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Renormalization of Self-Avoiding Walks on the Square Lattice

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Abstract

The complications encountered in direct renormalization approaches for the self-avoiding walk problem are discussed. Using a decimation transformation on the square lattice sequences of approximants to the critical exponent ν and to the inverse connective constant $K_c(1/K_c=\mu)$ are obtained.

1. Introduction

Recently [1,2] a renormalization method has been applied to the self-avoiding walk (SAW) problem on two dimensional lattices. The method is based upon direct comparison between SAW's on a lattice G and SAW's on another lattice G' isomorphic to the original lattice G . The lattice spacing of G' is larger by a scale factor ℓ . In order to study the SAW problem as a critical phenomenon, the correlation length ξ is introduced:

$$\xi^2 = \frac{\sum_W P(W) R^2(W)}{\sum_W P(W)} \quad (1)$$

The summation in (1) is extended over all possible SAW's W on G , $R(W)$ is the end-to-end distance of W and $P(W)$ its weight, which in the simplest case is $P(W)=k^N$ where N is the number of steps of W . In this case, it can be shown [1] that ξ diverges at some critical value $K_c (= 1/\mu)$, where μ is the connective constant of the lattice [3]) as

$$\xi \sim (1-K/K_c)^{-\nu} \quad (2)$$

where the critical exponent ν determines the asymptotic behaviour of the mean square end-to-end distance of N -stepped walks W_N , i.e.,

$$\langle R_N^2 \rangle = \frac{\sum_{W_N} R^2(W_N)}{\sum_{W_N} 1} \approx N^{2\nu} \quad (3)$$

The renormalization concept is introduced by assuming the existence of a mapping with the following properties: (i) Every SAW W' on G' is the image of a specific set $\{W\}_{W'}$ of SAW's

W on G (two such sets have no common elements). (ii) If the end-to-end distance of W' is R' (with respect to the spacing of G'), then the end-to-end distance of any SAW $W \in \{W\}_{W'}$ is $R = \ell R'$ (with respect to the spacing of G). (iii) For the walk-weights we can write:

$$P(W'; K') = \sum_{W \in \{W\}_{W'}} P(W; K) \quad (4)$$

(iv) The transformation (4) has a fixed point, such that $K = K' = K^*$. The correlation lengths are then related by

$$\xi(K') = \ell^{-1} \xi(K) \quad (5)$$

and ν is obtained by linearising the transformation (4) at the fixed point K^* , i.e.,

$$\nu = \ln \ell / \ln \lambda \quad (6)$$

where λ is the relevant ($\lambda > 1$) eigenvalue of the transformation (4) at K^* .

For the one-dimensional "chain" this procedure yields exact results for the SAW problem [2] as well as for the random walk problem [4]. However, in higher dimensionality one is confronted with serious difficulties when trying to calculate ν using these ideas. It is a puzzle to find a rule by which the mapping of SAW's from G to G' will not generate distant steps on G' . For instance, in the decimation transformation on the triangular lattice [1] some of the SAW's on G cannot be mapped into SAW's which are embedable on the decimated triangular lattice (G') unless links connecting distant sites are introduced on G' . In an approximation scheme one may neglect the configurations generating these distant steps or may choose to introduce distant steps

on both G and G' from the outset. In the latter case, step-weights L and L' for 2nd- neighbours, M and M' for 3rd- neighbours and so on, are introduced and (4) is replaced by

$$P(W'; K', L', M', \dots) = \sum_{W \in \{W\}_{W'}} P(W; K, L, M, \dots) \quad (4')$$

There are two more complications when trying to write down (4) in a form convenient for computations. The number of self-avoiding walks on G consistent with a SAW W' on G' will not depend only on a "simple" rule of mapping but also on the structure of W' , therefore, it is hard to see how (4) can be satisfied without taking account of the shape of the SAW's. In our opinion (4) cannot be satisfied for any non-trivial SAW problem and, it must be pointed out that, results obtained by such renormalization procedures should be looked for as approximations the validity of which is difficult to access. One may hope that by introducing gradually step-weights with memory (i.e. step-weights which take account of the structure of SAW's) the approximations will become better. To examine this point the step-weights $K, L, M, \dots$ will be replaced by a set of step-weights with memory: $\{K\} \equiv \{K \in \{K\}_n; n = 0, 1, 2, \dots\}$, where the set $\{K\}_n$ includes all possible step-weights that take the nature of up to n previous steps into account. For example, $\{K\}_0 \equiv \{K, L, M, \dots\}$ and $\{K\}_1 \equiv \{K_1, L_1, M_1, \dots\}$ where K_1 is the step-weight of a K -step making an angle, with its preceding step, characterized by the subscript i . The introduction of step-weights with memory is, of course, an unwanted complication, however, it should be realized that it reflects the essential property of the SAW problem, its long range nature.

