θ point of a linear polymer in 2 dimensions: a renormalization group analysis of Monte Carlo enumerations
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To cite this version:

HAL Id: jpa-00210750
https://hal.archives-ouvertes.fr/jpa-00210750
Submitted on 1 Jan 1988

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1. Introduction.

Most recently the collapse transition [1] of a linear polymer in two dimensions has been the object of considerable interest. Various methods have been used in order to characterize the scaling properties of polymer conformations at the θ temperature, marking the separation between self-avoiding chain and collapsed regimes.

Powerful numerical techniques, like Monte Carlo simulation [2], exact enumerations analysis [3, 4], or phenomenological renormalization group (RG) calculations on strips [5, 6], have given rather disperse predictions, which, together with an experimental estimate [7], are not yet sharp and consistent enough to allow a precise guess on the values of the exponents. As a consequence, it is also difficult to judge about the possible validity of very appealing recent theoretical conjectures concerning the fractal and entropic properties of polymer conformations at the θ point.

Indeed a non rigorous argument by Coniglio et al. [8], suggests that the statistics of polymer rings at the theta point in d = 2 could coincide with that of the external perimeter, or hull of a percolation cluster at threshold. This would lead to a value \(d_{\theta} = 7/4\) of the fractal dimension of polymers at the θ point, the dimension obtained recently on the basis of numerical investigations [9, 10], conjectures [11] and exact theoretical arguments [12] for the percolation hull. Such value of \(d_{\theta}\) has also been obtained for a model of self-avoiding walk on a hexagonal lattice with random forbidden hexagons [13]. For this model with vacancies explicit predictions have been made also for the tricritical entropic and cross-over exponents, \(\gamma_t\) and \(\phi_t\), respectively [13].

In this work we consider the standard model for polymers at the θ point, in which polymer configurations are represented by self-avoiding walks (SAW) on a (square) lattice and an attractive energy \(-e (e > 0)\) is associated with each pair of neighbour- ing visited sites, which are not adjacent along the walk.

Our purpose is to determine the θ point exponents by enumeration methods. The strategy we follow, however, is not standard, as we will show below. Its
power mostly derives from the circumstance that many advantages peculiar of very different and more standard methods, like exact enumeration, Monte Carlo simulation, and phenomenological renormalization group, are somehow optimally combined in our techniques.

The starting goal of our approach is a substantial extension of the existing exact enumeration data available for the problem, on the basis of a very accurate Monte Carlo strategy. In this way we more than double the length of the existing truncated series, with a relatively limited computational effort. Of course, the price we have to pay for this extension is unavoidable (small) fluctuations with respect to the exact data. It thus seems necessary to obtain more appropriate methods of analysis, as little sensible as possible to such fluctuations.

It is indeed with respect to this problem that we make the most original methodological proposal of this paper, namely an analysis of exact or approximate enumeration data, based on renormalization group ideas [14].

This paper is organized as follows. In section 2 we briefly report on our Monte Carlo enumeration technique and results, and start to apply some standard methods of analysis to our data.

In the next section we illustrate our new way of analyzing exact or approximate enumerations, based on the renormalization group idea. We apply this approach to the problem of locating the theta point and of determining its exponents in section four. In the last, fifth section we summarize our results and compare them with other numerical and theoretical predictions.

2. Exact and Monte Carlo enumerations.

For the interacting SAW model described in the introduction extensive exact enumerations in \( d = 2 \) have been produced very recently by Ishinabe, for the square lattice and walks up to 20 steps [3], and by Privman, for the triangular lattice and walks up to 16 steps [4]. In both these papers the analysis focuses on the asymptotic behaviour of the average square end-to-end distance for large number of steps, \( N \).

If we indicate by \( W \) a SAW with \( |W| \) steps, the average square end-to-end distance for walks with \( N \) steps is:

\[
R_N^2 = \sum_{|W|=N} r^2(W) \sum_{|W|=N} e^{wB(W)}
\]

where the sumsations are over all SAW of \( N \) steps, and \( r^2(W) \) and \( B(W) \) are, respectively, the square end-to-end distance, and the number of nearest neighbour attractive interactions of \( W \). In equation (2.1) the dimensionless energy \( \omega = \epsilon / k_B T \), measures the strength of the attractive interactions.

For large \( N \) one expects:

\[
R_N^2 \sim N^{2\nu}
\]

with \( \nu = \nu_{SAW} \) for \( \omega < \omega_t \), \( \nu = \nu_t \) for \( \omega = \omega_t \), and \( \nu = 1/d \) for \( \omega > \omega_t \). \( \omega_t \) is the value of the interaction parameter at the theta point. In two dimensions \( \nu_{SAW} = 3/4 \) [15]. \( \omega < \omega_t \) corresponds to the excluded volume regime, dominated by repulsive forces. For \( \omega > \omega_t \), we have the collapsed regime, in which attractive forces prevail. In this range of \( \omega \) values the polymer prefers compact configurations, with fractal dimension \((= 1/\nu)\) equal to the space dimensionality.

