# Scanning method as an unbiased simulation technique and its application to the study of self-attracting random walks

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(Received 28 September 1984; revised manuscript received 8 May 1985)

The scanning method proposed by us [J. Phys. A **15**, L735 (1982); Macromolecules **18**, 563 (1985)] for simulation of polymer chains is further developed and applied, for the first time, to a model with *finite* interactions. In addition to "importance sampling," we remove the bias introduced by the scanning method with a procedure suggested recently by Schmidt [Phys. Rev. Lett. **51**, 2175 (1983)]; this procedure has the advantage of enabling one to estimate the statistical error. We find these two procedures to be equally efficient. The model studied is an $N$-step random walk on a lattice, in which a random walk $i$ has a statistical weight $p^{M_i}$, where $p<1$ is an attractive energy parameter and $M_i$ is the number of distinct sites visited by walk $i$. This model, which corresponds to a model of random walks moving in a medium with randomly distributed static traps, has been solved analytically for $N\to\infty$ for any dimension $d$ by Donsker and Varadhan (DV) and by others. $\langle M\rangle$ and $\ln\phi$, where $\phi$ is the survival probability in the trapping problem, diverge like $N^{\alpha}$ with $\alpha=d/(d+2)$. Most numerical studies, however, have failed to reach the DV regime in which $d/(d+2)$ becomes a good approximation for $\alpha$. On the other hand, our results for $\alpha$ (obtained for $N\leq 150$) are close to the DV values for $p\leq 0.7$ and $p\leq 0.6$ for $d=2$ and 3, respectively. This suggests that the scanning method is more efficient than both the commonly used direct Monte Carlo technique, and the Rosenbluth and Rosenbluth method [J. Chem. Phys. **23**, 356 (1954)]. Our results support the conclusion of Havlin *et al.* [Phys. Rev. Lett. **53**, 407 (1984)] that the DV regime exists already for $\phi\leq 10^{-13}$ for both $d=2$ and 3. We also find that at the percolation threshold $p_c$ the exponents for the end-to-end distance are small, but larger than zero, and that the probability of a walk returning to the origin behaves approximately as $N^{-1/3}$ for both $d=2$ and 3.

## I. INTRODUCTION

The scanning method is a computer simulation technique for polymer chains suggested recently by the author.[1-3] So far the method has been applied only to models with hard-core interaction, such as self-avoiding walks (SAW's) on square and simple cubic lattices[1-3] and many-chain systems.[4] In this work the method is further extended to simulate chain models with *finite* interactions; we apply it to a model of self-attracting random walks on a lattice, which will be described later on. With the scanning method a SAW is constructed with a step-by-step procedure, based on scanning at each step all the possible continuations of the partial SAW in $b$ "future" steps (in practice, $b\leq 10$ for the square lattice[1-3]). Obviously, for walks with finite interactions, as those studied here, one should also take into account the Boltzmann factor of each future continuation. In this way the local environment of a step is taken into account *exactly*. Very recently the method has been significantly improved by taking into account *approximately* the remote environment of a step with the help of a mean field parameter.[3] It should be pointed out that the scanning method generates walks with a certain bias, which in principle can be removed by employing "importance sampling"[5,6] for very large samples. However, no criterion has been provided which enables one to determine the extent of convergence for a practical sample size. In order to overcome this difficulty we employ here, in addition to importance sampling, an alternative procedure, which enables one to extract from an originally biased sample of walks an effectively smaller sample of unbiased ones. Thus, the averages, as well as their statistical errors, can be obtained directly from the unbiased sample.[7]

The model of interacting random walks studied here has been recently investigated by Stanley *et al.*[8] In this model a random walk of $N$ steps that has visited $M$ distinct lattice sites has a statistical weight of $p^M=\exp(-KM)$, where $p$ is a parameter. For $p=1$ ($K=0$) the model corresponds to the purely random walk. If $p>1$ ($K<0$) walks that visit a new site at each step are weighted most heavily and the walk is self-repelling, becoming self-avoiding as $p\to\infty$. In the regime $p<1$ ($K>0$) the walker prefers to return to previously visited sites. This case, of self-attracting walks ($p<1$), is studied here.

The partition function $Z$ ($p<1$) has been solved analytically for any dimension $d$, by Donsker and Varadhan[9] (DV) in the limit of $N\to\infty$,

$$\lim_{N\to\infty}\ln[(2d)^{-N}Z]=-A\,[\ln(p^{-1})]^{2/(d+2)}N^{\alpha}\,,\qquad \alpha=d/(d+2) \quad (1)$$

where $A$ is a constant which depends on the lattice. It should be pointed out that this model ($p<1$) corresponds

 

to a model of random walks, moving on a lattice with randomly distributed static traps; for trap concentration $1-p$ the survival probability[8] $\phi$ (i.e., the average fraction of walks which survive after $N$ steps) equals $(2d)^N Z(p)$ [Eq. (1)] (see also Refs. 10–12). However, most numerical studies of this model for $d \geq 2$ have failed to obtain the DV asymptotic values of $\alpha$, which has raised the question of how large $N$ must be for Eq. (1) to be a useful approximation[13–17] (the DV regime). Stanley *et al.*[8] have employed series expansion techniques for the study of self-attracting walks at the percolation thresholds $p_c$ of the hypercubical lattices, $1 \leq d \leq 10$. Their values for $\alpha$, however, deviate significantly from the DV values, $d/(d+2)$, which is probably a consequence of using too-short series. Fixman[13] and Klafter *et al.*[15] (see also Ref. 16) investigated the trapping problem by computer simulation and concluded that the DV regime is obtained for $\phi \leq 10^{-67}$ and $10^{-21}$, respectively. On the other hand, Havlin *et al.*,[17] using their numerical techniques, have found a significantly higher estimate, $\phi \leq 10^{-13}$.

These discrepancies have motivated us to apply the scanning method to the model of self-attracting random walks. In order to compare our results to those of Ref. 8, we simulate walks on square and simple cubic lattices at $p_c$. We also study the model at $p \neq p_c$, which enables one to compare the efficiency of the scanning method to that of the other methods mentioned above. At $p_c$ we investigate the behavior of quantities, which have not been studied analytically by DV, such as the end-to-end distance, the radius of gyration, and the probability of a walk to return to the origin.

## II. THEORY

### A. Thermodynamic and geometrical properties of self-attracting walks

Assume a lattice of dimensionality $d$ with coordination number $q$ ($q=2d$) and a random walk $i$ of $N$ steps, which starts from the origin and visits $M_i$ distinct lattice sites. If the interaction parameter for a distinct site visited is $p=\exp(-K)$ the ensemble probability $P_i$ is

$$P_i = p^{M_i}/Z = \exp(-KM_i)/Z \ , \tag{2}$$

where $Z$, the partition function, is

$$Z = \sum_i \exp(-KM_i) \ . \tag{3}$$

The entropy $\langle S \rangle$ (in units of $k_B$, where $k_B$ is the Boltzmann constant) is

$$\langle S \rangle = -\sum_i P_i \ln P_i \ . \tag{4}$$

We shall be interested in $\langle M^l \rangle$, the ensemble average of $M_i$ and its $l$ moments,

$$\langle M^l \rangle = \sum_i P_i M_i^l, \quad 1 \leq l \leq 4 \tag{5}$$

and the fluctuation $\langle \Delta^2 M \rangle$, where

$$\langle \Delta^2 M \rangle = \langle M^2 \rangle - \langle M \rangle^2 \ . \tag{6}$$

$\langle M^l \rangle$ and $\langle \Delta^2 M \rangle$ are expected to scale, with exponents $\alpha_l$ and $\beta$, respectively,

$$\langle M^l \rangle \sim N^{l\alpha_l} \ , \tag{7}$$

$$\langle \Delta^2 M \rangle \sim N^{\beta} \ . \tag{8}$$

The free energy $\langle F \rangle$ (in units of $k_B T$, where $T$ is the absolute temperature) is given by

$$F = -\ln Z = K\langle M \rangle - \langle S \rangle \ . \tag{9}$$

For $N \to \infty$, $F$ can be obtained from Eq. (1) [using $p=\exp(-K)$],

$$F = AK^{2/(2+d)} N^{d/(d+2)} - N \ln(2d) \ . \tag{10}$$

This means that the entropy [the second term in Eq. (10)] is extensive, whereas $\langle M \rangle$ (the first term), which plays the role of energy, diverges with an exponent $\alpha = d/(d+2) < 1$. It should be pointed out that $\langle M^l \rangle$ [Eq. (7)] can be obtained by taking $l$ derivatives of $F$ with respect to the parameter $-K=\ln p$; therefore $\beta=\alpha_l = d/(d+2)$ for all $l$.

