Universality for interacting oriented self-avoiding walk: A transfer matrix calculation

A. Trovato [1] and F. Seno [2]
[1] *International School for Advanced Studies (SISSA), Via Beirut 2-4, 34014 Trieste, Italy*
[2] *INFM–Dipartimento di Fisica, Università di Padova, Via Marzolo 8, 35131 Padova, Italy*
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In this paper we perform transfer matrix calculations to study the two-dimensional problem of oriented self-avoiding walks on a square lattice where nearest neighbor interactions depend on the relative orientation (parallel or antiparallel) between different parts of the path. Our main purpose is to verify a conformal field theory conjecture that the entropic exponent γ, which is related to the number of such walks, varies continuously with the energy of the parallel interaction. We find no evidence of this behavior, but see many unexpected features for the model, such as the existence of a line of θ points belonging to the universality class of polymer collapse on a Manhattan lattice. Finally we study the phase diagram in the parallel and antiparallel interaction planes and we conjecture a crucial role for the standard θ point. [S1063-651X(97)05906-0]

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I. INTRODUCTION

The problem of a polymer chain collapsing at low temperatures due to the competition between the excluded volume and the attractive interactions between the monomers composing the chain has been of long-standing theoretical interest. The associated phase transition occurs at a tricritical θ point [1–4]. The basis for most lattice models is the self-avoiding walk (SAW), which, by construction, includes an excluded volume interaction, important in physical polymers. To mimic the complicated monomer-solvent interactions that give rise to the collapse transition, an energy is associated with nonconsecutive nearest neighbor portions (e.g., sites or bonds) of the walk [interacting self-avoiding walk (ISAW)].

A simple, but intriguing, modification of the ISAW model [5,6] has been recently introduced to study polymers with an intrinsic orientation. Such an orientation could be due to the presence of dipole moments on the monomers of the chain, or to a precise ordering in the sequence of monomer constituents, as in the case of the *A-B* polyester [7]. In this model a direction is attached to the whole walk, which in turn is associated to each step of the walk. Short-range interactions are divided in two types according to the relative orientation (parallel or antiparallel) of the monomers which are in contact.

Such a model, named the interacting oriented self-avoiding walk (IOSAW), has attracted considerable interest due to some unexpected results predicted for its critical behavior by conformal field theory. According to the most striking of these conjectured results, the entropic exponent γ, which relates to the total number c_N of open walks of length N via the formula $c_N \sim N^{\gamma-1}\mu^N$, is not a universal quantity. At least for a repulsive energy it would seem to depend continuously on the temperature [5].

Since the publication of these fascinating but unforeseen results, several attempts have been made to verify numerically their validity. Despite all of these efforts the situation is still quite controversial. It is numerically difficult to extract the exponent γ and to observe the predicted nonuniversality, which is expected to be small. Indeed, exact enumeration [6] and transfer matrix calculations [8] seem to confirm, although with some caution, the existence of such nonuniversality, whereas the authors of recent extensive Monte Carlo simulations [9,10] are much more doubtful on the validity of the conformal invariance hypothesis.

In this paper we try to get new insight into this problem by studying, using the transfer matrix (TM) technique, some parts of the phase diagram which have not yet been elucidated but that are crucial in order to clarify the validity of the conjecture.

We first estimate the values of the entropic exponent in the limit where the parallel interactions are completely forbidden. In this limit the effect of the predicted nonuniversality is most important while the absence of parallel contacts introduces a relevant simplification in the configurational analysis, allowing us to work with larger system sizes than in the previous calculations.

Secondly, we follow the behavior of γ along one of the θ lines present in the phase diagram. It is possible to apply heuristic arguments (confirmed by our numerical work) showing that there are different values of γ in at least two points of this line. It then turns out that such a θ line should be an optimal candidate for exhibiting a continuous variation of the entropic exponent.

The main result is that, while no evidence of a continuous variation of the critical index is found, the phase diagram presents an extremely rich variety of universality classes.

The paper is set out as follows. In the next section we introduce the IOSAW model and briefly review the results obtained thus far. We discuss the general features of the phase diagram as they emerge from previous papers and we recall the conformal field theory predictions and their numerical checks. In Sec. III we present the TM method together with the phenomenological renormalization group strategy used to compute the critical exponents. Section IV is devoted to presenting our results for the regime where parallel contacts are forbidden. As a by-product of this analysis we show how it is possible to improve previous TM calculations for the general problem and we present our estimate for the above mentioned θ line. We then map the phase diagram of the model (Sec. V). In the last section we sum-

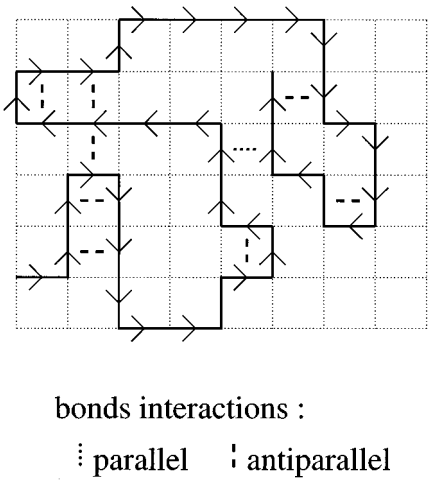

FIG. 1. An oriented self-avoiding walk on a square lattice with parallel and antiparallel interactions between nonconsecutive bonds which are nearest neighbors.

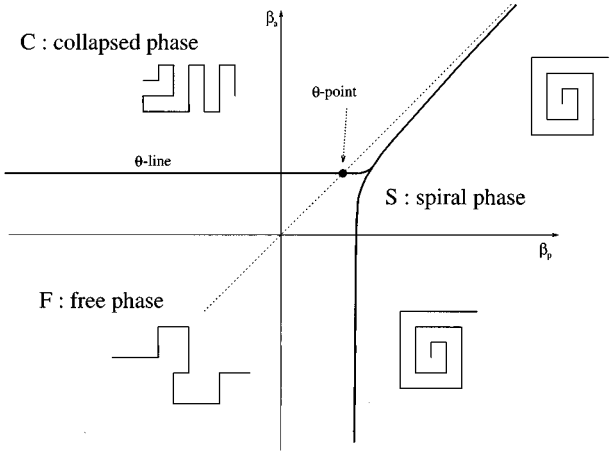

FIG. 2. A schematic illustration of a conjectured phase diagram in the (β_p,β_a) plane as proposed by Bennett-Wood *et al.* [6]. Three phases are shown: free (F), collapsed (C), and spiral (S). The dotted line is the normal (i.e., nonoriented) collapse problem with $\beta_p=\beta_a$ and contains the θ point.

marize our results and present possible further developments.

II. THE MODEL AND THEORETICAL PREDICTIONS

The IOSAW model [5,6,8–10] is an oriented SAW embedded on a square lattice. Interactions are assigned to bonds which are on opposite edges of the lattice plaquette (Fig. 1).

If we indicate by W one of these walks with $|W|$ steps, the partition function $Z_N(\beta_p,\beta_a)$ and the average end-to-end distance $R_N(\beta_p,\beta_a)$ for walks with N steps are

$$Z_N(\beta_p,\beta_a)=\sum_{|W|=N} e^{m_p(W)\beta_p+m_a(W)\beta_a}, \tag{2.1}$$

$$R_N^2(\beta_p,\beta_a)=\frac{\sum_{|W|=N} r^2(W)e^{m_p(W)\beta_p+m_a(W)\beta_a}}{Z_N(\beta_p,\beta_a)}, \tag{2.2}$$

where the sums are over all the oriented walks of length N; $m_p(W)$ and $m_a(W)$ are, respectively, the number of parallel and antiparallel contacts; $r^2(W)$ is the squared end-to-end distance for each walk and the parameters β_p and β_a are given by $\beta_p=\beta\epsilon_p$ and $\beta_a=\beta\epsilon_a$, where β is the inverse temperature and $-\epsilon_p$ and $-\epsilon_a$ are the energies for parallel and antiparallel interactions. For large N we expect

$$Z_N(\beta_p,\beta_a)\sim[\mu(\beta_p,\beta_a)]^N N^{\gamma(\beta_p,\beta_a)-1}, \tag{2.3}$$

$$R_N^2(\beta_p,\beta_a)\sim N^{2\nu(\beta_p,\beta_a)}. \tag{2.4}$$

Equation (2.3) is thought to be true at least for all the extended and θ phases, whereas in the collapsed regimes a more involved expression is needed [11].

