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F-model-type phase transition in the 2D Flory model of polymer melting

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Abstract. In this paper we perform a transfer matrix study of the F model and the Flory model of polymer melting. For the F model, which can be reformulated in terms of polymers, we calculate numerically the exponent $\eta(T)$ of the massless phase and our results are in good agreement with recent conjectures. For the Flory model we find a very similar behaviour suggesting that these two models have the same kind of transition. The discrepancy with Monte Carlo calculations where a first-order phase transition has been found is discussed.

1. Introduction

The problem of polymer melting has recently attracted renewed interest in the literature, mainly because of a recent disproof of the Flory theory (see Nagle *et al* (1984) for a review). The problem is to describe a possible transition from an extended chain crystalline state in which the internal degrees of freedom of molecules are well ordered to a fluid phase in which these internal degrees of freedom are disordered.

The simplest theoretical model for handling this problem is a lattice model which was proposed by Flory (1956) 30 years ago. In this model one considers a Hamiltonian walk (i.e. a self-avoiding walk which passes through all sites of a square or cubic lattice). This walk represents a polymer whose rigidity is taken into account by associating with each bond which is not collinear with the preceding one ('gauche' bond) an energy $\varepsilon > 0$ (see figure 1). One then has a competition between rigidity and entropy effects. In particular at $T = \infty$ one recovers the classical Hamiltonian walk while at $T = 0$ the polymer is completely ordered and all bonds are parallel to one axis of the lattice. This model is generally expected to contain the essential features of the physics of polymer melting although more sophisticated models have been introduced recently in 2D, presenting in particular the property of 'Gridlock' (Nagle 1985). We will not discuss such models here.

The first study of this model is due to Flory (1956). His method consists in evaluating with a kind of mean-field-type approximation the entropy per site $s(g)$ as a function of the fraction g of gauche bonds. The main result is that for g smaller than a finite non-zero value g_0, the entropy $s(g)$ is zero, i.e. the number of configurations grows slower than exponentially with the size of the system. This leads then to the prediction of a first-order phase transition, the low-temperature phase being completely ordered and inactive and g jumping from 0 to a finite value $g_c > g_0$ at $T = T_c$. In this Flory treatment the result is valid for all dimensionalities and for modified versions of the problem where one considers, for instance, a fixed concentration of polymers and of

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solvent molecules. A slightly modified treatment involving the Huggins (1942) approximation has also been given (Gibbs and di Marzio 1958). The approximation of Flory-Huggins gives the exact result when applied to another two-dimensional model, the KDP† model (Nagle 1974). While the Flory-Huggins result was also in agreement with experiments on real polymers in three dimensions, it has been considered for a long time that this treatment was at least qualitatively correct. The results have been applied in particular in the Gibbs-di Marzio (1958) theory of the glass transition.

Twenty years later however, Gujrati (1980, 1982) and Gujrati and Goldstein (1981) have shown the existence of an important failure in the Flory treatment. Their method consists in evaluating explicitly in the 2D or in the 3D case the number of a certain kind of Hamiltonian walk, obtaining in this way a lower bound to $s(g)$ which is not zero except at $g = 0$. This shows that the essential result of the Flory-Huggins approximation is wrong. There was then no more reason to believe in the results of the Flory treatment and the authors raised the question of the nature of the transition—if any—in the general case.

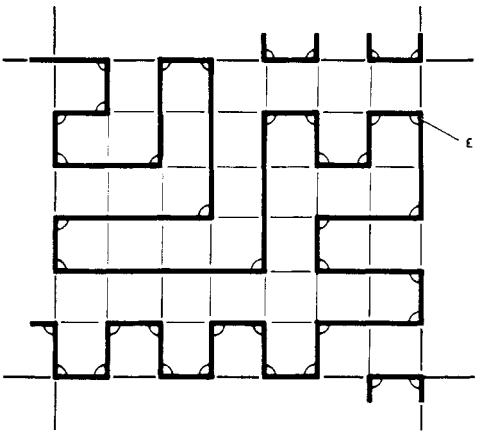

Figure 1. A typical piece of a Hamiltonian walk on the square lattice. In the Flory model an energy ε is associated with each corner of the polymer.

Recently, Baumgartner and Yoon (1983) performed Monte Carlo simulations of the model in two and three dimensions, obtaining indications of a first-order phase transition in each case, with a low-temperature phase which is almost completely ordered, the Flory-Huggins results becoming better when one goes from $D = 2$ to $D = 3$ as is expected for a mean-field-type approximation.

