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A Monte Carlo analysis of self-avoiding walks in three dimensions†

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Abstract. We present estimates for critical exponents of self-avoiding walks on a cubic lattice. We treat a grand canonical ensemble of walks with free ends in a Monte Carlo approach and make use of real space renormalisation ideas. Our estimate for ν is 0.59 ± 0.01. Our estimate for γ does not share the same degree of accuracy. However, we are able to pinpoint the source of this discrepancy. In addition, we define a quantity $\chi_L(\beta)$, the probability that a walk starting at the origin will end outside or at the border of a cube of side L. This quantity turns out to be quite suitable for a real space renormalisation group analysis.

1. Introduction

Self-avoiding walks (SAW) on a lattice are a suitable model for the conformational properties of long linear polymers in good solvents; the self-avoidance constraint simulates the excluded volume effect arising from short-range monomer–monomer repulsion (for a review, see the book by de Gennes (1979)). Although the experimental study of polymer solutions is almost entirely confined to the physically realisable space dimensionality $d = 3$ ($d = 2$ can be obtained through adsorption of a polymer monolayer on a surface, see, e.g., Villanove and Rondelez (1980)), there is no such restriction as regards the theoretical study of SAW. Further, since the statistics of SAW is obtained in the $n \to 0$ limit of the ferromagnetic n-component spin vector model (de Gennes 1972, des Cloizeaux 1975), concepts and methods initially devised for the study of thermal phase transitions can be (and actually have been) successfully applied in this case. From this viewpoint, one can see space dimensionality as a parameter (which can even be made to vary continuously, as in the ε expansion (de Gennes 1972)). In particular, the Flory formula (see de Gennes 1979) for the exponent ν (relating the average RMS end-to-end distance of a SAW to the number of steps N through $\langle R^2 \rangle^{1/2} \sim N^{\nu}$) is written as

$$\nu = 3/(d+2) \qquad 1 \leqslant d \leqslant 4. \tag{1}$$

For $d \geqslant 4$ the Flory approach correctly predicts the excluded volume to be irrelevant, so $\nu = \frac{1}{2}$ (as in a random walk). In spite of its approximate nature, the Flory formula works surprisingly well (this fact is often attributed to a fortuitous cancellation of errors): it is exact in $d = 1$ and, apart from logarithmic corrections, in $d = 4$ (although

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it is not exact in $d = 4 - \varepsilon$ (de Gennes 1972)), and is thought to be exact in $d = 2$ as well (Nienhuis 1982). However, in $d = 3$ there is a considerable amount of evidence pointing towards a value of ν slightly lower than the Flory estimate of $\frac{3}{5}$: from a field-theoretic approach, Le Guillou and Zinn-Justin (1977, 1980) obtain $\nu = 0.588 \pm 0.001$; Monte Carlo renormalisation group calculations by Kremer *et al* (1981) give $\nu = 0.59 \pm 0.01$; from a Monte Carlo approach, using the concept of 'local fractal dimensionality', Havlin and Ben-Avraham (1983) quote $\nu = 0.588 \pm 0.003$. Further, the analysis of experimental results from, say, light scattering in polymer solutions also seems to favour a value of ν smaller than 0.60; Cotton (1980) quotes $\nu = 0.586 \pm 0.004$. Recently, Obukhov (1984) has estimated that, for $1 < d < 4$, the accuracy $\delta\nu/\nu$ of the Flory approximation must be 10^{-1}-10^{-2}; although this gives ample room for the above estimates to be considered consistent with Flory's value, the question still persists as to what the precise value of ν is in $d = 3$. Thus, we feel that the use of a variety of methods to approach the SAW problem in $d = 3$ is justified, inasmuch as they can provide independent estimates of the quantities of interest. When added to the already existing numerical results, it is expected that the new ones can contribute towards a better understanding of the physical problem under study.

In this paper we report the results from a Monte Carlo (MC) study of SAW with free endpoints on a cubic lattice. The present study is an extension of the MC approach of Aragão de Carvalho and Caracciolo (1983) for SAW with fixed endpoints which incorporates the improvements proposed by Berretti and Sokal (1985). Both articles originate from a connection with field theory worked out by Aragão de Carvalho *et al* (1983), which, in turn, is a further development of the work of Brydges *et al* (1982).

