

Study of polymers with crossing bonds on the square lattice

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1997 J. Phys. A: Math. Gen. 30 1445

(<http://iopscience.iop.org/0305-4470/30/5/013>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.112

The article was downloaded on 02/06/2010 at 06:12

Please note that [terms and conditions apply](#).

Study of polymers with crossing bonds on the square lattice

Kleber D Machado and Jürgen F Stilck†

Departamento de Física, Universidade Federal de Santa Catarina, 88040-900 Florianópolis-SC, Brazil

Received 21 August 1996, in final form 15 November 1996

Abstract. Using the transfer matrix technique, finite-size scaling, phenomenological renormalization group and conformal invariance ideas, we studied the model of polymers with crossing bonds on the square lattice. We define an activity $x = e^{-\beta\mu}$ for bonds and an activity $y = e^{-\beta\epsilon}e^{-2\beta\mu}$ for a crossing of two bonds, where ϵ is the interaction energy between the two bonds. We calculated the correlation length for two strips of widths L and L' and we found the fixed points of the phenomenological renormalization group equations. Within this formalism, we obtained the phase diagram for this model which shows three phases, two of them being polymerized. The estimated values of the exponents ν and η along the transition between the non-polymerized phase and regular polymerized phase are consistent with $\nu = \frac{3}{4}$ and $\eta = \frac{5}{24}$, believed to be exact for $y = 0$.

1. Introduction

Polymers modelled as self- and mutually avoiding walks on regular lattices in two dimensions have been extensively studied using several techniques, such as series expansions [1] and finite-size scaling and phenomenological renormalization group ideas in models for linear polymers [2], or branched polymers [3, 4]. Here, we solve models defined on strips with different widths, L , and infinite length, calculating relevant thermodynamic quantities. Then we accomplish some process of extrapolation of the results for the two-dimensional limit $L \rightarrow \infty$. In particular, we consider models defined on strips of two widths, L and L' , and search for fixed points of the phenomenological renormalization group (PRG) equation [5]

$$\frac{\xi_L(\tau)}{L} = \frac{\xi_{L'}(\tau')}{L'} \quad (1)$$

where τ is some relevant parameter defined in the model and ξ is the correlation length. Furthermore, the exponent ν can be easily estimated through

$$1 + \frac{1}{\nu} = \frac{\ln\left[\frac{d\xi_L(\tau)}{d\tau} / \frac{d\xi_{L'}(\tau)}{d\tau}\right]_{\tau_c}}{\ln(L/L')} \quad (2)$$

where τ_c is the fixed point value obtained by equation (1).

In order to calculate the longitudinal correlation length of the model defined on strips, we use the transfer matrix technique, since the two largest eigenvalues of this matrix are related to ξ by [6]

$$\xi^{-1} = -\ln\left(\frac{\lambda_2}{\lambda_1}\right) \quad (3)$$

† E-mail address: jstilck@fsc.ufsc.br

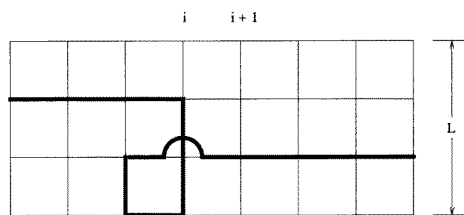


Figure 2. A strip of width $L = 4$ with a possible configuration of the polymer.

factor y is associated to each crossing of two bonds on an elementary square of the lattice. The equivalence of both models is easily shown since each configuration of the first model may be mapped into one configuration of the second model on the dual lattice, as may be seen in figure 1.

A model quite similar to the one we are considering here was solved on Bethe and Husimi lattices [11], and for lattices with coordination numbers larger than 4 only one polymerized phase was found, whose transition to the non-polymerized phase could be of first or second order, these two transition lines being separated by a tricritical point. For an Husimi lattice of coordination number four, however, a qualitatively different phase diagram was found, with two distinct polymerized phases. This result was one of the motivations of the present calculation, since one might ask if on the square lattice similar phase diagrams will be found for this model.