The reduced free energy per step $k(\beta_p,\beta_a)$ in the thermodynamic limit can be readily obtained from Eq. (2.3) through the following equation:

$$k(\beta_p,\beta_a)=\lim_{N\to\infty}\frac{\ln[Z_N(\beta_p,\beta_a)]}{N}=\ln[\mu(\beta_p,\beta_a)]. \tag{2.5}$$

When $\beta_p=\beta_a=0$, the model describes the free SAW and the critical exponents $\nu(0,0)=\nu_{\rm SAW}=\frac{3}{4}$ and $\gamma(0,0)=\gamma_{\rm SAW}=\frac{43}{32}$ are exactly known from Coulomb gas techniques [12]. The case when $\beta_p=\beta_a$ is the usual interacting walk problem: for $\beta_p=\beta_a<\beta_\theta$ the model falls in the universality class of the SAW, while μ depends on the temperature. At $\beta_p=\beta_a=\beta_\theta$ the system exhibits tricritical behavior (θ point) with $\nu(\beta_\theta,\beta_\theta)=\nu_\theta=\frac{4}{7}$ [2] and $\gamma(\beta_\theta,\beta_\theta)=\gamma_\theta=\frac{8}{7}$ [2]. Finally, for $\beta_p=\beta_a>\beta_\theta$, it collapses in its globule phase ($\nu=\frac{1}{2}$).

It is possible to argue that in the phase diagram there are at least three different regions (Fig. 2): a free phase (F) occurring for negative or small values of β_p and β_a where the asymptotic behavior of the walks should be governed by the SAW correlation length exponent; a spiral phase (S), for high values of β_p, where the most statistically important walks are tightly bound, compact spirals; and a ''normal'' collapsed phase (C) for high values of β_a and negative or moderate values of β_p.

Much information about the phase diagram can be derived from the simple, but important, fact that oriented loops (closed oriented walks) do not contain any parallel interactions. Then the transition between the free and the spiral phases cannot be the usual θ transition because it cannot occur for loops. The absence of parallel interactions in loops can also be used to rigorously prove that the free energy $k(\beta_p,\beta_a)$ [and therefore the connectivity constant $\mu(\beta_p,\beta_a)$ in Eq. (2.3)] is constant, for any fixed β_a, in the interval $-\infty<\beta_p\leqslant\beta_a$. This last statement implies that the θ line between the free and the collapsed phases is independent of β_p, at least for $\beta_p<\beta_\theta$, and is described by the equation $\beta_a=\beta_\theta$.

On the basis of these (and other) results and considerations, in conjunction with exact enumeration calculations, the authors of Ref. [6] predicted a phase diagram, schematically represented in Fig. 2. According to them, the transition to the spiral phase may well be first order from either one of the other two phases.

The latest numerical work on the IOSAW has dealt only with the line $\beta_a=0$. References [8,10] confirm the presence of a free-to-spiral transition, but disagree on its order. We will return later (Sec. V) to this point, and to the structure of the phase diagram.

In the introduction it was stated that the two-dimensional conformal invariance field theory predicts some new and unexpected results for the IOSAW model. The analysis follows from the fact that the oriented polymer problem can be derived as the limit $n\to 0$ of a complex $O(n)$ model [7,13]. In this context the orientation dependent interaction has been identified with a current-current coupling. Regarding this coupling as a perturbation of the SAW regime and by using the result that such a perturbation is truly marginal, it is possible to determine the critical exponents [5].

Following this scheme Cardy predicted that $\gamma(\beta_p,\beta_a)$ is a nonconstant function of β_p when $\beta_a=0$ (at least for negative values of β_p). More precisely, for $\beta_a=0$ the operator which corresponds to the source of a q-leg oriented SAW scales with an exponent

$$x_q(\beta_p,0)=\frac{9q^2-4}{48}+2\pi\lambda(\beta_p)q^2=x_q(0,0)+2\pi\lambda(\beta_p)q^2, \tag{2.6}$$

where $\lambda(\beta_p)$ is an unknown function of β_p having the opposite sign of its argument [i.e., $\lambda(0)=0$] and supposed to be monotonic [6]. These exponents are related to the entropic exponents γ_q through standard scaling [6], and for the linear polymers, e.g., $q=1$, it turns out that

$$\gamma(\beta_p,0)=\nu[2-2x_1(\beta_p,0)]=\nu\left(\frac{43}{24}-4\pi\lambda(\beta_p)\right). \tag{2.7}$$

It has to be pointed out that a dependence on β_p is not expected for ν, whereas a behavior similar to the one expressed by Eqs. (2.6) and (2.7) should be valid for the portion of the plane $\beta_p\leqslant\beta_a$ and $\beta_a<\beta_\theta$ where the unperturbed regime is that of the SAW model.

Two strategies have been employed to check this conjecture. One is based on the calculations of the two quantities

$$\Delta_q(\beta_p,0)=\gamma_q(0,0)-\gamma_q(\beta_p,0), \tag{2.8}$$

$$R_{q,q'}(\beta_p,0)=\frac{\Delta_q(\beta_p,0)}{\Delta_{q'}(\beta_p,0)}=\frac{q(q+1)}{q'(q'+1)} \tag{2.9}$$

for different values of q and q'. The gaps $\Delta_q(\beta_p,0)$ should increase as β_p goes to $-\infty$ while the ratios $R_{q,q'}(\beta_p,0)$ should be independent from β_p.

The second scheme follows from the fact that if γ depends on β_p then $\langle m_p\rangle$, the average number of parallel contacts, should grow at the SAW point logarithmically with the length of the walk N, otherwise it should be independent of N.

Earlier results obtained from exact enumerations [6] found very tiny values for $\Delta_1(-\infty)$ [0.0091(33) and 0.0115(15)], but a possible confirmation of the theory was found by looking at the two-legged case and by noticing that, up to length $N=27$, $\langle m_p\rangle$ was growing logarithmically with N [6]. Further support to Cardy's theory was given by the TM calculation of Ref. [8] where the scaling dimensions $x_q(\beta_p,0)$ were calculated for $q=1,2,3,4$ and for $\beta_p=-1,-2,-3$. However, more recent Monte Carlo enumerations [10] show that for large N (N up to 5000) $\langle m_p\rangle$ seems to saturate to a constant in clear contrast with the conformal field theory conjecture. In our opinion, this result cannot be considered definitive, because the nonuniversality effect would lead to a very tiny slope for $\langle m_p\rangle$ as a function of $\ln N$. This could still be present in the results of Ref. [10].

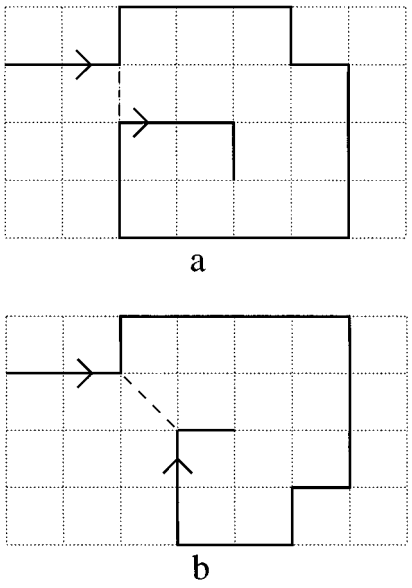

FIG. 3. (a) An oriented SAW configuration with a trapped end but without any parallel contact between bonds. (b) An oriented SAW configuration with a trapped end but without any parallel contact between sites.

To start our analysis of this puzzling problem we notice that Δ_q (if the theory is correct) reaches its maximum value for $\beta_p=-\infty$. The most convenient thing to do would be to work exactly in that limit where the calculation is even simpler than elsewhere in the phase diagram, because the absence of parallel contacts simplifies any numerical approach. This simplification will increase the size of the semi-infinite strips that can be studied through a TM approach.

It has been observed [5,6] that the presence of parallel contacts implies that at least one end of the walk is trapped. One may expect that for $\beta_p=-\infty$, when parallel contacts are strictly forbidden, the walks could not be trapped. (This fact has been used by Cardy to state that, if his conjecture is right, the fraction of untrapped walk, which goes with N as $N^{\gamma(-\infty)-\gamma(0)}$, is vanishingly small when $N\to\infty$). However, this is not the case for the IOSAW model with interactions between bonds on a square lattice. As shown in Fig. 3(a), it is possible to have a trapped walk without any parallel bond interactions.