In § 2 below we recall the definition of a few basic quantities which play important roles in our calculations, and the MC procedure is described; in § 3 we present our results and carry out their analysis in a standard way; then, in § 4 we show results obtained through a new real space renormalisation scheme from which it is possible to obtain accurate estimates from the analysis of our data; finally, in § 5 we summarise our findings.

2. Statistical ensemble and MC procedure

MC techniques are usually applied to perform averages over SAW configurations with a fixed number, N, of steps, which corresponds to a canonical ensemble. From MC simulations for a given lattice and different values of N, one is able to estimate the exponent ν defined previously. As regards the (lattice-dependent) effective coordination number μ and the susceptibility-like exponent γ, defined by

$$C_N \sim \mu^N N^{\gamma - 1} \tag{2}$$

where C_N is the number of N-step SAW starting at the origin on a given lattice, their values have been estimated to great accuracy mainly by exact enumeration techniques (see, e.g., the review by McKenzie (1976)). For $1 < d < 4$, $\gamma > 1$. Le Guillou and Zinn-Justin (1977, 1980) quote $\gamma_{3d} = 1.165 \pm 0.0011$.

On the other hand, if one draws upon the analogy between the SAW problem and Euclidean lattice field theory (Aragão de Carvalho *et al* 1983), the statistical ensemble which arises most naturally is the space of *all* SAW, with any number of steps (hereafter referred to as $\{\omega\}$), which means a 'grand canonical' ensemble. To an N-step walk one assigns a fugacity β^N, where β is the inverse temperature of the associated field

theory (de Gennes 1979). From (2) the grand partition function $\chi(\beta)$ (which is the susceptibility of the associated field theory) becomes critical at $\beta_c = \mu^{-1}$; with $\tau \equiv (\beta_c - \beta)/\beta_c$, $\chi(\beta)$ behaves as

$$\chi(\beta) \sim \tau^{-\gamma} \qquad \beta \to \beta_c^- (\tau \to 0^+). \tag{3}$$

Two other quantities of interest are the average number of steps in a SAW for a given β and the mean square end-to-end distance, respectively given by

$$\langle N \rangle_\beta = \chi^{-1} \sum_{\{\omega\}} N(\omega) \beta^{N(\omega)} \tag{4a}$$

and

$$\langle R^2 \rangle_\beta = \chi^{-1} \sum_{\{\omega\}} R^2(\omega) \beta^{N(\omega)}. \tag{4b}$$

Their critical behaviour is immediately seen to be

$$\langle N \rangle_\beta \sim \tau^{-1} \tag{5a}$$

$$\langle R^2 \rangle_\beta \sim \tau^{-2\nu} \qquad \tau \to 0^+. \tag{5b}$$

Finally, we introduce a quantity $Q(\beta)$, related to the four-point correlation function of the field theory problem, which is particularly useful to estimate the exponent γ (which cannot be obtained directly through χ without the large errors involved in computing partition functions via MC methods). $Q(\beta)$ is the probability that two independent walks starting from the origin will not intersect each other again

$$Q(\beta) = \chi^{-2} \sum_{\{\omega_1\}\{\omega_2\}} \beta^{N(\omega_1)+N(\omega_2)} \sigma(\omega_1, \omega_2) \tag{6}$$

where $\sigma(\omega_1, \omega_2) = 1$ if the walks do not intercept each other and is zero otherwise.

One can show (Aragão de Carvalho *et al* 1983) that

$$Q(\beta) = \frac{\partial \chi^{-1}}{\partial \ln \beta} \tag{7}$$

whence, from (3) and assuming $1 < d < 4$ (so $\gamma > 1$)

$$Q(\beta) \sim \tau^{\gamma - 1} \qquad \tau \to 0^+. \tag{8}$$

The MC procedure generates two independent sequences of SAW, both starting at the origin and having the other end free. From an initial arbitrary configuration, each sequence is generated by using two types of elementary deformations of the walks: (i) adding a link ($\Delta N = +1$) or (ii) deleting a link ($\Delta N = -1$) at the free end. Obviously, this latter possibility will only arise if the walk has not been previously reduced to a point ($N(\omega) = 0$). There may also be null transitions in which the walk is transformed into itself.

