Dynamic critical exponent of some Monte Carlo algorithms for the self-avoiding walk

This article has been downloaded from IOPscience. Please scroll down to see the full text article.
1986 J. Phys. A: Math. Gen. 19 L797
(http://iopscience.iop.org/0305-4470/19/13/008)
View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 129.252.86.83
The article was downloaded on 31/05/2010 at 10:01

Please note that terms and conditions apply.

## LETTER TO THE EDITOR

# Dynamic critical exponent of some Monte Carlo algorithms for the self-avoiding walk 

Sergio Caracciolo $\dagger$ and Alan D Sokal $\ddagger \S$<br>$\dagger$ Scuola Normale Superiore and INFN-Sezione di Pisa, Pisa, Italy<br>$\ddagger$ Courant Institute of Mathematical Sciences, New York University, 251 Mercer St, New York, NY 10012, USA

Received 23 May 1986


#### Abstract

We discuss the dynamic critical behaviour of some Monte Carlo algorithms for the self-avoiding walk (SAW). For algorithms with local $N$-conserving elementary moves, we argue that the autocorrelation time behaves as $\tau \sim N^{p}$ with $p \approx 2+2 \nu$. For the bFACF dynamics (a grand canonical algorithm), we present Monte Carlo data indicating that $p=2.2 \pm 0.5$ for two-dimensional non-reversal random walks and $p=3.0 \pm 0.4$ for twodimensional SAW, values which are significantly less than $2+2 \nu$.


The study of dynamic critical phenomena in statistical mechanical model systems is of interest for two reasons. First, and most obviously, to the extent that the mathematical dynamics is a reasonable model of a real physical dynamics, the conclusions are of direct physical interest. A second and more subtle reason arises out of the widespread use of dynamic Monte Carlo methods as a tool for studying the static properties of statistical mechanical systems (Binder 1979, 1984). Monte Carlo studies of critical phenomena have been greatly hampered by critical slowing down: the autocorrelation time $\tau$ of the Monte Carlo stochastic process grows to infinity as the critical point is approached, which leads to a corresponding growth in the statistical error bars $\|$. The rate of growth of $\tau$ is thus a crucial factor in determining the statistical efficiency of the Monte Carlo algorithm.

In this letter we investigate the dynamic critical behaviour of some Monte Carlo algorithms for lattice models of polymer chains-in particular, for the self-avoiding walk (SAW), the non-reversal random walk (NRRW) and the ordinary random walk (ORW). For these models 'criticality' corresponds to the long-chain limit. The mean square end-to-end-distance of an N -step chain behaves asymptotically as

$$
\begin{equation*}
\left\langle\boldsymbol{R}_{N}^{2}\right\rangle \sim N^{2 \nu} \tag{1}
\end{equation*}
$$

[^0]for $N \rightarrow \infty$. The relevant length scale is thus $\xi=\left\langle\boldsymbol{R}_{N}^{2}\right\rangle^{1 / 2} \sim N^{\nu}$. The autocorrelation time of the Monte Carlo stochastic dynamics behaves asymptotically as
\[

$$
\begin{equation*}
\tau \sim N^{p} \tag{2}
\end{equation*}
$$

\]

(or $\tau \sim\langle N\rangle^{p}$ for algorithms working with chains of variable length); this defines a dynamic critical exponent $p$, which is the object of our study $\dagger$.

We first consider algorithms whose elementary moves are local N -conserving deformations of the chain (some examples are shown in (a)-(g) of figure 1). Algorithms of this type have been proposed by Verdier and Stockmayer (1962) and subsequently by many others $\ddagger$. Some of these algorithms and their properties are listed in table 1.

Let us begin with a crude heuristic estimate of the autocorrelation time $\tau$ for this class of algorithms. Consider the motion of the centre-of-mass vector of the chain. Very crudely speaking, this quantity executes a random walk, moving a distance of order $1 / N$ at each elementary move. When it has finally moved a distance of order $\xi \sim N^{\nu}$, it seems reasonable to say that the chain has reached an 'essentially new' configuration. It takes about $(N \xi)^{2} \sim N^{2+2 \nu}$ elementary moves for this to occur. We predict, therefore, that $p=2+2 \nu$.