The second and fourth average moments of the end-to-end distance $R$ are

$$\langle R^l \rangle = \sum_i P_i R_i^l, \quad l=2,4 \ . \tag{11}$$

$\langle R^l \rangle$ is expected to scale with an exponent $\nu_{lR}$, i.e.,

$$\langle R^l \rangle \sim N^{l\nu_{lR}} \ . \tag{12}$$

Another quantity of interest is $G_i$, the radius of gyration of walk $i$, where

$$G_i^2 = (N+1)^{-1} \sum_{k=0}^{N} \sum_{m=1}^{d} (r_k^m - \bar{r}^m)^2 \ . \tag{13}$$

In Eq. (13) $r_k^m$ and $\bar{r}^m$ are the coordinates of step $k$ and of the center of mass, respectively, where

$$\bar{r}^m = (N+1)^{-1} \sum_{k=0}^{N} r_k^m \ . \tag{14}$$

We shall estimate $\langle G^l \rangle$ for $l=2$ and 4, where

$$\langle G^l \rangle = \sum_i P_i G_i^l \ . \tag{15}$$

The $\langle G^l \rangle$'s are expected to scale with exponents $\nu_{lG}$,

$$\langle G^l \rangle \sim N^{l\nu_{lG}} \ . \tag{16}$$

We shall also estimate $P^0$, the probability of a walk to return to the origin,

$$P^0 = \sum_i P_i l_i \ , \tag{17}$$

where $l_i$ equals 1 or 0 according to whether walk $i$ returns or does not return to the origin, respectively. $P^0$ is expected to scale with exponent $\gamma$,

$$P^0 \sim N^{\gamma} \ . \tag{18}$$

### B. The scanning procedure

Let us construct a walk of $N$ steps, which starts from the origin of the coordinate system. The first step is determined in one of the $q$ directions with equal probability $1/q$. In the next steps of the process ($k>1$) the probability to select a direction $\nu$ ($\nu=1,2,\ldots,q$) becomes a function of step $k$ in the following way. Assume that we are at the $k$th step of the process, i.e., $k-1$ directions of the walk, $\nu_1,\nu_2,\ldots,\nu_{k-1}$, have already been determined and we want to specify $\nu_k$. For that let us first introduce the notion of a future walk of $b$ steps. This is a continuation of the partial walk in the future, consisting of $b$ steps (i.e., $k,k+1,\ldots,k+b-1$) [more strictly, the number of steps of a future walk is $\min(b,N-k+1)$]. It should be pointed out that each direction $\nu$ ($\nu=1,q$) at step $k$ constitutes an origin of $q^{b-1}$ different future walks $j$, that visit (together with $\nu$) $m_j$ new distinct sites. One can therefore define a future partition function $Z_k(\nu,b)$, where

$$Z_k(\nu,b)=\sum_{j=1}^{q^{b-1}}\exp(-Km_j) \tag{19}$$

and thereby define a transition probability $p_k(\nu,b)$ for selecting a direction $\nu$,

$$p_k(\nu,b)=Z_k(\nu,b)\Big/\sum_{\nu=1}^{q}Z_k(\nu,b)\ . \tag{20}$$

Obviously $Z_k(\nu,b)$, as well as $p_k(\nu,b)$, depends on $\nu_1,\nu_2,\ldots\nu_{k-1}$ and on the interaction parameter $p=\exp(-K)$. $\nu_k$ is selected by a lottery according to the $p_k$'s and the process continues. Once a walk $i$ of $N$ steps has been constructed, one knows its construction probability $P_i(b)$,

$$P_i(b)=q^{-1}\prod_{k=2}^{N}p_k(\nu_k,b)\ , \tag{21}$$

which is the product of the $N$ sequential transition probabilities with which the directions $\nu_1,\nu_2,\ldots,\nu_N$ have been chosen. It should be pointed out that for practical values of $b$ ($b\ll N$) $P_i(b)$ [Eq. (21)] always approximates the exact probability $P_i$ [Eq. (2)] and one can show that it gives preference (as compared to $P_i$) to the noncompact (open) walks. This bias however, can systematically be reduced by increasing $b$ and in fact for $b=N-k+1$ (which means that the *whole* future is taken into account at each step $k$), $P_i(b)$ becomes equal to $P_i$ (see Ref. 3). However, increasing $b$ is not practical and therefore we shall introduce now a "mean-field" parameter, which improves $P_i(b)$ almost without further expenditure of computer time.

### C. The mean-field parameter

One can incorporate a mean-field parameter $m$ in the transition probability [Eq. (20)] in the following way:[3]

$$p_k(\nu,b,m)=Z_k(\nu,b)m^{-\bar{\nu}\cdot\bar{x}}\Big/\sum_{\nu}Z_k(\nu,b)m^{-\bar{\nu}\cdot\bar{x}}\ . \tag{22}$$

In this equation $\bar{\nu}$ is a unit vector in direction $\nu$ and $\bar{x}$ [$=\bar{x}(k)$] is a unit vector, which points from the center of mass of the partial walk (of $k-1$ steps) towards step $k-1$. Clearly, a direction $\nu$, which points towards the outer (inner) part of the walk will generally lead to $\bar{\nu}\cdot\bar{x}>0$ ($<0$), which means that for $m>1$ $p_k(\nu,b,m)$ will be smaller (larger) than $p_k(\nu,b)$ [Eq. (20)]. Therefore, the preference given by $P_i(b)$ to the open walks (mentioned in Sec. II B) weakens in $P_i(b,m)$ for $m>1$, where

$$P_i(b,m)=q^{-1}\prod_{k=2}^{N}p_k(\nu_k,b,m)\ . \tag{23}$$

In other words, with the mean-field parameter the effect of the remote steps from site $k$ (in space) is taken into account *approximately*, in addition to the effect of the local environment of step $k$, which is taken into account *exactly* by the scanning procedure. The effect of $m>1$ is to close the walk, i.e., to decrease its end-to-end distance and the radius of gyration. We shall now describe criteria for determining $m^*$, the optimal value of $m$. For that let us define the free-energy functional $\langle F\rangle_{b,m}$,

$$\langle F\rangle_{b,m}=K\langle M\rangle_{b,m}-\langle S\rangle_{b,m}\ , \tag{24}$$

where $\langle M\rangle_{b,m}$, the average number of distinct sites visited, and the entropy functional $\langle S\rangle_{b,m}$ are

$$\langle M\rangle_{b,m}=\sum_i P_i(b,m)M_i\ , \tag{25}$$

$$\langle S\rangle_{b,m}=-\sum_i P_i(b,m)\ln P_i(b,m)\ . \tag{26}$$

Obviously, $\langle F\rangle_{b,m}$ is never smaller than the true free energy $\langle F\rangle$ [Eq. (9)] but can be minimized with respect to $m$, at $m=m^*$, to give the best approximation for $\langle F\rangle$. $m^*$ can also be defined by the criterion of minimum fluctuation $\Delta F(b,m)$,[18] where

$$\Delta F(b,m)=\left[\sum_i P_i(b,m)[\langle F\rangle_{b,m}-(KM_i+\ln P_i(b,m)]^2\right]^{1/2}\ . \tag{27}$$

This fluctuation, which vanishes for the true free energy [Eq. (9)], is expected to decrease with improving $P_i(b,m)$.[18]

It should be emphasized that, since for a practical value of $b$ $P_i(b,m)$ is always approximate, any statistical average $\langle V\rangle_{b,m}$,

$$\langle V\rangle_{b,m}=\sum_i P_i(b,m)V_i\ , \tag{28}$$

of a random variable $V_i$ will always be *biased*. $\langle V\rangle_{b,m}$ can be estimated by $\bar{V}(b,m)$ from a sample of $n$ walks, generated with $P_i(b,m)$

$$\bar{V}(b,m)=n^{-1}\sum_{t=1}^{n}V_{i(t)}\ , \tag{29}$$

where $i(t)$ is walk $i$ obtained at time $t$ of the process. We shall describe now two methods for removing this bias, importance sampling[5,6] and a generalized Metropolis Monte Carlo procedure,[19] suggested by Schmidt,[7] which enables one to extract an unbiased sample from a biased one.

