cell is straightforward.

Generally, critical indices obtained by a small-cell renormalisation cannot be regarded as trustworthy by themselves. However, since much of the inherent approximation involved in this method derives from the inter-cell effects which should diminish as the cell size is increased, often large-cell extrapolations [11] are employed to obtain more accurate estimates of critical exponents. For the present question of the crossover exponent, it turns out that the exact evaluation is possible for all cell sizes and in all dimensions as follows. Consider any hypercubic cell of size b^d. The leading terms of recursion relations are given as

$$K' = K^b + bG^2K^{b-1} + \ldots \tag{11a}$$

$$G' = G(K^{b-1} + K^b + K^{b+1} + \ldots + K^{2b-2}) + G^3(\ldots) + \ldots . \tag{11b}$$

Linearising these near the one-dimensional fixed point at $(1, 0)$, we get $\lambda_{1,2} = b$ for all b. Thus, the *infinite* cell limit of the crossover exponent is *one*.

While the two-parameter renormalisation serves well in the above discussion, a simple scaling argument suggests that the rescaling of the stiff linear chain must also renormalise the extent of the excluded volume effect. Since this must be responsible for the differences exhibited between two- and three-dimensional stiff linear chains, we must also include the excluded volume parameter as the third parameter to be

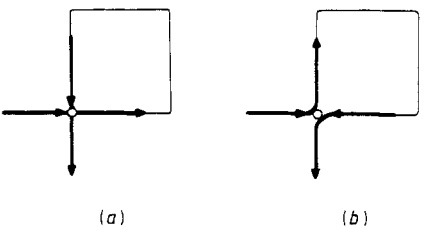

Figure 2. Two different configurations of self-intersection are shown. Renormalised fugacities are (*a*) $K'(K'+G')(1-u')$ and (*b*) $G'(K'+G')(1-u')$. The first step coming into the cell is constrained to be horizontal and the last step going out of the cell is chosen arbitrary.

renormalised if we were to be able to discuss the dimensional differences in the crossover behaviour. To incorporate this parameter we use the so-called Domb-Joyce model [13], in which a parameter u represents excluded volume, $u = 1$ corresponding to full excluded volume and $u = 0$, no excluded volume. To this effect, we extend the recent work [14] of Family and Gould which allows intersections of a flexible walk with itself, multiplying a weight $(1-u)$ for each intersection.

To find the recursion relations we must formulate some rule which corresponds to the *spanning rule* that was used above. In what follows, we will illustrate the results obtained using the following general rule.

(i) For the rescaled gauche and trans steps, we use the same rule as before, except for the inclusion of intersection. Thus we get

$$K' = \sum_{k,m,n} a_{k,m,n}(1-u)^k K^m G^n \tag{12a}$$

$$G' = \sum_{k,m,n} b_{k,m,n}(1-u)^k K^m G^n \tag{12b}$$

where $a_{k,m,n}$ and $b_{k,m,n}$ are the analogous quantities to those in $(8a)$ and $(8b)$, respectively, having k intersections.

(ii) To renormalise u, we must consider walks which rescale to an intersecting walk on the renormalised cell. For this, we count walks that first leave the cell along a particular direction and then re-enter along a different direction to self-intersect at the origin.

To obtain a concrete recursion formula, we have to make additional approximations since it is impossible to generate an infinite number of (self-intersecting) walks even on a small cell. We can, however, plausibly argue that keeping all possible outgoing and incoming walks of size up to the longest SAW (b^d steps) on the cell should be sufficient for our purpose. Also, to obtain (8) and (12) we have fixed an incoming step in a certain direction since, by symmetry of the cell, the choice of such a step does not make any difference for the resulting recursion relations. However, for the renormalisation of u, a different choice of the direction of the incoming step would result in a different recursion relation since the renormalised outgoing step would be different. Therefore arbitrary choice of incoming step is not adequate for our current purpose.