The purpose of this paper is to carry out a transfer matrix study of the Flory model on strips and to give evidence of an F-model-type† phase transition in the 2D case. The paper is organised as follows. In § 2 we study the F model on strips. This model, which is solvable only in the thermodynamic limit, can be interpreted in terms of a polymer problem similar to the Flory model, so our study will give a qualitative understanding of the finite-size effects in these polymer problems. We will in particular extract from the correlation lengths predictions for $\eta(T)$ which confirm recent conjectures. In § 3 we carry out a similar study of the Flory model, obtaining a strong

† This model is defined and studied in detail in Baxter (1982).

indication of the same kind of transition, with a non-diverging specific heat, a correlation length scaling as N for $T > T_c$ and a susceptibility scaling as a power of N in part of the high-temperature region. In § 4 we study modifications of the model and suggest that, as in the XY case, a small modification of the rules could give strong modifications of the nature of the transition. This could explain the discrepancy between our results and those of Monte Carlo simulations.

2. The F model on strips

In this section we present a numerical transfer matrix study of the F model on strips.

This model is a particular six-vertex model (see the energies in figure 2) which is almost completely solved in the thermodynamic limit only (Lieb and Wu 1972, Baxter 1982). As Nagle (1974) has pointed out, this model can be interpreted in terms of polymers. Let us choose one sublattice of the square lattice and put a link of polymer on each arrow which goes outwards from a site of this sublattice. Because of the allowed vertex configurations one gets in this way two polymer links attached to each site. The sites where these two links are not collinear correspond to vertices 1-4 and have an energy ε (see figure 3). The F model thus has many features in common with the Flory model. However because the polymer-arrow correspondence is defined locally one loses the connectivity constraint of a single Hamiltonian walk. If one considers a finite system with free boundary conditions as in figure 3 it is now filled by several non-intersecting self-avoiding walks of varying length whose extremities are on the boundary, and also by polymer loops. When the system becomes infinite, the main difference with the Flory model is the presence of these loops. This is an unphysical feature whose consequences are difficult to evaluate *a priori*. We have

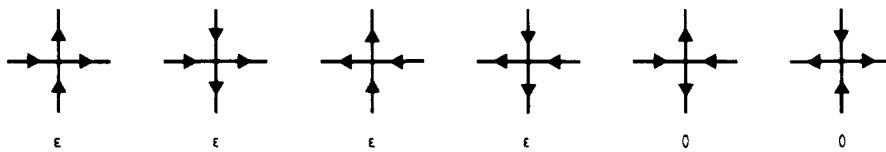

Figure 2. Energies of the F model. The two other possible vertices are forbidden by the ice rule.

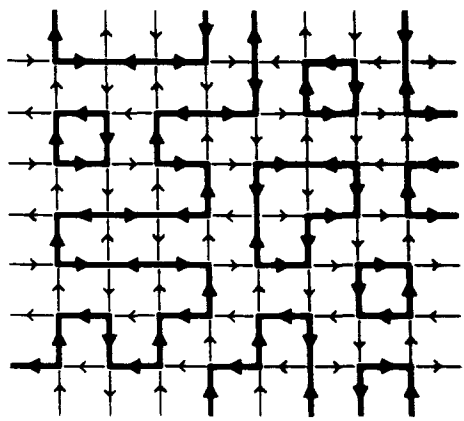

Figure 3. Example of a polymer version of a typical configuration of the F model. Bold lines represent polymer links.

carried out a study of this model by the transfer matrix method on strips of finite width N. The lattice is the square lattice with the strip axis parallel to the $(1, 0)$ direction (normal strip). We have taken periodic boundary conditions. The matrices have been written in this polymer representation. Transfer matrices for polymers are now well known (see Enting 1980, Derrida 1981, Derrida and Herrmann 1983).

The first quantities we will study are the thermodynamic ones. They are known in the thermodynamic limit where it has been shown that the model has a transition of infinite order at $T_c = (\log 2)^{-1}$ (with $k_B = \varepsilon = 1$). At this point all thermodynamic quantities have an essential singularity of the type $\exp(-\text{constant} \times |T - T_c|^{-1/2})$ (Lieb and Wu 1972, Baxter 1982). The specific heat does not diverge but has a maximum at a value $T > T_c$. The exponent α can be taken as negative and infinite. As an example of the efficiency of the study on strips we give in figure 4 the specific heat C_N per site on strips of width N. There are some parity effects which are often encountered in this kind of polymer model (Saleur 1986) but the results for each parity converge respectively in a regular and rapid way to their exact values.

