LETTER TO THE EDITOR

Phenomenological renormalisation of the self avoiding walk in two dimensions

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Abstract. Phenomenological renormalisation is used to calculate the exponent ν and the connective constant of the self-avoiding walk problem on a square lattice. A transfer matrix technique is developed for the polymer problem. The results indicate that Flory's value $\nu = 0.75$ is true in two dimensions to extremely high accuracy.

Trying to calculate the critical properties of the two-dimensional self avoiding walk (SAW) by a real space renormalisation is no longer a very new idea (Hilhorst 1976, 1977, Shapiro 1978, Coniglio and Daoud 1979). However since the phenomenological renormalisation (PR) is becoming more and more useful to study two-dimensional systems (Nightingale 1976, 1979, Sneddon 1978, 1979, Nightingale and Blöte 1980, Ràcz 1980, Derrida and Vannimenus 1980a), I found it interesting to use it in this case. The motivations for the present work were provided by the two following facts. First, the PR requires the calculation of the correlation lengths of strips of finite width. The standard technique to do so for spin systems is the transfer matrix method. It was therefore necessary to define a transfer matrix for the SAW. The procedure is similar to one proposed for percolation (Derrida and Vannimenus 1980a). The interest of the definition given here is that it can be generalised to other polymer problems (solution of polymers, branched polymers, vulcanisation). Secondly, the SAW is simple enough to allow calculations for strips of rather large width. The other purpose of this work was to study the convergence of the PR when the width n of the strip increases. Up to now, the convergence law is not well understood except in the Ising case where the critical temperature and the critical exponent ν calculated by the PR with strips of width n and $n - 1$ and periodic boundary conditions converge respectively like n^{-3} and n^{-2} to their exact values. (Nightingale 1976, Derrida and Vannimenus 1980b).

The PR method introduced by Nightingale (1976, 1979) is based on finite-size scaling arguments. I merely recall here the principle of the method without repeating its justifications. Suppose that one wants to study the critical properties of a two-dimensional model with coupling constant x. Using the transfer matrix one can calculate the correlation length $\xi_n(x)$ of a strip of width n. The PR consists in writing a renormalisation equation

$$(1/n)\xi_n(x) = (1/m)\xi_m(x') \tag{1}$$

which expresses the changes of the interaction x associated with the change of scale of ratio n/m. The critical point and the exponent ν of the two-dimensional problem can be

calculated from equations (2) and (3):

$$(1/n)\xi_n(x_c) = (1/m)\xi_m(x_c) \tag{2}$$

$$\frac{1}{\nu} = \frac{\ln[d\xi_n/dx|_{x_c}(d\xi_m/dx|_{x_c})^{-1}]}{\ln(n/m)} - 1. \tag{3}$$

Other exponents can be calculated by similar formulae.

As far as n and m are finite, the method is an approximation which can be improved by choosing n as large as possible and $m = n - 1$ (Nightingale 1976, Derrida and Vannimenus 1980b, dos Santos and Sneddon 1980).

In order to use the PR method for the SAW, one has to define the correlation length as a function of a parameter x in the same way as for spin models. This can be done using the famous $q \to 0$ limit of the classical q-component Heisenberg model (de Gennes 1972, des Cloizeaux 1975, Daoud *et al* 1975)

$$\lim_{q \to 0} \langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_R \rangle = \sum_{p=0}^{\infty} x^p \mathcal{N}_{0R}(p) = G_{0R}(x). \tag{4}$$

Equation (4) relates the correlation function $\langle \boldsymbol{S}_0 \cdot \boldsymbol{S}_R \rangle$ of Heisenberg spins located on sites 0 and R to the number of self-avoiding walks $\mathcal{N}_{0R}(p)$ of length p going from site 0 to site R, x is the nearest-neighbour interaction in the Heisenberg model. When the distance R between the two sites becomes large, the correlation function decreases exponentially in the high-temperature phase. In the $q \to 0$ limit this defines the correlation length $\xi(x)$ for the polymer problem as a function of x which is a chemical potential of monomers

$$G_{0R}(x) \sim \exp(R/\xi(x)). \tag{5}$$

It is now possible to explain how $\xi(x)$ can be calculated for a strip of any width. Suppose that sites 0 and R belong to two columns N_0 and N_R on the strip. If one cuts the strip at column N between N_0 and N_R, the part of the polymer at the left of column N is made of several branches: one site of column N is connected to site 0 of column N_0 whereas some of the other sites of column N are connected by pairs (figure 1). The writing of the transfer matrix needs two steps.