We first count each outgoing walk twice, considering it as if the walk with first step as gauche gives a different configuration from that with first step as trans. Applying this rule on the re-entering step as well, one complete walk intersecting at the origin results in four different configurations. This procedure leads to a recursion formula of the form

$$(K'+G')^2(1-u') = (K+G)^2 \sum_{k,m,n} c_{k,m,n}(1-u)^k K^m G^n \tag{13a}$$

where $c_{k,m,n}$ is the number of walks described above, having k intersections, m trans steps and n gauche steps excluding first and re-entering steps whose contributions are the prefactor $(K+G)^2$.

Equation $(13a)$ can also be obtained from the following rule with the incoming step fixed. Allow two types of intersecting configurations as shown in figure 2 and count the re-entering step in each case twice (once as trans and once as gauche equally). Walks leaving the cell along the right (top) edge and re-entering along the top (right) edge can be rescaled into the self-intersection of type figure $2(a)$ (figure $2(b)$). Having these two types of configurations and taking the simple average with equal weighting, we obtain $(13a)$.

We have counted, by computer, all possible walks of up to twelve steps (six outgoing and six re-entering) on the square lattice and sixteen steps on the simple cubic lattice, each of cell size $b = 2$, in order to obtain the recursion relations with these rules. As a result, we found two non-trivial isotropic SAW and RW fixed points (K^*, G^*, u^*) at (0.4656, 0.4656, 1), (0.4597, 0.4597, 0) for the square lattice and at (0.2972, 0.2972, 1), (0.2911, 0.2911, 0) for the simple cubic lattice. In addition we found a line of fixed points between (1, 0, 1) and (1, 0, 0). Since, without allowing immediate returns (or allowing but counting them as gauche steps), there is no difference between the one-dimensional RW and SAW, every point on the line connecting these two points describes the identical one-dimensional behaviour.

While the full flow diagram can be drawn in the three-dimensional parameter space, it is difficult to visualise three-dimensional flows on a piece of paper. Also since we are interested in how the chain crosses over from its one-dimensional limit to the isotropic SAW or RW limit, it is natural to look at the flows in the plane which contains these fixed points. In figures 3(a) and 3(b) we see clear differences between two and three dimensions. In three dimensions there is a bifurcation line connecting a point