For \( \omega \) in the neighborhood of \( \omega_t \) and \( N \) large enough, a tricritical sort of scaling is expected for \( R_N^2 \):

\[
R_N^2 \sim N^{2\nu_t} f \left( \frac{\Delta \omega}{N^{-\phi_t}} \right)
\]

where \( \Delta \omega = \omega - \omega_t \) and \( \phi_t \) is a crossover exponent [1].

Another important aspect of the theta point problem, which we investigate in this paper, is the entropic one. If we call \( C_{NM} \) the number of \( N \)-step self-avoiding walks with \( M \) nearest-neighbour attractive interactions, we expect:

\[
\sum_M C_{NM} e^{wM} = C_N(\omega) \sim N^{\gamma - 1} K_c(\omega)^{-N}
\]

for \( N \to \infty \). Also in this case the \( \gamma \) exponent should assume a peculiar tricritical value, \( \gamma_t \), for \( \omega = \omega_t \). \( K_c(\omega) \) is the effective connectivity constant of the walk, which for \( \omega = 0 \) (SAW case), has been estimated as \( = 0.3790 \) [16].

The Monte Carlo strategy we used in order to extend (approximately) the exact enumeration results is very simple and efficient. The presence of interaction \( \omega \neq 0 \) leads to the necessity of an importance sampling of the polymer configurations. A configuration with \( N \) steps and \( M \) nearest neighbour attractive interactions should occur with a probability proportional to \( e^{wM} \), the Boltzmann factor appropriate to the configuration itself. We do not achieve this by the introduction for the \( N \)-step chain of a markovian dynamics (e.g. a reptation dynamics [17]) relaxing to the correct canonical equilibrium. We choose instead to generate each configuration dynamically, with a growth process guaranteeing automatically the correct occurrence probability for each configuration.

Imagine a walk growing step by step. The first step is made by choosing at random among the 4 possible bonds connected with the starting point. The \( N \)-th step \((N > 1)\) can be made by walking along one of the three bonds different from that chosen for the \((N-1)\)-th step. We however include also the pos-
Table I. — Comparison of $R_i^2$ from our Monte Carlo method (right columns) with the exact values of reference [3] (left columns).

$$
\begin{array}{|c|c|c|}
\hline
N & R_i^2 \text{(exact)} & R_i^2 \text{(Monte Carlo)} \\
\hline
1 & 1.000000 & 1.000000 \\
2 & 2.666667 & 2.666679 \\
3 & 4.299065 & 4.299577 \\
4 & 6.633241 & 6.633317 \\
5 & 8.666068 & 8.665654 \\
6 & 11.406570 & 11.405511 \\
7 & 13.670183 & 13.668387 \\
8 & 16.722562 & 16.721195 \\
9 & 19.257318 & 19.256509 \\
10 & 22.538029 & 22.537776 \\
11 & 25.31682 & 25.32086 \\
12 & 28.82712 & 28.825884 \\
13 & 31.844266 & 31.842321 \\
14 & 35.553836 & 35.547345 \\
15 & 38.775188 & 38.773385 \\
16 & 42.670761 & 42.671431 \\
17 & 46.094535 & 46.095146 \\
18 & 50.171218 & 50.181653 \\
19 & 53.784422 & 53.794659 \\
20 & 58.032011 & 58.048096 \\
\hline
\end{array}
$$

Fig. 1. — Schematic representation of a cul de sac situation for the SAW.

(1) Here by nearest neighbours we mean sites which would feel a nearest neighbour attractive interaction with site $i$, if this would be visited.

sibility of abortion of the walk without performance of the $N$-th step.

Let us indicate by $n_i (0 \leq n_i \leq 3)$ the number of already visited sites which are nearest neighbours (1) of the $i$-th site ($i = 1, 2, 3$) accessible at the $N$-th step (with the convention $n_i = 0$ if this $i$-th site itself has been visited already). The step on the $i$-th site will be chosen with probability $\exp (n_i \omega_1)/3 \exp (3 \omega)$. Unless the three accessible sites are all in a cul de sac situation (all $n_i = 3$) for the SAW, like in the example of figure 1, abortion of the walk can occur with probability

$$
1 - \left[ \sum_{i=1}^{N} \exp (n_i \omega_1)/3 \exp (3 \omega) \right].
$$

Of course abortion also occurs if the walk steps on a site which has already been visited, and thus the SAW constraint is violated.

It is clear that all the $N$-steps SAW generated by this process occur with probabilities proportional to the correct Boltzmann factors due to their attractive interactions.