First, one needs the list of all the possible configurations $\mathscr{C}$ at column N. One configuration is defined by the site of column N connected to site 0 and by the pairs of sites connected by the part of the strip at the left of column N. Configurations A and B of figure 1 are examples of such configurations. One can notice that the different branches which reach column N will be connected together by the right part of the strip to form a single polymer. So, some configurations are eliminated (like configuration C of figure 1) where there are crossings between the different branches of the configuration.

For each allowed configuration $\mathscr{C}$, one can define the function $H_N(\mathscr{C})$ by

$$H_N(\mathscr{C}) = \sum_{p=0}^{\infty} x^p \mathcal{N}_N(p, \mathscr{C}) \tag{6}$$

where $\mathcal{N}_N(p, \mathscr{C})$ is the number of ways one can put p monomers at the left of column N in order to realise configuration $\mathscr{C}$ at column N. The transfer matrix T is defined by the
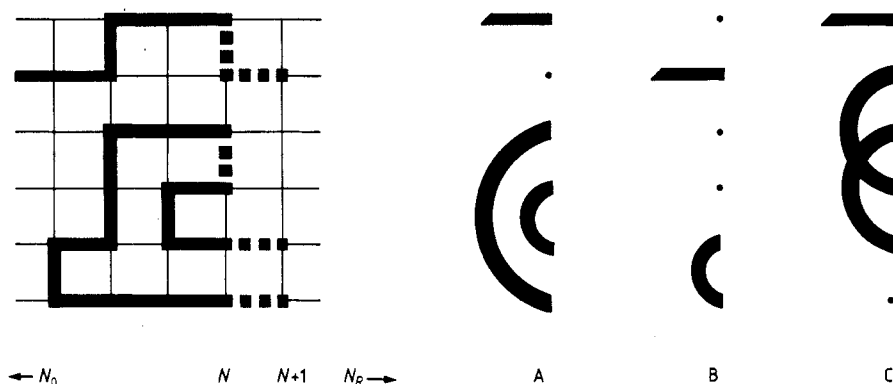
Figure 1. The configurations A and B represent the part of the polymer on the strip at the left of columns N and $N + 1$ respectively. The dashed links are the monomers one has to add to configuration A at column N to give rise to configuration B at column $N + 1$. The number of these monomers is here five. So the matrix element between these configurations A and B is x^5. Configuration C is an example of a forbidden configuration.

set of linear relations which allow the calculation of the $H_{N+1}(\mathscr{C})$ as functions of the $H_N(\mathscr{C})$:

$$H_{N+1}(\mathscr{C}) = \sum_{\mathscr{C}'} T(\mathscr{C}, \mathscr{C}') H_N(\mathscr{C}'). \tag{7}$$

Obviously $T(\mathscr{C}, \mathscr{C}') = x^{t(\mathscr{C}, \mathscr{C}')}$ where $t(\mathscr{C}, \mathscr{C}')$ is the number of monomers one has to add to configuration $\mathscr{C}'$ at column N to give rise to configuration $\mathscr{C}$ at column $N + 1$. If there is no way to connect two configurations $\mathscr{C}$ and $\mathscr{C}'$, the matrix element $T(\mathscr{C}, \mathscr{C}')$ is zero.

