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Survival Probabilities for Random-Walks on Lattices with Randomly Distributed Traps.

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Abstract: I present here a numerical procedure to compute survival probabilities for random walks on lattices with randomly distributed traps. The procedure has some advantages over existing methods, and its performance is evaluated for the 1D simple random walk, for which some exact results are known. Thereafter, I apply the procedure to 1D random walks with variable step length and to 3D simple random walks.

Key words: Lattice random walk; trapping; number of distinct lattice points visited; survival probabilities.

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1. Introduction.

Random walks on lattices with randomly distributed traps serve as models for many physical processes in which absorption and emission occur [1,2]. In spite of their conceptual clarity and simplicity, these models often defy exact mathematical analysis. Indeed, most of the existing exact results are limited to 1D random walks with transitions to nearest neighbours only.

Apparently, the stochastic nature of these models makes them well-suited to brute-force Monte Carlo simulations, but in this case useful studies take up an enormous amount of computer time. In fact, the probability that a random walker survives an n-step walk is a fast decreasing function of n, and to explore the large-n behaviour one must generate a huge amount of random walks and random trap configurations. Moreover, the lower the concentration of traps, the higher the probability that the random-walker is trapped at large n, therefore the scope of the method is rather limited.

The gap between exact results and brute-force simulations has been filled by several workers who have produced approximate results. Those studies concentrate mainly on two quantities: the number $\{S_n\}$ of distinct sites visited by a random walker in an n-step unrestricted walk, and the n-step survival probabilities $\{f_n\}$ in presence of traps.

Basically, the relevance of the S_n's comes from their relationship with the f_n's:

$$f_n = \langle (1-c)^{S_n} \rangle \quad . \qquad (1)$$

Here c is the concentration of traps and $\langle\ \rangle$ denotes the average over all n-step unrestricted walks (in formula (1) the average over all trap configurations has already been taken). In his original paper on luminescent emission in organic solids with traps [3] Rosenstock approximated (1) moving the average to the exponent:

$$f_n \approx (1-c)^{<S_n>} \quad . \qquad (2)$$

The Rosenstock approximation (2) has been shown to work reasonably well only for very small concentrations (see e.g. [4]).

It turns out that (2) is just the first of a series of approximations derived after truncation of the so-called "cumulant expansion" [2], where the "cumulants" are simply expressed in terms of the central moments of the distribution $P(S_n)$ of the S_n's. Only the first moment $<S_n>$ can be computed without too much trouble using the generating function formalism [5], and analytic results also exist for the second central moment. However, to compute the higher moments one must resort to Monte Carlo simulation of unrestricted walks. This is no longer a direct simulation of the trapping problem, hence it is free from the simulation time problems mentioned above. These expansions work quite well for short walks, but they all break-down badly for longer walks [2].

In addition, I wish to mention a wealth of asymptotic formulas, both for the S_n's [6] and for the f_n's [7,8,9]: these formulas set the goal for all numerical efforts (cfr. [8] and [10]).

In this paper I present a numerical approximation which is in some way similar to the cumulant expansion and to the work of Blumen and Zumofen [5], but which is much better behaved. In section 2 I describe the approximation, apply it to 1D simple random walk and compare the numerical results with the asymptotic formula of Anlauf [8]. In section 3 I give numerical results for the 1D random walk with transitions to nearest neighbours (NN) and next-nearest-neighbours (NNN) and for the 3D simple random walk.

2. The procedure.

Consider a simple random walker which has already taken n-1 steps on the lattice. Some of the lattice sites that can be reached at the next step have already been visited, while others may be new to the walker. Let p_n be the fraction of new sites. Then p_n is also the probability of visiting a new site at the n-th step, and cp_n is the probability of falling on a trap at the n-th step. Therefore the probability that this walker is still free after the n-th step is:

$$\tilde{f}_n = (1-cp_n)\,\tilde{f}_{n-1} \ . \qquad (3)$$

Thus

$$\tilde{f}_n = \prod_{k=0}^{n} (1-cp_k) \ , \qquad (4)$$

where it is assumed that the origin may also be a trap, and one defines $p_0 \equiv 1$. Then, taking the average over all walks

$$f_n = <\tilde{f}_n> = <\prod_{k=0}^{n} (1-cp_k) > \ . \qquad (5)$$

Equation (5) can also be written as a recurrence formula:

$$f_n = f_{n-1} - c<p_n\tilde{f}_{n-1}> \ . \qquad (6)$$

Notice also that $<p_n>$ *is* just the average *number* of new sites visited by the random walker at the n-th step, and therefore $<p_n> = \Delta_n$ in the usual notation of Montroll and Weiss (cfr. [11] and [1]).