In order to accomplish the study, we define the model on strips of width L and infinite length (see figure 2) and, building the transfer matrix (that is defined in the appendix) for a pair of widths, L and L' , we are able to calculate the correlation length on the strips and then, using equation (1), to find x_c for a fixed value of y . Since the size of the transfer matrix increases quickly with growing values of L , computational limitations force us to restrict our calculations to $L \leq 9$. Before performing the numerical computations, we use the symmetries of the model to block-diagonalize the transfer matrix, thus reducing the size of the matrices whose eigenvalues we need to obtain. It is known that usually the best results with the phenomenological renormalization group are obtained if one chooses $L' = L + 1$. However, in our calculations we notice parity problems which lead us to choose $L' = L + 2$. So, we study the pairs 3-5, 4-6, 5-7, 6-8 and 7-9, obtaining the phase diagrams for each pair of widths. We calculate the values of the exponents ν and η and compare them with results in the literature. The need to study pairs of widths with the same parity can be understood to be related to our choice of boundary conditions for the walk as follows. For a strip with an odd width L a column may be connected to the previous column through all the horizontal bonds between them, but this is not possible for strips of even widths. Thus, there exists a frustration effect which forces us to compare strips of widths with the same parity.

3. Results and discussion

All phase diagrams we obtained show three distinct phases: a non-polymerized phase, NP, a usual polymerized phase, UP, and a dense polymerized phase that has a predominance of crossing bonds, DP. In this last phase, the polymer becomes more compact. The two first phases were expected to appear, since one point of this boundary between them, that corresponds to $y_c = 0$, is the usual polymerization transition and was studied by a variety of techniques, including the one we are employing here [2]. In relation to the third phase,

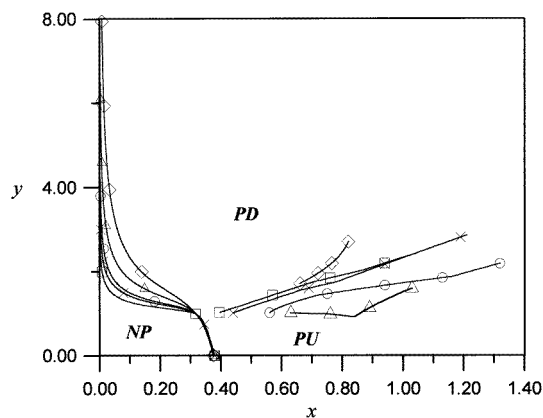


Figure 3. Phase diagrams for pairs 3–5 (\diamond), 4–6 (Δ), 5–7 (\circ), 6–8 (\times) and 7–9 (\square).

Table 1. Results obtained for the first transition for two values of y_c .

L	L'	$x_c(y_c = 0)$	$\nu(y_c = 0)$	$x_c(y_c = 0.1)$	$\nu(y_c = 0.1)$
3	5	0.375 076 84	0.741 718 65	0.371 227 81	0.733 821 96
4	6	0.377 291 28	0.746 214 55	0.373 352 55	0.738 366 57
5	7	0.378 185 87	0.748 252 62	0.374 266 59	0.740 852 21
6	8	0.378 575 97	0.749 207 20	0.374 698 38	0.742 372 91
7	9	0.378 764 52	0.749 667 81	0.374 927 28	0.743 407 78

Table 2. Extrapolation of x_c and ν to the two-dimensional system.

y_c	x_c	ν
0	$0.379\,047 \pm 0.000\,006$	$0.750\,03 \pm 0.000\,05$
0.1	$0.375\,353 \pm 0.000\,003$	0.751 ± 0.001

we had an indication of its existence, since it appears in the solution of the model on a four-coordinated Husimi lattice [4]. Figure 3 shows the phase diagrams.

From the observation of the phase diagrams, it may be noted that the tendency for asymptotic behaviour of the boundary between the non-polymerized and the usual polymerized phases (henceforth called first boundary) is much more regular than the one for the other boundary (indicated by second boundary). This affects the results for the critical exponents ν and η as well. A consequence is that, for the first boundary the exponents show a regular asymptotic behaviour. This can be noted if we look at table 1 which presents the values of x_c and the exponent ν obtained for $y_c = 0$ and $y_c = 0.1$ for all widths studied. To calculate the exponent η , we extrapolated the sequence of estimates for x_c first and then applied equation (4) for each width. Therefore, we obtained a sequence of estimates for η that may itself be extrapolated. To accomplish the extrapolations we use the ideas presented in [12]. Table 2 shows the values of x_c and ν extrapolated for the two values of y_c given above. From this table, it may be noted that the exponent ν remains constant on different points of the boundary, that is, the estimates indicate that the whole boundary belongs to the same universality class. Table 3 presents the values of the exponents η calculated using the estimates for x_c extrapolated from the values in table 2 in equation (4), while table 4 shows

Table 3. Values of η obtained using the x_c as extrapolated in table 2.