So the size of the transfer matrix is the number of configurations $\mathscr{C}$ and its elements are either zeros or integral powers of x. Clearly, when the two columns N_0 and N_R are very far from one another, one has

$$G_{0R}(x) \sim [\lambda(x)]^R \tag{8}$$

where $\lambda(x)$ is the largest eigenvalue of the matrix T. So the correlation length $\xi(x)$ can be calculated by

$$\xi(x) = -\frac{1}{\ln(\lambda(x))}. \tag{9}$$

From a practical point of view, the size of the matrix can be reduced using the symmetries of the strip. These reduced sizes S_n for strips of width n with periodic boundary conditions and free boundary conditions are given in tables 1 and 2 respectively. The general expression of these sizes is too complicated to be given here. Let me just mention that for large n, S_n increases like 3^n.

The self avoiding walk was studied here on a square lattice. The results shown in table 1 were obtained by calculating $\xi_n(x)$ for strips with periodic boundary conditions and by using formulae (2) and (3) with $m = n - 1$. The values of ν are in much better agreement with Flory's value $\nu = 0.75$ (Domb 1969) than previous real-space renormalisations ($\nu = 0.740$ by Hilhorst 1977 and $\nu = 0.70$ by Shapiro 1978). The discrepancy between those previous works and Flory's value is however, recovered here for narrow strips and is probably due to small size effects.

Table 1. Results of the phenomenological renormalisation for the SAW problem using strips of width n and $n-1$ with *periodic boundary conditions*. S_n is the size of the transfer matrix for a strip of width n once the symmetries have been used. The uncertainty on x_c and ν calculated for all the choices of n and m is less than 10^{-7} for x_c and 10^{-6} for ν. The error bars indicated for the extrapolated values come only from the extrapolation procedure.

n	m	x_c	ν	S_n
2	1	0.347 8104	0.668 473	1
3	2	0.365 3048	0.724 477	2
4	3	0.373 3995	0.739 124	3
5	4	0.376 6329	0.745 005	7
6	5	0.377 9095	0.747 680	13
7	6	0.378 4477	0.748 928	32
8	7	0.378 6984	0.749 527	70
9	8	0.378 8280	0.749 826	179
10	9	0.378 9013	0.749 983	435
11	10	0.378 9459	0.750 067	1142
12	11			2947
Extrapolation		0.379 05 ± 0.000 03	0.7503 ± 0.0002	
Flory's value			0.75	

Table 2 contains the results of the PR for strips with free boundary conditions. The results are worse than in the periodic case and the convergence of ν is not even monotonic. However, for large width the agreement with the periodic case seems to take shape.

The extrapolation of the results of table 1 leads to

$$\nu = 0.7503 \pm 0.0002$$
$$x_c = 0.37905 \pm 0.00003 \tag{10}$$

and the convergence law is well described by a power law $(n^{-3.5})$ for ν and x_c. The Flory value $\nu = \frac{3}{4}$ and the connective constant $x_c = 0.37900$ given by McKenzie (1976) are out of the error bars of equations (10). However, one cannot be sure that the asymptotic regime in n has been reached. Non-monotonic convergence might occur for larger sizes

Table 2. As table 1 but with *free boundary conditions*. Note that the results for ν do not converge monotonically.

n	m	x_c	ν	
2	1	0.465 5712	0.715 312	1
3	2	0.414 6801	0.745 306	3
4	3	0.398 2330	0.753 958	6
5	4	0.390 8852	0.756 904	16
6	5	0.387 0023	0.757 908	38
7	6	0.384 7187	0.758 139	100
8	7	0.383 2708	0.758 037	256
9	8	0.382 3000	0.757 790	681
10	9	0.381 6200	0.757 483	1805
11	10			4867

as was the case in table 2. In any case, even if Flory's values were not exact, it would be an extremely good approximation to the true exponent.

This work has shown once more that phenomenological renormalisation is a very powerful tool. Small calculations ($n \leq 5$) lead to satisfactory results whereas longer ones give very accurate numbers. It would be of great interest to be able to predict the convergence law of the results for making very accurate extrapolations.

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