Equation (5) or (6) shows that if one neglects correlations then

$$f_n \approx \prod_{k=0}^{n} (1-c\Delta_k) \ , \qquad (7)$$

or, equivalently,

$$f_n \approx (1-c\Delta_n)f_{n-1} = f_{n-1}-c\Delta_n f_{n-1} \ . \qquad (8)$$

Moreover, if $c \ll 1$, then

$$\log f_n \approx \sum_{k=0}^{n} \log(1 - c\Delta_k) \approx -c \sum_{k=0}^{n} \Delta_k = -c \langle S_n \rangle \approx \langle S_n \rangle \log(1-c) \ , \qquad (9)$$

and one recovers the Rosenstock approximation (2)[1].

Equation (7) or (8) is still only an approximate formula, but one can do better by including some of the missing correlation, namely applying the recurrence formula (3) twice, so that

$$\tilde{f}_n = (1-cp_n)(1-cp_{n-1})\,\tilde{f}_{n-2}$$

$$= \tilde{f}_{n-2} - c(p_n+p_{n-1})\tilde{f}_{n-2} + c^2 p_n p_{n-1}\tilde{f}_{n-2} \ . \qquad (10)$$

After averaging, if one still neglects the correlations between the p_n's and the f_n's, this gives

$$f_n \approx f_{n-2} - c(\Delta_n+\Delta_{n-1})f_{n-2} + c^2\langle p_n p_{n-1}\rangle f_{n-2}$$

$$= [\,1 - c(\Delta_n+\Delta_{n-1}) + c^2\langle p_n p_{n-1}\rangle\,]\, f_{n-2} \ . \qquad (11)$$

---

[1] It is also quite easy to see that (8) is an approximate lower bound for (6). In fact when p_n is large it is easy to find - on average - a trapping site, and f_{n-1} must be small, and conversely if p_n is small then f_{n-1} is large.

Therefore $\langle p_n \tilde{f}_{n-1}\rangle < \Delta_n f_{n-1}$ and then $f_n > (1-c\Delta_n)f_{n-1}$.

Though still approximate, (11) displays explicitly the correlation between the two last steps; moreover this correlation involves only probabilities that may be computed from unrestricted random walks. It is difficult to compute this correlation analytically, but it can be found by Monte Carlo simulation of unrestricted walks, just like the moments $\langle S_n^k \rangle$ required for the cumulant expansions. It must also be remarked that in order to compute (11) one needs two starting values for the survival probabilities:

$$f_0 = (1-c)$$
$$f_1 = (1-c)(1-c\Delta_1) \qquad (12)$$

(f_1 is exact, since for all random walks $p_1 = \Delta_1$).

It is now possible to proceed further, and include the correlations among the last three steps, and so on. Then one obtains recurrence formulas similar to (11). Three or more starting values are required, and they must be found by direct enumeration.

In what follows the procedure shall be denoted by PFP (probability factorization procedure), and the "j-th order" PFP is the approximation obtained by expanding the first j factors in expression (5). E.g. (11) is the second order approximation. The j-th order approximation requires j starting values.

To test PFP I used the asymptotically exact expression [8] for the survival probabilities of the 1D simple random walk

$$f_n = \frac{8}{\pi}\sqrt{\frac{2}{3\pi}}\; x^{3/2} \exp\left(\frac{-3x}{2}\right)\left\{1 + \frac{17}{18}\frac{1}{x} + \frac{205}{648}\frac{1}{x^2} - \frac{3115}{34992}\frac{1}{x^3} + O\left(\frac{1}{x^4}\right)\right\}$$

$$\text{with } x = [-\pi \log(1-c)]^{2/3}\; n^{1/3} . \qquad (14)$$

I computed the Δ_n's exactly, using a series inversion method similar to that used by Blumen and Zumofen [5], and the averages $\langle p_n p_{n-1} \cdots p_{n-j+1} \rangle$ with a Monte Carlo simulation of the unconstrained walks. The starting values for the survival probabilities are easily found from direct enumeration of short walks[2].

