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Chaos, pseudo-random number generators and the random walk problem

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Résumé. — Nous proposons un test expérimental de la nature du chaos engendré par l'itération de systèmes dynamiques discrets en développant des simulations de Monte-Carlo de marches aléatoires sur un réseau uni-dimensionnel périodique contenant un site absorbant. Nous considérons en particulier l'application logistique comme un générateur de nombres pseudo-aléatoires. La comparaison avec des résultats analytiques généralisés aux cas de marches asymétriques et de marches faiblement non markoviennes apporte de fortes évidences expérimentales de la validité de la conjecture selon laquelle la sensibilité sur les conditions initiales implique, pour l'application, l'existence d'une mesure invariante absolument continue par rapport à la mesure de Lebesgue.

Abstract. — To test the nature of the deterministic chaos generated by the iteration of discrete dynamical systems, we perform Monte-Carlo random walk experiments on a one-dimensional periodic lattice with a trapping site using the logistic map as a generator of pseudo-random numbers. Comparison with analytical results derived for asymmetric and also for weakly non-Markovian random walks lend strong experimental support to the conjecture that sensitive dependence on the initial conditions implies for the map the existence of an absolutely continuous invariant measure with respect to Lebesgue's measure.

1. Introduction.

Iterations of continuous maps of an interval onto itself provide the simplest examples of models for dynamical systems [1]. In spite of their structural simplicity, such models exhibit a variety of behaviours, including limit points, limit cycles and chaotic attractors. In the present work, we focus our attention on those regimes where the behaviour (although fully deterministic) appears as chaotic, i.e. shows profound similarities with the sample function of a random process.

From a mathematical point of view a random process involves random variables whose values cannot be predicted in advance. In other words, a realization of a given random variable is completely uncorrelated with previous and future realizations. This amounts to defining with J. N. Franklin [2] that a sequence (of numbers) is random if it has every property that is shared by all infinite sequences of independent samples of random variables. In this sense the random behaviour of a deterministic sequence is highly suspect. To justify this terminology, one must examine in what sense the generated numbers behave as if they were truly random. Since Franklin's statement can be shown to be impossible to fulfil in practice, one has to turn to a more pragmatic definition: « A random sequence is a vague notion embodying the

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idea of a sequence in which each term is unpredictable to the uninitiated and whose numbers pass a certain number of tests, traditional to statisticians and depending somewhat on the uses to which the sequence is to be put [2] ». A fundamental test is the existence of a limit probability density function ρ which, for iterative processes of the type

$$x_{n+1} = f(x_n) \tag{1.0}$$

where f is a scalar function, can be defined as the time average:

$$\rho(x) = \lim_{n \to \infty} \frac{1}{n} \sum_{k=1}^{n} \delta(x - f^{k}(x_{0}))$$
 (1.1)

with $\delta(x)$ the Dirac measure at x. Equation (1.1) defines what mathematicians call an invariant measure on the orbit of x_0 . If one starts from another number x'_0 , the measure defined by (1.1) is in general different. For a process defined by the iterative procedure (1.0) to be called random, one would further require that the measure be independent of the starting point, or in other words, be «absolutely continuous with respect to Lebesgue measure». However, the existence of such absolutely continuous measures has been proved only in a limited number of cases. No general theorem is available but a conjecture by Ruelle for general dynamical systems states that if a system possesses sensitive dependence on initial conditions (i.e. a system with positive Liapunov characteristic exponents), then invariant measure(s), when conditioned onto the unstable manifold(s), should be absolutely continuous [3] (1).

Now restriction to maps of the interval makes the problem easier because, when there is an unstable direction, then there is no space for a stable direction. When the map is everywhere expanding, the Liapunov characteristic exponent is clearly positive, and in this case the existence of an absolutely continuous invariant measure was shown [4, 5]. A map of the interval with a critical point is of course not uniformly expanding; however it was proved that there is an absolutely continuous invariant measure when the critical points have orbits which eventually land on unstable fixed points [6, 7]. This result holds for maps whose critical points have orbits that do not come close to the critical point [8, 9]. Very recently, it was shown that an absolutely continuous invariant measure exists when the Liapunov exponent is positive and the inverse of the map is contracting [10].

These rigorous results appear to converge and lend support to Ruelle's conjecture. However a dissonant claim [11] was recently presented on the basis of a numerical study of the logistic map of the interval [0, 1]:

$$x_{n+1} = f(x_n) = Rx_n(1 - x_n)$$
 (1.2)

Kozak, Musho and Hatlee [11] considered this map as a pseudo-random number generator and they used Monte-Carlo simulation to calculate the average walk length for trapping on a periodic one-dimensional lattice with a centrosymmetric trap. They arrived at the conclusion that comparison with exact results suggests that the only truly chaotic sequence is the one for R = 4.

This conclusion is obviously misleading since it has been proved that there exists infinity of R-values for which the logistic map possesses an absolutely continuous invariant measure. We argue that the failing of the random walk test comes from short-range correlation effects stemming from the deterministic character of the sequences of numbers generated by the iteration of (1.2). When these correlations are taken into account, either by introducing them in a reformulation of the theory, or by numerically removing them by using some iterate of f, we show that good agreement is obtained between the Monte-Carlo experiment and the exact theoretical results for all R's yielding sensitive dependence on the initial conditions. This indicates that with some caution the logistic map can be used as a good pseudo-random number generator. This conclusion recently announced in a short letter [12], lends experimental support to Ruelle's conjecture.