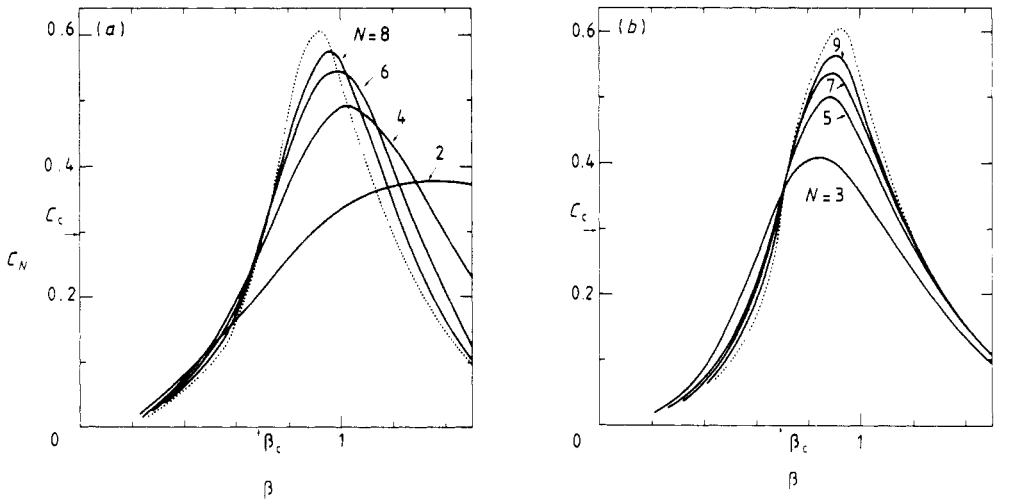

Figure 4. Plot of the specific heats per site C_N in the F model. (*a*) N even, (*b*) N odd. C_c and β_c are the critical specific heat and critical temperature, respectively. The dotted curves are the results for the infinite system.

More interesting and generally not exactly known are the electric quantities of the F model to which we turn now.

The F model is an antiferroelectric model. At $T = 0$ it is completely ordered with vertices of type 5 and 6 only. The order parameter is a staggered polarisation. In terms of polymers the two ground states correspond to the situation where all polymer links are aligned parallel to one of the two axes of the lattice. In terms of polymers the order parameter can be taken:

$$m = n_h - n_v \tag{1}$$

where n_h and n_v are respectively the number of horizontal (vertical) links per site. This order parameter grows as $T = T_c$ with an exponent β which can be taken as infinite. Its general form is exactly known (Baxter 1973). On a strip of width N the two ground states correspond to the polymer links aligned parallel to the axis of the

strip or perpendicular to it, forming in this way loops around the strip (we work with periodic boundary conditions). For N even, one can go from a region which is in one ground state to a region which is in the other ground state by creating an interface of energy N. This is not possible for N odd. In this case the transfer matrix breaks into two equal submatrices, each corresponding to one preferred orientation. By working with one of these submatrices one can observe curves m_N as a function of temperature which give a good idea, when N grows, of the variation of the order parameter in the infinite system, as can be seen in figure 5. For N even, on the contrary, the symmetry between the two directions is respected by the transfer matrix and m_N is always zero. This effect of breaking the symmetry for N odd could be easily suppressed by working on strips in a diagonal direction, as will be done for the Flory model case. However, we have obtained better results by working on normal strips with N even where the symmetry is also respected, so we will study this case only in the following.

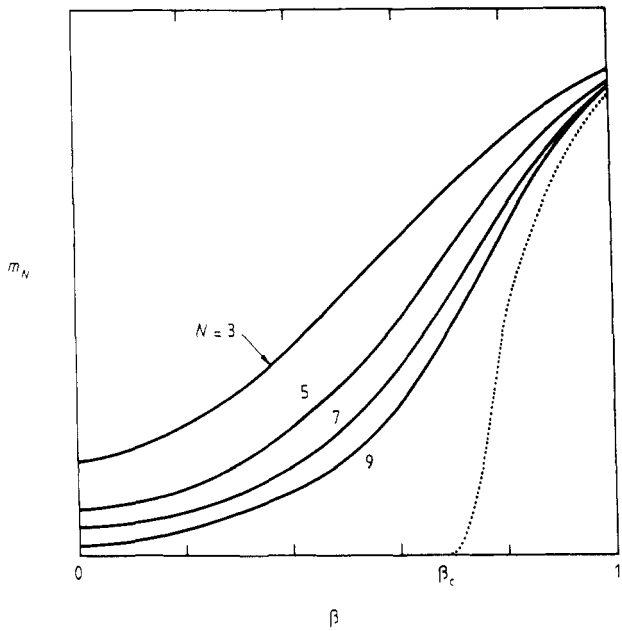

Figure 5. Shape of the order parameter variations on strips with N odd where the symmetry between the two directions of the lattice is broken (see the text). The dotted curve is the order parameter in the infinite system.

When $T \to T_c^-$, the correlation length diverges as $\exp[\text{constant} \times (T_c - T)^{-1/2}]$ (this corresponds to $\nu = \infty$). It is generally supposed (den Nijs 1979, Baxter 1982) that the correlation length remains infinite in all the high temperature phase $T > T_c$ where the correlation functions have an algebraic decay.

The correlation function for the staggered magnetisation is exactly known for $T = 2T_c$ where Baxter (1973) has shown that it decays as $1/r^2$. A general form has been conjectured by Black and Emery (1981) which is $1/r^\eta$ with

$$\eta = \left[1 - \frac{1}{\pi}\cos^{-1}\left(\frac{4^{T_c/T}}{2} - 1\right)\right]^{-1}. \tag{2}$$

This gives in particular $\eta(T_c) = 1$, $\eta(2T_c) = 2$ and $\eta(\infty) = 3$. The correlation lengths

on strips of finite widths have been calculated by

$$\xi_N = -\frac{1}{\log|\lambda_2/\lambda_1|} \tag{3}$$

where λ_1 and λ_2 are the two largest eigenvalues of the transfer matrix. It can easily be checked, using the polymer arrows correspondence, that this correlation length corresponds to the staggered magnetisation correlations. Our results are given in figure 6 where we have given the curves N/ξ_N as a function of β.