We then propose two changes to the model. The first one is to consider interactions between nearest neighbor sites (rather than bonds) of the oriented walk which are not directly linked. As can be seen in Fig. 4, this makes it more difficult to assign the type of energy contact (parallel or antiparallel), however, the model is still well defined and in the limit $\beta_p\to-\infty$ we no longer have the undesired configura-

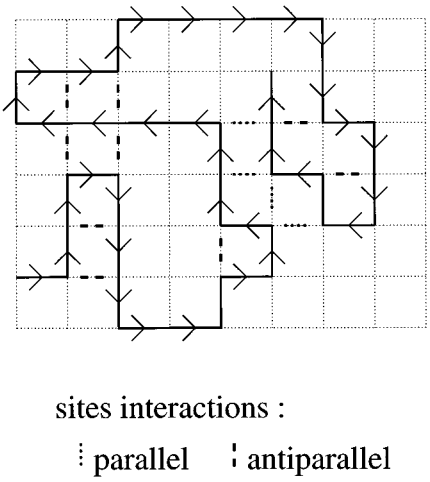

FIG. 4. An oriented SAW on the square lattice with parallel and antiparallel interactions between sites which are nearest neighbors not directly linked by the walk.

tions of Fig. 3(a). However, this is not enough: Fig. 3(b) shows a trapped configuration without any parallel contacts between sites. A third version of the model is then necessary, which takes into account also next-nearest neighbor interactions (we call it the plaquette model because, from a computational point of view, it is convenient to consider single plaquettes of the lattice and to verify whether they are visited by different portions of the walk). In this way the problem of trapped walks is completely solved, although the definition of parallel or antiparallel contacts is quite cumbersome. Both for the site and for the plaquette model it is possible to rederive [14] all the rigorous results obtained in Ref. [6].

Before returning our attention to the free-to-collapsed phase line of θ points we recall an argument due to Bennett-Wood *et al.* [6]. There is a close analogy between the IOSAW problem for $\beta_p=-\infty$ and that of interacting walks on a Manhattan lattice. The Manhattan lattice is a two-dimensional square lattice on which bonds are directed, so that there is no overall directional bias (Fig. 5). On this lattice a SAW is oriented by default, but in the interacting case there are no parallel interactions (in the spirit of the plaquette model).

This model has been exactly solved at its collapse transition [15]. It turns out that the exponent ν is unchanged compared to the standard θ-point value of $\frac{4}{7}$, while the exponent γ is $\frac{6}{7}$ instead of $\frac{8}{7}$. Although this mapping between IOSAW at $\beta_p=-\infty$ and ISAW on the Manhattan lattice is not rigorous, it is quite plausible that the point $(\beta_p=-\infty,\beta_a=\beta_\theta)$ in the oriented polymer phase diagram falls in the same universality class as the θ point of Manhattan walks. If this conjecture is verified, two points along the θ line have very distinct values of the γ exponent: $\gamma(-\infty,\beta_\theta)=\frac{6}{7}$ and $\gamma(\beta_\theta,\beta_\theta)=\frac{8}{7}$. It is then intriguing to think that Cardy's hypothesis may also hold along the free-to-collapse line where, due to the quite clear difference between the extremal values, it should be much easier to see a continuous variation of the exponent γ. In order to study these questions we decided to use the TM technique.

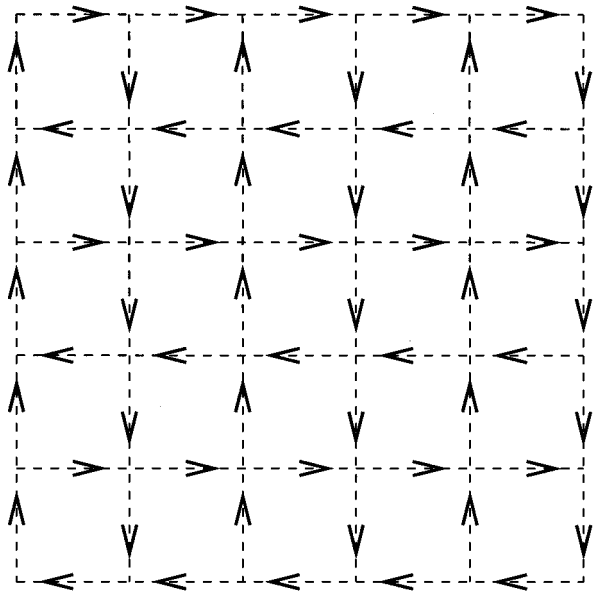

FIG. 5. The Manhattan lattice: an oriented square lattice.

III. THE TRANSFER MATRIX CALCULATION

The TM has proven to be a useful tool for problems in statistical mechanics. It has been extremely effective in the study of models of interacting polymers in two dimensions [16–20].

It is convenient to define a two point correlation function as

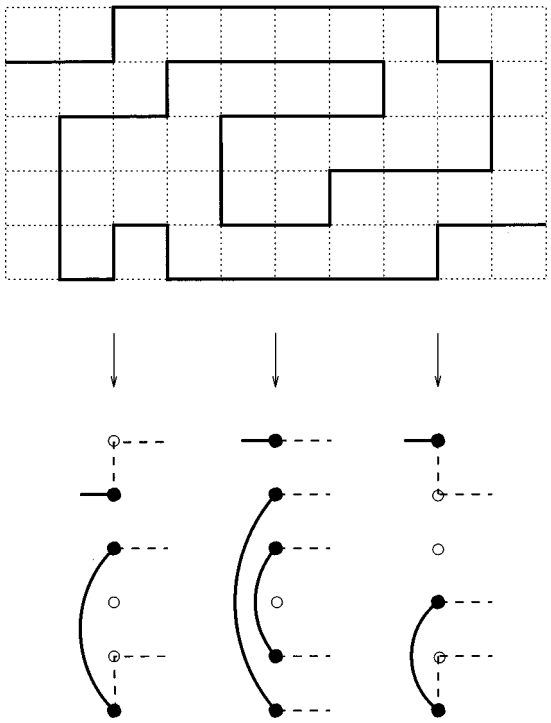

FIG. 6. Example of possible configurations defined for a SAW on a strip of width $L=6$, in the simple case without either orientation or interaction.

TABLE I. Transfer matrixes size S_L of q-legged walks for different values of the strip width L at $\beta_p=-\infty$ in the case of site (or plaquette) interaction.

Strip width L	S_L for q-legged walks $q=1$	$q=2$
1	1	
2	1	
3	2	
4	6	1
5	23	2
6	95	10
7	398	41
8	1716	200
9	7487	932
10	33121	4470
11	147909	21212
12		101090

$$G(x,\beta_p,\beta_a,r)=\sum_{N=1}^{\infty}\sum_{m_p,m_a} x^N e^{m_p\beta_p+m_a\beta_a} c_N(m_p,m_a,r)\ , \tag{3.1}$$

where x is the step fugacity and $c_N(m_p,m_a,r)$ is the number of different oriented walks, made up with N steps and m_p (m_a) parallel (antiparallel) contacts which connect the origin with an arbitrary point at distance r. For fixed values of β_p and β_a, a definite value $x_c(\beta_p,\beta_a)=1/\mu(\beta_p,\beta_a)$ exists, called critical fugacity, such that $G(x,\beta_p,\beta_a,r)$ decreases at long distances exponentially with r for $x<x_c(\beta_p,\beta_a)$, defining in this way a correlation length $\xi(x,\beta_p,\beta_a)$:

$$G(x,\beta_p,\beta_a,r)\underset{r\to\infty}{\sim}\exp\left[-\frac{r}{\xi(x,\beta_p,\beta_a)}\right]. \tag{3.2}$$

$\xi(x,\beta_p,\beta_a)$ diverges when $x\nearrow x_c(\beta_p,\beta_a)$ and the way in which it breaks away gives the exponent ν of Eq. (2.4):

$$\xi(x,\beta_p,\beta_a)\sim[x_c(\beta_p,\beta_a)-x]^{-\nu(\beta_p,\beta_a)}\ . \tag{3.3}$$

The TM approach consists of calculating exactly the correlation length $\xi_L(x,\beta_p,\beta_a)$, defined in Eq. (3.2), on an $L\times\infty$ strip, that is to say, a lattice strip of infinite length and finite width L. The idea is to write recursion relations between a strip of length r and a strip of length $r+1$. If we consider a walk on a strip which goes from the left to the right and we cut the strip at column r (see Fig. 6), the part of the path at the left of column r realizes a connectivity configuration $\mathcal{C}$ of the sites at column r. Giving $\mathcal{C}$ is the same as knowing the occupied sites of column r and how these occupied sites are connected with each other by the part of the walk at the left of r. In order to consider the interacting case, we have to take care, in the definition of a given configuration $\mathcal{C}$ at column r, also about the bonds occupied by the walk between columns $r-1$ and r.

The number of possible configurations $\mathcal{C}$ corresponds to the size S_L of the TM; this size can be strongly reduced by considering symmetry operations.