With the possible deformations restricted to the free end of the walk, this algorithm has two important properties: (i) it is ergodic (any walk in the ensemble can be transformed into any other walk) and (ii) it is *local* in the sense that, except for the SAW restriction, the MC transition probability $W(\omega \to \omega')$ depends on a very small number of links. We can then write

$$W(\omega \to \omega') = P(\Delta N) \sigma(\omega') \tag{9}$$

where $\sigma(\omega') = 1$ if ω' is a SAW, and zero otherwise.

The local term $P(\Delta N)$ must satisfy the condition

$$P_0(\omega)+\sum_{\hat{e}} P(\Delta N)=1 \tag{10}$$

where $P_0(\omega)$ is the probability of a null transition and the sum extends over all unitary lattice vectors $\hat{e}$ from a site to its nearest neighbours.

The detailed balance equation is

$$\beta^{N(\omega)}P(\Delta N)=\beta^{N(\omega')}P(-\Delta N) \tag{11}$$

where ω and ω' are SAW and $N(\omega)-N(\omega')=\Delta N$. Thus

$$P(+1)=\beta P(-1). \tag{12}$$

We now specialise to a d-dimensional hypercubic lattice. One has to consider two possibilities separately:

$$N(\omega)\neq 0: \qquad P_0(N(\omega)\neq 0)+(2d-1)P(1)+P(-1)=1 \tag{13a}$$

$$N(\omega)=0: \qquad P_0(N(\omega)=0)+2dP(1)=1. \tag{13b}$$

Since there are three equations (12), (13a) and (13b) and four unknown quantities, we must make a choice. In order that the phase space be spanned as thoroughly as possible in a MC sweep, we choose $P_0(N(\omega)\neq 0)$ equal to zero. Then, we have

$$P(1)=\frac{\beta}{1+(2d-1)\beta} \qquad P(-1)=\frac{1}{1+(2d-1)\beta}$$

$$P_0(N(\omega)=0)=\frac{1-\beta}{1+(2d-1)\beta}. \tag{14}$$

Once we have the transition probabilities, the process of generating the MC sequence of walks follows the usual steps. It is to be noted that, if the transition $\omega\to\omega'$ corresponds to the addition of a new link, it has to be checked whether ω' is a SAW or not; if it is then ω' is the next walk in the sequence, whereas if it is not then the next walk is ω again. Since links can be deleted as well as added, a walk can always get out of a trap, by tracing back on previous steps. This, coupled to the fact that in the grand canonical ensemble all walks (and not only those with a given number of steps) contribute to the averages, makes our procedure more efficient than the usual ones in terms of 'per cent of phase space spanned per sweep'. Although the constraint that deformations can only take place at the extremity of the walk works slightly against efficiency, in the critical region ($\beta\sim\beta_c<1$) the probability of deletion of a link is high enough (see (14)), so a walk will be frequently reduced to a point and then start again with no memory of previous steps. For a discussion of the interplay between different features of MC, see Berretti and Sokal (1985).

It may be of interest to note that a grand canonical ensemble has also been used in a MC study of SAW (in two dimensions) by Redner and Reynolds (1981b). While our method for generating walks is a dynamic one, theirs is a quasistatic method which used an enrichment algorithm (see appendix A of Berretti and Sokal (1985)) in which all possible next steps of a walk are systematically tested. This latter aspect of their algorithm makes it somewhat similar, although not identical, to exact enumeration techniques. In spite of the differences in walk-generating algorithms, both methods share the advantages of the grand canonical formulation: walks of all lengths enter the averages, and configurational properties are calculated in terms of the temperature-like variable β (instead of N), which makes it easier to probe the vicinity of the asymptotic regime (Redner and Reynolds 1981b, Berretti and Sokal 1985).

3. Numerical results

We have developed an MC computer program for SAW with free endpoints which calculates the averages $\langle N\rangle_\beta$, $\langle R^2\rangle_\beta$ and $\langle Q\rangle_\beta$, respectively defined by (4*a*), (4*b*) and (6) above. Although our program is in principle suitable for application to a generic *d*-dimensional hypercubic lattice, we have up to now restricted ourselves to $d=3$.

We have made use of (5*a*) above in order to determine the extent of the critical region. Our approach consisted of the following steps.