### D. Importance sampling

The *exact* statistical average $\langle V\rangle$ of $V_i$ can be expressed as a ratio of two statistical averages with the probability $P_i(b,m)$ [Eq. (23)],

$$\langle V\rangle=\sum_i P_i V_i=\sum_i \exp(-KM_i)V_i \Big/ \sum_i \exp(-KM_i)$$
$$=\sum_i P_i(b,m)[\exp(-KM_i)V_i P_i^{-1}(b,m)] \Big/ \sum_i P_i(b,m)[\exp(-KM_i)P_i^{-1}(b,m)] \ . \quad (30)$$

The expressions in the brackets can be considered as random variables and therefore an estimation $\bar{V}_{\rm IS}$ of $V$ [where walks are selected with $P_i(b,m)$, see Eq. (28)] is

$$\bar{V}_{\rm IS}=\sum_{t=1}^{n} \exp(-KM_{i(t)})V_{i(t)} \times P_{i(t)}^{-1}(b,m) \Big/ \sum_{t=1}^{n} \exp(-KM_{i(t)})P_{i(t)}^{-1}(b,m) \ , \quad (31)$$

where IS denotes importance sampling.

In particular, the free energy and the entropy are estimated by $\bar{F}_{\rm IS}$ and $\bar{S}_{\rm IS}$, respectively, where

$$\bar{F}_{\rm IS}=-\ln\left[n^{-1}\sum_{t=1}^{n} \exp(-KM_{i(t)})P_{i(t)}^{-1}(b,m)\right] , \quad (32)$$

$$\bar{S}_{\rm IS}=-\bar{F}_{\rm IS}+K\bar{M}_{\rm IS} \ . \quad (33)$$

Let us now discuss the efficiency of the importance sampling procedure. It should first be stressed that for an infinite sample, $\bar{V}_{\rm IS}$ [Eq. (31)] will be equal to $\langle V\rangle$ even for $b=1$ and $m=1$ (in contrast to $\bar{V}(b,m)$ [Eq. (29)], which is always biased). However, for a finite sample size $n$ the extent of convergence of $\bar{V}_{\rm IS}$ to $\langle V\rangle$ is determined by the standard deviations of the two averages defining $\langle V\rangle$ [Eq. (30)], which are functions of $N$, $b$, and $m$ via $P_i(b,m)$. As $b/N$ increases, $P_i(b,m^*)\to P_i$ and hence these standard deviations become smaller. In other words, in order to become a good estimation of $\langle V\rangle$, the sample generated with $P_i(b,m^*)$ should contain a sufficiently large number of the typical equilibrium walks (i.e., those which are most probable with the exact probability $P_i$ [Eq. (2)]). These walks, which are relatively improbable with $P_i(b,m^*)$, will dominate the summations defining $\bar{V}_{\rm IS}$ by their large factors $1/P_i(b,m^*)$ (see Ref. 21 and a discussion in Ref. 20).

It should be pointed out that the present procedure, with $b=1$ only and without employing a mean-field parameter, was suggested long ago by Rosenbluth and Rosenbluth [for self-avoiding walks (SAW's)].[21] Their method (with $b=1$) has been extended to self-interacting SAW's (Refs. 22–24) and to adsorption problems[25] by Mazur, McCrackin, and Guttman. These authors have also employed parameters (different from our mean-field parameter), however, they have not provided a criterion for optimizing their parameters.

To summarize, importance sampling, even though it guarantees convergence for infinite samples, does not provide a criterion for estimating the extent of convergence for a finite sample size $n$. This difficulty can partially be solved by the generalized Monte Carlo procedure suggested by Schmidt[7] that enables one to determine the number of walks in a biased sample which effectively contribute to the correct averages.

### E. Schmidt's generalized Monte Carlo procedure

Schmidt[7] has recently suggested an approximate simulation technique, based on renormalization-group ideas, in which he interprets the configurations produced as trial configurations in a generalized Metropolis Monte Carlo procedure.[6,19] This enables one to select from an originally biased sample a partial equivalent sample of *unbiased* configurations. Let us describe this procedure, as applied to the present model of self-attracting walks. Assume that walk $i$ has been obtained in the $n$th iteration of a Monte Carlo procedure. To determine a walk for the $(n+1)$st iteration a trial walk $j$ is first selected with probability $T_{ij}$. $j$ is accepted as the $(n+1)$st walk with probability $A_{ij}$; otherwise the current ($n$th) walk is kept for the $(n+1)$st walk. In the usual Monte Carlo procedure $T_{ij}$ is taken to be a symmetric matrix.[6] For a general stochastic matrix $T_{ij}$ Schmidt defines

$$A_{ij}=\min(1,\ T_{ji}P_j/T_{ij}P_i) \ , \quad (34)$$

where $P_i$ is the ensemble probability [Eq. (2)]. Obviously, this definition of $A_{ij}$ satisfies the detailed balance condition

$$T_{ji}A_{ji}P_j=T_{ij}A_{ij}P_i \ . \quad (35)$$

If $T_{ij}\equiv P_j$, then all the trial walks $j$ become independent of $i$ and are *always* accepted. Similarity, one can sample trial walks independently with an aproximate probability such as $P_i(b,m^*)$. In this case, however, the acceptance rate $\mathscr{R}$ is smaller than 1, where

$$\mathscr{R}=n_{\rm accepted}/n_{\rm total} \ , \quad (36)$$

where $n_{\rm accepted}$ is the numer of trial walks accepted and $n_{\rm total}$ is the total number of trial walks. Therefore, $\mathscr{R}$ is expected to constitute a measure of the extent of approximation of $P_i(b,m^*)$. As $P_i(b,m^*)\to P_i$, $\mathscr{R}$ is expected to increase. The sample of accepted walks (AW's) obtained by $n$ iterations of the generalized MC process is unbiased and therefore one can estimate $\langle V\rangle$ [see Eq. (30)] from this sample (denoted A) by $\bar{V}_{\rm A}$ [see Eq. (29)],

$$\bar{V}_{\rm A}=n^{-1}\sum_{t=1}^{n}{}' V_{i(t)} \ , \quad (37)$$

where $i(t)$ is walk $i$ defined for iteration $t$ and the prime denotes summation over the unbiased sample. $\bar{V}_{\rm A}$, in contrast to $\bar{V}(b,m)$ [Eq. (29)], is unbiased. It should be pointed out that, in contrast to importance sampling, with the generalized Monte Carlo procedure the entropy can be obtained only approximately, by estimating $\langle S\rangle_{\rm A}$, where

$$\langle S\rangle_{\rm A}=-\sum_i P_i \ln P_i(b,m^*) \ . \quad (38)$$

This is because the value of the exact probability $P_i$ [Eq. (2)] is unknown. The free energy $\langle F\rangle_{\rm A}$ is

$$\langle F\rangle_A = K\langle M\rangle_A - \langle S\rangle_A \ . \tag{39}$$

The entropy $\langle S\rangle_A$ is estimated by the $\bar{S}_A$,

$$\bar{S}_A = -\sum_{t=1}^{n}{}' \ln P_{i(t)}(b,m^*) \ . \tag{40}$$

$\langle S\rangle_A$ always overestimates the true entropy $\langle S\rangle$ [Eq. (4)]; this is proved rigorously in the theory section and in Refs. 24 and 25 of the following paper.[26]

Finally, it should be pointed out that we use the number of AW's, rather than the total number of walks in the biased sample, as an effective sample size for the importance sampling averages. This number enables one to estimate the statistical accuracy of the importance sampling results.