L	3	4	5	6	7	8	9
$\eta (y_c = 0)$	0.233 039 40	0.221 552 35	0.216 246 27	0.213 580 79	0.212 097 65	0.211 193 38	0.210 601 20
$\eta (y_c = 0.1)$	0.243 012 92	0.231 097 74	0.225 078 66	0.221 730 87	0.219 669 81	0.218 297 16	0.217 333 28

Table 4. Values of η obtained for the two-dimensional system for the values of y_c of table 3.

y_c	η
0	0.2084 ± 0.0004
0.1	0.212 ± 0.004

the extrapolated values for η . It may be seen that the exponent η also remains constant, within the error bars, along the boundary.

After a comparison of the values obtained in this work with previous results, we can conclude that they are in very good agreement. The best value of x_c (for $y_c = 0$) in the literature was found using series expansions in [1] and is $x_c = 0.379\,0523 \pm 0.000\,0002$. The value obtained in by us is $x_c = 0.379\,047 \pm 0.000\,006$. The exact values of the exponents are believed to be $\nu = \frac{3}{4}$ and $\eta = \frac{5}{24}$ [10]. We found $\nu = 0.750\,03 \pm 0.000\,05$ and $\eta = 0.2084 \pm 0.0004$ for $y = 0$.

With respect to the second boundary, it is interesting to note in figure 3 that it approaches the first one, but does not touch it. These boundaries will only touch in the $L, L' \rightarrow \infty$ limit, that is, when we reach the two-dimensional system. For finite widths there are limitations in the technique. From equation (3), we can observe that we must compare the two largest eigenvalues of the transfer matrix. These eigenvalues are related to the phases which become critical at the boundary. The eigenvalue associated to the non-polymerized phase is equal to 1 (corresponding to the empty lattice), while the other phases have eigenvalues calculated using the transfer matrix. When we are on the second boundary, the two largest eigenvalues of the matrix are larger than 1. However, if we walk on this frontier in direction of decreasing values of x , the eigenvalues become smaller, until one of them becomes smaller than 1. Thus, we are unable to obtain results below this limiting value of x .

The nature of the transitions on the two boundaries may not be known directly from our calculations. Although PRG calculations should lead to reasonable results on second-order transitions only, fixed points may also be present where the transition is of first order [13]. The solution of the model on the four-coordinated Husimi lattice [4] displays a tricritical point and a critical endpoint. These higher-order critical points might be found using three widths renormalization [3], but we found no solutions for the corresponding fixed point equations. It should be mentioned that the same situation also occurs for the model of an attractive walk on the square lattice [14–16].

One way to study the nature of the three phases of the model is to look at the thermodynamic properties of the model on strips of large widths. Although the second transition is not present in those one-dimensional models, it is possible to know at least qualitatively what the behaviour of the two-dimensional model is, by finding a sequence of values for the relevant densities for the model defined on strips of increasing widths L and then performing some extrapolation on them. The densities are defined as

$$\rho_x = \frac{\langle N_x \rangle}{N} \quad (5)$$

and

$$\rho_y = \frac{\langle N_y \rangle}{N} \quad (6)$$

where $\langle N_x \rangle$ is the average number of bonds, ρ_x is the density of bonds, $\langle N_y \rangle$ is the average number of crossing bonds and ρ_y is the density of crossing bonds in a strip of width L , N sites and length $M = \frac{N}{L}$. These average numbers are related to the largest eigenvalue, λ_1 , of the transfer matrix by

$$\langle N_x \rangle = Mx \frac{\partial}{\partial x} \ln \lambda_1 = \frac{Mx}{\lambda_1} \frac{\partial \lambda_1}{\partial x} \quad (7)$$

and

$$\langle N_y \rangle = My \frac{\partial}{\partial y} \ln \lambda_1 = \frac{My}{\lambda_1} \frac{\partial \lambda_1}{\partial y}. \quad (8)$$

Thus, the densities are

$$\rho_x = \frac{1}{L} \frac{x}{\lambda_1} \frac{\partial \lambda_1}{\partial x} \quad (9)$$

and

$$\rho_y = \frac{1}{L} \frac{y}{\lambda_1} \frac{\partial \lambda_1}{\partial y}. \quad (10)$$