(i) We plotted $\langle N\rangle_\beta$ against β, ignoring the fact that the exponent in (5*a*) is already known. The range of values of β for which the fitted exponent was closest to -1 was assumed to be the region in which (5*a*), (5*b*) and (8) above hold.

(ii) Using this range of values of β and fixing the exponent to unity, we plotted $\langle N\rangle_\beta$ against β in order to obtain β_c.

(iii) Using the range of values of β given by (i) and β_c as given by (ii) we plotted $\langle R^2\rangle_\beta$ and $Q(\beta)$ against τ in order to obtain ν and γ.

Note that the value of β_c obtained from (ii) is outside (and above) the region defined in (i), which in the present case is estimated to be the interval $0.1925 \leqslant \beta \leqslant 0.2075$ (figure 1), whereas $\beta_c \simeq 0.2133$. The reason for this is that, since our Monte Carlo runs have a finite (although large) number of iterations (typically 8×10^6), our results are expected to be properly thermalised only as long as we do not get too close to the critical point. Thus, step (i) above is a self-consistency condition: it establishes a subregion of the critical region where critical fluctuations are not strong enough to prevent MC data from stabilising by the end of a run. Typical times were of order 2×10^{-4} seconds per Monte Carlo step ($\sim 1.6\times10^3$ seconds per run) on a Cyber 170/800 computer.

The values obtained for the critical quantities are

$$\mu = \beta_c^{-1} = 4.689 \pm 0.003$$
$$\nu = 0.58 \pm 0.02 \qquad (15)$$
$$\gamma = 1.0 \pm 0.1.$$

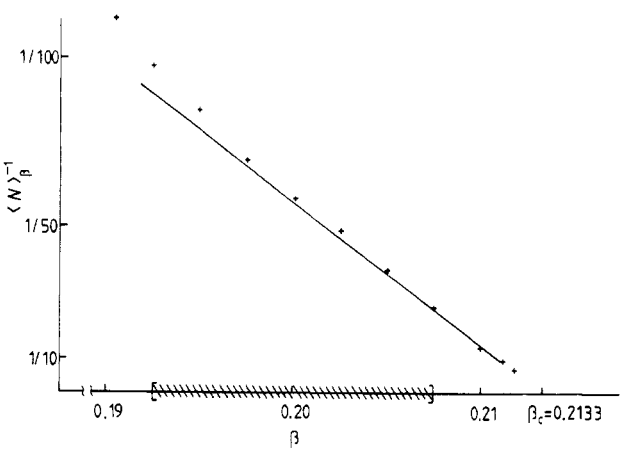

Figure 1. Plot of $(\langle N\rangle_\beta)^{-1}$ against β; the hatched region is that in which $(\langle N\rangle_\beta)^{-1} \sim \beta +$ constant with least deviation. The straight line is a guide to the eye.

The value of β_c thus obtained agrees with, and is more precise than, that quoted by Aragão de Carvalho and Caracciolo (1983) for SAW with fixed ends, namely 4.66 ± 0.04. It is also in very good agreement with the series results $\mu = 4.6838$ quoted by McKenzie (1976). We note that our result for β_c did not change appreciably when we enlarged the range of values of β used as the 'critical region' mentioned above.

The estimate obtained for ν (see figure 2) does seem to be lower than the Flory value of 0.6; however, the standard deviation is still large (although smaller than the corresponding one given by Aragão de Carvalho and Caracciolo (1983), who quote $\nu \neq 0.62 \pm 0.05$ for fixed-end SAW).

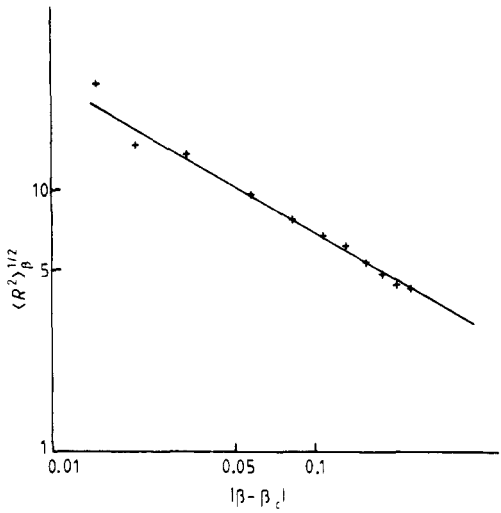

Figure 2. Logarithmic plot of $\langle R^2 \rangle_\beta^{1/2}$ against τ; only the best fit is shown. The straight line has slope -0.58 and we have used $\beta_c = 0.2133$.