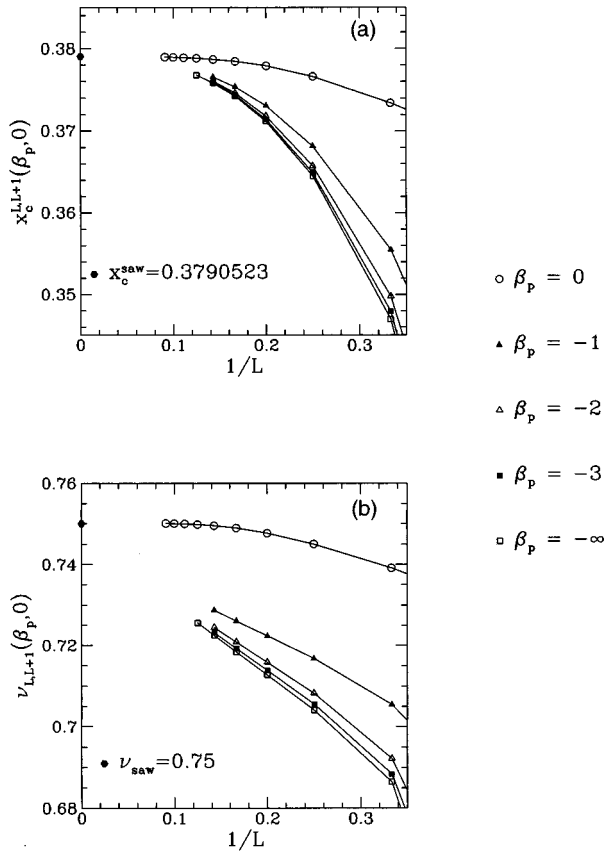

FIG. 7. (a) Critical fugacity $x_c^{L,L+1}(\beta_p,0)$ for the site model against the inverse of the strip width L at $\beta_p=-1,-2,-3,-\infty$. (b) Plot of the critical exponent $\nu_{L,L+1}(\beta_p,0)$ at the same values of β_p and with the same conventions as in (a).

For each couple of allowed configurations $\mathcal{C}$ and $\mathcal{C}'$, thought to correspond to adjacent columns, the TM is set up by calculating the quantity

$$\mathcal{T}_{\mathcal{C}\mathcal{C}'}=x^{t(\mathcal{C}')}e^{\beta_p[u_p(\mathcal{C}')+v_p(\mathcal{C}',\mathcal{C})]}e^{\beta_a[u_a(\mathcal{C}')+v_a(\mathcal{C}',\mathcal{C})]}\ , \tag{3.4}$$

where $t(\mathcal{C})$ is the number of occupied bonds in $\mathcal{C}$, $u_{p(a)}(\mathcal{C})$ the number of parallel (antiparallel) contacts in $\mathcal{C}$, and $v_{p(a)}(\mathcal{C}',\mathcal{C})$ the number of parallel (antiparallel) contacts between the monomers in $\mathcal{C}'$ and those added to obtain configuration $\mathcal{C}$. If there is no way to connect the two configurations $\mathcal{C}$ and $\mathcal{C}'$, the matrix element $\mathcal{T}_{\mathcal{C}\mathcal{C}'}$ is zero.

Once the matrix $\mathcal{T}$ has been computed for a strip of width L, it is trivial to extract the statistical quantities of interest. As $r\to\infty$, the expression of $G_L(x,\beta_p,\beta_a,r)$ is dominated by the largest eigenvalue of the TM, $\lambda_L^{\max}(x,\beta_p,\beta_a)$:

$$G_L(x,\beta_p,\beta_a,r)\underset{r\to\infty}{\sim}[\lambda_L^{\max}(x,\beta_p,\beta_a)]^r. \tag{3.5}$$

This means that for a strip of width L the correlation length is given by

$$\xi_L(x,\beta_p,\beta_a)=-\frac{1}{\ln\lambda_L^{\max}(x,\beta_p,\beta_a)}. \tag{3.6}$$

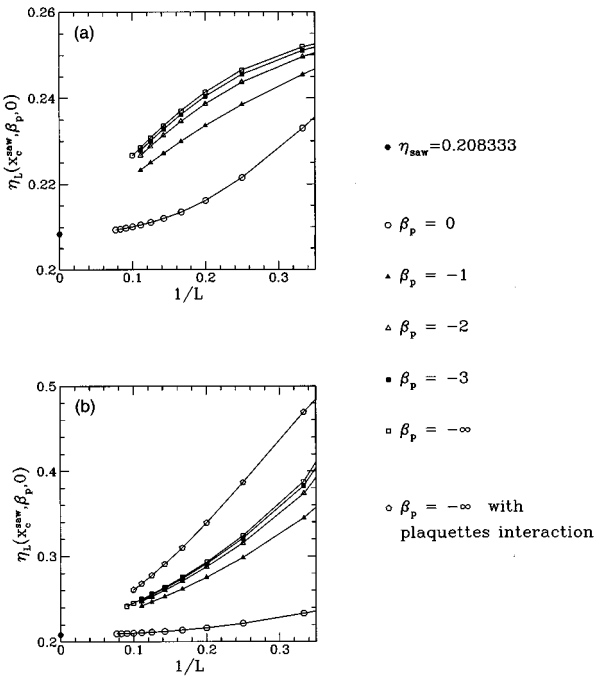

FIG. 8. (a) Critical exponent $\eta_L(x_c^{\mathrm{SAW}},\beta_p,0)$ against the inverse of the strip width L at $\beta_p=-1,-2,-3,-\infty$ for the bond model. (b) As in (a) but for the site model, and for the plaquette model in the case $\beta_p=-\infty$.

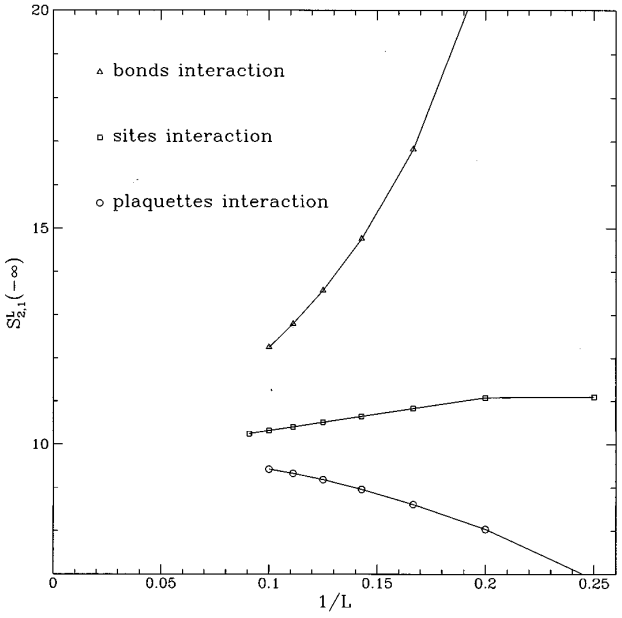

FIG. 9. Plot of the quantity $S^L_{2,1}(-\infty)$, defined in Eq. (4.1) of the text, against the inverse of the strip width L for all the considered models (bond, site, and plaquette).

A one-parameter phenomenological renormalization group approach can be used to obtain finite size approximations to the critical fugacity, $x_c^{L,L+m}(\beta_p,\beta_a)$, by comparing the correlation lengths of strips of different widths, L and $L+m$:

$$\frac{\xi_L(x_c^{L,L+m},\beta_p,\beta_a)}{L}=\frac{\xi_{L+m}(x_c^{L,L+m},\beta_p,\beta_a)}{L+m}, \quad (3.7)$$

where m is an integer number (usually $m=1$ or $m=2$). Linearizing around the fixed point of Eq. (3.7) gives a series of approximations for the correlation length exponent ν:

$$1+\frac{1}{\nu_{L,L+m}(\beta_p,\beta_a)}=\ln\left[\frac{\left.\frac{d\xi_L(x,\beta_p,\beta_a)}{dx}\right|_{x=x_c^{L,L+m}(\beta_p,\beta_a)}}{\left.\frac{d\xi_{L+m}(x,\beta_p,\beta_a)}{dx}\right|_{x=x_c^{L,L+m}(\beta_p,\beta_a)}}\right]\frac{1}{\ln\left(\frac{L}{L+m}\right)}. \quad (3.8)$$

To examine the exponent γ one can use the scaling relation $\eta=2x=2-\gamma/\nu$, where η is the exponent governing the decay at long distances of the critical correlation function. Finite size approximations to η can be obtained from the conformal invariance result [21]:

$$\eta_L(x,\beta_p,\beta_a)=2x_L(x,\beta_p,\beta_a)=\frac{L}{\pi\xi_L(x,\beta_p,\beta_a)}, \quad (3.9)$$

where the correlation length is evaluated for a strip with periodic boundary conditions.

The previous analysis can easily be adapted for any kind of IOSAW model (bond, site, or plaquette interactions) and for any q-leg type of oriented polymers. Of course the whole procedure is not a trivial task since, in our model, the walk carries an orientation. As explained in Ref. [8] this implies a larger TM than for the standard ISAW problem. Moreover, it is much more complicated to keep track of the noncrossing constraint: some configurations have to be disregarded if the orientations of the different parts of the walk are not consistent with this constraint.