We studied the behaviour of these densities for fixed values of x as functions of the activity y . Two values of x were considered: $x = 1.0$ and $x = 0.4$. It may be noticed in figure 3 that the results for the densities show a clear parity effect, which prevents us from attempting any extrapolation of the full data set for $L \rightarrow \infty$. Since at least four values are needed to perform an extrapolation [12], only the set of data for odd widths could lead us to any result. Unfortunately even this set did not provide meaningful extrapolations in the whole range of the activity y , so we will limit ourselves to consider the behaviour of the densities for odd widths, as shown in figures 4 and 5. It may be noticed from the behaviour of the densities as functions of y that for $x = 1.0$ the increase of the densities in the region of the transition is rather smooth, while a much steeper increase is obtained for $x = 0.4$. These results indicate the possibility that the transition between the two polymerized phases could be of first order for low values of x , turning into a second-order transition as x increases.

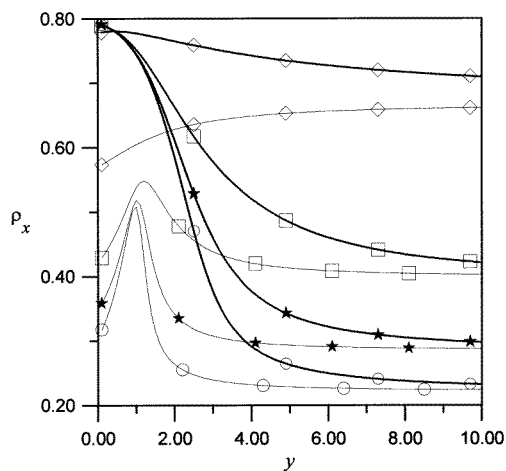


Figure 4. Density of bonds ρ_x for widths 3 (\diamond), 5 (\square), 7 (\star) and 9 (\circ). Heavy curves correspond to $x = 1.0$ and light curves to $x = 0.4$.

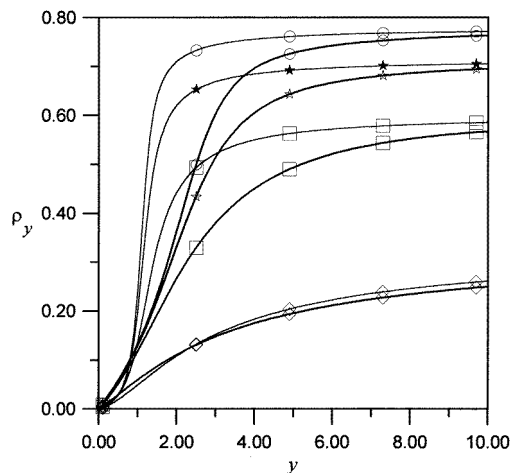


Figure 5. Density of crossing bonds ρ_y for widths 3 (\diamond), 5 (\square), 7 (\star) and 9 (\circ). Heavy curves correspond to $x = 1.0$ and light curves to $x = 0.4$.

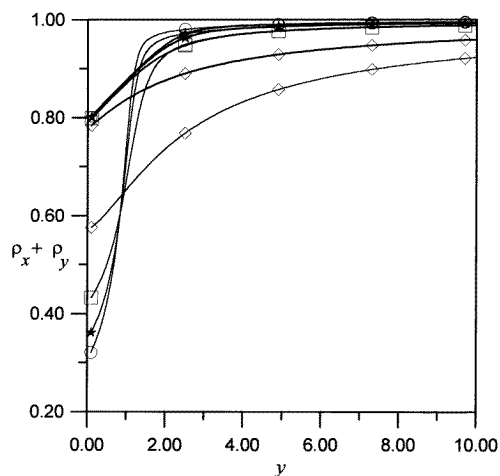


Figure 6. Sum of densities $\rho_x + \rho_y$ for widths 3 (\diamond), 5 (\square), 7 (\star) and 9 (\circ). Heavy curves correspond to $x = 1.0$ and light curves to $x = 0.4$.