On the other hand, our estimate for γ is rather poor. This is because the configurational space available to *two* walks with one *free end* each (whose probability of non-intersection, $Q(\beta)$, yields γ) is very large; consequently, our MC results for $Q(\beta)$ are much less accurate than those for $\langle R^2 \rangle_\beta$ or $\langle N \rangle_\beta$ (quantities related to a *single* walk) obtained from the same simulation. We note that, for SAW with fixed ends, in which case the configurational space involved in the calculation of $Q(\beta)$ is much smaller, Aragão de Carvalho and Caracciolo (1983) quote $\gamma = 1.17 \pm 0.013$ in $d = 3$, which is both more accurate than the present result and closer to other estimates, which give $\gamma = 1.165 \pm 0.0011$ (Le Guillou and Justin, 1977, 1980). In order to have a deeper understanding of the reasons for our result, we have plotted the average number of intersections $\langle N_I \rangle$ between the two walks (apart from their common origin) as a function of β (figure 3). The fact that this quantity is close to one, and fluctuates strongly about this central value, is a key point: what defines the quantity $\sigma(\omega_1, \omega_2)$ in (6) above is whether the walks do not intersect each other *at all* or whether they intersect *any* number of times. Thus, the border is at *one* intersection, and it is understandable that fluctuations of $\langle N_I \rangle$ about this value induce strong fluctuations in the estimates of quantities calculated through $Q(\beta)$.

Within the framework of this section, more precise results could possibily be obtained by extending our calculations to longer runs. However, we shall not try to

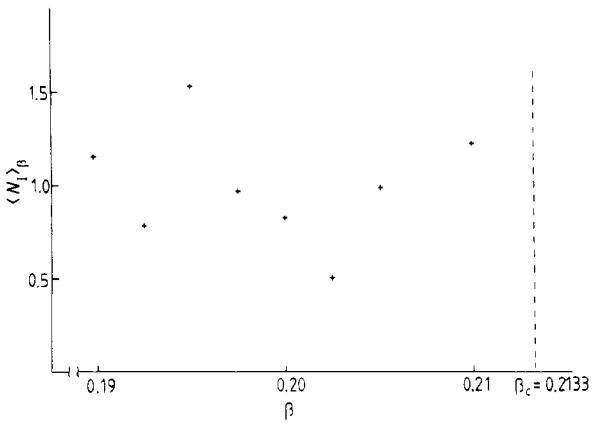

Figure 3. Average number of intersections $\langle N_1 \rangle$ (apart from the common origin) of two SAW, as a function of β.

do so; instead, in the next section we show that an alternative analysis of our present data can be carried out with good results, as regards the accuracy of extrapolated estimates.

4. Real space renormalisation group analysis

Consider the quantity

$$G_\beta(\boldsymbol{x}) \equiv \sum_{\{\omega: 0 \to \boldsymbol{x}\}} \beta^{N(\omega)} \tag{16}$$

where $\{\omega: 0 \to \boldsymbol{x}\}$ is the set of all SAW which start at the origin and end at $\boldsymbol{x}$. $G_\beta(\boldsymbol{x})$ is the two-point correlation function in the associated field theory, and behaves as

$$G_\beta(0, \boldsymbol{x}) \sim \begin{cases} |\boldsymbol{x}|^{-(d-2+\eta)} & |\boldsymbol{x}| \ll \xi(\beta) \qquad (17a) \\ \exp(-|\boldsymbol{x}|/\xi(\beta)) & |\boldsymbol{x}| \gg \xi(\beta) \qquad (17b) \end{cases}$$

where $\xi(\beta) \sim (\beta_c - \beta)^{-\nu}$ is the correlation length of the field theory and corresponds to the mean square end-to-end distance of the polymer problem.