With respect to the SAW without attractive interactions, the computational cost of this strategy, in terms of aborted walks, increases with higher $\omega$ values. Due to the large amount of abortions, we found it convenient, for $\omega > 0$, to prevent abortion due to violations of the SAW constraint or to the other prescriptions above, by standard tricks, well known in the literature [18, 19].

With our importance sampling method we computed $R_i^2$ for $N \leq 40$ and for several different values of $\omega$. For each $\omega$ value our program, realizing the above importance sampling for the calculation of $R_i^2$, took about 8 hours of CPU time with a VAX 8600 Digital computer. In table I we report our results for three $\omega$ values and compare them with the exact data for $N \leq 20$ [3].

At $\omega$ strictly equal to 0, errors with respect to the
exact values [16] are extremely small (≈ 0.05 % for \( N = 27 \)). As clearly shown in table I, fluctuations remain rather limited also for relatively high values of \( \omega \) (≈ 0.13 % for \( N = 20 \) and \( \omega = 1.1 \), about twice the estimated \( \omega_t \)).

In order to get an idea of the accuracy of our Monte Carlo calculations for \( N > 20 \) and \( \omega > 0 \), we made several independent runs for \( \omega = 0.8 \) and we estimated fluctuations of \( R_N^2 \) still within ≈ 0.1 % for \( N \leq 30 \), and within ≈ 1 % for \( 30 < N \leq 40 \).

For an accurate evaluation of \( C_N(\omega) \) in the theta region, we also made use of our importance sampling method. In principle, to get \( C_{NM} \), one could study simply the noninteracting SAW (\( \omega = 0 \)). A standard method consists in generating a large number \( N' \), of \( N \)-step walks with a known entropy (e.g. random walks in which each step is free, apart from the constraint of not going opposite to the preceding one; these walks are of course \( 4.3^N - 1 \) in \( d = 2 \)).

One then obtains \( C_{NM} \) as the product of the total number of SAW with \( M \) interactions present in the sample times the ratio \( 4.3^N - 1 / N' \).

This method reveals accurate enough for computing \( C_N(\omega) \) in the theta region, i.e. the total number of \( N \) step SAW. However, fluctuations in the \( C_{NM} \) with large \( M \), due to the difficulty of sampling very compact configurations, lead to poorer results if equation (2.4) is used to obtain \( C_N(\omega) \) for \( \omega \) in the theta region. To this purpose we found it more convenient to use again our importance sampling procedure. Once a reasonably accurate value for \( C_N(\omega) \) is obtained, it is easy to get an estimate of the various \( C_{NM} \) from a given sample of interacting SAW (generated with some \( \omega \) in the range where we are actually interested to evaluate (2.4)). In this way the \( C_{NM} \) with \( M \) high, improve substantially and the results for \( C_N(\omega) \) improve even more. We give an example in table II, where comparison is made with exact enumeration data for \( N = 20 \) [3].

Altogether the accuracy of our Monte Carlo results is rather high. In the rest of this paper we try several methods of analysis of these results, with the purpose of determining the theta point multicritical properties.

A very immediate way of analyzing exact or approximate results for \( R_N^2 \) consists in computing effective exponents of the type

\[
2 \nu_N = \ln \left( \frac{R_N^2 / R_{N-2}^2}{\ln \left( \frac{N}{N-2} \right)} \right).
\]  

This definition turns out to be more appropriate with respect to one in which \( R_N \) and \( R_{N-1} \) are involved, due to the relatively strong odd-even oscillations determined by square lattice data. Of course, since expression (2.5) depends on only two values of the average end-to-end distance, we should be prepared to possibly large effects of the errors if Monte Carlo data are used for \( R_N \).

Table II. — Comparison of our Monte Carlo \( C_N(\omega) \) coefficients for \( \omega = 0.65 \) (right column) with the exact ones from reference [3] (left column).