Figure 1. Some examples of local elementary moves. $(a)-(g)$ are $N$ conserving. One-bead moves: (a), $180^{\circ}$ kink-jump; (b), $90^{\circ}$ end-bond rotation; (c), $180^{\circ}$ end-bond rotation; two-bead moves: ( $d$ ), $180^{\circ}$ crankshaft; ( $e$ ), $90^{\circ}$ crankshaft ( $d \geqslant 3$ only); ( $f$ ), two-bead kink-jump; a three-bead move: (g), three-bead L flip; non- $N$-conserving moves: $(h)$, plaquette insertion ( $\Delta N=+2$ ); (i), plaquette deletion ( $\Delta N=-2$ ).

[^1]Table 1. Some local $N$-conserving Monte Carlo algorithms
\(\left.$$
\begin{array}{llll}\hline & & & \begin{array}{l}\text { Autocorrelation } \\
\text { time } \tau \\
\text { (in elementary } \\
\text { moves) }\end{array}
$$ <br>

(see figure 1)\end{array}\right]\)| Scheme |
| :--- |

This heuristic estimate has numerous limitations.
(i) It could be wrong if there are modes which relax essentially more slowly (i.e. with a larger dynamic critical exponent) than the centre-of-mass vector.
(ii) It could be wrong if there are special conservation laws or quasi-conservation laws which inhibit the relaxation. This indeed occurs for the Verdier-Stockmayer (vs) and Verdier-Kranbuehl (vk) algorithms for the saw and nrrw (but not the orw); see Hilhorst and Deutch (1975) and Boots and Deutch (1977). It may also occur for some or all of the algorithms in dimension $d=3$ as a result of 'quasi-knots' (Sokal 1986).
(iii) In the saw and NRRW cases, the centre-of-mass vector does not in fact execute a pure random walk; its successive moves are correlated. There are three a priori possibilities.
(a) The successive moves are strongly positively (resp negatively) correlated, due to some important (probably local) physical mechanism which our argument fails to take into account. Then $p$ could be significantly smaller (resp larger) than $2+2 \nu$. This is what causes $p>2+2 \nu$ in the vs and vk models.
(b) The successive moves are positively (resp negatively) correlated for global reasons arising out of the excluded-volume effect. In this case one would expect $p$ to be slightly smaller (resp larger) than $2+2 \nu$, with the error being roughly of order $\nu-\frac{1}{2}$.
(c) The correlation between successive moves is irrelevant for the critical behaviour. Then $p$ would be exactly equal to $2+2 \nu$; only the critical amplitude would be affected by the correlation.

Note, however, that what is relevant is not the correlation per se, but whether it gets radically stronger or weaker as $N \rightarrow \infty$.

Despite these limitations, this heuristic estimate also has some successes.
(i) It is exact in the orw case ( $\nu=\frac{1}{2}, p=3$ ); see Verdier (1966a,b, 1970, 1973), Iwata and Kurata (1969), Orwoll and Stockmayer (1969) and Stockmayer et al (1971). It is probably also exact in the NRRW case.
(ii) It agrees with a heuristic estimate of $p$ based on the balance between the elastic restoring force and viscous friction (De Gennes 1976).
(iii) It agrees with renormalisation group calculations in dimension $d=4-\varepsilon$ to first order in $\varepsilon$ (Jasnow and Moore 1977, Al-Noaimi et al 1978, Oono and Freed 1981, Shiwa and Kawasaki 1982 $\dagger$, Muthukumar 1983). Calculations to order $\varepsilon^{2}$ have apparently not yet been done. However, Oono and Freed (1981) and Muthukumar (1983) claim that $p=2+2 \nu$ holds exactly.
(iv) It agrees roughly with the results of most Monte Carlo studies in dimension $d=3$ (Birshtein et al 1977, Ceperley et al 1978, 1981, Baumgärtner 1980, Gurler et al 1982, Meirovitch 1984). However, some studies differ (Kranbuehl and Verdier 1979, 1980, Romiszowski and Stockmayer 1984).

Remark 1. These models simulate the dynamics of a single polymer chain in a good solvent in the 'free-draining' limit i.e. neglecting hydrodynamic interactions. This limit does not correspond to any physically realisable situation, for in fact the hydrodynamic interactions always dominate the dynamics. For our present purposes this objection is irrelevant.

Remark 2. Very recently, Madras and Sokal (1986a) have proved that every dynamic algorithm for the SAW (but not the NRRW or ORW) based on a finite repertoire of local $N$-conserving elementary moves is non-ergodic. It follows that the autocorrelation time $\tau$, defined with respect to the usual (equal weight) saw distribution, is infinity: the correct equilibrium distribution is never reached. In these cases the foregoing heuristic argument has to be reinterpreted as referring to the relaxation time within one of the ergodic classes. The meaning of $\nu$ has to be reinterpreted analogously.