The situation is slightly simpler if we restrict ourselves to the case where parallel bonds are forbidden ($\beta_p=-\infty$). In this case a configuration $\mathcal{C}$ such that $u_p(\mathcal{C})\neq 0$ cannot exist. By using suitable symmetry and periodic boundary conditions we could work for the bond, site, and plaquette mod-

TABLE II. Critical exponent $\eta_L(x_c^{\mathrm{SAW}},-\infty,0)$ for different values of the strip width L in the three models considered, with final extrapolations in the thermodynamic limit $L\to\infty$; the power-law convergence exponent used in the Bulirsch-Stoer algorithm is $\omega=1$. The error bars have a purely statistical meaning.

	$\eta_L(x_c^{\mathrm{SAW}},-\infty,0)$		
Strip width L	Bonds	Sites	Plaquettes
1	0.308786	0.308786	0.308786
2	0.258368	0.617572	0.617572
3	0.251908	0.387552	0.469266
4	0.246514	0.323980	0.386670
5	0.241406	0.293070	0.339154
6	0.237080	0.275156	0.309874
7	0.233584	0.263574	0.290700
8	0.230786	0.255490	0.277438
9	0.228524	0.249526	0.267818
10	0.226670	0.244940	0.260560
11		0.241300	
Extrapolations	0.2094(32)	0.2096(10)	0.2085(14)

els with strips up to $L=10$, $L=11$, $L=10$, respectively, in the case of one-leg polymers. The sizes of the different matrices are listed in Table I.

For the general IOSAW model, without any configurational simplification, we could operate with widths up to $L=9$ for each of the models considered. This corresponds to an improvement of two units compared to the previous analysis of the same problem [8].

IV. ANALYSIS OF THE NONUNIVERSALITY PREDICTION

We start our numerical analysis by considering the line $\beta_a=0$ for $\beta_p\leqslant 0$, where the theoretical predictions of conformal invariance should hold in the form expressed by Eq. (2.7). For fixed values of β_p and β_a and for any type of IOSAW (site, bond, plaquette) we first compute $x_c^{L,L+m}(\beta_p,\beta_a)$ (the case $m=1$ is the most used) by using Eq. (3.7). We then estimate the correlation length exponent $\nu_{L,L+m}(\beta_p,\beta_a)$ through Eq. (3.8) and the exponent $\eta_L(x,\beta_p,\beta_a)$ by means of Eq. (3.9). In this last case the most natural strategy is to compute $\eta_L(x,\beta_p,\beta_a)$ at the critical value $x=x_c^{L,L+m}(\beta_p,\beta_a)$ obtained with the phenomenological renormalization group law (3.7).

TABLE III. Critical exponent $\eta_L(x_c^{\theta},-\infty,\beta_\theta)$ for different values of the strip width L in the sites model, with final extrapolation in the limit $L\to\infty$; the power-law convergence exponent used in the Bulirsch-Stoer algorithm is $\omega=2$. The error bars have a purely statistical meaning.

Strip width L	$\eta_L(x_c^{\theta},-\infty,\beta_\theta)$
1	0.371570
2	0.743138
3	0.582390
4	0.555390
5	0.537908
6	0.528058
7	0.521530
8	0.517070
9	0.513858
10	0.511496
11	0.509748
Extrapolations	0.5010(20)

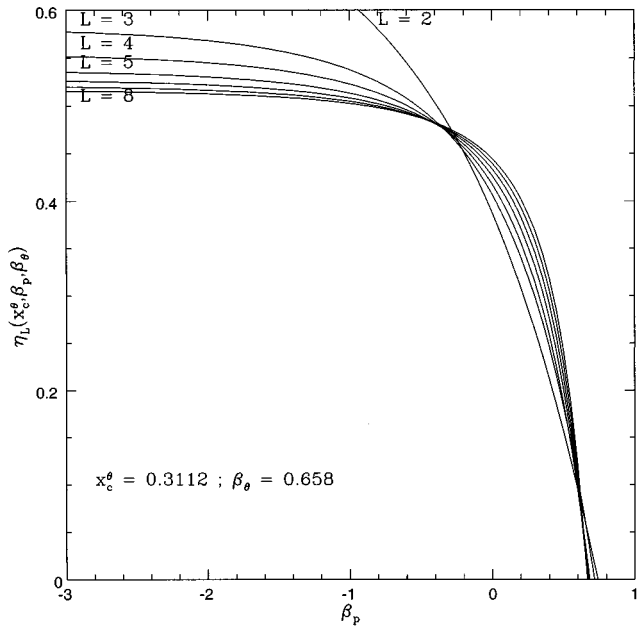

FIG. 10. Critical exponent $\eta_L(x_c^{\theta},\beta_p,\beta_\theta)$ against the parallel interaction parameter β_p, for different strip widths L.

However, it is more efficient to explicitly use the fact that $x_c(\beta_p,0)$ is constant and equal to $x_c(0,0)$ for any value of β_p less than 0. Along this line we can then calculate η_L at $x=x_c(0,0)=x_c^{\mathrm{SAW}}$ using the estimate $x_c^{\mathrm{SAW}}=0.379\,052\,3$ [22]; in this way it turns out that these estimates of η_L are more asymptotic than with the standard approach.

We repeated this procedure for $\beta_p=-1,-2,-3$ where some measurements have already been made in Ref. [8] with the bond model, but where our calculation adds two extra terms for the strip width L, and for the more significant case $\beta_p=-\infty$ where our TM can work with strips up to $L=11$ or $L=10$, depending on the model.

As a check of the quality of our approach and to understand the kind of convergences in $1/L$ to expect, we consider the critical fugacity $x_c^{L,L+1}(\beta_p,0)$ and the thermal exponent $\nu_{L,L+1}(\beta_p,0)$. Both these two quantities should maintain their SAW values ($\nu_{\mathrm{SAW}}=\frac{3}{4}=0.75$ and $x_c^{\mathrm{SAW}}=0.379\,052\,3$) for any value of β_p. In Fig. 7 we plot these results for the site model. In order to make a comparison we insert the estimates for the SAW case where we can work with strip widths up to $L=13$.

Although the convergence is much slower than for the SAW , it is quite clear that the different sets of points approach the expected values. This can easily be confirmed by an extrapolation of the data with one of the sophisticated techniques that are used with TM calculations, such as the Bulirsch-Stoer algorithm [23,24].

We can then look at the entropic exponent

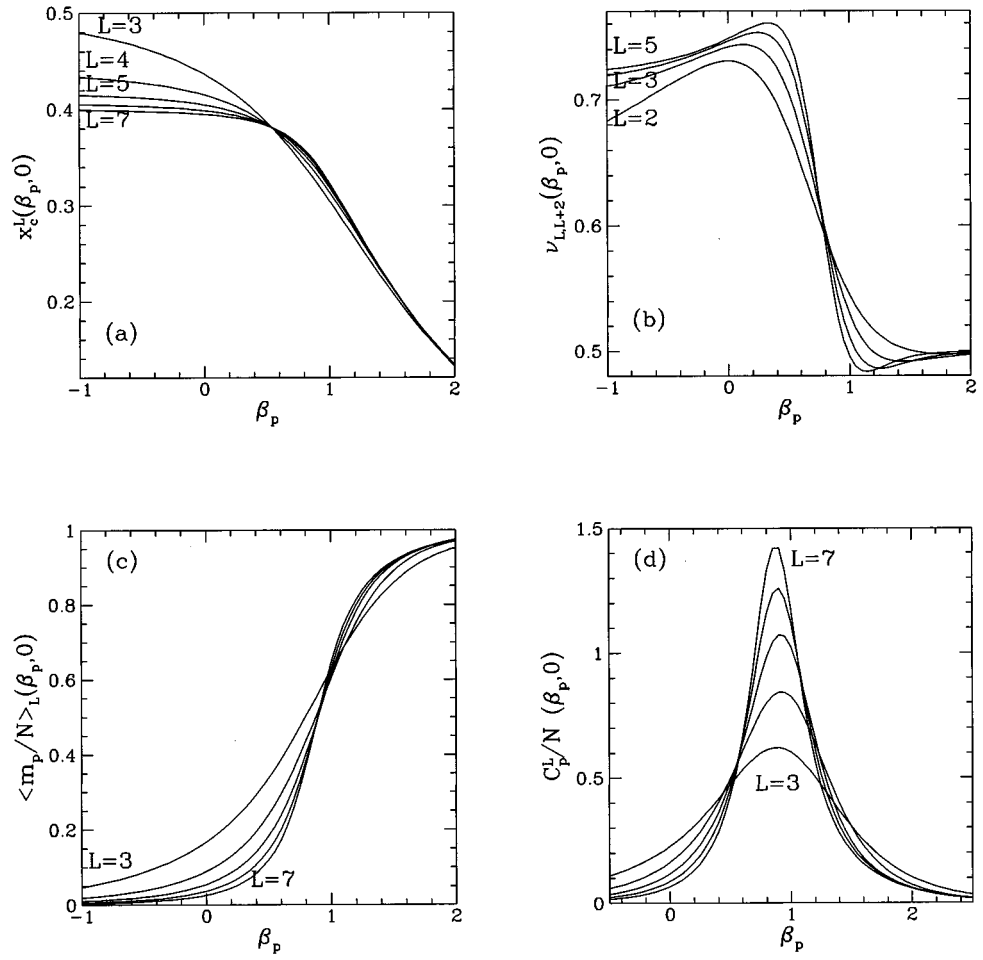

FIG. 11. One-strip critical fugacity $x_c^L(\beta_p,0)$ (a), correlation length exponent $\nu_{L,L+2}(\beta_p,0)$ (b), average number of parallel contacts $\langle m_p/N\rangle_L(\beta_p,0)$ (c), and step specific heat $(C_p^L/N)(\beta_p,0)$ (d) against the parallel interaction parameter β_p for different strip widths L.