<table>
<thead>
<tr>
<th>( C_{(0)} )</th>
<th>( C_{(0)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4000E+01</td>
<td>0.4000E+01</td>
</tr>
<tr>
<td>0.1200E+02</td>
<td>0.1200E+02</td>
</tr>
<tr>
<td>0.4323E+02</td>
<td>0.4323E+02</td>
</tr>
<tr>
<td>0.1293E+03</td>
<td>0.1293E+03</td>
</tr>
<tr>
<td>0.4499E+03</td>
<td>0.4499E+03</td>
</tr>
<tr>
<td>0.1356E+04</td>
<td>0.1356E+04</td>
</tr>
<tr>
<td>0.4680E+04</td>
<td>0.4680E+04</td>
</tr>
<tr>
<td>0.1431E+05</td>
<td>0.1431E+05</td>
</tr>
<tr>
<td>0.4838E+05</td>
<td>0.4838E+05</td>
</tr>
<tr>
<td>0.1503E+06</td>
<td>0.1503E+06</td>
</tr>
<tr>
<td>0.5017E+06</td>
<td>0.5017E+06</td>
</tr>
<tr>
<td>0.1568E+07</td>
<td>0.1568E+07</td>
</tr>
<tr>
<td>0.5205E+07</td>
<td>0.5205E+07</td>
</tr>
<tr>
<td>0.1631E+08</td>
<td>0.1631E+08</td>
</tr>
<tr>
<td>0.5392E+08</td>
<td>0.5392E+08</td>
</tr>
<tr>
<td>0.1695E+09</td>
<td>0.1695E+09</td>
</tr>
<tr>
<td>0.5580E+09</td>
<td>0.5580E+09</td>
</tr>
<tr>
<td>0.1759E+10</td>
<td>0.1759E+10</td>
</tr>
<tr>
<td>0.5773E+10</td>
<td>0.5773E+10</td>
</tr>
<tr>
<td>0.1822E+11</td>
<td>0.1822E+11</td>
</tr>
</tbody>
</table>

Plotted as a function of \( \omega \) the estimates (2.5) obtained on the basis of the exact enumeration data have the general trend already described in reference [4] for the case of the triangular lattice. The curves with different \( N \) have a clear tendency to intersect each other in a restricted region between \( \omega = 0.6 \) and \( \omega = 0.7 \).

In view of equation (2.3) it is natural to interpret the abscissas and ordinates of these intersection points as approximations to \( \omega_t \) and \( \nu_t \), respectively [4, 5].

Since the sequence of intersection coordinates of the above curves for increasing \( N \) is not extrapolable with standard methods [20] at this stage, we only attempted a preliminary determination of \( \omega_t \) and \( \nu_t \). We looked at the intersections among \( \omega_N \) curves with e.g. \( N = 10, 11, \ldots, 20 \) and, in view of the fact that the relatively large number of intersections (23) have a rather peaked distribution on the \( \omega \) axis, we took their average abscissa, \( \omega = 0.64 \) and the root mean square deviation around it, \( \Delta \omega = 0.02 \), as an approximation for \( \omega_t \) and as a tentative estimate of its uncertainty, respectively.

The corresponding value of \( \nu_t \) can be taken as the average of the various \( \nu_N \) for \( \omega = \omega_t \approx 0.64 \), i.e. \( \nu_t \approx 0.59 \).

Of course, as we will show below, a more conclusive location of \( \omega_t \) and determination of \( \nu_t \) could only be guessed after verifying how the values selected in this way would possibly shift upon replacement of the above set of \( \nu_N \) curves with more asymptotic ones (e.g. \( N = 15, 16, \ldots, 25 \), etc.). In other words, we plan to operate an extrapolation on
the statistical properties of intersections sets like that described above, and not on the individual intersections.

Once accepted the above one as an approximation for \( \omega_t \), we can also analyse the enumeration data with different techniques. Padé approximations are very useful for a determination of \( \nu \) exponents alternative to (2.5). These approximants also offer the great advantage of a much less pronounced sensibility to fluctuations of the \( R_{2N} \), than the ratio estimates (2.5). This will help us later in the analysis of our Monte Carlo enumerations.

In order to apply Padé analysis in this case, we considered the following function, constructed with \( R_{2N}^2 \) at \( \omega = 0.64 \):

\[
R^2(X) = \sum_{N=1}^{\infty} R_{2N}^2 X^N.
\] (2.6)

In this series the first 20 coefficients are exactly known. In view of equation (2.2) we expect

\[
R^2(X) \sim A \frac{1}{(1 - X)^{2\nu + 1}}
\] (2.7)

where \( A \) is some constant. By evaluating Padé approximations for the quantity \((1 - X) \frac{d}{dX} R^2(X)\) at \( X = 1 \), we thus get estimates of \( 1 + 2 \nu \). In the present case the Padé estimates (\( \nu = 0.57 \)) are not inconsistent with the value obtained above with the ratios.

We verified, by substitution of the exact data with our Monte Carlo generated \( R_{2N}^2 \) with \( N \leq 20 \), that the above results would remain essentially unaffected by the small Monte Carlo errors. In particular the Padé table becomes only slightly more dispersed, but still centered around the same value.

A central problem connected with this analysis is however the determination of \( \omega_{\nu} \). More confidence on the assumed value of \( \omega_{\nu} \), can only come only by testing its stability under replacement of the data used above with more asymptotic ones.

The same stability has of course to be studied for the average of \( \nu_N \) considered above and taken as an estimate of \( \nu \).