Next, we consider algorithms which append and/or delete bonds at the endpoint(s) of the chain, such as the 'slithering-snake' (reptation) algorithm (Kron 1965, Kron et al 1967, Wall and Mandel 1975, Mandel 1979) and the 'slithering-tortoise' algorithm (Berretti and Sokal 1985). In these algorithms the centre-of-mass vector moves a distance of order $\left|\mathbf{R}_{N}\right| / N \sim \xi / N$ per elementary move, so that it takes a time of order $N^{2}$ for the centre-of-mass vector to diffuse a distance of order $\xi$. The autocorrelation time $\tau$ is thus expected to be of order $N^{2}$ (or $\langle N\rangle^{2}$ ), which is indeed what is observed (Mandel 1979, Berretti and Sokal 1985).

Finally, we consider an algorithm proposed by Berg and Foerster (1981), Aragão de Carvalho and Caracciolo (1983) and Aragão de Carvalho et al (1983) (henceforth referred to as BFACF ). This algorithm generates SAW (or NRRW) of variable length N which begin at the origin and end at a fixed lattice site $x \neq 0 \ddagger$. Its elementary moves are ( $a$ ), ( $h$ ) and (i) of figure 1 , which have $\Delta N=0,+2$ and -2 , respectively. The algorithm satisfies detailed balance with respect to a modified grand canonical ensemble in which each $N$-step walk gets relative weight $N \beta^{N}$. Here $\beta$ is a user-chosen parameter satisfying $0 \leqslant \beta \leqslant \beta_{\text {crit }} \equiv 1 / \mu$, where $\mu$ is the connective constant of the lattice $Z^{d}$ for SAW (or NRRW). This algorithm is of considerable interest, as it is the most efficient known way of generating SAW with fixed endpoints; such SAW are required for

[^2]determining the critical exponent $\alpha_{\text {sing }}$ and thereby testing the conjectured hyperscaling relation $\mathrm{d} \nu=2-\alpha_{\text {sing }}$.

The analysis of the bFACF dynamics appears to be quite subtle, even for the NRRW case. A $\Delta N=0$ move causes the centre-of-mass vector to move a distance of order $1 / N$. On the other hand, a $\Delta N= \pm 2$ move causes the centre-of-mass vector to move an average distance of order $S_{N} / N \sim \xi / N$, where $S_{N} \sim \xi \sim N^{n}$ is the radius of gyration of the chain. One might assume, therefore, that the $\Delta N= \pm 2$ moves dominate the relaxation, so that $p=2$. But it is not so clear that the $\Delta N= \pm 2$ moves, which deform the chain perpendicular to itself, are as effective in promoting relaxation of the chain as the 'slithering-snake' and 'slithering-tortoise' moves, which extend and contract the chain along itself. So perhaps $p \approx 2+2 \nu$ after all. Nor is it clear that the centre-of-mass vector is the slowest relaxing mode (see below).

There is a further subtlety in the bFACF dynamics, but to explain it we must first define more precisely what we mean by 'autocorrelation time'. Let $A$ be an observable and let

$$
\begin{equation*}
\rho_{A A}(t)=\frac{\langle A(0) A(t)\rangle-\langle A(0)\rangle^{2}}{\left\langle A(0)^{2}\right\rangle-\langle A(0)\rangle^{2}} \tag{3}
\end{equation*}
$$

be its normalised time-autocorrelation function in the stationary stochastic process (i.e. 'in equilibrium'). Typically $\rho_{\mathrm{AA}}(t)$ decays exponentially ( $\sim \mathrm{e}^{-t / \tau}$ ) for large $t$; we define the exponential autocorrelation time

$$
\begin{equation*}
\tau_{\exp , A}=\limsup _{t \rightarrow \infty} \frac{t}{-\log \left|\rho_{A A}(t)\right|} \tag{4}
\end{equation*}
$$

and

$$
\begin{equation*}
\tau_{e \times p}=\sup _{A \in L^{2}} \tau_{\exp , A} . \tag{5}
\end{equation*}
$$

(In (5) the supremum is taken over all observables $A$ with finite second moment.) Thus $\tau_{\text {exp }}$ is the relaxation time of the slowest mode in the system and $\tau_{\text {exp, } A}=\tau_{\text {exp }}$ for all observables $A$ which are not 'orthogonal' to this slowest mode. We also define the integrated autocorrelation time

$$
\begin{equation*}
\tau_{\mathrm{int}, A}=\frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_{A A}(t)=\frac{1}{2} \tilde{\rho}_{A A}(0) \tag{6}
\end{equation*}
$$

It is this quantity which determines the statistical error bars in Monte Carlo measurements of $\langle A\rangle$ (Binder 1979, ch 1, Berretti and Sokal 1985).