We now define the quantity

$$\chi_L(\beta) \equiv \chi_{(\beta)}^{-1} \sum_{\{\boldsymbol{x} \text{ out } L^d\}} G_\beta(\boldsymbol{x}) \tag{18}$$

where $\{\boldsymbol{x} \text{ out } L^d\}$ is the set of all points $\boldsymbol{x}$ outside or at the border of a hypercube of volume L^d centred at the origin. It is easy to see that:

$$\chi_L(\beta) < 1 \qquad 0 < \beta < \beta_c$$

$$\lim_{L \to 0} \chi_L(\beta) = 1$$

$$\lim_{L \to \infty} \chi_L(\beta) = 0 \qquad \lim_{\beta \to \beta_c} \chi_L(\beta) = 1$$

In other words, $\chi_L(\beta)$ is the probability that a walk starting at the origin will end outside (or at the border of) the hypercube L^d.

If we consider the real space renormalisation group procedure in which the hypercube L^d is renormalised into the elementary hypercube 1^d, probability invariance demands that

$$\chi_L(\beta) = \chi_1(\beta') = \beta'. \tag{19}$$

In (19), which defines a renormalised bond fugacity β', we are making use of the fact that in the region of interest $0 < \beta < \beta_c < 1$, a *fugacity* can be interpreted as a *probability* of existence of a link (see the discussion in Redner and Reynolds (1981a, b)). Note that our procedure is not the same as the usual constant fugacity Monte Carlo renormalisation group (Redner and Reynolds 1981b). There, an MC sampling is done on a *finite cell* from the start, and only walks that traverse the cell are counted for the renormalised fugacity.

Following the standard renormalisation group ideas (Wilson and Kogut 1974), we search for the fixed point of recursion relation (19)

$$\beta^*(L) = \chi_L(\beta^*(L)) \tag{20}$$

at which an estimate for the critical exponent is obtained through

$$\nu(L) = \ln L / \ln(\mathrm{d}\beta'/\mathrm{d}\beta)_{\beta^*(L)}. \tag{21}$$

It is expected that

$$\lim_{1/L \to 0} \beta^*(L) = \beta_c \tag{22a}$$

and

$$\lim_{1/L \to 0} \nu(L) = \nu. \tag{22b}$$

The values of β for which (20) holds, for a range of values of L (in the region where $\langle N \rangle^{-1}$ scales linearly with β, see § 3), are displayed in table 1, together with the respective estimates for ν. For cubes with $L > 11$, the fixed point is expected to be located deeper inside the critical region, where critical fluctuations make it impractical for us to obtain accurate estimates, as discussed in § 3.

Instead of pushing our calculations for larger cubes, we have taken advantage of the fact that the simulations described in § 4 provided us with a wealth of data for a number of (fixed) values of β. Thus, we have turned (20) inside out, i.e. for a given β we would interpolate to obtain the (non-integer) value of L which would make (20) hold. The derivative in (21) was also obtained by a similar interpolation procedure.

Table 1. Values of $\beta^*(L)$, $(\partial\beta'/\partial\beta)_{\beta^*(L)}$ and $\nu(L)$ obtained from our renormalisation group analysis for different values of L

L	$\beta^*(L)$	$(\partial\beta'/\partial\beta)_{\beta^*(L)}$	$\nu(L)$
5	0.191 27	11.6940	0.6545
6	0.197 73	16.9009	0.6337
7	0.201 63	22.6701	0.6235
8	0.204 08	28.5072	0.6207
9	0.205 84	36.0099	0.6131
10	0.207 15	41.5422	0.6179
11	0.208 21	49.6746	0.6140

Our data are displayed in table 2. Although the region of β space thus probed is roughly the same as the one swept by keeping L fixed, we feel that comparing both procedures is important as a check on the self-consistency of our renormalisation group scheme.

Indeed, we have checked that the quality of our data is very much the same, whether one picks results from table 1 or table 2, or both. This means not only that the average square deviation from a suitable extrapolating curve (see below) is about the same either way, but also that an undesirable small jump in the exponent estimate is present in both calculational procedures (from $L=9$ to $L=10$ in table 1; from $\beta=0.203\,75$ to $\beta=0.2050$ in table 2). While we have no explanation for this discontinuity at the moment, it seems comforting that our data exhibit a monotonic behaviour everywhere else. This may be an argument for viewing the causes of the jump as fortuitous, instead of a structural failure of our renormalisation group scheme.