I have generated 10^5 1D unrestricted simple random walks, 1000 steps long. To choose the direction of each step I have used a Tausworthe-type random bit generator [12] with p=9689, q=4187, where p and q are the exponents in the (irreducible) polynomial associated with the random bit recurrence formula [13]. With such a generator one can safely simulate random walks less than 10^4 steps long, since linear relationships among bits appear only after p=9689 steps. Figure 1 some of the correlation terms $\langle p_n p_{n-1} \cdots p_{n-j+1} \rangle$ obtained from the Monte Carlo program and used by PFP. The same program was used to compute the averages $\langle S_n^k \rangle$ (up to k=4) needed for the cumulant expansion. The first 4 cumulant approximations of f_n are shown in figure 2, while the results of PFP up to 4th order are shown in figure 3.

---

[2] It turns out that for all simple random walks on D-dimensional cubic lattices the first four p_n's are constant

$$p_0 = \Delta_0 = 1, \qquad p_1 = \Delta_1 = 1, \qquad p_2 = \Delta_2 = \frac{2D-1}{2D}, \quad p_3 = \Delta_3 = \frac{2D-1}{2D},$$

and therefore for these walks the calculation of the first five f_n's is trivial

$$f_0 = \tilde{f}_0 = 1-c, \qquad f_1 = \tilde{f}_1 = (1-c)^2,$$

$$f_2 = \tilde{f}_2 = (1-c)^2 \left(1 - c\,\frac{2D-1}{2D}\right) \qquad f_3 = \tilde{f}_3 = (1-c)^2 \left(1 - c\,\frac{2D-1}{2D}\right)^2,$$

$$f_4 = \langle (1-cp_4)\tilde{f}_3 \rangle = \langle (1-cp_4) \rangle\, f_3 = (1-c\Delta_4)\, f_3 .$$

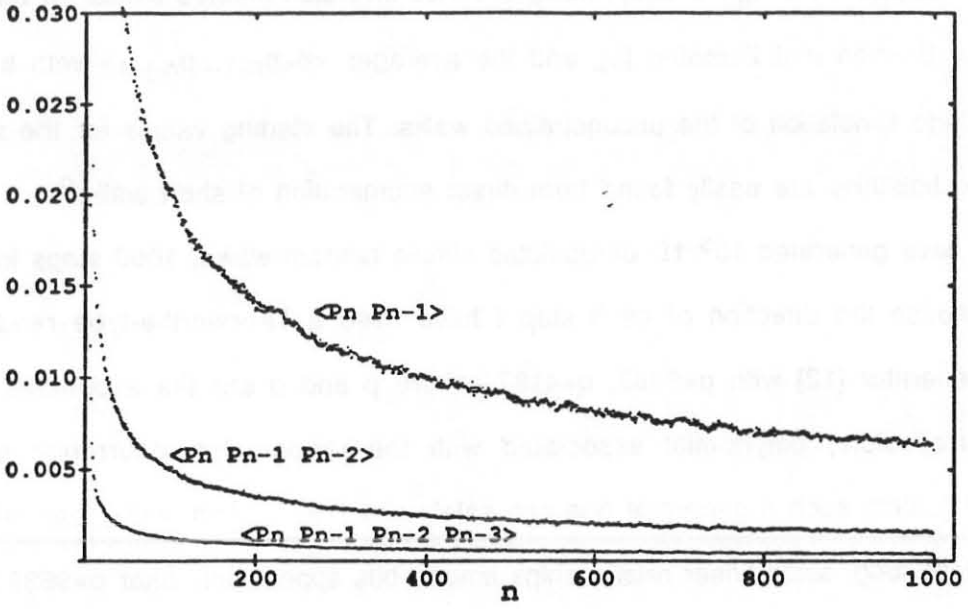

Figure 1: Some of the correlation terms from the Monte Carlo simulation of the unrestricted 1D simple random walk. $\langle P_n P_{n-1} \rangle$, $\langle P_n P_{n-1} P_{n-2} \rangle$ and $\langle P_n P_{n-1} P_{n-2} P_{n-3} \rangle$ appear respectively, as the top, middle and bottom data points.