A straightforward extension to higher values of \( N \) of the above analysis, based on the effective exponents (2.5), encounters however serious difficulties, which are arising also from the fact that Monte Carlo errors become more and more substantial.

If we look at the intersections of \( \nu_N \) curves from equation (2.5) for \( N > 20 \), Monte Carlo errors

\[
\Delta \omega \text{ becomes of the order of } 0.2.
\]

In the forthcoming section we describe a new method for obtaining \( \nu \) estimates, which fortunately does not suffer of the above limitations, and allows an unambiguous extension of the analysis to Monte Carlo enumeration results.

3. Renormalization group analysis of truncated series.

Here we present our new method of analysis of truncated series. To be concrete let us consider the case of SAW (\( \omega = 0 \)) for which one can define a quantity like

\[
\xi^2(K) = \sum_{i=1}^{\infty} K^i R^2 C_i(0) / \sum_{i=0}^{\infty} K^i C_i(0)
\] (3.1)

i.e. the grand-canonical average end-to-end distance. We know that this quantity has a singularity

\[
\xi(K) \sim (K_c - K)^{-\nu}
\] (3.2)

where \( K_c = 0.3790 \) [16] for the square lattice and \( \nu = 3/4 \) [15].

Let us call \( \xi_N(K) \) the quantity given by expression (3.1) with both infinite summations truncated after \( N \) terms.

Equation (3.2) tells us that \( \xi_N(K) = \xi(K) \sim (K_c - K)^{-\nu} \). On the other hand it is also easy to show that [21]

\[
\xi_N(K_c) = N^\nu.
\] (3.3)

If we consider also the case \( (K_c - K) \to 0 \), \( N \to \infty \) the leading parts of various sums in equation (3.1) can be well approximated by integrations and the property

\[
\xi_N(K_c + (K - K_c)) = \ell^\nu \xi \left( K_c + \ell (K - K_c) \right)
\] (3.4)

is easily deduced. Indeed, taking into account the asymptotic expression (2.4) of \( C_i \), the dependence on \( K \) and \( K_c \) in the integrands comes from the factors \( (K/K_c)^i \), whose leading contribution can be approximated by \( \exp [\ell (K - K_c)/K_c] \). The homogeneity property (3.4) thus follows by a simple substitution of integration variable.

Equation (3.4) is reminiscent of finite size scaling (FSS) homogeneity equations [20]. One would indeed write the same equation if \( \xi_N(K) \) would represent the SAW correlation length on an infinite
lattice strip of width $N^v$, with $\ell^v$ representing a length rescaling of this width.

It is possible to look at (3.4) as at a sort of FSS homogeneity property. Indeed a truncation at $i = N$ of the summation in (3.1) amounts, in some sense, to a finite size effect of the order $\sim N^v$, since we know that typical distances covered by $N$ step walks (the maximum length of walks included in (3.1)) are growing like $N^v$. Properties like (3.4) are however more general, and can be established also for different quantities and different models.

The starting point of our method of analysis of truncated series is equation (3.4). In the spirit of a renormalization group approach we try to implement equation (3.4) on our finite $N$ results by looking for mappings of $K$ into a renormalized fugacity $K'$, such that:

$$\xi_N(K) = \left(\frac{N}{N'}\right)^{\nu_N} \xi_N(K'(K)).$$  

We fix the unknown $\nu_N$ (\footnote{We omit the explicitate the $N'$ dependence for $\nu_N$ and $K^*_N$, in order to avoid heavy notations. In the cases of interest to us $N' = N - 1$ or $N' = N - 2$.}) in equation (3.5) by the supplementary condition that $\frac{\partial K'}{\partial K}|_{K^*} = \frac{N}{N'}$ at the fixed point $K^*_N$ (if any) of the mapping defined by (3.5). Thus, for $N, N' \to \infty$, we expect $K^*_N$ and $\nu_N$ to approach $K_c$ and the correct SAW $\nu$ exponent, respectively. In other words equation (3.5) should reduce to equation (3.4) under these conditions.

The reader will recognize the usual RG postulates in the above assumptions, e.g., in the regularity of the mapping; in particular our method, in view of the already stressed formal analogy with FSS, is similar to the phenomenological renormalization group widely applied to finite lattice calculations [22].

In our example application of the above RG strategy gives very satisfactory results. For a given $N$, the best $K^*$ and $\nu$ estimates are obtained, like usual in phenomenological RG, for $N' = N - 1$ or $N - 2$ ($N - 2$ again is sometimes suggested by the presence of odd-even oscillations, which are however less strong than in the case of (2.5)).