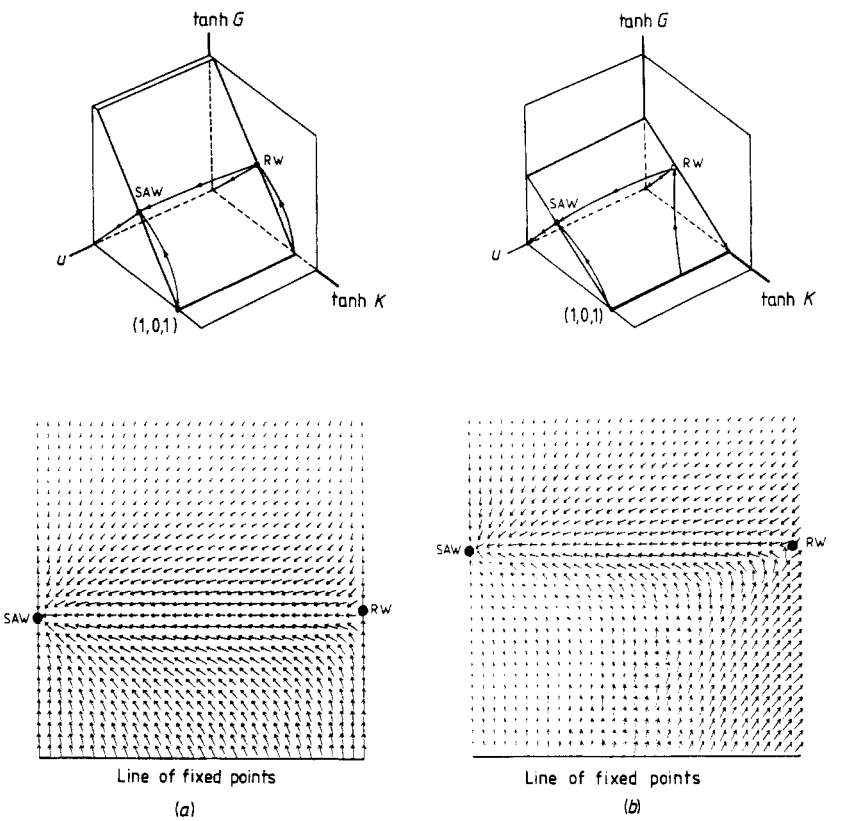

Figure 3. Flow diagram from a three-parameter cell renormalisation of the biased self-avoiding walk is illustrated for a 2×2 cell on (a) the square lattice and (b) the simple cubic lattice. (See text for rules used.) At top, isotropic self-avoiding walk (SAW) and isotropic random walk (RW) fixed points are marked and flows between fixed points are indicated with arrowed full lines. At bottom, the local directions of flow for the points on the plane as shown at top are indicated by arrows.

with $u>0$ and the flexible RW fixed point. Close to this line, the flows are first to the RW fixed point and then to the SAW fixed point, showing that the chain will eventually cross over to the SAW limit. In two dimensions, however, this line lies in the plane of $u=0$ and for any $u>0$ flows are directly to the SAW fixed point. This difference is consistent with our earlier observation based on Monte Carlo simulations.

In the above discussions we have presented one of the most reasonable ways of weighting among many possible ways for the first and re-entering steps. We have, however, also examined other types of weighting, some of which we introduce in the following.

(A) The first step is weighted as gauche $(2d-2)$-times more than as trans. This is because there are $(2d-2)$ different ways of having the incoming step in a different direction from the first step in the cell while there is only one way in the same direction. Applying the same rule on the re-entering step as well, we obtain a recursion relation for u of the form

$$(K'+(2d-2)G')^2(1-u')=(K+(2d-2)G)^2\sum_{k,m,n}c_{k,m,n}(1-u)^kK^mG^n \tag{13b}$$

where $c_{k,m,n}$ is the same quantity as in (13*a*).

(B) With the first step fixed, taking either one of the two loop configurations shown in figure 2, and counting the re-entering step as gauche and trans once each equally, we obtain a corresponding recursion formula.

(C) With the first step fixed along the horizontal direction, we count the re-entering step gauche if all other steps are trans, and otherwise as trans. This is because for $G=0$, the chain is strictly one dimensional and a loop configuration is not possible and also because, for a stiff chain, trans steps have much higher statistical weight than gauche. In this case, the recursion relation takes the form of

$$K'G'(1-u')=\sum_{k,m,n}c'_{k,m,n}(1-u)^kK^mG^n \tag{13c}$$

where $c'_{k,m,n}$ is the number of walks described above.

Counting all walks of up to twelve steps for two dimensions and sixteen steps for three dimensions, appropriate recursion relations have been obtained for these and other possible rules and the fixed points and the flows have been calculated as usual. We find unexpectedly that the flow diagrams are quite sensitive to the weight of the first step, as follows.

Rule (A) does not show any dimensional difference and all flows are from the one-dimensional fixed points to the SAW fixed point without showing RW behaviour. However, we can argue that by this rule the same configuration with the first step as gauche has been counted more than necessary resulting in a chain more likely to be flexible. In rule (B) in three dimensions, missing some of the possible loop configurations results in the bifurcation line moving closer to the $u=0$ plane. The flow diagram still shows a RW behaviour, though weaker than figure 3(*b*), and then finally flows are to the SAW fixed point. Finally, rule (C) produces, although there is no rigorous justification of weighting for the first step, the most clear-cut dimensional difference in the crossover behaviour. There is no one-dimensional line of fixed points, but rather the two fixed points are different in this case. The bifurcation line is strictly from the one-dimensional SAW fixed point to the RW fixed point and all flows from the one-dimensional limit are first to the RW fixed point and finally to the SAW fixed point in three dimensions. In any of these cases, the immediate return, allowed and counted as a gauche step, does not affect the final result.

We have presented a simple cell renormalisation scheme for the BSAW model, and showed that (i) the stiff-to-flexible crossover exponent is exactly one in all dimensions and for all cell sizes, and that (ii) the RW-to-SAW crossover behaviour is clearly different in two and three dimensions. While somewhat different results have been obtained depending on how the first step is weighted, the most acceptable rule produces clearly different crossover behaviour in the limit $N \to \infty$ in two and three dimensions supporting our earlier observations.

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