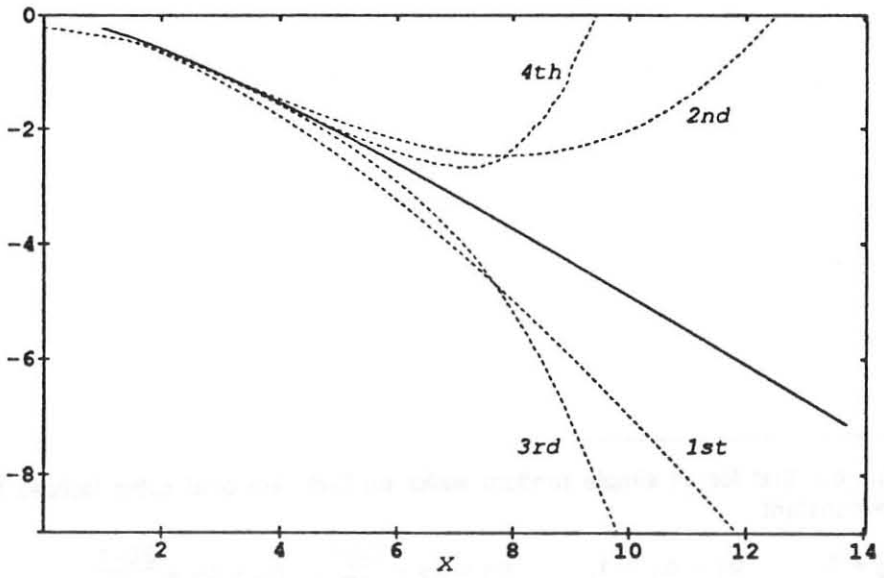

Figure 2: $\log_{10} f_n$ from the first four cumulant approximations for the 1D simple random walk. The solid line is the asymptotically exact expression (14) (for c=0.4), while the dashed lines show the first four cumulants. The data are plotted vs. the scaling variable x (see text). The irregularities in the fourth cumulant are due to the statistical fluctuations of Monte Carlo data. The first cumulant is the Rosenstock approximation.

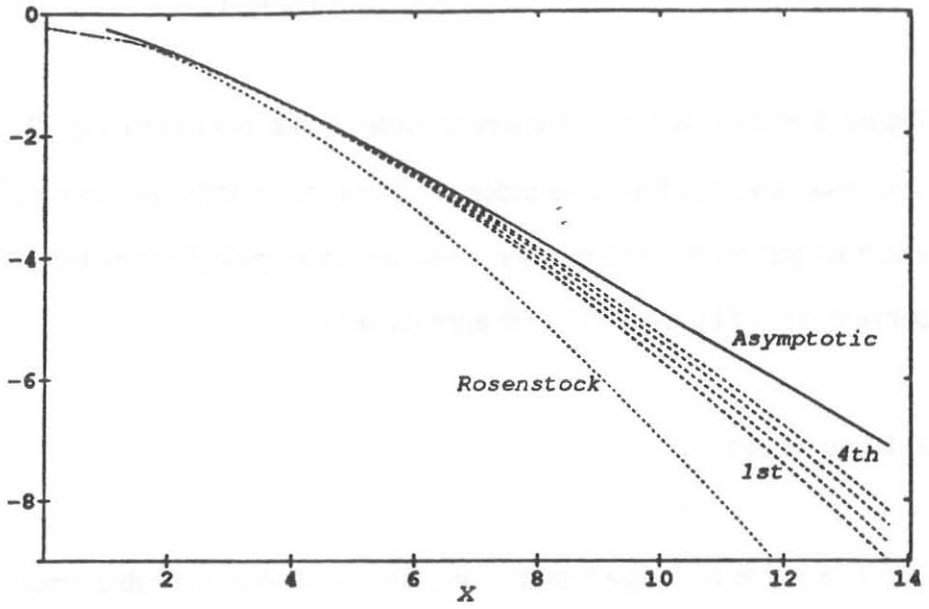

Figure 3: $\log_{10} f_n$ obtained from 1st to 4th order PFP for the 1D simple random walk (dashed lines). The solid line is the asymptotically exact expression (14) (for c=0.4). The data are plotted vs. the scaling variable x (see text). The Rosenstock approximation (dots) is also shown for comparison.