## III. RESULTS AND DISCUSSION

In order to compare our results to the series expansion results of Ref. 8, we study the model of self-attracting walks on square and simple cubic lattices at the percolation threshold values $p_c = 0.592\,77$ (Ref. 27) and 0.3117 (Ref. 28), respectively. We also present results for $\langle M\rangle$ and for the entropy $\langle S\rangle$ obtained at $p \neq p_c$ and $p < 1$. These results enable us to compare the efficiency of the scanning method to that of the simulation technique employed by Zumofen, Blumen, and Klafter[14–16] and by Fixman.[13] Biased samples of walks have been generated with the scanning method, using several values of the scanning parameter $b$. The bias has been removed in two ways, by importance sampling (see Sec. II D) and by defining unbiased samples of AW's using Schmidt's procedure (see Sec. II E). In order to obtain the critical exponents with sufficient accuracy it has been found necessary to generate samples which consist, at least, of $\sim 20\,000$ AW's. Such a relatively large sample size has restricted us to study walks of $N \leq 400$ steps on the square lattice at $p_c$. For $d=3$, however, the interactions are significantly stronger [since $p_c(d=3) < p_c(d=2)$] and hence the bias is stronger too; for that reason the walks studied at $p_c$ are relatively short, $N \leq 150$. In order to determine $m^*$, the optimal value of the mean-field parameter, we have first generated relatively small samples of walks for different values of $m$ and minimized $\langle F\rangle_{b,m}$ [Eq. (24)–(26)] with respect to $m$. We have found that the minimal values of $\langle F\rangle_{b,m}$ are obtained if for the first 17 steps $k$, $m$ is taken to be 1 and $m = m^*$ only for $k > 17$. (This stems from the fact that the global shape of a very short walk is not well defined.) It should be pointed out that the introduction of the mean-field parameter increases computer time by a factor of $\sim 1.8$ for $b=1$. However, this factor decreases sharply as $b$ increases, since most of the computer time is then spent on calculating the future walks.

In Table I results are presented for the free energy, its fluctuation, the entropy, and the acceptance rate obtained at $p_c$. We also provide the number of AW's in the sample and the average computer time $t$ required to generate 1000 AW's. Each result in the table is an average of results obtained for two samples, based on different random number sequences. For $d=2$ we employ $b=1$, 2, and 4 whereas for $d=3$ we utilize $b=1$, 2, and 3. The table reveals that $m^* \geq 1$ always, which means that the effect of $m^*$ is to decrease the values of $\langle M\rangle_{b,1}$, i.e., to form more-compact walks. The optimal mean-field parameter $m^*$ turns out to be more effective (i.e., larger) as the approximation worsens (i.e., $b/N$ decreases). For that reason the values of $m^*$ are also significantly larger for $d=3$ than for $d=2$ (see previous discussion in this section). For each $N$ the three results for the free energy $\langle F\rangle_{IS}$ [Eq. (32)] (for the different values of $b$), obtained by importance sampling, are equal, in most cases, within the statistical error. The same occurs with the results for the entropy $\langle S\rangle_{IS}$ [Eq. (33)]. This indicates that the estimation of $\langle F\rangle_{Is}$ and $\langle S\rangle_{IS}$ is statistically reliable. As expected, the results for $|\langle F\rangle_{b,m^*}|$ [Eq. (24)] are always smaller than those for $|\langle F\rangle_{IS}|$ (which we consider as the exact values) and they improve (i.e., increase) with increasing $b$. It should be pointed out that the deviation of the results for $\langle F\rangle_{b,m^*}$ from the (correct) values of $\langle F\rangle_{IS}$ is not larger than 1.6% for $d=2$ but 1.5–4.5% for $d=3$. This again reflects the fact that, for the values of $b$ studied, the results for $d=2$ are less biased then those for $d=3$. Another measure of this bias is the fluctuation $\Delta F(b,m^*)$ [Eq. (27)], which, as expected, decreases as $b$ increases and has significantly larger values for $d=3$ than for $d=2$. As is also expected (see Sec. II E), the results for $\langle S\rangle_A$ are always larger than the correct values of $\langle S\rangle_{IS}$, and they decrease with increasing $b$. For that reason the results for $|\langle F\rangle_A|$ always overestimate the correct values of $|\langle F\rangle_{IS}|$. The results for the acceptance rate $\mathscr{R}$ [Eq. (36)] increase as the approximation improves. The table reveals that, for $d=2$, $\mathscr{R}$ decreases from 0.636 for $N=50$ and $b=4$, to 0.008 for $N=400$ and $b=1$; as expected, for $d=3$ the corresponding values of $\mathscr{R}$ are smaller, decreasing from 0.345 (for $N=50$ and $b=3$) to 0.005 (for $N=150$ and $b=1$). The efficiency of the simulation can be measured by the average computer time $t$ required to generate 1000 AW's. The table shows that for $d=2$ and $N=50$, $t(b=2) \sim t(b=1)$; these simulations are significantly more efficient than those using $b=4$, where $t(b=4)/t(b=1) \sim 5$. As $N$ increases to 200 and 400, the ratio $t(b=1)/t(b=2)$ increases to 1.11 and 2 whereas $t(b=4)/t(b=1)$ decreases to 2.7 and 1.2, respectively. A similar behavior is observed for $d=3$. This means that to each value of $N$ there corresponds an optimal value $b^*$ which leads to the highest efficiency, i.e., to the shortest time $t$; $b^*$ increases as $N$ increases. It should be pointed out that a similar conclusion has also been drawn for the generation of self-avoiding walks, with the scanning method.[1–3] In order to compare between the scanning method and the Rosenbluth and Rosenbluth (RR) technique[21] we have simulated on the simple cubic lattice walks of $N=100$ steps using $b=1$ and $m=1$. The table reveals that the value for $|\langle F\rangle_{1,1}|$ is significantly lower than that obtained for $b=1$ and $m=m^*$ (1.169 versus 1.226, respectively) and the fluctuation $\Delta F(1,1)$ is 2 times larger than that obtained for $b=1$ and $m=m^*$. The acceptance rate for the RR simulation is 10 times lower than that obtained for $b=1$ and $m=m^*$, and $t(m=1)/t(m=m^*) \sim 8$. The RR technique is therefore significantly less efficient than the scanning method.