The dynamic scaling hypothesis (Hohenberg and Halperin 1977) predicts that $\tau_{\text {exp }}$, $\tau_{\text {exp,A }}$ and $\tau_{\text {int,A }}$ diverge at the critical point with the same dynamic critical exponent, at least for 'reasonable' observables $A$. However, this behaviour can fail for observables which are orthogonal to the slowest mode (typically by virtue of some symmetry) or asymptotically orthogonal to it (this typically occurs in models having a broad spectrum of relaxation times; see, e.g., Binder and Stauffer 1984, Madras and Sokal 1986b). In fact, as we now explain, the bFACF model falls into this latter category.

Very recently, Sokal and Thomas (1986) have proved the surprising result that $\tau_{\text {exp }}=\infty$ for the bFACF model at all $\beta>0$. Their proof uses a minimum hitting time argument: the transition between a fixed short walk and an approximately square $N$-step walk ( $N$ large) takes a minimum time of order $N^{2}$, but it turns out that the rarity of such long walks $\left(\sim N \beta^{N}\right)$ 'justifies' only a time of order $N$. From this it can
be shown that $\tau_{\text {exp }}=\infty$ : there are arbitrarily slowly relaxing modes associated with transitions to very long walks. Consequently, one expects that for 'most' observables $A$, the autocorrelation function $\rho_{\text {AA }}(t)$ will decay non-exponentially as $t \rightarrow \infty$ (e.g. as a power law), so that $\tau_{\text {exp.A }}=\infty$. However, there is nothing to prevent $\tau_{\text {int }, A}$ from being finite and indeed one expects that $\tau_{\mathrm{int}}<\infty$ for 'reasonable' observables $A$, i.e. those that are not too strongly coupled to very long walks. It then makes sense to study the dynamic critical exponent $p_{A}$ defined by $\tau_{\text {int }, A} \sim\langle N\rangle^{p_{A}}$ for $\beta \uparrow \beta_{\text {crit }}$.

To investigate this question, we performed a high precision Monte Carlo study of the bFACF dynamics for two-dimensional SAW and NRRW (with endpoint $|x|=1$ ) over a range of values of $\beta$. We used the following variant of the BFACF algorithm: link $l$ is chosen at random and its direction is compared with that of the preceding ( $p$ ) and following ( $f$ ) links in the walk. We distinguish four cases (figure 2 of Argão de Carvalho and Carcciolo (1983)):
(I) $p$ and $f$ are both perpendicular to $l$, and $p$ is not antiparallel to $f$;
(II) $p$ is antiparallel to $f$ (in this case, due to the constraints on our models, $p$ and $f$ are necessarily both perpendicular to $l$ );
(III) either $p$ or $f$ is parallel to $l$, but not both;
(IV) $p, l$ and $f$ are parallel.

We then consider the two possible deformations of the link $l$ by one unit parallel to itself, and propose them with probabilities $p(\Delta N)$ given by

$$
\begin{aligned}
& p(-2)=1 /\left(1+\beta^{2}\right) \\
& p(0)=\frac{1}{2} \\
& p(+2)-\beta^{2} /\left(1+\beta^{2}\right)
\end{aligned}
$$

(In cases III and IV these probabilities sum to less than one, and so a null transition is made with probability $c_{0}(\mathrm{III})=\left(1-\beta^{2}\right) / 2\left(1+\beta^{2}\right)$ or $c_{0}(\mathrm{IV})=\left(1-\beta^{2}\right) /\left(1+\beta^{2}\right)$, respectively.) If, however, the proposed new walk would violate the constraint of the model (self-avoidance or non-immediate reversal, as the case may be), the proposal is rejected and a null transition is also made. There will, therefore, be two types of null transitions: those arising out of failure to propose a new configuration (cases III and IV only) and those arising because the proposed new configuration violates the constraints of the model. We call these Monte Carlo rejections and constraint rejections, respectively. (It is important to realise that in the NRRW as well as the sAw there are constraint rejections: see figure 2 for a $\Delta N=-2$ transition which is forbidden by the NRRW constraint.)