The computed values of f_n are plotted versus x, the scaled step number of (14): the advantage of using x instead of n is that the plots, at least asymptotically, do not depend on the concentration (for the record, I always used c=0.4 in these simulations).

PFP is free from the divergence problems of the cumulant expansion and seems to reproduce reasonably well the asymptotic behaviour (14), at least for step numbers that are not too large. For large step numbers the correlation terms approach constant values, so that the approximated survival probabilities eventually behave like simple exponentials.

The difference between the second and the first order approximations (expressions (11) and (7), denoted by $f_n^{(2)}$ and $f_n^{(1)}$) can be expressed by

$$\log f_n^{(2)} - \log f_n^{(1)} \approx c^2 \left(\langle p_n p_{n-1} \rangle - \Delta_n \Delta_{n-1} \right)$$

$$= c^2 \, \mathrm{Cov}(p_n p_{n-1}) \, . \qquad (17)$$

Figure 3 shows that with increasing order k the difference $\log f_n^{(k+1)} - \log f_n^{(k)}$ decreases and has the same order of magnitude as (17), therefore the asymptotic value of the covariance may be used as an empirical estimator of the rate of convergence of the series of PFP approximations.

3. Some results.

PFP is a rather fast algorithm: the only step that takes a sizable amount of time is the Monte Carlo program used to compute the averages $\langle p_n p_{n-1} \ldots p_{n-j+1} \rangle$. If n is the length of each random walk, N is the total number of walks generated and j is the order of the approximation, then the program takes a time proportional to $2^j N n^2$, and a memory space proportional to $2^j n$ for any lattice dimension (the run time is proportional to n^2 because at each step during the generation of the random walk one must scan the previous steps to count the number of free adjacent sites).

PFP is affected by two kinds of errors: statistical errors in the Monte Carlo used to compute the averages, and systematic errors intrinsic in the method. Statistical errors can be minimized by generating a large number of unrestricted random walks. The systematic errors can be reduced by going to higher orders and using the covariance (17) as a heuristic estimator of the accuracy of PFP.

I have applied PFP to symmetric 1D random walks with transitions to nearest-neighbours and next-nearest-neighbours, and to simple 3D random walks.

Take the 1D random walk first, and let p be the probability that the random walker steps to one of its nearest neighbours (NN) and q the probability of

stepping to one of the next-nearest-neighbours (NNN) (p+q=0.5). This walk becomes a simple random walk if p=0.5 or q=0.5.

I have generated 10^5 unrestricted walks, 100 steps long, for each of 21 uniformly spaced values of the parameter p

Figure 4 shows the "asymptotic" covariance - i.e. the covariance at n=100 - which estimates the rate of convergence of PFP. The covariance decreases for both low and high p's, indicating that the procedure is more reliable when the random walk approximates a 1D simple random walk.

Figure 5 shows $\log_{10}(f_{100})$ from third order PFP as function of the parameter p. Since q=0.5-p, it is easy to see that there is no symmetry between p and q.

Then I generated 10^5 unrestricted 3D simple random walks, 200 steps long. In this case there are no asymptotic formulas for the survival probabilities, so I used then a Monte Carlo procedure like that of Anlauf [4,8] to estimate the quality of PFP. The results of the simulation are shown in figure 6, together with the Rosenstock approximation, and the first and fourth order PFP. I wish to stress that the simple first order PFP seems to be much better than the Rosenstock approximation (cfr. [4]), even though the computational effort is exactly the same[3].

Unfortunately the simple exponential behaviour is reached quite early even by the 4th order approximation, and therefore it cannot be used to find the onset of the Donsker-Varadhan asymptotic regime having stretched exponential behaviour (cfr. [7] and [10]).