Let us discuss now the results for $F_{IS}$ and $S_{IS}$ in more detail. The table reveals that the results for $S_{IS}$ (which

TABLE I. Results for the free energy, the entropy, and the parameters of efficiency obtained for self-attracting walks on a square lattice ($d=2$) and a simple cubic lattice ($d=3$) at the percolation threshold $p_c$. $N$ is the number of steps, $b$ is the scanning parameter, and $m^*$ is the optimal mean-field parameter. $\langle\ \rangle_{\rm IS}$ and $\langle\ \rangle_{\rm A}$ denote averages obtained by importance sampling and from the unbiased samples defined by Schmidt's procedure (Ref. 7), respectively. Free energy is estimated by $\langle F\rangle_{b,m}$ [Eq. (24)], $\langle F\rangle_{\rm IS}$ [Eq. (32)], and $\langle F\rangle_{\rm A}$ [Eq. (39)]. $\Delta F(b,m)$ [Eq. (27)] is the fluctuation of $\langle F\rangle_{b,m}$; its results are rounded off to three significant figures. All these results are expresed in units of $Nk_BT$ where $k_B$ is the Boltzmann constant and $T$ is the absolute temperature. Entropy (expressed in units of $Nk_B$) is estimated by $\langle S\rangle_{\rm IS}$ [Eq. (33)] and $\langle S\rangle_{\rm A}$ [Eqs. (38) and (40)]. Acceptance rate is defined in Eq. (36). Statistical error is denoted by parentheses, e.g., 1.675(6)=1.675±0.006.

| $N$ | $b$ | $m^*$ | $-\langle F\rangle_{b,m^*}$ | $-\langle F\rangle_{\rm IS}$ | $-\langle F\rangle_{\rm A}$ | $10^6\times\Delta F(b,m^*)$ | $\langle S\rangle_{\rm IS}$ | $\langle S\rangle_{\rm A}$ | Acceptance rate $\mathscr{R}$ | $t(s)$ (1000 AW's) | No. of AW's in sample |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | $d=2$ | | | | | |
| 50 | 1 | 1.25 | 1.144 46(9) | 1.154 89(6) | 1.165 05(7) | 436 | 1.133 93(1) | 1.349 5(2) | 0.472(2) | 12 | 56 400 |
| | 2 | 1.15 | 1.147 93(3) | 1.154 89(6) | 1.161 6(1) | 288 | 1.339 24(6) | 1.345 8(2) | 0.558(2) | 13 | 62 720 |
| | 4 | 1.0 | 1.150 33(1) | 1.154 86(4) | 1.159 17(6) | 188 | 1.339 0(2) | 1.343 3(2) | 0.636(2) | 60 | 81 920 |
| 200 | 1 | 1.35 | 1.225 89(1) | 1.242 92(5) | 1.255 6(3) | 238 | 1.340 5(2) | 1.353 1(1) | 0.093(3) | 390 | 11 400 |
| | 2 | 1.25 | 1.229 79(1) | 1.243 05(2) | 1.253 8(1) | 167 | 1.340 6(2) | 1.351 3(2) | 0.125(1) | 350 | 45 360 |
| | 4 | 1.15 | 1.232 82(1) | 1.243 05(6) | 1.251 6(1) | 123 | 1.340 5(2) | 1.348 9(1) | 0.173(1) | 1075 | 54 400 |
| 400 | 1 | 1.35 | 1.256 76(2) | 1.277 0(4) | 1.293(1) | 142 | 1.346(2) | 1.362(2) | 0.008(1) | 7315 | 2300 |
| | 2 | 1.25 | 1.261 11(2) | 1.276 89(8) | 1.288 8(2) | 110 | 1.347 5(4) | 1.359(1) | 0.020(1) | 3650 | 16 000 |
| | 4 | 1.15 | 1.264 76(3) | 1.277 01(7) | 1.286 9(2) | 85 | 1.347 7(7) | 1.357 6(5) | 0.040(1) | 8830 | 8060 |
| | | | | | | $d=3$ | | | | | |
| 50 | 1 | 1.7 | 1.134 01(7) | 1.174 3(1) | 1.211 8(3) | 1700 | 1.584 8(4) | 1.621 7(4) | 0.162(3) | 49 | 30 900 |
| | 2 | 1.25 | 1.147 79(7) | 1.174 52(5) | 1.199 5(2) | 1090 | 1.584 5(2) | 1.609 5(4) | 0.253(1) | 53 | 60 000 |
| | 3 | 1.15 | 1.156 52(7) | 1.174 43(5) | 1.191 8(3) | 730 | 1.585 0(2) | 1.602 4(3) | 0.345(2) | 134 | 43 500 |
| 100 | 1 | 1.0 | 1.169 36(2) | 1.277 8(6) | 1.341(3) | 2495 | 1.583(2) | 1.650(2) | 0.004(1) | 5600 | 1030 |
| | 1 | 1.8 | 1.225 63(1) | 1.278 4(4) | 1.320(2) | 1280 | 1.585(1) | 1.627(2) | 0.029(1) | 720 | 25 100 |
| | 2 | 1.4 | 1.235 38(2) | 1.278 9(3) | 1.314(1) | 1030 | 1.586 1(4) | 1.622(3) | 0.048(2) | 670 | 28 800 |
| | 3 | 1.25 | 1.246 40(1) | 1.279 0(1) | 1.306(1) | 770 | 1.586 7(7) | 1.613 5(6) | 0.086(2) | 1160 | 20 000 |
| 150 | 1 | 1.9 | 1.276 97(2) | 1.337(4) | 1.39(2) | 1020 | 1.594(4) | 1.64(2) | 0.005(2) | 7500 | 26 000 |
| | 2 | 1.4 | 1.284 73(1) | 1.335 54(2) | 1.372(2) | 920 | 1.594(3) | 1.632(2) | 0.011(2) | 4880 | 12 100 |
| | 3 | 1.25 | 1.295 84(1) | 1.336 1(4) | 1.368(2) | 730 | 1.596(2) | 1.627 0(1) | 0.022(1) | 7160 | 7600 |

TABLE II. Results for geometrical properties of self-attracting walks obtained at the percolation threshold $p_c$. $\langle\ \rangle_{IS}$, $\langle\ \rangle_A$, $N$, $d$, and the statistical error are defined in the caption of Table I. $\langle M\rangle$ and $\langle M^2\rangle$ are the first and second moments of the number of distinct sites visited, respectively [Eq. (5)]. $\langle \Delta^2 M\rangle$ is the fluctuation of $M$ [Eq. (6)]. $\langle G^2\rangle$ and $\langle G^4\rangle$ are the second and fourth moments of the radius of gyration, respectively [Eqs. (13)–(15)]. $\langle R^2\rangle$ and $\langle R^4\rangle$ are the second and fourth moments of the end-to-end distance, respectively [Eq. (11)] and $P^0$ is the probability for a walk to return to the origin [Eq. (17)].

| $N$ | $\langle M\rangle_{IS}$ | $\langle M\rangle_A$ | $\langle M^2\rangle_{IS}/N$ | $\langle \Delta^2 M\rangle_{IS}$ | $\langle \Delta^2 M\rangle_A$ | $\langle G^2\rangle_{IS}/N$ | $\langle G^4\rangle_{IS}/N$ | $\langle R^2\rangle_{IS}/N$ | $\langle R^4\rangle_{IS}/N^2$ | $P^0_{IS}$ | $P^0_A$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | $d=2$ | | | | | | |
| 50 | 17.623(7) | 17.66(4) | 6.462(5) | 12.49(3) | 12.48(3) | 0.057 29(3) | 0.214 9(4) | 0.245 9(5) | 0.148 0(5) | 0.068 0(7) | 0.068 3(7) |
| 100 | 25.791(3) | 25.81(2) | 6.865(9) | 21.6(2) | 21.1(2) | 0.034 98(5) | 0.144 6(4) | 0.1372(3) | 0.0439(3) | 0.0542(5) | 0.0533(7) |
| 150 | 31.990(9) | 31.99(3) | 7.002(3) | 26.9(2) | 26.9(2) | 0.026 19(2) | 0.114 6(5) | 0.096 8(5) | 0.208(2) | 0.047 8(4) | 0.048 3(8) |
| 200 | 37.28(3) | 37.27(4) | 7.11(1) | 31.51(8) | 31.4(3) | 0.021 9(3) | 0.100 5(4) | 0.077 3(4) | 0.012 87(8) | 0.044(2) | 0.044(2) |
| 400 | 54.03(6) | 54.07(4) | 7.43(1) | 50(3) | 50(3) | 0.013 95(3) | 0.081 3(7) | 0.050(3) | 0.005 2(6) | 0.035(5) | 0.034(3) |
| | | | | | $d=3$ | | | | | | |
| 50 | 17.594(8) | 17.596(7) | 6.374(6) | 9.17(2) | 9.15(4) | 0.031 19(3) | 0.055 0(2) | 0.114 2(3) | 0.026 7(3) | 0.074 3(9) | 0.076(2) |
| 70 | 21.38(2) | 21.38(3) | 6.69(1) | 11.36(5) | 11.41(7) | 0.023 13(4) | 0.040 3(1) | 0.081 4(5) | 0.012 8(2) | 0.068(3) | 0.069(3) |
| 100 | 26.35(4) | 26.34(3) | 7.08(2) | 14.0(2) | 13.8(2) | 0.017 17(3) | 0.030 8(1) | 0.057 8(4) | 0.006 16(9) | 0.060(2) | 0.060(3) |
| 150 | 33.4(2) | 33.4(2) | 7.53(7) | 18(1) | 18.3(4) | 0.012 41(6) | 0.023 6(3) | 0.042(2) | 0.003 1(2) | 0.053(8) | 0.055(6) |