$\eta_L(x_c^{\rm SAW},\beta_p,0)$. In Figs. 8(a) and 8(b) the obtained results for the three models are plotted together with those for the SAW case. Again, at first sight, the data seem to converge to the SAW value ($\eta_{\rm SAW}=\frac{5}{24}=0.2083\overline{3}$) for every value of β_p, but this time we have to be more careful because the absolute values of the estimates are still quite far from the final results (Table II); this means that the convergence is much slower than for x_c and ν. Nevertheless the application of extrapolation techniques again confirms an asymptotic value for η very close to the SAW one for any value of β_p. Looking at Table II, we see that the extrapolated values of $\eta(-\infty)$ for the three models are slightly higher than the SAW value. If we want to be conservative and consider only the site model which gives the highest estimate of the exponent, we cannot completely rule out the prediction of nonuniversality, but if we calculate the gap $\Delta_1(-\infty)$, defined by Eq. (2.8), we find that it is around 0.001, nine times smaller than observed by exact enumeration [6]. In other words, if the nonuniversality exists it must give rise to an extremely tiny effect. Indeed, from our numerical data, we can estimate an upper bound for the undetermined function $|\lambda(\beta_p)|$ [defined in Eq. (2.6)] equal to $|\lambda_{\rm max}|=|\lambda(-\infty)|=0.0001$. This conclusion has been confirmed with the other two models (bond and plaquette).

As a further check we consider two-leg oriented walks. Instead of the quantity described in Eq. (2.9), it is more convenient to look at the variable $S_{q,q'}(\beta_p)$ defined by (in the following equation we have neglected the dependence on β_a and on x_c, since they are fixed to the values $\beta_a=0$ and $x_c=x_c^{\rm SAW}$)

$$S_{q,q'}(\beta_p)=\frac{\Delta\eta_q(\beta_p)}{\Delta\eta_{q'}(\beta_p)}=\frac{\eta_q(\beta_p)-\eta_q(0)}{\eta_{q'}(\beta_p)-\eta_{q'}(0)}, \qquad (4.1)$$

which, for any value of β_p less than zero, should give $(q/q')^2$ according to Eq. (2.6).

In Fig. 9 we plot our estimates of $S_{2,1}^L(\beta_p=-\infty)$ as a function of $1/L$, for the three models. We can see that the data do not approach the expected value 4, but seem to be approaching three distinct values as is possible from Eq. (4.1) if $\eta_q(-\infty)=\eta_q(0)$.

These results seem to be in clear contrast with Eq. (2.6), and we conclude this part of the analysis by saying that the nonuniversality effects are unlikely along the $\beta_a=0$ line.

To verify the other possibility, mentioned in Sec. II, that a continuous variation of the entropic exponent γ could occur along the θ line between the free and the collapsed phases, we first check that the point ($\beta_p=-\infty$, $\beta_a=\beta_\theta$) really falls in the universality class of the interacting SAW on a Manhattan lattice. To this end, it is convenient to work with the site model because in the nonoriented case, $\beta_p=\beta_a$, it corresponds to the model usually employed to study the θ transition, for which the location of transition and the relative critical fugacity have been determined very accurately by

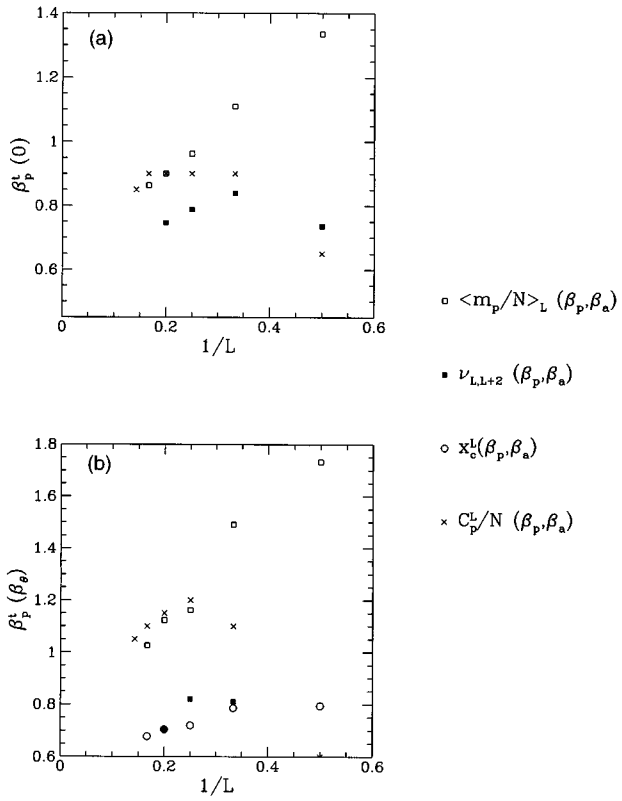

FIG. 12. (a) Values of the parallel interaction parameter β_p at the intersection of two successive L estimates of $x_c^L(\beta_p,0)$, $\nu_{L,L+2}(\beta_p,0)$, and $\langle m_p/N\rangle_L(\beta_p,0)$, and at the maxima of the step specific heat $(C_p^L/N)(\beta_p,0)$, against the inverse of the strip width L. (b) As in (a), but at $\beta_a=\beta_\theta$.

means of Monte Carlo calculations [4] at the values $\beta_p=\beta_a=\beta_\theta=0.658(4)$ and $x_c(\beta_\theta,\beta_\theta)=x_c^\theta=0.3112(13)$.

Our estimates for $\eta_L(x_c^\theta,-\infty,\beta_\theta)$ with strips up to $L=11$ are listed in Table III. They converge towards $\frac{1}{2}$, as expected for the Manhattan θ point where $\gamma=\frac{6}{7}$ and $\nu=\frac{4}{7}$.

To explore the θ line we have to use the standard TM, the one implemented for the whole phase diagram, which allows us to work with strips up to $L=8$. (For each single point we can work with strip widths up to 9, as said in the preceding section, but the time required to study the full line would be prohibitive.) The exponent $\eta_L(x_c^\theta,\beta_p,\beta_\theta)$ is plotted in Figure 10 as a function of β_p for different sizes of the strips. We can see that the values of η_L become constant, as the size of the system grows, for negative values of β_p. Only when β_p is bigger than zero does the exponent start to decrease abruptly towards the expected value $\eta_\theta=0$. More than a continuous variation of the exponent, this behavior indicates that only for $\beta_p=\beta_a=\beta_\theta$ is the critical regime governed by the standard θ point, while for $\beta_p\leqslant\beta_\theta$ the system immediately flows to the universality class of the Manhattan θ point. This scenario is also supported by the fact that the different lines $\eta_L(x_c^\theta,\beta_p,\beta_\theta)$ are crossing each other twice (apart from the less asymptotic case $L=2$) in connection with values close to $\eta=0.5$ and $\eta=0$, as one can expect if there are only two universality classes.

We then conclude this part of our calculation with strong evidence of the absence of any nonuniversal behavior, both for $\beta_a=0$ and $\beta_a=\beta_\theta$, but with the very important result

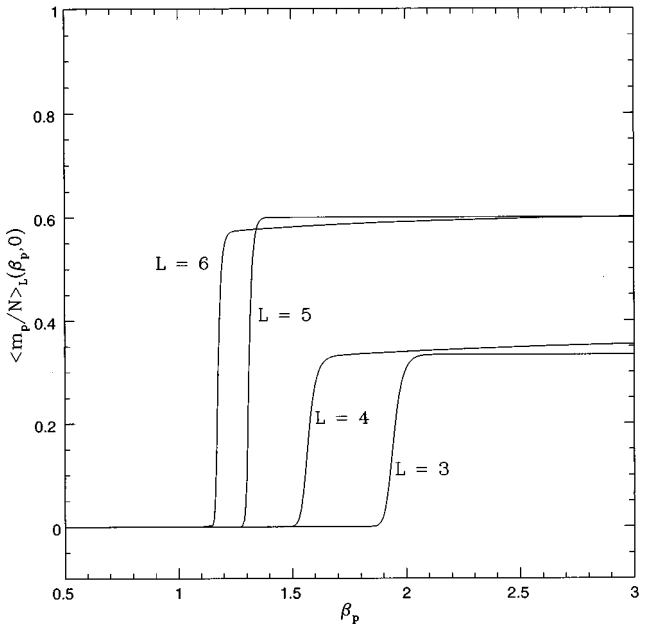

FIG. 13. Plot of the order parameter $\langle m_p/N\rangle_L(\beta_p,0)$, as a function of the parallel interaction parameter β_p, obtained by using a transfer matrix with free boundary conditions, for different strip widths L. With these boundary conditions the value $\langle m_p/N\rangle=1$ expected in the spiral phase cannot be reached with strips of finite width L.

that the θ line between the free and the collapsed phases is entirely governed (when $\beta_p<\beta_\theta$) by the universality class of the Manhattan θ point. This implies that in the enlarged phase diagram (β_p,β_a) the standard θ point acquires another relevant direction, becoming more properly a multicritical point. The question whether the θ line continues for $\beta_p\geqslant\beta_\theta$ (as drawn in Fig. 2 by the authors of Ref. [6]), and eventually with which value for the exponent η, or whether it stops at $\beta_p=\beta_\theta$, will be investigated in the next section.