The analysis applied to the exact SAW enumeration data with $N = 27$ [16] leads to successions of both $K^*_N$ and $\nu_N$ values which are not so well behaved to allow standard extrapolations, often used in FSS or phenomenological renormalization group widely applied to finite lattice calculations [20]. A satisfactory way of handling the data turns out to be a best fit of the standard form:

$$\nu_N = \nu_{\infty} + \frac{A}{N^\rho},$$

and

$$K^*_N = K_c + \frac{B}{N^\sigma},$$

where the dependences on $N'$ on the left hand sides are omitted and the exponents $\rho$ and $\sigma$ describe power law corrections. In this way we obtained $\nu_{\text{SAW}} = 0.7575$ and $K_c \approx 0.3780$, which compare extremely well with the values expected on the basis of other standard analysis [16]. A similar procedure applied to exact enumeration data ($N = 20$) for the cubic lattice gave $\nu_{\text{SAW}} = 0.59$ and $K_c \approx 0.2131$, to be compared with most recent estimates by other methods of series analysis: $\nu_{\text{SAW}} = 0.592 \pm 0.002$ and $K_c \approx 0.2134$ [16].

An interesting feature of the $\nu_N$ determinations based on the mapping in (3.5), is their global dependence on all the enumeration data up to the orders considered. It is thus legitimate to hope for a relatively low sensibility of the results to the introduction of fluctuations in the enumeration data. This is indeed what we verified, e.g., in the case of the two-dimensional SAW. By employing our accurate Monte Carlo data for $R_t$ and $C_t(0)$ up to $N = 40$ we could finally obtain $\nu_{\text{SAW}} = 0.755$ and $K_c \approx 0.3784$ as optimal estimates.

As we will see in the next section, the low sensibility to fluctuations is also revealed by the rather high localization of the intersections of $\nu_N$ plots with different $N$ on the $\omega$ axis, when the RG analysis is applied to the $\theta$ point problem.

Indeed, from the above discussion, it is obvious that the method illustrated for the SAW example can be generalized to the case $\omega \neq 0$, if the appropriate $C_{i}(\omega)$ coefficients are substituted in equation (3.1). In this case the fixed point of the mapping (3.5) approximates $K_c(\omega)$, and, by looking again at the intersections of the various curves for $\nu_N$, one can estimate $\omega_t$, $\nu_t$ and $K_c(\omega_t)$, along lines similar to those followed in the previous section, as we will discuss below.

In view of the relative difficulty to get very accurate estimates of $C_i(\omega)$ by Monte Carlo, one can also adopt a RG strategy which determines $\omega_t$ and the $\nu_t$ exponent only, and makes use of the Monte Carlo results for $R_N$ alone. For the function

$$\xi^2(X) = \sum_{i=1}^{\infty} X^i R_i^2 / \sum_{i=1}^{\infty} X^i,$$  

which can be defined both for $\omega = 0$ and $\omega \neq 0$, one expects a singular behaviour

$$\xi^2(X) \sim \frac{1}{X - 1} \frac{1}{(1 - X)^{2\nu + 1}}.$$  

So, by using truncated series in (3.8) we can implement renormalization mappings for $X$, whose

\footnote{\textit{A more detailed discussion of the RG method of series analysis and the modalities of its application will be given elsewhere [23].}}
fixed points should converge to unity (no information on $K_c(\omega)$ can be obtained in this case) and whose $\nu_N$ exponents should approach that appearing in equation (2.2).

By applying this second scheme to our data for $R_i^2$ up to $i = 40$ we could obtain the $\nu_N$ values reported in table III which can be extrapolated according to equation (3.1) to $\nu_{SAW} = 0.7504$.

Table III. — Values of $2\nu_N$ for the SAW ($N$ is reported in the first column on the left, while $N'$ appears in the second) obtained with our RG analysis of Monte Carlo coefficients. In the third column we report fixed point values for $X$, which should converge to 1.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$N'$</th>
<th>$2\nu_N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>13</td>
<td>1.02529</td>
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The $\gamma$ exponent and $K_c(\omega)$ can also be obtained by our RG strategy, as illustrated below. We consider the function

$$\chi(K, \omega) = \sum_{i=1}^{\infty} C_i(\omega) K^i$$

(3.10)

which should diverge as

$$\chi(K, \omega) \sim \frac{1}{K - K_c(\omega)} (K_c(\omega) - K)$$

(3.11)

according to equation (2.4). For $\chi_N(K_c, \omega)$, the truncated version of (3.10), the homogeneity corresponding to equation (3.4) becomes

$$\chi_N(K_c(\omega) + K - K_c(\omega), \omega) = \ell^\gamma \chi_N(K_c(\omega) + K - K_c(\omega), \omega)$$

(3.12)

which is again analogous to a FSS equation.

A mapping of the type (3.5) thus gives an approximation to $\gamma$ and $K_c(\omega)$.