Step-weights with memory were introduced by M.Napiórkowski, E.H.Hauge and P.C.Hemmer [2], in the present work we shall try to explore this concept by extending the memory as far as possible, and observe the effect of this extension on the approximants.

Another complication concerns the number of configurations on G generating a single step on G' . In both the "decimation transformation" [1] and in the "majority rule cell-transformation" [2] there is an infinite number of configurations on G generating a single step on G' . For practical purposes one must restrict these configurations by using a "simple" rule. Shapiro [1] uses a "cluster approximation", i.e., the configurations on G generating a single step on G' are restricted within a "small" cluster of points. Napiórkowski et al.[2] use a "cumulant-like" method, in their n^{th} order approximation only configurations which use at most n "intercell" steps are considered.

In the next section we consider a decimation transformation on the square lattice (scale factor $\ell=\sqrt{2}$), the configurations on G generating a single step on G' are restricted to use at most a specified number of steps on G . In particular, in the two-steps approximation the configurations on G generating a single step on G' involve at most two steps on G . Three-steps approximants will also be considered.

2. Decimation transformation on the square lattice

Figure 1 shows the square lattice, G , before (broken lines) and after, G' , (full lines) a decimation transformation by a dilation factor $\ell = \sqrt{2}$. In the two-steps approximation a single step of a SAW on G' is generated by using at most two steps on G . A 2nd neighbour step L' is thus generated on G' (two colinear steps on G) so that an L -step should be included from the outset on both lattices. Figure 2 shows all possible ways a K' -step can be generated. The renormalization equations are

$$\left. \begin{aligned} K' &= 2K^2 + L \\ L' &= K^2 \end{aligned} \right\} \quad (7)$$

(7) has a non-trivial fixed point ($K^* = 1/3, L^* = 1/9$) with a relevant eigenvalue yielding $\nu = 0.6385 \dots$.

Within the two-steps approximation we may include in (7) step-weights from the set $\{K\}_1$. In order to describe the structure of a KK-configuration (i.e. a configuration of two successive K-steps) we must introduce two new parameters (K_1 and K_2) which correspond to the second K-step according to the angle they form with their preceding step (0° and 90° , respectively). Similarly, two new parameters are needed for each of the configurations: KL (L_1 corresponding to 45° and L_2 corresponding to 135°), LK (K_3 and K_4 corresponding to 45° and 135° , respectively) and LL (L_3 and L_4 corresponding to 0° and 90° , respectively). Instead of introducing these parameters in (7) all at once, we may follow a step by step procedure. We first consider the parameters corresponding to the "shortest" two-steps configuration which is the KK-configuration.

Introducing K_1 and K_2 we find:

$$K' = 2KK_2 + L$$

$$L' = KK_1 \quad (7')$$

$$K'K'_1 = 2KK_2(K_1K_2 + K_2^2 + L) + L(2KK_2 + L)$$

$$K'K'_2 = KK_2(K_1K_2 + 2K_2^2 + 2L) + L(2KK_2 + L)$$

From (7') we find a non-trivial fixed point ($K^*=0.3709$, $L^*=0.1327$, $K_1^*=0.3579$, $K_2^*=0.3210$) with a relevant eigenvalue corresponding to $\nu=0.6755\dots$. We go further and introduce combinations of one K' - and one L' -step. The transformation now reads:

$$K' = 2KK_2 + L$$

$$L' = KK_1$$

$$K'K'_1 = 2KK_2(K_1K_2 + K_2^2 + L_1) + L(2KK_2 + L)$$

$$K'K'_2 = KK_2(K_1K_2 + 2K_2^2 + L_1 + L_2) + L(K_3 + K_4)K_2 + L$$

$$K'L'_1 = KK_1K_2(K_1 + K_2) + LK_3K_1 \quad (7'')$$

$$K'L'_2 = KK_1K_2^2 + LK_4K_1$$

$$L'K'_3 = KK_1K_2(K_1 + K_2) + KK_1L_1$$

$$L'K'_4 = KK_1K_2^2 + KK_1L_2$$

The eigenvalue corresponding to the fixed point ($K^*=0.6205$, $L^*=0.2409$, $K_1^*=0.3883$, $K_2^*=0.3058$, $L_1^*=0.1348$, $L_2^*=0.0594$, $K_3^*=0.3471$ and $K_4^*=0.1529$) yields $\nu=0.7386\dots$.

If we proceed to introduce the LL-configuration (L_3 and L_4), then at this stage the renormalization equations do not have a fixed point. The sequence of two-steps approximations is thus discontinued here.