The results for the total densities $\rho_x + \rho_y$ shown in figure 6 also show similar behaviours, indicating that the total density has a value very close to 1 in the dense polymerized phase. Also, our calculations indicate that the transition between the non-polymerized phase and the regular polymerized phase is of second order, while the transition between the non-polymerized phase and the dense polymerized phase is discontinuous. The model may be solved exactly on the square lattice for $x = 0$, since in this case only two configurations are possible: the empty lattice (whose dimensional free energy per site is equal to 0) and the configuration for which there is a crossing of two bonds at every site of the lattice (with $f = -\ln y$). Therefore, a first-order transition occurs at $y = 1$ from the non-polymerized phase to a phase with $\rho = \rho_y = 1$. This result, together with the PRG results, suggest that the transition line between the non-polymerized and dense polymerized phases may be approximated by $y \approx 1$. Consistently, a critical endpoint should be located close to $y_{\text{cep}} \approx 1$ and $x_{\text{cep}} \approx 0.31$.

Despite our effort to obtain estimates for the critical endpoint and the tricritical point using methods such as the three widths renormalization and considering the next largest eigenvalue [3], no consistent results were obtained. Possibly better results at these special points would be obtained if larger widths could be considered. Although it might be expected

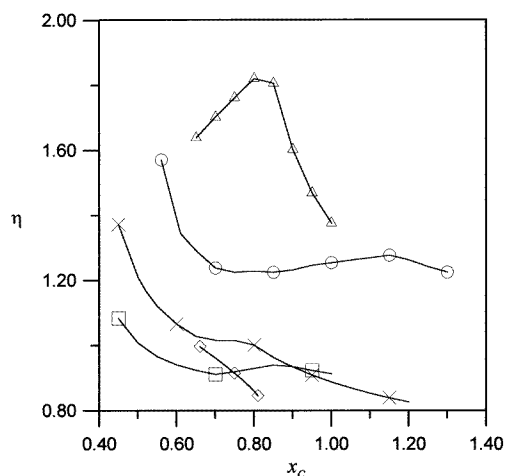


Figure 7. Exponent η for the second boundary for widths 3–5 (\diamond), 4–6 (Δ), 5–7 (\circ), 6–8 (\times) and 7–9 (\square).

that the PRG should not give meaningful results for the location of a first-order transition, this is not the case in our calculations and also in studies of other models [13].

As expected, the estimates for the exponents ν and η at the transition between the two polymerized phases, are quite poor. We show in figure 7, the exponent η as function of x . The behaviour of the exponent ν is quite similar. The particularly irregular behaviour for small values of x may be due to the fact that the transition there is of first order. Again better results should be expected if it were possible to consider strips of larger widths L .

4. Conclusion

As final observations, we can conclude that the model of polymers with crossing bonds on the square lattice shows a phase diagram with three phases: a non-polymerized phase, corresponding to the empty lattice; a usual polymerized phase, which corresponds to the linear polymers with some crossing bonds; and finally a dense, or saturated, phase in which the polymer has a predominance of crossing bonds, being more compact and having the following properties: $\rho_x + \rho_y \approx 1$ and $\rho_x = 0$ and $\rho_y = 1$ in the $x \rightarrow 0$ and $y \rightarrow \infty$ limits. The transition between the non-polymerized and dense polymerized phases is of first order and may be approximated by a horizontal straight line located at $y = 1$. In the case of the boundary between the non-polymerized and the usual polymerized phases, the transition is a second order one, which ends at a critical endpoint at $x_{\text{cep}} \approx 0.31$ and $y_{\text{cep}} \approx 1$. Finally, the transition between the two polymerized phases is a first order one from $(x_{\text{cep}}, y_{\text{cep}})$ to $(x_{\text{tcp}}, y_{\text{tcp}})$. At this point, there is a tricritical point that should have $0.4 \leq x_{\text{tcp}} \leq 1.0$. We used the phenomenological renormalization method of three widths and another method considering the next largest eigenvalue [3] to obtain some estimate of this tricritical point but we were not successful. Beyond the tricritical point the transition is of second order. It is important to note that the usual phenomenological renormalization method in principle should apply only to second-order transitions, but in other models meaningful results were obtained for first-order transitions as well [13]. In figure 8 we show a sketch of the conjectured phase diagram for the model on the square lattice.