We performed the calculations on an IBM 3033 computer, using the CERN pseudorandom number generator RNDM2. Each Monte Carlo step took roughly $20 \mu \mathrm{~s}$ CPU


Figure 2. A $\Delta N=-2$ move which is forbidden by the NRRW constraint.
time for the NRRW or $30 \mu \mathrm{~s}$ for the SAW; the entire study used about 600 h of cPU time. We took data once every $\approx \tau / 10 \mathrm{mc}$ step (based on a guess for $\tau$ ). We discarded the data from the first $\approx 100 \tau$ MC steps in order to guarantee that complete equilibrium (i.e. a stationary stochastic process) had been reached.

In table 2 we report the parameters of our runs and the observed rejection rates. In table 3 we report the estimated mean value $\langle N\rangle$ and autocorrelation times $\tau_{\text {int, } A}$ for the observables $A=N, N^{2}$ and $N^{3}$; the final columns of table 3 give the estimated dynamic critical exponents $p_{A}$.

Table 2. Parameters of our runs and observed rejection rates. All times are measured in MC steps. Data discarded at the beginning of the run equal 1000 times the data-taking interval.

| Beta | Run length | Data-taking <br> interval | Monte Carlo <br> rejection (\%) | Constraint <br> rejection (\%) |
| :--- | :---: | :---: | :--- | :--- |
| NRRW |  |  |  |  |
| 0.278 | $1.25 \times 10^{7}$ | 50 | 63.80 | 16.30 |
| 0.303 | $1.25 \times 10^{8}$ | 500 | 51.20 | 21.25 |
| 0.318 | $7.5 \times 10^{8}$ | 3000 | 41.54 | 24.00 |
| 0.323 | $1.75 \times 10^{9}$ | 7000 | 37.66 | 24.86 |
| 0.325 | $3.0 \times 10^{9}$ | 12000 | 36.02 | 25.15 |
| 0.3268 | $3.75 \times 10^{9}$ | 15000 | 34.29 | 25.39 |
| 0.3278 | $5.5 \times 10^{9}$ | 22000 | 33.39 | 25.53 |
|  |  |  |  |  |
|  |  | $5 A W$ |  |  |
| 0.335 | $2.5 \times 10^{7}$ | 50 | 64.10 | 13.20 |
| 0.355 | $3.0 \times 10^{8}$ | 400 | 56.57 | 14.86 |
| 0.369 | $3.5 \times 10^{9}$ | 7000 | 47.91 | 15.66 |
| 0.3728 | $8.5 \times 10^{9}$ | 17000 | 44.32 | 15.67 |
| 0.3744 | $1.65 \times 10^{10}$ | 22000 | 42.42 | 15.60 |
| 0.376 | $3.5 \times 10^{10}$ | 140000 | 39.98 | 15.45 |

Let us explain briefly our statistical methods. We estimate the mean value $\langle A\rangle$ by the sample mean $\bar{A}=(1 / N) \sum_{i=1}^{N} A(i)$, the unnormalised autocorrelation function $C_{A A}(t)=\langle A(0) A(t)\rangle-\langle A\rangle^{2}$ by the sample unnormalised autocorrelation function

$$
\begin{equation*}
\hat{C}_{A A}(t)=\frac{1}{N-|t|} \sum_{i=1}^{N-|t|}\left[A(i) A(i+|t|)-\bar{A}^{2}\right] \tag{7}
\end{equation*}
$$

and the normalised autocorrelation function $\rho_{A A}(t)=C_{A A}(t) / C_{A A}(0)$ by the sample normalised autocorrelation function $\hat{\rho}_{A A}(t) \equiv \hat{C}_{A A}(t) / \hat{C}_{A A}(0)$. Here $A(1), \ldots, A(N)$ are the observed values of the observable $A$ for the non-discarded part of the run. We then estimate $\tau_{\mathrm{in}, \mathrm{A}}$ by

$$
\begin{equation*}
\hat{\tau}_{\mathrm{int}, \mathrm{~A}} \equiv \frac{1}{2} \sum_{t=-T}^{T} \hat{\rho}_{A A}(t) \tag{8}
\end{equation*}
$$

where the 'window width' $T$ is chosen self-consistently to be equal to $5 \hat{\tau}_{\text {int }, A}$. The standard deviation of the estimator $\hat{\tau}_{\text {int }, A}$ is roughly $2 \tau_{\mathrm{int}, A}(T / N)^{1 / 2}$; this formula is based on the very crude assumption that the stochastic process $\{A(t)\}$ is approximately

Table 3. Estimates of $p_{N}, p_{N^{2}}$ and $p_{N^{3}}$ are based on a weighted least-squares fit to the data from the indicated and all higher values of $\beta$. Error bars are $\pm 2$ standard deviations.