Following standard finite-size scaling arguments (see, e.g., Redner and Reynolds (1981b) and references therein), we have extrapolated the finite-L estimates of ν against $1/\ln L$, and the finite-L estimates of β_c against $L^{-1/\nu}$, where a trial value of $\nu=0.59$ (our central estimate, see below), has been used throughout. In both cases we have made use of a quadratic term, besides the linear one, to take curvatures into account, and performed a least-squares fit. Our results for β_c extrapolate much more smoothly than those for ν, as can be seen from the estimated error bars (see below); certainly one of the reasons for the relatively bad performance for ν is the jump in the data referred to above.

Below we quote our extrapolations, obtained by using all data, both from tables 1 and 2. The error bars are given by the points at which the summed square deviations are twice those at their respective minimum (central estimates). Thus, we have

$$\begin{aligned} &\beta_c = 0.2133 \pm 0.0001 \\ &(\mu = \beta_c^{-1} = 4.688 \bullet 0.002) \\ &\nu = 0.59 \pm 0.01. \end{aligned} \tag{23}$$

Once again, our central estimate for ν is lower than the Flory value, though the error bar is just not narrow enough to exclude it.

Table 2. Values of L, $(\partial\beta'/\partial\beta)_{\beta^*(L)}$ and $\nu(L)$ obtained from our renormalisation group analysis for different temperatures $\beta^*(L)$.

$\beta \equiv \beta^*(L)$	L	$(\partial\beta'/\partial\beta)_{\beta^*(L)}$	$\nu(L)$
0.190 0	4.8488		
0.192 5	5.1546	13.2639	0.6348
0.195 0	5.5031	15.4407	0.6230
0.197 5	5.9610	17.6168	0.6223
0.200 0	6.5331	21.1862	0.6147
0.202 5	7.3362	26.7818	0.6061
0.203 75	7.7965	29.6831	0.6057
0.205 0	8.5242	32.8451	0.6137
0.206 25	9.2264	37.4504	0.6133
0.207 50	10.3926	45.6748	0.6126
0.208 75	11.6174	57.4933	0.6053

Although we have made no effort to separate statistical errors (e.g. from the Monte Carlo itself) from those originated from the extrapolation procedure, we feel that the error bars attributed to the latter are generous enough to cover variations arising from the former (for instance, we have decided to round up our estimate and error bar for ν, which actually gives $\nu = 0.590 \pm 0.007$ on the basis of the above-mentioned criterion).

Finally, we point out that the quantity $\chi_L(\beta)$ can be used in order to provide an estimate for the susceptibility exponent γ in the following way.

If we take into account the long distance behaviour of the correlation function $G_\beta(x)$ as given by (17*b*) and transform the sum in (18) into an integral (which is justified close to the critical point), the following expression is obtained for $\chi_L(\beta)$ near criticality:

$$\chi_L(\beta) \sim \tau^{\gamma-\nu} \exp(-L\tau^\nu). \tag{24}$$

If we use the central estimates for ν and β_c, namely 0.59 and 0.2133, (24) gives a value for γ. Indeed from an average over several values of β, with $L = 8$, 9 and 10, we have obtained $\gamma \cong 1.25$. Although the error bar is possibly as large as 0.1 in this case, this is reasonably closer than the corresponding result of § 3 to $\gamma \simeq 1.17$ as obtained by Aragão de Carvalho and Caracciolo (1983).

5. Conclusions

We have shown that a Monte Carlo calculation for a grand canonical ensemble of SAW with free ends provides good estimates for the critical fugacity and for the correlation length exponent ν in three dimensions. In particular, our estimate for ν is close to 0.59, thus giving independent support to the (by now, widely held) view which points towards a value lower than the Flory result of 0.60. Although our result for the susceptibility exponent γ is poorer than the corresponding one obtained for SAW with fixed ends by Aragão de Carvalho and Caracciolo (1983), we have succeeded in pinpointing the cause for this difference.

In addition, we have given results obtained from a new real space renormalisation group approach to the analysis of our data, which show that the quantity $\chi_L(\beta)$ is indeed a very suitable one for this sort of calculational scheme.

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