Let us consider a three-steps approximations by restricting

the configurations on G generating a single step on G' to use at most three K or/and L steps. In this case higher order steps M' and N' are generated on G' and these will be also included on G (see figure 3) from the outset. However, M and N will be considered as second-order quantities so that at most one of these and one K - or L -step may be combined to yield a single step on G' . Figure 3 shows all possible ways a K' step may be generated within this approximation. The weights for simple steps are now coupled by:

$$\begin{aligned}
 K' &= 2K^2 + L + 6K^2L + 4KN \\
 L' &= K^2 + M + 4K^2L + 4KN \\
 M' &= 2K^2L + 4KN \\
 N' &= K^2L + 2KN
 \end{aligned} \tag{8}$$

(8) has a fixed point ($K^* = 0.2218$, $L^* = 0.0898$, $M^* = 0.0159$, $N^* = 0.0079$) with a relevant eigenvalue corresponding to $v = 0.5686$. The first approximant to v is again very low. However, it is now possible to extend the memory, in the same way as in the two-steps approximation, at least until an $N'N'$ combination is included. Introducing K_1 , and K_2 in (8) we find:

$$\begin{aligned}
 K' &= 2KK_2 + L + 6K^2L + 4KN \\
 L' &= KK_1 + M + 4K^2L + 4KN \\
 M' &= 2K^2L + 4KN \\
 N' &= K^2L + 2KN \\
 K'K'_1 &= LC_0 + 2KK_2C_1 + 2K^2L(C_1 + C_2 + C_3) + 2KN(C_0 + C_4) \\
 K'K'_2 &= LC_0 + KK_2(C_1 + C_4) + K^2L(C_1 + C_2 + C_3 + C_4 + C_5 + C_6) + KN(2C_0 + C_1 + C_4)
 \end{aligned} \tag{8'}$$

with $C_0 = L + 2KK_2 + 6K^2L + 4KN$, $C_1 = L + K_2^2 + K_1K_2 + 2(K_1 + K_2)LK + K_2LK + K_2N + 2NK$,
 $C_2 = C_1 - K_2(LK + N)$, $C_3 = C_2 + K_1(N - K_2) - (K_1 + K_2)LK$, $C_4 = C_3 + K_2N$,

$$C_5 = L + (K_2 + K_1)N + 2NK, \quad C_6 = C_3 + K_1 K_2 - K_2^2 + K_2 N - K_1 N.$$

(8') yields for the critical exponent $\nu = 0.5801$. Ten parameters are involved in the third approximant ($K, L, M, N, K_1, K_2, L_1, L_2, K_3$, and K_4), whereas in the fourth approximant two more need to be introduced L_3 and L_4 . These two approximants were also calculated on a computer, they are tabulated in table I where all our results are listed.

As mentioned earlier, within the three-steps approximation it is possible to continue the sequence of approximants by including "longer" configurations. However, since the status of the convergence question of such a sequence is unclear, it seems wise to consider the three-steps approximation as a second-order approximation (since second-order quantities M' and N' are generated) and discontinue the sequence at this point where all second-order configurations on G' have been included (a similar practice is followed in the renormalization approach for the spin-Ising model [5]).

Then, the final approximants to $\nu(0.7538)$ and to $K_c(0.378)$ in the three-steps approximation are seen to be in good agreement with the best estimates from the "exact enumeration" [6] method, this indicates the usefulness of step-weights with memory for the SAW problem. We finally note that, K_c is obtained as the intersection of the "K-axis" (i.e. $K=K_1=K_2$, all other parameters zero) with the corresponding critical surface.

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TABLE I

Two-steps approximants			Three-steps approximants		
no. of parameters	ν	K_c	no. of parameters	ν	K_c
2	0.6385	0.3921	4	0.5686	0.3337
4	0.6755	0.4220	6	0.5886	0.3465
8	0.73863	0.4469	10	0.6268	0.3772
			12	0.7538	0.3780

				0.75*	0.3790 [†]

* Conjectured value of $\nu[6]$, [†] $K_c = 1/\mu$, where μ is the connective constant of the lattice which from the exact enumeration method is estimated $\mu \sim 2.6385[7]$.

Figure captions

Fig.1. Decimation transformation of the original square lattice G (broken lines) to a new square lattice G' (full lines). Steps on G are classified as follows: (Ok) is a K -step, (OL) is an L -step, (OM) is an M -step and (ON) is an N -step.

Fig.2 Graphical representation of the expression (7) for K' .

Fig.3 Graphical representation of the expression (8) for K' .
The last four terms are combinations of one K - and one N -step.

Figure 1.

Figure 2.

Figure 3.