| Beta | $\langle N\rangle$ | $\tau_{\text {int }, N}$ | $\tau_{\text {int, } N^{2}}$ | $\tau_{\mathrm{int}, N^{3}}$ | $p_{N}$ | $p_{N^{2}}$ | $p_{N^{3}}$ |
| :--- | ---: | :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  | NRRW |  |  |  |  |
| 0.278 | $5.87 \pm 0.08$ | $(6.9 \pm 0.5) \times 10^{2}$ | $(8.6 \pm 0.7) \times 10^{2}$ | $(8.5 \pm 0.7) \times 10^{2}$ | $2.42 \pm 0.06$ | $2.42 \pm 0.07$ | $2.42 \pm 0.08$ |
| 0.303 | $10.91 \pm 0.11$ | $(3.3 \pm 0.2)+10^{3}$ | $(5.9 \pm 0.5) \times 10^{3}$ | $(8.1 \pm 0.8) \times 10^{3}$ | $2.38 \pm 0.08$ | $2.24 \pm 0.11$ | $2.11 \pm 0.12$ |
| 0.318 | $21.76 \pm 0.21$ | $(1.8 \pm 0.1) \times 10^{4}$ | $(2.7 \pm 0.2) \times 10^{4}$ | $(3.0 \pm 0.2) \times 10^{4}$ | $2.30 \pm 0.14$ | $2.19 \pm 0.18$ | $2.14 \pm 0.18$ |
| 0.323 | $32.67 \pm 0.35$ | $(5.1 \pm 0.3) \times 10^{4}$ | $(7.0 \pm 0.6) \times 10^{4}$ | $(8.7 \pm 0.7) \times 10^{4}$ | $2.10 \pm 0.25$ | $1.88 \pm 0.30$ | $1.72 \pm 0.34$ |
| 0.325 | $40.92 \pm 0.43$ | $(8.7 \pm 0.5) \times 10^{4}$ | $(1.3 \pm 0.1) \times 10^{5}$ | $(1.5 \pm 0.1) \times 10^{5}$ | $1.95 \pm 0.42$ | $1.71 \pm 0.46$ | $1.34 \pm 0.57$ |
| 0.3268 | $51.81 \pm 0.63$ | $(1.4 \pm 0.1) \times 10^{5}$ | $(2.0 \pm 0.1) \times 10^{5}$ | $(2.2 \pm 0.2) \times 10^{5}$ | $1.72 \times 1.19$ | $1.45 \times 1.29$ | $0.98 \pm 1.51$ |
| 0.3278 | $59.69 \pm 0.66$ | $(1.8 \pm 0.1) \times 10^{5}$ | $(2.5 \pm 0.2) \times 10^{5}$ | $(2.6 \pm 0.2) \times 10^{5}$ | - | - | - |


| SAW |  |  |  |  |  |  |  |
| :--- | ---: | :--- | :--- | :--- | :--- | :--- | :--- |
| 0.335 | $5.73 \pm 0.07$ | $(6.0 \pm 0.3) \times 10^{2}$ | $(1.0 \pm 0.1) \times 10^{3}$ | $(1.2 \pm 0.1) \times 10^{3}$ | $3.15 \pm 0.05$ | $3.15 \pm 0.07$ | $3.16 \pm 0.07$ |
| 0.355 | $9.70 \pm 0.19$ | $(6.0 \pm 0.2) \times 10^{3}$ | $(1.3 \pm 0.06) \times 10^{4}$ | $(1.5 \pm 0.08) \times 10^{4}$ | $2.95 \pm 0.06$ | $2.88 \pm 0.09$ | $2.89 \pm 0.09$ |
| 0.369 | $21.51 \pm 0.31$ | $(5.7 \pm 0.2) \times 10^{4}$ | $(1.1 \pm 0.05) \times 10^{5}$ | $(1.3 \pm 0.07) \times 10^{5}$ | $3.09 \pm 0.13$ | $3.09 \pm 0.17$ | $3.02 \pm 0.19$ |
| 0.3728 | $33.53 \pm 0.53$ | $(2.3 \pm 0.1) \times 10^{5}$ | $(4.8 \pm 0.3) \times 10^{5}$ | $(5.9 \pm 0.4) \times 10^{5}$ | $3.09 \pm 0.25$ | $2.92 \pm 0.36$ | $2.84 \pm 0.39$ |
| 0.3744 | $44.39 \pm 0.86$ | $(5.0 \pm 0.3) \times 10^{5}$ | $(9.0 \pm 0.7) \times 10^{5}$ | $(1.0 \pm 0.1) \times 10^{6}$ | $3.36 \pm 0.49$ | $3.55 \pm 0.67$ | $3.64 \pm 0.70$ |
| 0.376 | $65.74 \pm 1.64$ | $(1.9 \pm 0.14) \times 10^{6}$ | $(3.6 \pm 0.4) \times 10^{6}$ | $(4.3 \pm 0.5) \times 10^{6}$ | - | - | - |