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[3] As a side remark, notice that by combining the 1st order approximation (7) with the fitting curve of Zumofen and Blumen [14]

$$\langle S_n \rangle \approx 0.662\, n + 0.525\, n^{1/2} + 0.501,$$

and recalling that $\Delta_n = \langle S_n \rangle - \langle S_{n-1} \rangle$, one obtains the approximation

$$\log f_n \approx \sum_{k=0}^{n} \log[1 - c(0.662 + 0.2625\, n^{-1/2})],$$

which turns out to be practically indistinguishable from the first order approximation shown in figure 6.

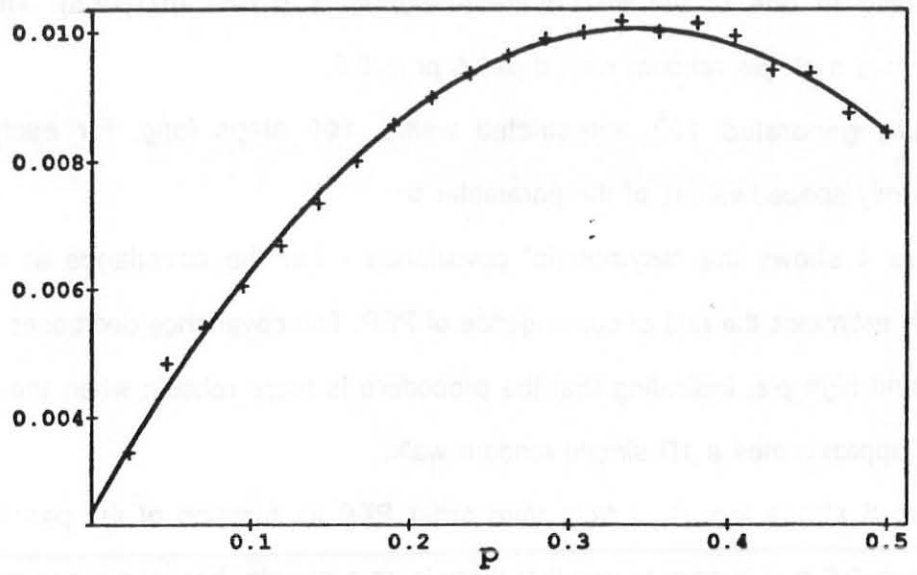

Figure 4: "Asymptotic" covariance $Cov(p_{100}p_{99})$ from the Monte Carlo data for the 1D random walk with NN and NNN transitions. The crosses show the covariance vs. p, and the solid curve is only meant to guide the eye.

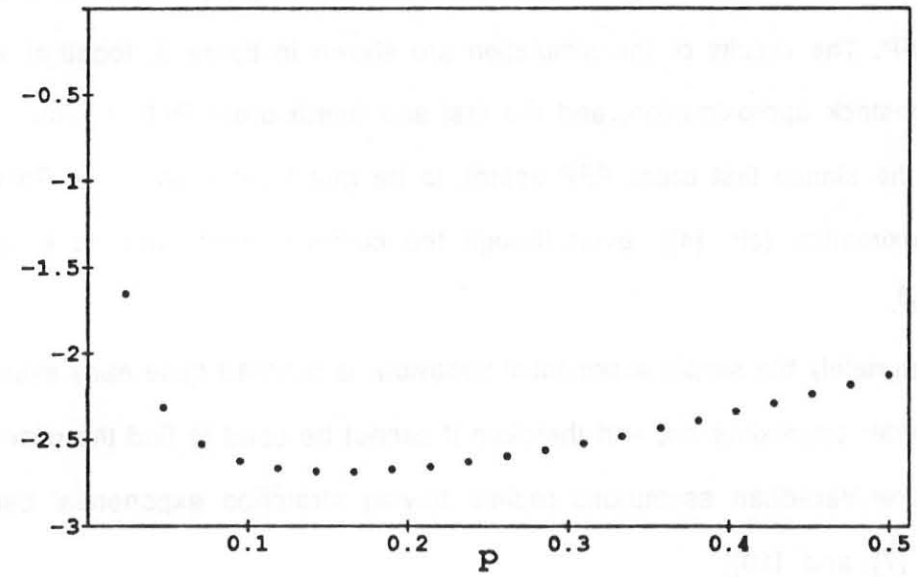

Figure 5: Plot of $\log_{10}(f_{100})$ vs. p for the 1D random walk with NN and NNN transitions obtained from the 3rd order PFP (for c=0.4).