The curves collapse in the high-temperature region. This is consistent with the existence of a massless high-temperature phase since the finite-size scaling gives $\xi_N \sim N$ at any critical point. For $T < T_c$ the curves do not collapse but rather move apart. A study of $\log \xi_N$ in this region confirms the general expression

$$\xi_N \sim \exp(N\beta s) \tag{4}$$

where s is the interfacial tension (Baxter 1982).

The curves intersect themselves at values of T which go rapidly to T_c when N grows as can be seen in table 1. The slopes of ξ_N/N do not stabilise to a finite power

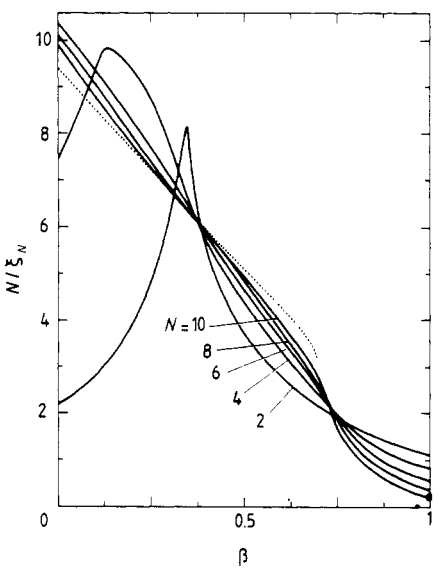

Figure 6. Plot of N/ξ_N against β in the F model. The dotted curve is $\pi\eta(T)$ where η comes from formula (2). (The cusps are due to the second eigenvalue changing of sign.)

Table 1. Estimates of the critical temperature T_c of the F model obtained by the relations $\xi_N/N = \xi_{N-2}/N - 2$.

N	$T_c(N)$
4	1.282
6	1.352
8	1.408
10	1.430
Expected value	$1.443 = (\ln 2)^{-1}$

of N, as expected since ν can be taken as infinite. (We note that the phenomenological renormalisation equations should not *a priori* give T_c since ξ_N is proportional to N in all the high-temperature region. This is probably an effect of corrections to scaling.)

A more complete use of these results can be made using the relation

$$\xi_N \sim N/\pi\eta \tag{5}$$

which is valid by conformal invariance at any critical point (Cardy 1984). This relation gives us estimates of the values $\eta(T)$ which are in reasonable agreement with the values conjectured by Black and Emery (1982) from relation (2). This can be seen in figure 6 where we have represented the values $\pi\eta(T)$ with η deduced from (2) as the broken curve. A better agreement is obtained around $T = 2T_c$. For T around T_c or T going to infinity the results for the smallest sizes do not agree well, but when N grows the correct shape is recovered. Successive estimates of η for various values of T are given in table 2.

Another interesting quantity which is not exactly known in general and related to the correlation length is the staggered susceptibility, which can be interpreted in terms of polymers as

$$\chi = \beta \lim_{\mathbb{N}\to\infty} \frac{\langle(\mathbb{N}_h - \mathbb{N}_v)^2\rangle}{\mathbb{N}}. \tag{6}$$

(Here $\mathbb{N}$ is the total number of links of a two-dimensional system.) It is exactly known only at $T = 2T_c$ where Baxter (1973) has shown that it diverges logarithmically with the staggered field. If we believe in the prediction of formula (2), however, we have that χ is finite for $T > 2T_c$ and infinite for $T \in [T_c, 2T_c]$. On a strip of width N this gives the behaviour

$$\chi_N \sim N^{2-\eta(T)} \tag{7}$$

in this region of temperature (Barber 1983). We have studied the scaling behaviour of susceptibilities in figure 7. One observes a saturation of χ_N for $T > 2T_c$. For $T \in [T_c, 2T_c]$ $\log \chi_N$ grows linearly with $\log N$. The slopes are in reasonable agreement with the values $2 - \eta(T)$ where η is taken from formula (2) as is shown in table 3 for several values.

The rather slow convergence (particularly for T around $2T_c$) is due to the corrections to (7). For example Baxter (1973) has conjectured that at T_c, χ goes as $\xi \log^2 \xi$ and this kind of logarithmic correction makes convergence to scaling rather slow.

Table 2. Values of η deduced from the correlation lengths at several temperatures. The expected values are those of formula (2).