Gaussian. Further details on the statistical analysis of autocorrelated time series can be found in the books of Priestley (1981), Anderson (1971) and Jenkins and Watts (1968), among others. Finally, we estimate the exponent $p_{A}$ by a weighted least-squares fit to the data, using the ansatz

$$
\begin{equation*}
\log \tau_{\mathrm{int}, \mathrm{~A}}=p_{A} \log \langle N\rangle+c_{A} \tag{9}
\end{equation*}
$$

and using weights inversely proportional to the estimated variances (squared standard deviations) of $\log \hat{\tau}_{\mathrm{int}, A}$. In this analysis we ignore the statistical errors in $\langle N\rangle$, since they are negligible compared to those in $\tau_{\text {int, } A}$.

The results of this analysis (table 3) are at least consistent with the idea that the exponents $p_{A}$ are the same for $A=N, N^{2}, N^{3}$; only the proportionality constant $c_{A}$ depends on the particular observable $A$. Our final estimates are

$$
\begin{equation*}
p=2.2 \pm 0.5 \quad \text { (NRRW) } \tag{10a}
\end{equation*}
$$

and

$$
\begin{equation*}
p=3.0 \pm 0.4 \quad \text { (SAW) } \tag{10b}
\end{equation*}
$$

( $95 \%$ subjective confidence limits). We have not attempted to specify separate systematic and statistical errors, because they seem hopelessly entangled. These estimates for $p$ are significantly below $2+2 \nu$, which is 3.0 for the NRRW and 3.5 for the saw.

In conclusion, we find that the expected relation $p=2+2 \nu$, although not completely ruled out, seems to be highly unlikely. As a result, the dynamic critical behaviour of the bFACF model remains somewhat mysterious. We hope that this letter could encourage further studies, both numerical and theoretical, in the difficult area of dynamic critical scaling.

The research of one of the authors (ADS) was supported in part by NSF grant DMS-8400955.

## References

Al-Noaimi G F, Martinez-Mekler G C and Wilson C 1978 J. Physique Lett. 39 L373
Anderson T W 1971 The Statistical Analysis of Time Series (New York: Wiley)
Aragão de Carvalho C and Caracciolo S 1983 J. Physique 44323
Aragão de Carvalho C, Caracciolo S and Fröhlich J 1983 Nucl. Phys. B 215[FS7] 209
Baumgärtner A 1980 J. Chem. Phys. 72871
Baumgärtner A and Binder K 1979 J. Chem. Phys. 712541
Berg B and Foerster D 1981 Phys. Lett. 106B 323
Berretti A and Sokal A D 1985 J. Stat. Phys. 40483
Binder K (ed) 1979 Monte Carlo Methods in Statistical Physics (Berlin: Springer)

- 1984 Applications of the Monte Carlo Method in Statistical Physics (Berlin: Springer)

Binder K and Stauffer D 1984 Applications of the Monte Carlo Method in Statistical Physics ed K Binder (Berlin: Springer) ch 8
Birshtein T M, Gridnev V N, Gotlib Yu Ya and Skvortsov A M 1977 Vysokomol. Soyed. A 191398 (Engl. transl. Polymer Sci. USSR 19 1612)
Boots H and Deutch J M 1977 J. Chem. Phys. 674608
Ceperley D, Kalos M H and Lebowitz J L 1978 Phys. Rev. Lett. 41313