4. Results for the $\theta$ point.

As remarked in section 2, an extension based on our Monte Carlo results of the analysis of the effective exponents given by (2.5) is not satisfactory.

In order to locate the theta point and to determine its exponents we try now a similar analysis, in which $\nu_N$ curves can be obtained on the basis of renormalization group mappings of the type (3.5).

To start, we repeat the analysis of the exact enumerations by considering the set of RG $\nu_N$ exponents for $N = 10, 11, \ldots, 20$. The intersection pattern for the various curves turns out to be very similar to that discussed in section 2. The average abscissa of intersections can be located at $\omega = 0.64$ and its width is rather small, $\Delta \omega = 0.01$. The average $\nu_N$ exponent for $\omega = 0.64$ is $\nu_t = 0.575$, and individual $\nu_N$ are very little dispersed around this average.

Since in this case we use our RG scheme with the exact $\omega$ dependent $C_i$ in the definition of $\xi_N$ (see Eq. (3.1)) we can also extrapolate $K_N(\omega)$ values at $\omega = \omega_t$, according to equation (3.7). We obtain in this way $K_c(\omega_t) = 0.312$.

A similar analysis can be performed on the exact data for $R_i^2$ according to the scheme based on equations (3.8) and (3.9). In this case $K_c(\omega)$ can, of course, not be obtained. The results for $\omega_t$ and $\nu_t$ are however rather consistent with those of the more complete analysis, and $\Delta \omega$ is of the same order. More precisely we obtain $\omega_t$ between 0.64 and 0.65 and the average $\nu_N$ at this $\omega_t$ is $\nu_t = 0.57$. A crucial question at this stage is to which extent such results for $\omega_t$ and $\nu_t$ would change when considering more asymptotic sets of data from our Monte Carlo enumerations.

Using a RG analysis involving Monte Carlo data for $R_i$ alone at many different $\omega$ values (13) in the range 0.55-0.75, we could locate with reasonable approximation most intersections among $\nu_N$ curves, for progressively more asymptotic sets of $N$ values.

We started with $N = 10, 11, \ldots, 20$, and, shifting by 1 step each time we arrived up to the set with $N = 30, 31, \ldots, 40$.

In figure 2a, we report plots of the average intersection abscissae for three fully independent extensive runs as a function of the maximum $N$ in the various groups considered, to be indicated by $N_{\max}$.
For \( N_{\text{max}} \) equal to 20 the average \( \omega \) of intersections falls very close to the value previously obtained with exact data for all three runs. The \( \Delta \omega \) in these cases is slightly larger than for the analysis of the exact \( R_i \), i.e. about 0.02. Besides the errors affecting the \( R_i \), certainly also the approximate procedure (linear interpolation) used to locate the intersections can be seen as responsible of these discrepancies with respect to the exact case.

Figure 2a shows very clearly that, within fluctuations due to the Monte Carlo data and to the approximations inherent to the procedure, the average \( \omega \) of the \( \nu_N \) intersections in the theta region remains substantially constant over the whole range \( 20 \leq N_{\text{max}} \leq 40 \). The variances \( \Delta \omega \) increase rather slowly with \( N_{\text{max}} \): we estimated \( \Delta \omega = 0.03 \) at \( N_{\text{max}} = 40 \). By repeating the whole analysis with e.g. groups of 15 \( \nu_N \) curves, the results are only slightly modified, as also shown in figure 2b.

The essential stability of \( \omega_t \) upon variation of \( N_{\text{max}} \) in the range explored, the estimated \( \Delta \omega \)'s and the discrepancies among the independent runs considered, naturally suggest \( \omega_t \approx 0.65 \pm 0.03 \) as an extrapolation of our data. This conclusion is further supported by an analysis of the variance of the various \( \nu_N \) with respect to their average as a function of \( \omega \). For all \( N_{\text{max}} \) this variance indeed displays a sharp minimum for \( \omega = \omega_t \).

For the groups of curves considered above one can also plot as a function of \( N_{\text{max}} \) the average \( \nu_N \) (see Fig. 2c, d) computed for \( \omega \) equal to the average intersection abscissa in each group (as reported in Fig. 2a, b). One finds that these average \( \nu_N \) have only little oscillations as a function of \( N_{\text{max}} \), and appear to remain sensibly constant in the explored range of \( N_{\text{max}} \). This constant value of the average \( \nu_N \) can be estimated as \( \nu_t = 0.57 \). To estimate the limits of confidence in this \( \nu_t \), we have to take into account that the root mean square deviations around the average \( \nu_N \) in each group considered above, and the oscillations in the plot 2c, d are both small compared to the deviation effects due to the uncertainty in \( \omega_t \). We consider these effects after reporting the Padé estimates for \( \nu_t \) below.