N	T_c	$2T_c$	∞
2	0.6978	—	0.6994
4	0.7717	2.218	2.358
6	0.8035	2.084	3.460
8	0.8402	2.042	3.295
10	0.8921	2.019	3.217
Expected values	1	2	3

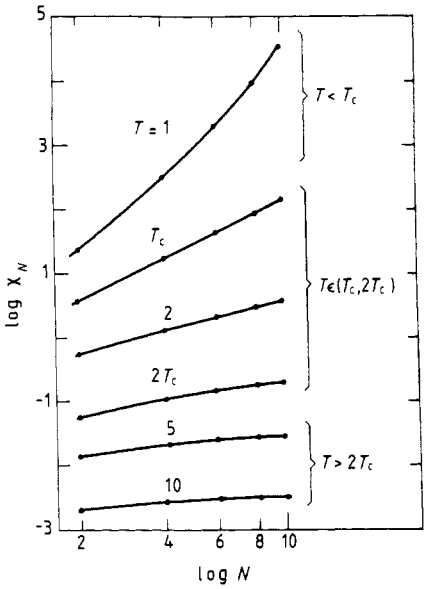

Figure 7. Scaling study of the susceptibilities in the F model. One can see three regions. For $T > 2T_c$ we have $\eta > 2$. The susceptibility is finite in the thermodynamic limit and we observe here a saturation of $\log \chi_N$. For $T \in [T_c, 2T_c]$ the susceptibility is infinite for the infinite system and scales as $N^{2-\eta}$ on strips. For $T < T_c$ the system is ordered. The susceptibility on strips grows exponentially with N.

Table 3. Values of η deduced from the slopes $\log(\chi_N/\chi_{N-2})/\log(N/N-2)$ for several values of T. The expected values are $2-\eta(T)$ where η comes from formula (2). The rather slow convergence (particularly for T around $2T_c$) is due to logarithmic corrections (see the text).

	T		
N	$2T_c$	2	T_c
4	0.5003	0.7285	1.152
6	0.4056	0.6338	1.131
8	0.3583	0.5957	1.120
10	0.3296	0.5680	1.112
Expected values	0	0.3790	1

We conclude that the transfer matrix method gives a good picture of the infinite order transition and of the massless phase properties in the F model. The results that we have obtained will be compared to those for the Flory model to which we turn now.

3. Transfer matrix study of the Flory model on strips

The aim of this section is to present a similar transfer matrix study in the case of the Flory model.

Some technical remarks first have to be made. Because the loops are now forbidden one has to decide whether one works with one extremity of the polymer on each side of the strip or the two on the same side. For N odd the free energy on the strip is obtained with the first case, while for N even, at least for N large enough and T fixed, it is given by the second case. For clarity we will present the results for N odd only, while the results for N even are very similar.

As the loops are forbidden, the symmetry between the two directions of the square lattice is broken for normal strips. This effect of breaking the symmetry could perhaps modify some properties of the model (it is well known that one must be careful when choosing a finite geometry for studying Hamiltonian walks (see for instance Gordon *et al* 1976)). We will thus present results mainly for strips whose axis is parallel to the (1, 1) direction (diagonal strips). Such strips have already been introduced in transfer matrix calculations (Derrida and Herrmann 1983). For these strips the symmetry between the two directions is respected and the order parameter is always zero. We will work with periodic boundary conditions (free boundary conditions give results which are similar but which converge more slowly when N increases). The size of the transfer matrices grows very rapidly for these diagonal strips so we will be limited to widths $N \leqslant 7$.

As a first step we present our results for the entropy per site as a function of the fraction g of gauche bonds $s_N(g)$ in figure 8. In this figure we have also given the best prediction of the Flory–Huggins theories and the two bounds obtained by Gujrati and Goldstein (1981). One can check the general failure of the mean-field theories while the better bound $\tilde{s}'_H(g)$ of Gujrati–Goldstein gives a good idea of the real curve

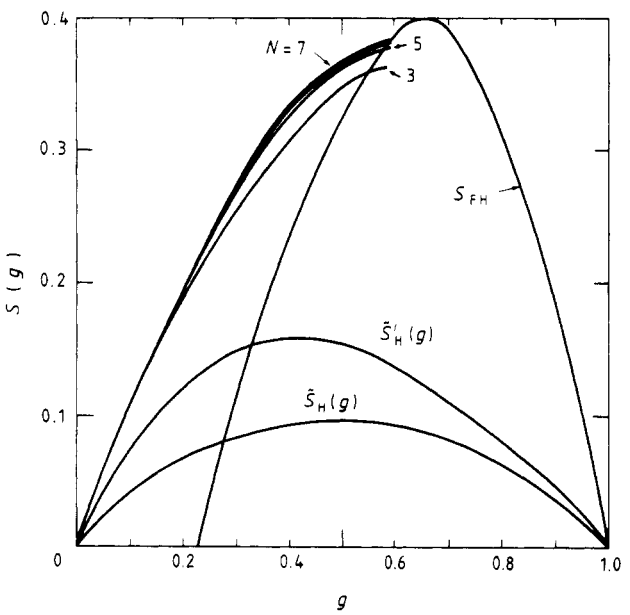

Figure 8. Study of the entropy per site as a function of the fraction g of gauche bonds in the Flory model. We give the results for diagonal strips. Results obtained with normal strips where the symmetry between the two directions of the lattice is broken (see the text) are very similar. The curve S_{FH} is the better result of Flory–Huggins-type theories while $\tilde{s}_H(g)$ and $\tilde{s}'_H(g)$ are the two bounds of Gujrati and Goldstein (1981). The physical region stops at $g = 0.602 \pm 0.0005$ on the infinite system.

in the low-temperature region. To determine the nature of the transition—if any—we turn to other quantities.