are in units of $k_B N$) almost do not increase as $N$ increases; for $d=2$ and $N=400$ the value for $\langle S\rangle_{IS}$ is $\sim 1.348$ (ln 3.85), whereas for $d=3$ and $N=150$, $\langle S\rangle_{IS}\sim 1.600$ (ln 4.95). These results, however, are smaller (by 3% and 11%) than the corresponding DV asymptotic values [Eq. (10)], $\ln(2d)\sim 1.386$ (ln4) and 1.792 (ln6), a fact that can be accounted for on the basis of geometrical considerations. The entropy can crudely be calculated from the total number of $N$-step random walks, which are limited to $\langle M\rangle$ distinct sites; thus, each of the "surface" sites (in contrast to the "inner" ones) contributes less degrees of freedom to a random walk than the maximum value $2d$, yielding thereby lower results for the entropy. Obviously, as $N$, and hence $\langle M\rangle$, increases, the "surface to volume" ratio decreases and $\langle S\rangle_{IS}$ is therefore expected to approach the DV asymptotic value. For that reason $\langle S\rangle_{IS}$ is also expected to increase as $\langle M\rangle$ increases as a result of increasing the interaction parameter $p$. The fact that $\langle M\rangle$ is not an extensive variable requires that $F\to S$ as $N\to\infty$, which means that asymptotically $F$ is only a function of $d$. Stanley *et al.*, [8] however, have found a superuniversal behavior for $F$, i.e, that $\lambda(p_c)=\lim_{N\to\infty}(-\langle F\rangle/N)\sim\ln 3.4$ for all $d$ (Ref. 8 mistakenly gives the value of $\exp\lambda$). We argue that this discrepancy stems from the fact that they have been extrapolated series expansion data of too-short walks ($N\leq 16$), which behave significantly different than the longer ones. To show this we have simulated walks of $N=13$ steps, which have also been studied in Ref. 8 by series expansion. Our results for $N\langle F\rangle_{IS}$ are approximately equal to those appearing in Fig. 2(a) of Ref. 8; in particular, we obtain (as in Ref. 8) that $|\langle F(d=3)\rangle| < |\langle F(d=2)\rangle|$, in contrast to the result $|\langle F(d=3)\rangle| > |\langle F(d=2)\rangle|$ obtained for the longer walks in Table I. The results for the entropy per step are 1.35 and 1.63 for $d=2$ and 3, respectively, which are very close to the corresponding values obtained for the longer walks in Table I. However, the result for $\langle M\rangle/N$ (which vanishes for $N\to\infty$) is relatively large for $N=13$, $\langle M\rangle/N\sim 0.60$ for both $d=2$ and 3. This relatively large value of $\langle M\rangle/N$ for the shorter walks leads to the family of lines $\langle F(N)\rangle$ with the same slope [Fig. 2(a) of Ref. 8]. In fact, for $N=13$ the slopes can approximately be calculated from the expression $0.6K-\langle S\rangle/N$ which yields $\simeq 1$ and 0.93 for $d=2$ and 3, respectively. Obviously, for larger $N$, $\langle M\rangle/N$ decreases and $\langle F(N)\rangle$ changes its behavior.

In Table II results obtained at $p_c$ are presented for $\langle M\rangle$ [$l=1$ and 2 only, see Eq. (5)]; the fluctuation $\langle \Delta^2 M\rangle$ [Eq. (6)]; the radius of gyration $\langle G^l\rangle$ [$l=2$ and 4, Eqs. (13)–(15)]; the end-to-end distance $\langle R^l\rangle$ [$l=2$ and 4, see Eq. (11)]; and $P^0$, the probability of a walk to return to the origin [Eq. (17)]. The results are weighted averages of results obtained for six different samples: two samples, based on different random number sequences, for each of the three values of $b$. The weights have been determined according to the number of AW's obtained in each sample. Each quantity has been estimated by importance sampling and from the unbiased samples of AW's defined with the generalized Monte Carlo procedure (Sec. II E). However, these last results are presented in the table only for $\langle M\rangle$, $\langle \Delta^2 M\rangle$, and $P^0$. From this table, and other

data not presented, it turns out that the results obtained by the two methods are equal within the statistical error and the errors themselves are approximately the same. The results of Table II (and results for $\langle M^l \rangle$ using $l=3$ and 4, which do not appear in the table) are used to calculate the various critical exponents, summarized in Table III. It should first be pointed out that log-log plots of the results of $\langle M^l \rangle$ (Table II) versus $N$ have always yielded straight lines. For $d=2$ the results for $\alpha_2$–$\alpha_4$ [Eq. (7)] are equal, within the statistical error, to $\alpha_1=0.533(6)$, which is 6.6% above the DV result $\alpha=0.5$ (the statistical error is defined in the caption of Table I). For $d=3$ $\alpha_1=0.584(5)$, which is 2.7% below the DV value $\alpha=0.6$. However, in this case only $\alpha_2$ is equal to $\alpha_1$ whereas $\alpha_3$ and $\alpha_4$ are smaller. These results are significantly better than those found in Ref. 8, i.e., that $\langle M^l \rangle \sim N^{\alpha l}$ where $\alpha=0.6$ for all $d$. Stanley *et al.*[8] have also pointed out that the data for $\langle M \rangle$ at $p_c$ lie on essentially the same locus of points for all $d$. This is indeed satisfied approximately by our results for small values of $N$; however, for larger $N$ $\langle M(d=3) \rangle > \langle M(d=2) \rangle$ as one would expect. The statistical error for the values of $\beta$ [Eq. (8)] is significantly larger than that observed for $\alpha$. For $\alpha=2$ the value $\beta=0.66(4)$ is significantly larger than the DV value 0.5. However, for $d=3$ the result $\beta=0.61(6)$ is close to the DV value 0.6.

At $p_c$ we have also obtained results for several critical exponents, which have not been solved analytically. The exponents $\nu_R$ [Eq. (12)] and $\nu_G$ [Eq. (16)], for the end-to-end distance and the radius of gyration, respectively, are very close to zero, which means that the shape of the walk expands very slightly with increasing $N$. These results do not agree with the preliminary results of Ref. 8, which reports that the values of $R$ appear to saturate at a finite value. In this context it should be emphasized that in some cases the results for the longest walks have deviated from a straight log-log line (see Table III). These deviations, however, have always been found to be in the direction which would increase the values of $\nu_R$ and $\nu_G$. It should also be pointed out that for self-avoiding walks ($p=\infty$), as well as for a pure random walk ($p=1$), the values of $\nu$ for each $d$ have been found to satisfy $\nu_{2R}=\nu_{4R}=\nu_{2G}=\nu_{4G}$. Our results, however, do not satisfy this relation; in particular, for $d=2$ the values of $\nu_G$ are significantly larger than those for $\nu_R$. We have also estimated the exponent $\gamma$ [Eq. (18)] for $P^0$, the probability of a walk to return to the origin. We obtain $\gamma(d=2) \simeq (d=3) \simeq -\frac{1}{3}$, within a relatively large statistical error.