V. THE PHASE DIAGRAM

We try to map out the phase diagram for the site model where we are able to work with the largest sizes [in this case L up to 7 because the computation of $x_c^L(\beta_p,\beta_a)$ through Eq. (5.4) is very time consuming]. In order to localize the transition lines we can look at different quantities, such as the critical step fugacity $x_c(\beta_p,\beta_a)$, that stay constant, at fixed β_a, for any β_p which belongs to the SAW universality class, and the related order parameters $\langle m_p/N\rangle(\beta_p,\beta_a)$, the average number of parallel contacts per step, and $\langle m_a/N\rangle(\beta_p,\beta_a)$, the average number of antiparallel contacts per step, that can be easily computed by

$$\left\langle\frac{m_p}{N}\right\rangle(\beta_p,\beta_a)=\frac{1}{N}\frac{\partial\ln[Z_N(\beta_p,\beta_a)]}{\partial\beta_p}\underset{N\to\infty}{\to}-\frac{\partial\ln[x_c(\beta_p,\beta_a)]}{\partial\beta_p} \tag{5.1}$$

and

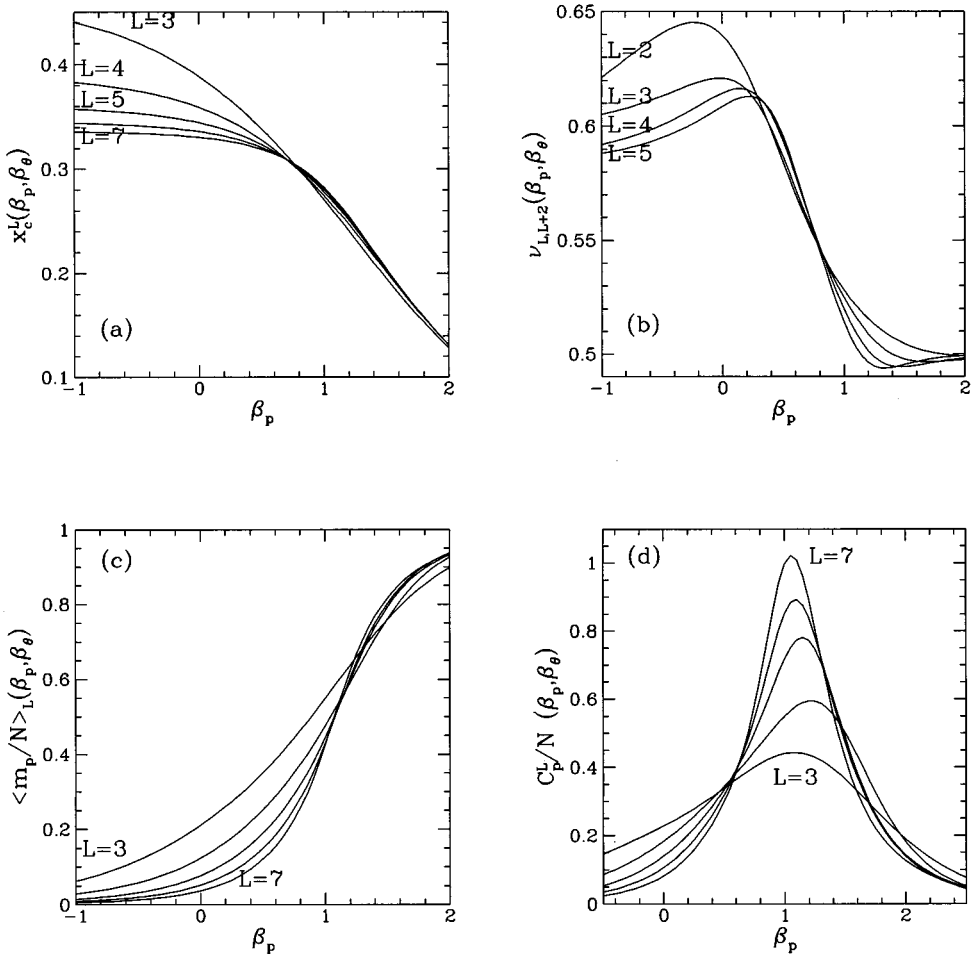

FIG. 14. As in Fig. 11, but at $\beta_a=\beta_\theta$.

$$\left\langle \frac{m_a}{N} \right\rangle (\beta_p,\beta_a) = \frac{1}{N}\frac{\partial \ln[Z_N(\beta_p,\beta_a)]}{\partial \beta_a} \underset{N\to\infty}{\to} -\frac{\partial \ln[x_c(\beta_p,\beta_a)]}{\partial \beta_a}. \tag{5.2}$$

It is also useful to consider the specific heat per step

$$\frac{C_p}{N}(\beta_p,\beta_a) = \frac{\langle m_p^2\rangle(\beta_p,\beta_a) - \langle m_p\rangle^2(\beta_p,\beta_a)}{N} \underset{N\to\infty}{\to} -\frac{\partial^2 \ln[x_c(\beta_p,\beta_a)]}{\partial \beta_p^2}, \tag{5.3}$$

which is a sort of ''partial'' specific heat regarding only the parallel interaction energy, and the correlation length exponent ν.

To compute the order parameters and the specific heat by means of the preceding equations, we have to derive finite size estimates $x_c^L(\beta_p,\beta_a)$ of the critical fugacity using only the L-wide strip. We have then to avoid the phenomenological renormalization group equation (3.7), so we take $x_c^L(\beta_p,\beta_a)$ as the value at which the correlation length (3.6) diverges:

$$\lambda_L^{\max}(x_c^L(\beta_p,\beta_a),\beta_p,\beta_a)=1. \tag{5.4}$$

Of course we still use Eqs. (3.7) and (3.8) to calculate $\nu_{L,L+m}(\beta_p,\beta_a)$ where we take $m=2$ to avoid the strong parity effects typical of compact phases.

In Fig. 11 all these quantities are plotted, in the case $\beta_a=0$, for different sizes of the strips. Signals of the free-to-spiral transition are evident. The critical fugacity is constant for negative or small values of β_p and then it is dropping down very quickly. The exponent ν crosses over from the SAW value $\frac{3}{4}$ to the compact phase value $\frac{1}{2}$. The average number of parallel contacts per site rises from 0 to 1 when β_p increases and the specific heat is presenting a well defined peak. A well known and often used method [25–27] to determine the transition consists in pinpointing the crossing points between the different lines drawn in Figs. 11(a)–11(c) and in following their behavior when the size of the strip increases. These crossing points, together with the position of the specific heat maxima, are plotted in Fig. 12(a). We can try to localize the transition $\beta_p^t(\beta_a=0)=\beta_p^t\ (0)$ to the spiral phase at

$$\beta_p^t(0)=0.6(15).$$

The order of this transition is harder to determine. There are many indications that it could be of second order, for example, $\langle m_p/N\rangle$ does not jump as abruptly as expected for a discontinuous transition and there are no strong movements of the heights of the specific heats. However, we feel that in the study of this point the effects of the boundary conditions