In figure 9(a) we give the energy per site u_N for diagonal strips. We give the corresponding specific heat c_N in figure 9(b). Contrary to what has been found in the Monte Carlo calculation of Baumgartner and Yoon (1983) (see in particular figure 1(a)) we do not find any indication of a first-order phase transition. The energy remains continuous, the specific heat saturates rapidly when N grows and simply has a smooth maximum. In figure 10, we give u_N and c_N for normal strips. We have explained why these results must be considered with some caution because the symmetry between the two directions is broken. However, as was the case for the F model where this symmetry was also broken for normal strips and N odd, these results confirm in fact the results obtained with diagonal strips. The maxima of the specific heat for each

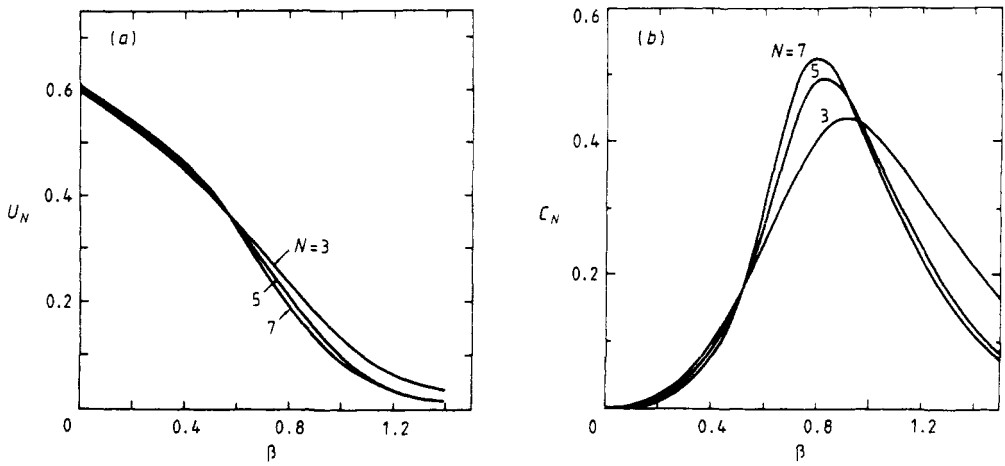

Figure 9. (a) Energy per site u_N in the Flory model calculated on diagonal strips. (b) Specific heats c_N. These curves can be compared with figure 1(a) of Baumgartner and Yoon (1983) where a first-order phase transition has been found.

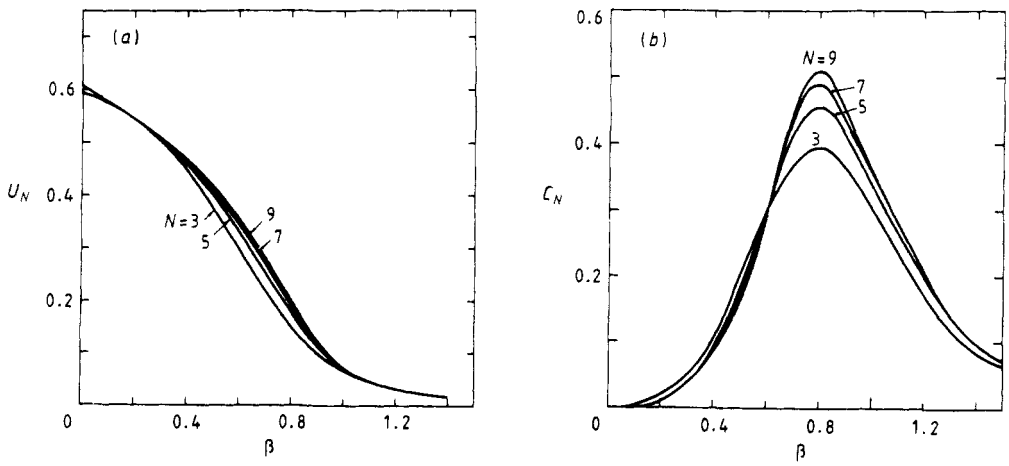

Figure 10. The same as in figure 9 but for normal strips. The results are very similar to those of figure 9.

geometry (figures 9(b) and 10(b)) occur at values of the temperature which surround our estimate

$$T_M = 1.20 \pm 0.02. \tag{8}$$

This value is slightly higher than the corresponding value in the F model.