Simulations have been also performed at $p \neq p_c$ for relatively short walks ($N \leq 150$), and results for $\langle S \rangle_{IS}$ [Eq. (33)], $\langle M \rangle_{IS}$ [Eqs. (5) and (31)], and the exponent $\alpha$ ($=\alpha_1$) are presented in Table IV. However, these results, in contrast to those of Tables I and II, are based on a single sample and therefore the calculated statistical errors are expected to underestimate the correct ones. The results for the entropy have been calculated for $N=150$ and 100 for $d=2$ and 3, respectively. These results monotonically approach (from below) the corresponding DV values [$\ln(2d)$], $\sim 1.386$ and 1.792, as $p$ increases. For $p=0.8$, for example, the deviation is relatively small, only 2.2% and 0.3% for $d=2$ and 3, respectively. Obviously, this behavior is a consequence of the monotonic increase of $\langle M \rangle$ as the attraction between steps weakens for $p \to 1$ (see preceding discussion). An opposite trend is observed for the results of $\alpha$, which approach the DV values as $p$ is decreased. For $d=2$ the deviation of our results from $\alpha=0.5$ increases from 2.8% for $p=0.4$ to 48% for $p=0.9$. For $d=3$ and $p=0.2$–$0.4$ the results for $\alpha$ are slightly smaller than 0.6 (by 2.2% for $p=0.4$), becoming significantly greater than 0.6 for $p=0.8$ (deviation of 43%). This behavior is in accord with numerical studies of random walks on lattices with randomly distributed static traps, which have found that as the density of traps $(1-p)$ decreases, longer walks are required in order to reach the DV regime.[14–17] It should be pointed out, however, that this need to generate longer walks is compensated, to some extent, by the fact that the bias vanishes for $p \to 1$, which means that smaller samples would be required with the scanning method. Indeed we have found that larger values of $p$ have always led to larger values of the acceptance rate $\mathcal{R}$ [Eq. (36)]. For example, for $d=3$, $N=100$ and $b=2$ we have obtained $\mathcal{R}=0.048$ at $p_c \approx 0.31$, as compared to $\mathcal{R}=0.71$ at $p=0.8$.

Let us compare now our results to results obtained for the trapping problem with other numerical techniques.[11,13–17] Zumofen, Blumen, and Klafter[14–16] have studied this problem using a direct (MC) technique in which a sample of $N$-step random walks is initially generated on a lattice *without* traps; the effect of traps is taken into account in the calculation of the averages by multiplying each term by $p^{M_i}$ ($1-p$ is the trap concentration). This method is expected to become inefficient for large $N$ since the typical size $\langle M \rangle$ of a random walk on a lattice without traps grows as $\sim N/\ln N$ and $N$ for $d=2$ and 3, respectively,[29] whereas self-interacting walks are significantly more compact since $\langle M \rangle \sim N^{d/(d+2)}$. Therefore, in the case of long walks one should simulate with the

TABLE III. Results for critical exponents of self-attracting walks at the percolation threshold $p_c$. $\alpha_l$, $l=1,4$ are the exponents of $\langle M^l \rangle$ [Eq. (7)]. $\beta$ is the exponent of $\langle \Delta^2 M \rangle$ [Eq. (8)]; $\nu_{lR}$ and $\nu_{lG}$, for $l=2$ and 4, are the exponents of the $l$ moments of the end-to-end distance [Eq. (12)] and the radius of gyration [Eq. (16)], respectively. $\gamma$ is the exponent of $P^0$, the probability for a walk to return to the origin [Eq. (18)]. $d$ and the statistical error are defined in the caption of Table I. The asterisk means that the result for the longest walk in Table II is not taken into account in the calculation of the exponent.

| $d$ | $\alpha_1$ | $\alpha_2$ | $\alpha_3$ | $\alpha_4$ | $\beta$ | $\nu_{2G}$ | $\nu_{4G}$ | $\nu_{2R}$ | $\nu_{4R}$ | $\gamma$ |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 0.533(6) | 0.530(8) | 0.527(8) | 0.523(8) | 0.66(4) | 0.145(5)* | 0.11(1)* | 0.080(5)* | 0.058(5)* | −0.32(3) |
| 3 | 0.584(5) | 0.58(1) | 0.570(7) | 0.565(8) | 0.61(6) | 0.08(1) | 0.040(3)* | 0.035(15) | 0.00(8) | −0.32(8) |

TABLE IV. Results for $\langle M \rangle_{IS}$ [Eq. (5)] and its exponent $\alpha$ [Eq. (7)], and the entropy $\langle S \rangle_{IS}$ [Eq. (33)] obtained for several values of the interaction parameter $p$. Values of $p_c$ are taken from Refs. 27 and 28. $N$, $d$, and the statistical error are defined in the caption of Table I.

| | | | $d=2$ | | | |
|---|---|---|---|---|---|---|
| $N$ | $p=0.4$ | $p=0.5$ | $p_c=0.59277$ | $p=0.7$ | $p=0.8$ | $p=0.9$ |
| 50 | 14.03(1) | 15.79(1) | | 20.041(5) | 22.587(5) | 25.248(1) |
| 100 | 20.03(1) | 22.81(1) | | 30.143(6) | 35.584(7) | 42.37(1) |
| 150 | 24.7(2) | 28.31(3) | | 37.74(1) | 45.55(2) | 56.753(1) |
| $\alpha$ | 0.514(4) | 0.531(2) | 0.533(6) | 0.579(1) | 0.642(1) | 0.739(1) |
| $\langle S \rangle_{IS}$ | 1.305 | 1.324 | 1.340 | 1.355 | 1.367 | 1.382 |
| | | | $d=3$ | | | |
| $N$ | $p=0.2$ | $p_c=0.3117$ | $p=0.4$ | $p=0.6$ | $p=0.8$ | |
| 50 | 14.34(3) | | 20.250(3) | 27.153(1) | 33.439(2) | |
| 70 | 17.33(8) | | 24.75(1) | 34.313(3) | 44.754(4) | |
| 100 | 20.9(5) | | 30.40(2) | 43.001(8) | 60.92(2) | |
| $\alpha$ | 0.54(4) | 0.584(5) | 0.587(1) | 0.665(1) | 0.860(1) | |
| $\langle S \rangle_{IS}$ | 1.514 | 1.586 | 1.640 | 1.735 | 1.788 | |