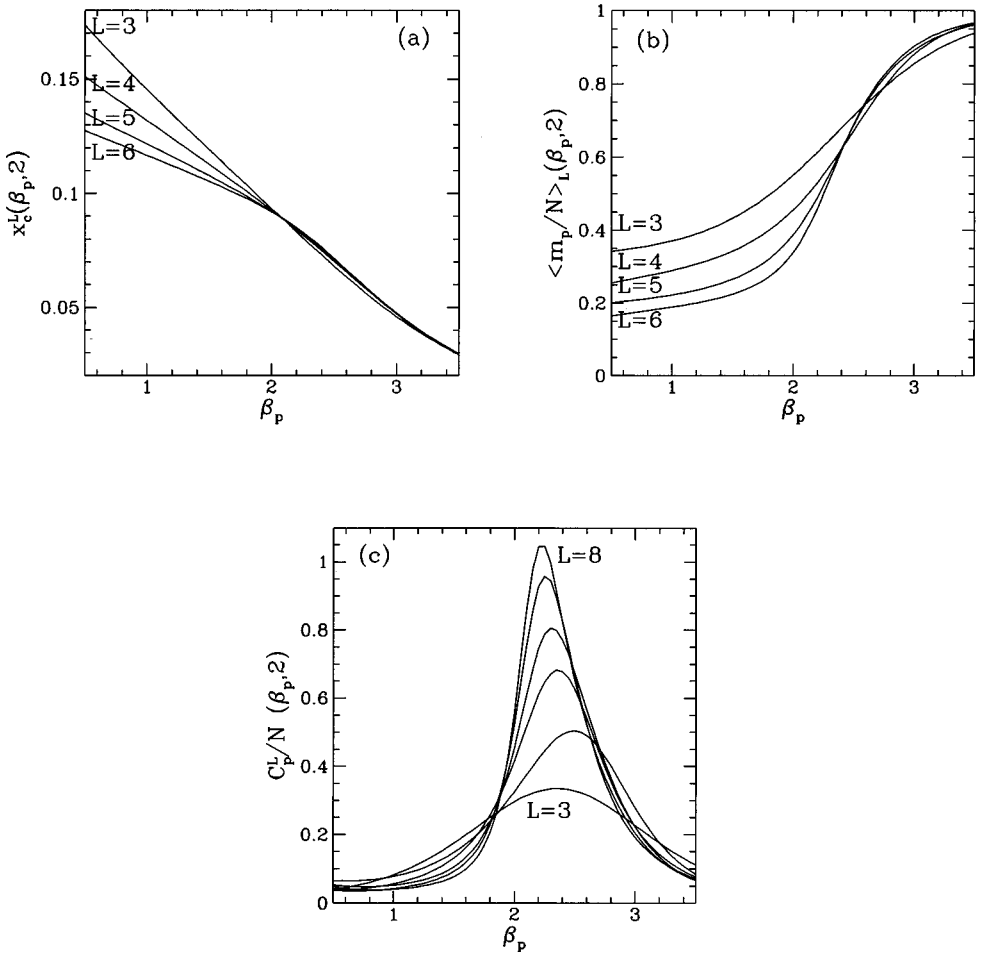

FIG. 15. As in Fig. 11, but at $\beta_a=2$, in order to evidence the collapsed-to-spiral transition. In this case we do not plot the correlation length exponent ν: it is always $\frac{1}{2}$ in compact phases.

can be strong. With the periodic boundary conditions we have used we see that there are parallel contacts which do not trap the walk. This fact, which is insignificant for negative or small values of β_p, can round the effects of the free-to-spiral transition for small sizes of the strips. To verify this hypothesis we build a TM with free boundary conditions. In this way we avoid any unwanted parallel interaction, but unfortunately this limits the system size (only up to $L=6$). Still we can see that the order parameter now increases more rapidly (Fig. 13), confirming the conjecture of Refs. [6,10] of a first order transition. This analysis is consistent with this conclusion for any line $\beta_p=k$, such that $k<\beta_\theta$.

The study along the θ line becomes even more complicated and uncertain because we are moving along a set of unstable points. Moreover, the jump in the exponent ν is now reduced because we are going from a regime with $\nu=\frac{4}{7}$ (for $\beta_p<\beta_\theta$) to another one with $\nu=\frac{1}{2}$ (for β_p sufficiently large). All the quantities already calculated in the case $\beta_a=0$ are now plotted in Fig. 14 at $\beta_a=\beta_\theta$. The position of the crossing points and of the specific heat peaks [Fig. 12(b)] suggests that the transition takes place at the point

$$\beta_p^t(\beta_a=\beta_\theta)=0.70(2).$$

This estimate is not very sharp and we are not able to determine if the θ point is the ending point of the θ line between the free and the collapsed phases or not.

The analysis of the collapsed-to-spiral transition for $\beta_a>\beta_\theta$ helps to elucidate this problem. This kind of transition is very hard to find by numerical methods because many of the critical indices are the same in the two phases (e.g., the exponent ν). This can create many false indications, as has been seen for other polymer models [20,28,29]. Fortunately for this problem the plot of the specific heat seems to present a clear peak [Fig. 15(c)] the position of which appears to converge towards the diagonal $\beta_p=\beta_a$, for all the values $\beta_a>\beta_\theta$ considered. This means that the collapsed-to-spiral transition merges with the θ point and, since we expect [6] the entire spiral transition line $\beta_p^t(\beta_a)$ to be continuous, we can conclude that the three critical lines all join together at the θ point, which becomes a fully repulsive point in the renormalization group language. While we do not have clear evidence of the order of the collapsed-to-spiral transition, the fact that for large β_a the transition takes place at large β_p could be an indication of a discontinuous transition, as explained in Ref. [6].

We end this section by conjecturing a phase diagram, shown schematically in Fig. 16. Once again we must caution

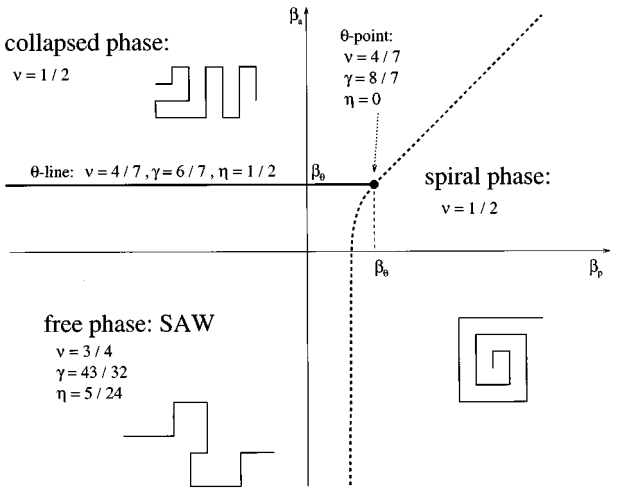

FIG. 16. A schematic illustration of the conjectured phase diagram for the site model. Dashed lines represent first order transition lines. The main critical indices are summarized.

the reader about the numerical difficulties that we have to deal with, when working near the θ point, and in the compact phases. In such conditions the sizes of the strip are not big enough to give definitive answers. Nevertheless, on the basis of other checks we have done varying β_a at β_p fixed, and of preliminary results of renormalization group calculation in position space, we believe our phase diagram to be trustworthy. We recall that our conclusions were reached with a numerical analysis of the site model, and therefore some nonuniversal features, such as the location of the transition lines, will not be the same for the other models.

VI. SUMMARY AND CONCLUSIONS

We have numerically studied the critical properties of IOSAW in the plane of parallel and antiparallel interactions by means of a TM calculation. We decided to give particular attention to the case in which parallel contacts are forbidden because in such a situation some of the theoretical predictions of nonuniversality of the entropic exponent γ, obtained by Cardy, should be more evident than in other parts of the phase diagram. Moreover, the absence of parallel interactions allowed us to enlarge the system sizes that could be studied. We devoted some care to choosing more adequate models with which to study these nonuniversal effects.

Despite these efforts, we found no evidence to support Cardy's theory, but, on the contrary, many indications of its invalidity. We could also see that along the θ line, the extremes of which we have verified to belong to different universality classes, the entropic exponent stays constant, changing its value only at the θ point. According to us, our results are more robust than those obtained by Monte Carlo enumeration [9,10], because the TM approach allows us to work with really infinite polymers, although restricted in a strip, whereas with other approaches one is always limited by the finiteness of the walk. If the nonuniversality effect predicted for this model, as now believed [30], turned out only for polymers with a large number of steps, the Monte Carlo method would miss it, while the TM one would not. Of course the extrapolation analysis in this last case must be extremely careful and sophisticated.

In the second part of the paper we tried to work out the full phase diagram for the model with interactions between the sites. In this case the numerical accuracy is not as good as for the determination of the γ exponent, but we were able to see clearly the existence of the three expected phases (free, collapsed, spiral) and of the three lines which are separating them. One of these lines is the above mentioned θ line, which falls in the universality class of the collapse transition of ISAW on a Manhattan lattice, while the other two are probably of the first order. On the basis of our numerical checks we suppose that these three lines are merging at the standard θ point ($\beta_p = \beta_a = \beta_\theta$). We think that some new large Monte Carlo simulations are necessary to verify this last hypothesis, whereas we believe that our results for the entropic exponent should open a new debate on the nonuniversality conjecture presented in Ref. [5] in order to clarify whether the directed application of conformal invariance fails or why the undetermined function $\lambda(\beta_p)$ defined in Eq. (2.6) is so small.

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