The study of normal strips where the symmetry is broken can also give an idea of the shape of the order parameter as was the case for the F model with normal strips and N odd. Our results are given in figure 11. They do not indicate any discontinuity (compare with figure 1(b) of Baumgartner and Yoon (1983)). The study of these quantities thus shows that there is no first-order phase transition in the Flory model case. The discrepancy with Monte Carlo calculations will be discussed later. Our results suggest rather that the transition of the Flory model is of the same nature as in the F model, as can be seen by comparing figures 4, 9, 10, and figures 5 and 11. We will confirm this point by studying the electric properties. From now on we work on diagonal strips only where the total symmetry is conserved.

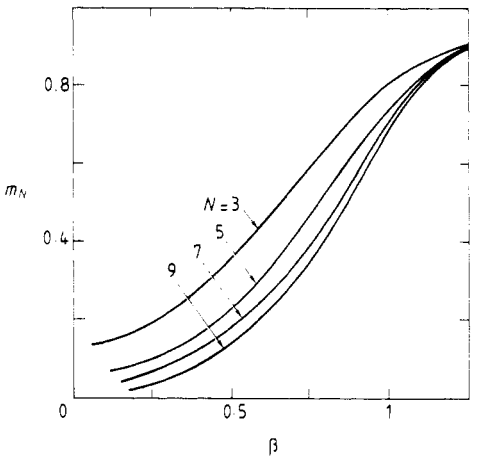

Figure 11. Order parameter in the Flory model. The calculation is done on strips in the normal direction where the symmetry between the two directions is broken. These curves do not seem to indicate a discontinuity (compare with figure 1(b) of Baumgartner and Yoon (1983)).

We have given the correlation lengths for the staggered polarisation in figure 12. We have represented $2N/\xi_N$ in this case because when one takes a strip in diagonal direction the unit of length along the strip is half of the unit of length in a perpendicular direction. Despite the fact that we have studied just three sizes we think that these curves present a collapse in the high-temperature phase which is similar to that of figure 6 for the F model, suggesting that in this case the high-temperature phase is also massless. The intersections of the curves give an estimate

$$T_c = 1.55 \pm 0.05 \tag{9}$$

for the critical temperature which is slightly higher than in the F model. The order of magnitude for the quantity $\pi\eta(T)$ is the same as in the F model. In particular the value of η_c is likely to equal 1 as will be confirmed by the study of susceptibilities. In the same way for T infinite we obtain values of η compatible with the value $\eta = 3$ of the F model. This suggests that Hamiltonian walks are critical objects with angular correlations decaying as $1/r^3$.

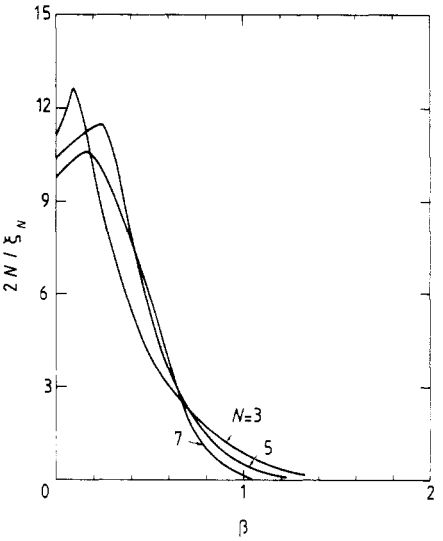

Figure 12. Plot of $2N/\xi_N$ against β in the Flory model (strips in the diagonal direction).

One can find the value where $\eta = 2$ at $T \simeq 2.50$ although this value is not very accurate.

Finally, we have studied the susceptibilities which are defined as in the F model case. The scaling behaviour is given in figure 13. For T high enough χ_N saturates when N grows. For values of T in the region $[1.55, 2.50]$ $\log \chi_N$ is linear against $\log N$. In particular at our estimate of T_c the slopes of $\log \chi_N$ suggest that $\eta_c = 1$

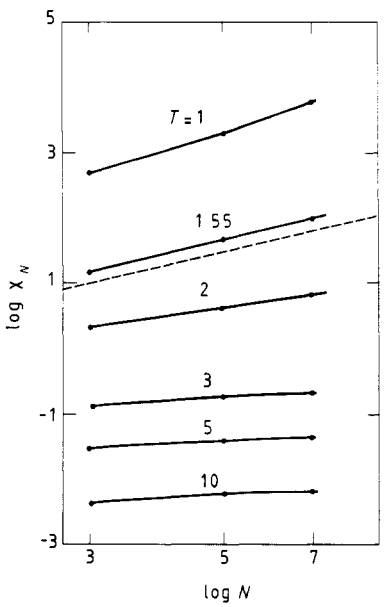

Figure 13. Study of the scaling behaviour of susceptibilities for the Flory model (strips in the diagonal direction). The broken curve indicates the slope corresponding to $\eta_c = 1$. It compares well with our curve $\log \chi_N$ against $\log N$ at our estimate of T_c.

although it would be necessary to do calculations on wider strips to confirm this hypothesis.