The estimated value of the critical activity x when $y = 0$ is $x_c = 0.379\,047 \pm 0.000\,006$ in agreement with the known value $x_c = 0.379\,0523 \pm 0.000\,0002$ [1]. The values obtained for the exponents ν and η at the first transition (between the non-polymerized and the

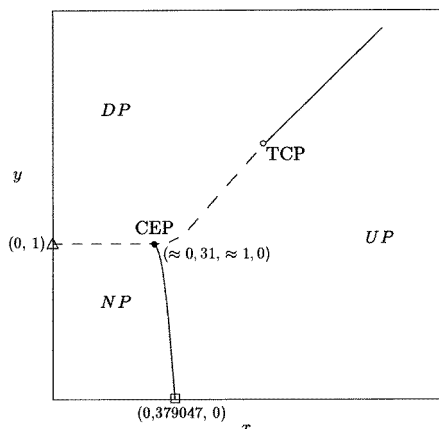


Figure 8. Sketch of the phase diagram for our model on the square lattice. Full curves represent second-order transitions and broken curves indicate first-order transitions.

usual polymerized phase) are $\nu = 0.75003 \pm 0.00005$ and $\eta = 0.2084 \pm 0.0004$, again in agreement with the expected values $\nu = \frac{3}{4}$ and $\eta = \frac{5}{24}$ [10]. The exponents of the first boundary remain constant, within the error bars, as functions of y , as expected from universality.

The calculations for the second transition (between the two polymerized phases) did not show good convergence at the widths we were able to consider, and therefore it was not possible to obtain any reasonable estimates for the critical exponents on this boundary. This problem may also be associated to the fact that in part of this boundary the transition should be of first order. We found evidence of this boundary for the solution of the model on square lattice, and it was found before in the solution on the four-coordinated Husimi lattice [4]. It is remarkable that the solution of a model for interacting polymers on a four-coordinated Husimi lattice leads to similar phase diagrams [17]. This might be understood since the presence of crosslinks favours more compact configurations of the polymer, as do the interactions in the attractive polymer model. Evidence has been found [18] that two polymerized phases may also be present in the phase diagrams for self-attracting branched polymers in two dimensions, with phase diagrams which resemble the ones we obtained in this work and in [17]. Actually, all configurations of the polymer we considered in this work are also present in the model of branched polymers, but since we only accept configurations that correspond to a single walk with crossings at sites of the lattice, some branched polymer configurations are not allowed in the model we considered here. In view of the results presented here, one might ask if two polymerized phases may also be found without self-attraction of the branched polymers. We are presently investigating this possibility.

Acknowledgments

We thank the Centro Nacional of Supercomputação (UFRGS) for the use of their computational resources and the Brazilian agency CNPq for partial financial support. Pablo Serra and Sérgio L A de Queiroz are gratefully acknowledged for helpful conversations. We acknowledge Nilton da S Branco for a critical reading of the manuscript.

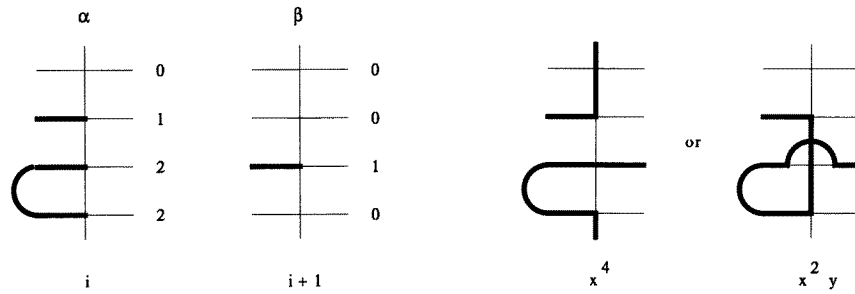


Figure A1. α and β , possible configurations of the columns i and $i + 1$ on a strip of width $L = 4$.

Figure A2. One element of the transfer matrix. The statistical weights are explained in the text.

Appendix. Some elements of the transfer matrix

We will illustrate how the transfer matrix is built by an example: the calculation of one element of this matrix for $L = 4$. To build the necessary configurations to the calculation of the transfer matrix, we associate indexes to the sites of the strips of width L (see figure A1). These indexes are assigned in the following way.

- If a bond arrives at a site from the left which is directly linked to the origin, this site will have the index 1. Since we want the polymer to pass through the whole strip, always one site in each column will have this index (the origin is at the left end of the strip). In the above example, the second site in the α configuration and the third site in the β configuration have this index.