- 1981 Macromol. 141472

De Gennes P G 1976 Macromol. 9587
Gurier M T, Crabb C C, Dahlin D M and Kovac J 1983 Macromol. 16398
Heilmann O H 1968 K. Dansk Vidensk. Selsk. Mat. Fys. Meddr. 37 no 2
Heilmann O H and Rotne J 1982 J. Stat. Phys. 2719
Hilhorst H J and Deutch J M 1975 J. Chem. Phys. 635153
Hohenberg P C and Halperin B I 1977 Rev. Mod. Phys. 49435
Iwata K and Kurata M 1969 J. Chem. Phys. 504008
Jasnow D and Moore M A 1977 J. Physique Lett. 38 L467
Jenkins G M and Watts D G 1968 Spectral Analysis and Its Applications (San Francisco: Holden-Day)
Kranbuehl D E and Verdier P H 1979 J. Chem. Phys. 712662
—— 1980 Polymer Preprints (ACS) 21195
Kremer K, Baumgärtner A and Binder K 1981 J. Phys. A: Math. Gen. 152879
Kron A K 1965 Vysokomol. Soyed. 71228 (Engl. transl. Polymer Sci. USSR 7 1361)
Kron A K, Ptitsyn O B, Skvortsov A M and Fedorov A K 1967 Molek. Biol. 1576 (Engl. transl. Molec. Biol. 1 487)
Lax M and Brender C 1977 J. Chem. Phys. 671785
Madras N and Sokal A D 1986a J. Stat. Phys. to be submitted

- 1986b in preparation

Mandel F 1979 J. Chem. Phys. 703984
Meirovitch H 1984 Macromol. 172038
Muthukumar M 1983 J. Stat. Phys. 30457
Oono Y and Freed K F 1981 J. Chem. Phys. 751009
Orwoll R A and Stockmayer W H 1969 Adv. Chem. Phys. 15305
Priestley M B 1981 Spectral Analysis and Time Series 2 vol (New York: Academic)
Romiszowski P and Stockmayer W H 1984 J. Chem. Phys. 80485
Shiwa Y and Kawasaki K 1982 J. Phys. C: Solid State Phys. 155345
Sokal A D 1986 in preparation
Sokal A D and Thomas L E 1986 in preparation
Stockmayer W H, Gobush W and Norvich R 1971 Pure Appl. Chem. 26537
Taran Yu A and Stroganov L B 1978 Vysokomol. Soyed. A 201787 (Engl. transl. Polymer Sci. USSR 20 2007)
Verdier P H 1966a J. Chem. Phys. 452118

- 1966b J. Chem. Phys. 452122
- 1970 J. Chem. Phys. 525512
- 1973 J. Chem. Phys. 596119

Verdier P H and Kranbuehl D E 1976 Polymer Preprints (ACS) 17148
Verdier P H and Stockmayer W H 1962 J. Chem. Phys. 36227
Wall F T and Mandel F 1975 J. Chem. Phys. 634592


[^0]:    § Address after 1 September 1986: Department of Physics, New York University, 4 Washington Place, New York, NY 10003, USA.
    $\|$ Each block of data of length $\approx 2 \tau$ can be considered, roughly speaking, to contribute one statistically independent' data point. Therefore, the 'effective sample size' from a Monte Carlo run of length $N$ is $\approx N / 2 \tau$, resulting in statistical error bars of order $(\tau / N)^{1 / 2}$. For a more detailed treatment, see Binder (1979) §§ 1.2.3 and 1.2.4, and Berretti and Sokal (1985) §4.1.

[^1]:    $\dagger$ In this letter we measure time in units of attempted elementary moves of the Monte Carlo algorithm (sometimes called 'bead cycles'). Much of the literature on dynamic polymer chain models uses a timescale of attempted elementary moves per bead; autocorrelation times expressed in this way should be multiplied by $N$ (or $N+1$ ) before comparing them to the present letter. The conventional exponent $z$ is defined by $p=z v+1$.
    $\ddagger$ See, e.g., Heilmann (1968), Hilhorst and Deutch (1975), Verdier and Kranbuehl (1976), Birshtein et al (1977), Taran and Stroganov (1978), Kranbuehl and Verdier (1979), Kremer et al (1981), Heilmann and Rotne (1982), Meirovitch (1984), Madras and Sokal (1985a) and references cited therein. Similar algorithms have been employed for continuum polymers; see, e.g., Baumgärtner and Binder (1979) and Baumgärtner (1980).

[^2]:    $\dagger$ Shiwa and Kawasaki do not explicitly mention the free-draining excluded-volume fixed point at $u^{*}=\pi^{2} \varepsilon / 2$, $\lambda^{*}=0$, but it is easily deduced from their formulae that $z=4-\varepsilon / 4$ there, in agreement with the other RG studies.
    $\ddagger$ For SAw in dimension $d=3$, the algorithm is ergodic only if $|x|_{\infty} \equiv \max \left(\left|x_{1}\right|,\left|x_{2}\right|,\left|x_{3}\right|\right) \geqslant 2$ (Sokal 1986): if $|x|_{\infty}=1$ there exist knotted configurations which cannot be untied.