The last prediction for \( \nu_t \) is very consistent with the Padé estimates, based on the \( R_i \) for \( i \leq 40 \) and \( \omega = \omega_t = 0.65 \), which also give \( \nu_t = 0.57 \) rather sharply. The most substantial source of uncertainty on \( \nu_t \) is, as we said above, the indetermination of
ωt. Considering RG and Padé estimates for ω = 0.68 and ω = 0.62, we finally guessed

\[ \nu_t = 0.570 \pm 0.015 \]  \hspace{1cm} (4.1)

After obtaining ωt and νt in this way, we can easily extend our analysis to the other critical properties.

A RG calculation at ω = 0.65 with Ri and Ci(ωi) obtained from our Monte Carlo method (i ≤ 30) gives an estimate of νt well compatible with (4.1) and Kc(ωt) = 0.312, which corroborates our previous estimate based on the exact series.

This value of Kc(ωt) is also rather consistent with what can be obtained from an analysis of the γt exponent based on our Ci(ωt) up to i = 30.

With the method illustrated at the end of section 3 renormalization group analysis of our data at ω = 0.65, ω = 62 and ω = 0.68, yields, upon extrapolation of the type (3.6),

\[ \gamma_t = 1.10 \pm 0.04 \]  \hspace{1cm} (4.2)

which is our RG estimate for γt. Extrapolation of the fixed point connectivities according to (3.7) for those three ω values gives

\[ K_c(\omega_t) = 0.312 \pm 0.004 \]  \hspace{1cm} (4.3)

A Padé analysis of γt based on the same data is somewhat less consistent with the RG analysis than in the case of νt.

By computing Padé approximants for \( \frac{d \ln x}{dK} \) (K, ω), for ω = 0.62, 0.65 and 0.68, we get γt = 1.06 ± 0.04 and connectivities consistent with (4.3).

The final quantity we study is the crossover exponent φt appearing in equation (2.3). By our Monte Carlo technique we could get reasonably accurate values for \( \frac{\partial R^2_t}{\partial \omega} \) up to i = 40. Since \( \frac{\partial R^2_t}{\partial \omega} \) is expected to diverge like \( N^{2\gamma_t + \phi_t} \) at the theta point, we perform RG calculations of this exponent following a scheme like that described for the function in equation (3.8). Our final estimate based on RG calculations at ω = 0.62, ω = 0.65 and ω = 0.68 is

\[ \phi_t = 0.52 \pm 0.07 \]  \hspace{1cm} (4.4)

which is less sharp than for νt and γt. Padé approximants are also consistent with (4.4).

5. Conclusions.

With our RG analysis of Monte Carlo enumerations we were able to predict location and tricritical exponents of the theta point in two dimensions.

In most cases our predictions were further supported by independent Padé analysis of the data.

For νt previous analysis of exact enumerations gave νt = 0.535 ± 0.025 [4], while the phenomenological RG calculations of references [5] and [6] gave νt = 0.55 ± 0.01. Our prediction (4.1) is rather sharp and appears to be well compatible with the experimental result νt = 0.56 ± 0.01 [7].

Even more important, equation (4.1) supports rather strongly the conjecture by Coniglio et al. [8], according to which νt should be equal to the reciprocal of the percolation hull fractal dimension. This fractal dimension is known to be equal to 7/4 in d = 2 [12]. νt = 4/7 was also derived by Duplantier and Saleur on the basis of a Coulomb gas treatment for the tricritical point of a SAW on the hexagonal lattice with random forbidden hexagons [13].

As to the γ exponent, this was not discussed in previous work on exact enumerations. In reference 6 phenomenological strip calculations were suggesting γt = 1 ± 0.05. At variance with this result our estimate (4.2) seems to indicate a substantial deviation from unity for γt. This rules out the possibility γt = 1, which could be suggested by a no sufficiently careful extension of the connection between polymers at the theta point and indefinitely growing SAW (IGSAW) [24] discussed in reference [8].

Even if not fully consistent with the Padé analysis, our γt in (4.2) appears compatible with the value proposed in reference [13], i.e. γt = 8/7.

Our φt exponent is definitely lower than the value previously obtained in reference [4]. φt = 0.64 ± 0.05, and more consistent with φt = 0.48 ± 0.07 as predicted on the basis of phenomenological RG calculations [6]. The spread in (4.3) is definitely larger than in the other cases. The value proposed by Duplantier and Saleur is φt = 3/7 = 0.4286... [13].

Acknowledgments

We are indebted to R. Dekeyser for his interest in this work and for useful comments on several technical aspects of our analysis. We also thank A. Maritan for useful discussions.

References

[21] IGLOI, F., *J. Phys. A* **19** (1986) 3077. In this paper equations of the type (3.3) were used as a basis of an analysis of series for problems in which \( K \) was already known.