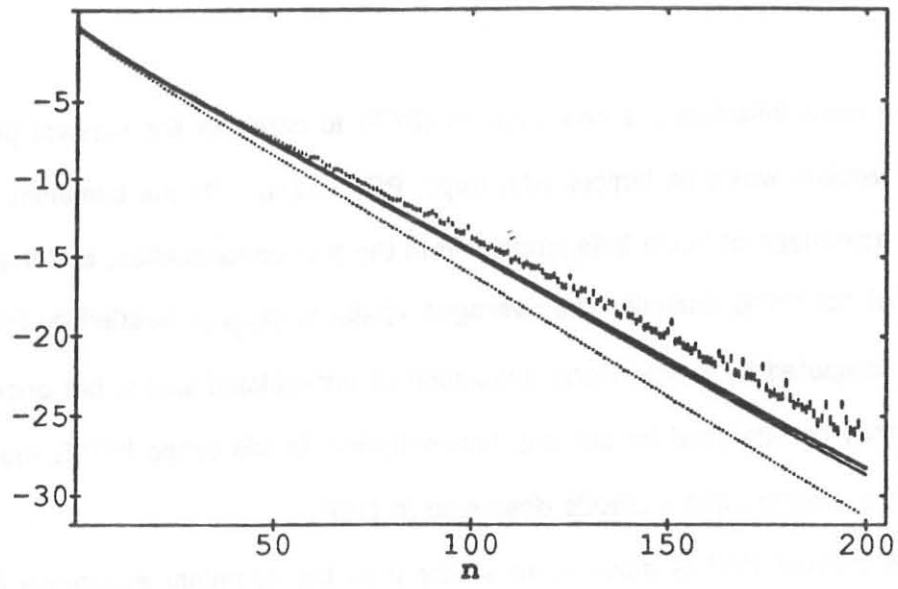

Figure 6: $\log_{10} f_n$ for the 3D simple random walk: the dots are the results of the Monte Carlo simulation "á la Anlauf" [8] with c=0.4, the dotted curve is the Rosenstock approximation, while the solid lines show the 1st (lower curve) and the 4th order (upper curve) PFP.

All the numerical calculations have been carried out on an Apple Macintosh IIfx and on a Digital VAX 900. The simulation of the 1D unrestricted random walks with transitions to NN and to NNN to compute the averages needed by the 3rd order PFP was one of the longest, and it took 40 minutes of CPU time on the VAX.

4. Conclusions

I have introduced a new method (PFP) to compute the survival probabilities for random walks on lattices with traps. PFP shares with the cumulant expansion the advantage of being independent from the trap concentration, and the disadvantage of not being analytic. The averages $\langle p_n p_{n-1} \cdots p_{n-j+1} \rangle$ needed by PFP have to be computed by Monte Carlo simulation of unrestricted walks, but once this is done they can be used for any trap concentration. In this sense PFP is much faster than the enumeration methods described in [10][4].

Moreover PFP is much more stable than the cumulant expansion (cfr. figures 2 and 3).

The PFP algorithm is easily adapted to widely different lattice topologies, neither run time nor memory space depend on the lattice dimensionality, and the 1st order approximation (7) is so simple and performs so much better than the Rosenstock approximation that it might replace it.

Just as it happens for the other methods, it is quite difficult to estimate the systematic error of the PFP approximation. However, it is possible to reduce this systematic error by going to higher order approximations, and to estimate empirically the rate of convergence of this series of approximations.

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[4] While these methods are actually much faster than brute-force Monte Carlo methods, they require a large amount of memory space. For a given trap concentration one can easily estimate the run time and the memory space to be proportional respectively to $n^D N_c$ and to n^D, where N_c is the number of simulated configurations with the given trap concentration, n is the length of the random walk and D is the lattice dimension.