direct MC technique extremely large samples, otherwise the values of $\alpha$ are expected to overestimate the correct ones. Obviously, this technique differs from the scanning method which, by taking into account the attraction between steps, gives a strong preference for generating the most probable compact walks. Also, with the scanning method the statistical accuracy can be estimated from the acceptance rate (see Sec. II) whereas no similar criterion is known to exist for the direct MC technique. For $d=2$ Klafter *et al.*[15] have studied walks of up to $N=10^4$ steps on the square lattice for several values of the trap concentration $(1-p)$ from 0.005 to 0.3. However, in spite of this relatively large $N$, the corresponding results for $\alpha$ (0.69—0.86) are significantly larger than the DV value 0.5; this has led them to the conclusion that the regime in which the DV value [Eq. (1)] becomes a good approximation is obtained for survival probability $\phi \leq 10^{-21}$, a value which is too small to be detected experimentally. However, our results show that this value is probably an underestimation: at $p=0.7$ Klafter *et al.*[15] have obtained $\alpha=0.69$, whereas we have obtained, already from very short walks ($N \leq 150$), a significantly lower estimate, $\alpha=0.573$. This suggests that the relatively large values of $\alpha$ obtained in Ref. 15 are, at least partially, a consequence of employing two-small samples and not only a result of studying insufficiently long walks. Indeed, Havlin *et al.*,[17] who have employed their own numerical techniques, have estimated, for both $d=2$ and 3, that the DV regime exists already for $\phi \leq 10^{-13}$. It should be pointed out, however, that this conclusion is based on calculations carried out only in the extreme regions of very low and very high trap concentration. They have also shown[17] that for both $d=2$ and 3, $\phi$ scales nicely as a function of $\rho=[\ln(p^{-1})]^{2/(2+d)}N^{d/(d+2)}$ for $\rho \geq 10$, which is in accord with the conclusion (see Refs. 15 and 16) that as $p$ increases longer walks are required in order to reach the DV regime. The direct MC technique[14–16] turns out to be relatively inefficient for $d=3$, where calculations of Zumofen and Blumen[14] did not show a significant deviation from exponential decay and those carried out by Fixman have led to the conclusion that the DV regime is obtained only for $\phi \leq 10^{-69}$.[30] On the other hand, our results for $\alpha$ in the range $p=0.2$—$0.6$ (Table IV) are already close to the DV value 0.60 for $N \leq 100$. This agrees with the scaling result of Havlin *et al.*,[17] which for $\rho \geq 10$ and $p=0.4$ yields $N \geq 115$. A similar agreement between our results and those of Ref. 17 is also found for $d=2$. This supports the conjecture of Havlin *et al.* that the condition $\rho \geq 10$ defines the DV regime for all values of $p$.

## IV. SUMMARY

In this work the scanning method has been applied, for the first time, to a chain model with finite interactions. We study self-attracting random walks[8] on a square and simple cubic lattices, which correspond to a model of random walks moving on a lattice, with randomly distributed static traps. The free energy of the self-attracting walks (which is related to the survival probability in the trapping problem) has been solved analytically for large $N$ by Donsker and Varadhan[9] and by others.[10–12] However, the question has been raised as to how long the walks should be (or how small $\phi$ should be) in order that the DV results become a good approximation (the DV regime). We study this problem by the scanning method.

The scanning method generates chains with a certain bias, which so far has been removed by importance sampling; in this paper we have also tested an alternative procedure, suggested by Schmidt,[7] which enables one to select from a biased sample an equivalent partial sample of *unbiased* walks. The acceptance rate $\mathcal{R}$ of the unbiased AW's is expected to constitute a measure of the bias and indeed it has been always found to increase (towards 1) as the bias has been decreased by increasing the scanning parameter $b$. Also, the averages obtained from the unbiased samples have been found to be equal, within the statistical error, to those obtained with importance sampling. However, with importance sampling, the entropy and hence the free energy can, in principle, be obtained *exactly* whereas from the unbiased samples they can be estimated

only with a certain approximation. We have found that to each value of chain length $N$ there corresponds an optimal value $b^*$ which leads to the highest efficiency; $b^*$ increases with increasing $N$. The Rosenbluth and Rosenbluth simulation procedure[21] (i.e, $b=1$ and $m=1$) turns out to be significantly less efficient than the scanning method.

At the percolation threshold $p_c$ our results for $\alpha$ deviate by $\sim 6\%$ from the DV asymptotic values. The probability for a walk to return to the origin leads to the exponent $\gamma \simeq -\frac{1}{3}$ for $d=2$ and 3 and the exponents for the end-to-end distance and the radius of gyration are very small, but still larger than zero for both $d=2$ and 3; these three quantities have not been studied by other techniques.

Calculations at $p \neq p_c$ for relatively short walks show that the entropy approaches the DV value $\ln(2d)$ (from below) as the interaction parameter $p$ increases. The values of $\alpha$, on the other hand, increase monotonically to 1 as $p \to 1$, which means that longer walks should be studied in order to reach the DV regime. Our results are closer to the DV values than results obtained by Klafter *et al.*,[15] which suggests that the scanning method is more efficient than their direct Monte Carlo technique. Our calculations support the conclusion of Havlin *et al.*[17] that the DV regime is reached for survival probability $\phi \leq 10^{-13}$, for both $d=2$ and 3.

## ACKNOWLEDGMENT

I thank Dr. J. Klafter for helpful discussions.

[1]H. Meirovitch, J. Phys. A **15**, L735 (1982).
[2]H. Meirovitch, J. Chem. Phys. **79**, 502 (1983); **81**, 1053 (1984).
[3]H. Meirovitch, Macromolecules **18**, 563 (1985).
[4]H. C. Öttinger, Macromolecules **18**, 93 (1985); **18**, 1348 (1985).
[5]H. Kahn, in *Symposium on Monte-Carlo Methods,* edited by H. A. Meyer (Wiley, New York, 1956), p. 146.
[6]J. M. Hammersley and D. C. Handscomb, *Monte Carlo Methods* (Methuen, London, 1964).
[7]K. E. Schmidt, Phys. Rev. Lett. **51**, 2175 (1983).
[8]H. E. Stanley, K. Kang, S. Redner, and R. L. Blumberg, Phys. Rev. Lett. **51**, 1223 (1983); **54**, 1209 (1985).
[9]M. D. Donsker and S. R. S. Varadhan, Commun. Pure Appl. Math. **28**, 525 (1975); **32**, 721 (1979).
[10]B. Ya. Balagurov and V. G. Vaks, Zh. Eksp. Teor. Fiz. **65**, 1939 (1973) [Sov. Phys.—JETP **38**, 968 (1974)].
[11]P. Grassberger and I. Procaccia, J. Chem. Phys. **77**, 6281 (1982); R. F. Kayser and J. B. Hubbard, Phys. Rev. Lett. **51**, 79 (1983).
[12]B. Movaghar, G. Sauer, D. Würtz, and D. L. Huber, Solid State Commun. **39**, 1179 (1981); J. Stat. Phys. **27**, 473 (1982); S. Redner and K. Kang, Phys. Rev. Lett. **51**, 1972 (1983); D. Y. C. Chan and B. D. Hughes, J. Phys. A **17**, L121 (1984).
[13]M. Fixman, Phys. Rev. Lett. **52**, 791 (1984); J. Chem. Phys. **81**, 3666 (1984).
[14]G. Zumofen and A. Blumen, Chem. Phys. Lett. **83**, 372 (1981); **88**, 63 (1982).
[15]J. Klafter, G. Zumofen, and A. Blumen, J. Phys. (Paris) **45**, L49 (1984).
[16]G. Zumofen, A. Blumen, and J. Klafter, J. Phys. A **17**, L479 (1984).
[17]S. Havlin, M. Dishon, J. E. Kiefer, and G. H. Weiss, Phys. Rev. Lett. **53**, 407 (1984).
[18]H. Meirovitch and Z. Alexandrowicz, J. Stat. Phys. **15**, 123 (1976).
[19]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[20]F. L. McCrackin, J. Res. Natl. Bur. Stand. USA **3&4**, 193 (1972).
[21]M. N. Rosenbluth and A. W. Rosenbluth, J. Chem. Phys. **23**, 356 (1954).
[22]J. Mazur and F. L. McCrackin, J. Chem. Phys. **49**, 648 (1968).
[23]F. L. McCrackin, J. Mazur, and C. M. Guttman, Macromolecules **6**, 859 (1973).
[24]J. Mazur, C. M. Guttman, and F. L. McCrackin, Macromolecules **6**, 872 (1973).
[25]F. L. McCrackin, J. Chem. Phys. **47**, 1980 (1966).
[26]H. Meirovitch, following paper, Phys. Rev. A **32**, 3709 (1985).
[27]T. Gebele, J. Phys. A **17**, L51 (1984).
[28]D. W. Heermann and D. Stauffer, Z. Phys. B **44**, 339 (1981).
[29]E. W. Montroll and G. H. Weiss, J. Math. Phys. **6**, 167 (1965).
[30]It should be pointed out that Fixman's result has been obtained for spherical traps in a continuum. Much larger values are suggested by him for walks on a lattice.