To conclude this study, we have given strong evidence that the Flory model has a behaviour very similar to that of the F model. There are only minor numerical differences due to the presence of loops. In particular our results suggest that $\eta_c = 1$ in this model as in the F model. It remains to be understood why Monte Carlo simulations have given different results.

4. Comparison with Monte Carlo simulations

Our result of an F-model-type phase transition disagrees with the first-order phase transition found by Baumgartner and Yoon (1983). A first possible explanation is that our strips are too narrow to show evidence of such a transition. We think that the study of the F model that we have carried out in parallel should eliminate this hypothesis. A second possible explanation is that the Monte Carlo simulations have observed a kind of gel transition due to the very long relaxation times of the system so it would be perhaps interesting to carry out longer simulations. However, we think that another explanation is also possible.

We first recall that Baumgartner and Yoon (1983) have simulated the Flory model in a way which is slightly different to that of the original model. They have considered a polymer system of 21 chains of 20 segments each on a 21×21 square lattice. This introduction of 5% of voids and several polymers was *a priori* expected not to modify the nature of the transition and allowed the authors to use the reptation algorithm. They have found a jump in energy and magnetisation at $T_c \simeq 0.93$. The shift in critical temperature when compared with our results of $T_c \simeq 1.55$ is easily explained by the modifications of the system. (As Baumgartner and Yoon have calculated, a Flory approximation for a system with 5% of voids gives a critical temperature shifted by $\Delta T \simeq 0.50$ when compared with the result for the original Flory model.)

We think that an explanation of the discrepancy between our result and the first-order phase transition found by these authors could also be given by these modifications. It is well known that in the XY case, for example, a modification of the precise form of the interactions can drive the system to a first-order phase transition. (For example, Domany *et al* (1984), taking as the interaction between spins a power of a cosine high enough have given evidence of a first-order phase transition.)

The first modification of the original Flory model in the simulation of Baumgartner and Yoon (1983) is the presence of empty sites. We have thus studied by the transfer matrix method a system where voids are authorised. This is easily done by working in a grand canonical ensemble with a potential conjugated to the empty sites. This potential is adjusted at any temperature to give a fixed density of voids. We give in figure 14 a typical example with a density of voids equal to 10%. As can be seen in this figure, the specific heats have in fact a behaviour very similar to figure 9(b), the curves being simply shifted toward the low-temperature region. We have studied in this way different densities between 0 and 1 without any indication of a possible first-order phase transition.

A second more important modification is that in the simulation of Baumgartner and Yoon (1983) there are several polymers, each of a size comparable with the sample size. Because the polymers can move with respect to each other this gives corrections to the free energy of the original Flory model which are in fact very important for the

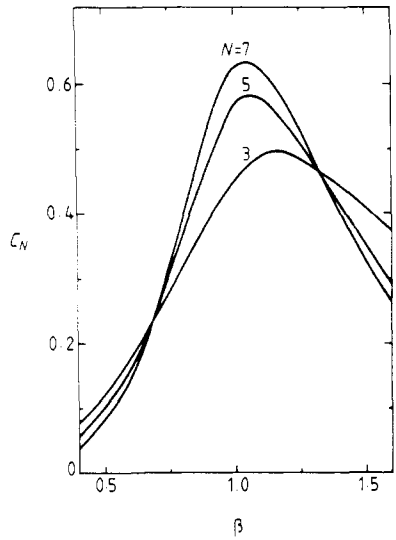

Figure 14. Specific heat per occupied site for a system with 10% of empty sites (strips in the diagonal direction). The curves are shifted toward low temperatures when compared to figure 9. There is no evidence of a first-order phase transition.

lengths of the chains which have been used (Petschek 1984). These corrections could explain the observed first-order phase transition as a finite (chain) size artefact (Petschek 1984). We have thus also studied the case where several polymers are present. However by varying the mean length of the chains up to values comparable with the strip width we have not observed any indication of a first-order phase transition.

The drawback of the transfer matrix in this case is that one can fix only the mean length of the chains but one cannot avoid the dispersity. It is not clear whether this dispersity could have an influence on the transition. More complete Monte Carlo simulations with a study of different distributions of chain lengths should clarify the situation. An attempt in this direction has already been made by Baumgartner (1984).

5. Conclusion

In conclusion our transfer matrix study of the Flory model gives evidence of an F-model-type phase transition, with only minor numerical differences. We have proposed that the discrepancy between this result and the results of Monte Carlo simulations could be due to the modifications of the model that the authors have been constrained to do for studying it by the reptation algorithm in an efficient way. As in the XY case, certain modifications of the precise form of the potential could perhaps drive the system to a first-order phase transition. We think that it would be interesting to carry out more complete Monte Carlo simulations to elucidate this point.

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