- If the site is not connected to another site to the left, it has the index 0. The first site in the α configuration and the first, second and fourth sites in the β configuration have this index.

- Finally, if two sites of the column are connected through a walk to the left, both will be given the same, index larger than 1. The third and fourth sites in the α configuration have the index 2 and in the β configuration there is no pair of sites like this.

From the observation of figure A1 we note that there are two possible ways for a polymer to have the α configuration in column i and the β configuration in column $i + 1$. These possibilities are shown in figure A2. One of them has four bonds (statistical weight x^4) while the other has two bonds and one crossing bond (statistical weight x^2y). The element of the transfer matrix associated with these configurations will be

$$\langle \alpha | T | \beta \rangle = x^4 + x^2y \quad (\text{A1})$$

where T is the transfer matrix.

To accomplish the calculations we need all elements of the transfer matrices up to the largest widths we considered. As the size of the transfer matrix increases quickly, computational limitations fix the largest width we were able to consider. We may calculate the number of configurations, N_s , for a column of width L having the index 1 on the first site and a number of pairs N_p of sites linked together, through the expression

$$N_s = \frac{(L-1)!}{2^{N_p} N_p! N_z!} \quad (\text{A2})$$

in which $N_z = L - 1 - 2N_p$ is the number of sites in the column with index equal to zero. The total number of configurations, N_s , is obtained by summing over all possible numbers

Table A1. Number of states and size of the transfer matrix for the studied widths L .

L	3	4	5	6	7	8	9	10
N_S	2	4	10	26	76	232	764	2620
N	6	16	50	156	532	1856	6876	26200

of pairs, that is

$$N_S = \sum_{N_p=0}^{\text{int}(\frac{L-1}{2})} N_S. \quad (\text{A3})$$

The size N of the matrix is obtained by

$$N = L \times N_S. \quad (\text{A4})$$

The sizes of the matrices for the widths we studied are shown in table A1. As an example, we show below the transfer matrix for $L = 3$:

$$T = \begin{pmatrix} x & x^2 + x^3 & x^2 + x^3 & x^3 + x^2y & 0 & 0 \\ x^2 + x^3 & x & x^2 + x^3 & 0 & x^3 + x^2y & 0 \\ x^2 + x^3 & x^2 + x^3 & x & 0 & 0 & x^3 + x^2y \\ 0 & x^3 + x^2y & x^3 + x^2y & x^3 & 0 & 0 \\ x^3 + x^2y & 0 & x^3 + x^2y & 0 & x^3 & 0 \\ x^3 + x^2y & x^3 + x^2y & 0 & 0 & 0 & x^3 \end{pmatrix}. \quad (\text{A5})$$

References

- [1] Guttmann A J and Wang J 1991 *J. Phys. A: Math. Gen.* **24** 3107
- [2] Derrida B 1981 *J. Phys. A: Math. Gen.* **1** L5
- [3] Derrida B and Herrman H J 1983 *J. Physique* **44** 1365
- [4] Banchio A J and Serra P 1995 *Phys. Rev. E* **51** 2213
- [5] Nightingale M P 1976 *Physica* **83A** 561
- [6] Domb C 1960 *Adv. Phys.* **9** 149
- [7] Cardy J L 1984 *J. Phys. A: Math. Gen.* **17** L385
- [8] Wheeler J C, Kennedy S J and Pfeuty P 1980 *Phys. Rev. Lett.* **45** 1748
- [9] Wheeler J C and Pfeuty P 1981 *Phys. Rev. A* **24** 1050
- [10] Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
- [11] Stilck J F and Wheeler J C 1992 *Physica* **190A** 24
- [12] Henkel M and Schütz G 1988 *J. Phys. A: Math. Gen.* **21** 2617
- [13] Alcaraz F C, Drugowich J R, Köberle R and Stilck J F 1985 *Phys. Rev. B* **32** 7469
- [14] Derrida B and Saleur H 1985 *J. Phys. A: Math. Gen.* **18** L1075
- [15] Saleur H 1986 *J. Stat. Phys.* **4** 419
- [16] Saleur H 1986 *J. Phys. A: Math. Gen.* **19** 2409
- [17] Stilck J F, Machado K D and Serra P 1996 *Phys. Rev. Lett.* **76** 2734
- [18] Henkel M and Seno F 1996 *Phys. Rev. E* **53** 3662 and references therein