The paper is organized as follows. In section 2, we introduce the random-walk experiment as a test of pseudo-random number generators and discuss its relation with classical statistical tests. To implement the random walk test requires knowledge of exact analytical results. Recently, problems of solid state physics have stimulated either explicitly or implicitly a number of investigations on diffusion processes modelled by lattice random walks. The theory on infinite lattices was first discussed by Polya [13] who was especially concerned with the effect of dimensionality on the probability that a walker starting at a given point eventually returns to that point. Some other types of problems which are of special interest involve the average time required by a walker to go from a given lattice point to another preassigned point for the first time. Results on these topics as well as the effect of a small number of lattice defects on random walks have been discussed in a series of papers by Montroll and co-workers [14]. In section 3 we extend the analysis of Montroll [14] to anisotropic random walks and derive the average walk length of a walker starting from an arbitrary site on a periodic onedimensional lattice with a centro-symmetric trapping site. In section 4 we present the numerical results obtained from the Monte-Carlo random-walk experiment. Comparison with theory requires the estimate of the statistical error which is derived in the Appendix B.

⁽¹⁾ For a revised version on the problem of the measures describing Turbulence, see D. Ruelle, *Suppl. Prog. Theor. Phys.* **64** (1978) 339.

2. The Monte-Carlo random walk experiment as a « statistical test » of pseudo-random generators.

As outlined in the introduction, when confronted with an apparent « chaotic » sequence of numbers obtained by iterating (1.0), one has to invent procedures to test the nature of its randomness. Workers interested in Monte-Carlo computations i.e. using extensively pseudo-random number generators, have been aware of this problem for a long time. They have introduced several empirical tests some of which we will recall briefly [2]. One can roughly divide these tests into two categories. Those of the first one check that the generated numbers are distributed according to a welldefined probability distribution ρ (Kolmogorov-Smirnov and frequency tests) (see Fig. 1). Tests of the second category are devised to essentially detect correlations in the sequence of numbers. For example, the serial correlation test computes the usual correlation function C(j) defined by

$$C(j) = \frac{\sum_{i=1}^{n} x_i x_{i+j} - \frac{1}{n} \left(\sum_{i=1}^{n} x_i\right)^2}{\sum_{i=1}^{n} (x_i^2 - \langle x \rangle^2)}$$
(2.0)

where
$$\langle x \rangle = \frac{1}{n} \sum_{i=1}^{n} x_i$$
.

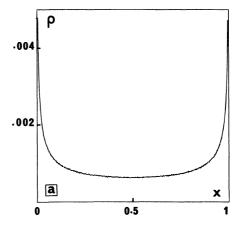
A small value of C(j) indicates that quantities x_i , x_{i+j} ... are roughly speaking independent of each other. Another example is the so-called run-test which examines the length of monotonic subsequences of the original sequence (i.e. segments which are increasing or decreasing) and compares the length distribution to that one should observe for a true random variable. Let us finally mention the test on subsequences: after extracting a subsequence (for example by taking one number out of every two numbers in the initial sequence) one can apply to it the set of tests mentioned above.

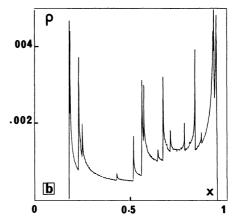
The need for many tests, when theorems on the generator are not available, stems from the fact that it has been reported that some pseudo-random sequences have passed some tests successfully and failed others.

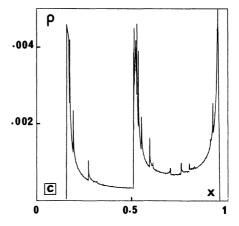
We now present a new statistical test, the random walk test introduced in a recent study on the chaotic orbits of the logistic map [11, 12].

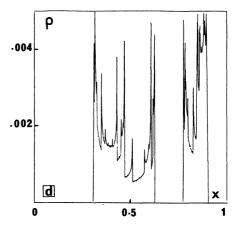
The underlying idea is that the most useful test to apply to a given pseudo-random sequence of numbers is just the calculation for which the pseudo-random numbers are needed and, if the correct answer to this problem is known theoretically, then it provides a

Fig. 1. — Probability density $\rho(x)$ obtained by plotting the \rightarrow histogram of 5×10^6 iterates of $x_0 = 0.4$ by equation (1.2), in 1 000 intervals [i/1 000, i + 1/1 000], i = 0, ..., 999. R = 4(a), 3.8(b), 3.8275(c), 3.62(d).









straightforward test of the generator. In this spirit, the random walk test uses the non-linear map (1.0) (for example (1.2)) as a random number generator for a Monte-Carlo random walk experiment on a one-dimensional periodic lattice (of period N) with a trapping site. The Monte-Carlo experiment is performed as follows: knowing the interval explored by the

successive iterates of (1.2), namely
$$\left[\frac{R^2}{4}\left(1-\frac{R}{4}\right), \frac{R}{4}\right]$$

we choose arbitrarily a cut-off separating this interval into two sub-intervals. One then makes the random walker step either to the right or to the left depending on which subinterval the iteration lies in. Counting the relative number of iterates which fall on the right, { left }, subinterval allows to define and experimentally measure the average probability p, $\{1-p\}$, for the walker to step to the right, { left }. Simulations are performed for \mathcal{N} (= 2000 to 800.000) walkers starting from each of the N-1 non-trapping lattice sites (N = 13). The numerical average $\langle n_T(s) \rangle_{exp}$ is obtained by calculating the walk length of each walker starting from a given site placed at s steps from the trap (counting clockwise) and averaging over the ${\mathcal N}$ walkers. Then by comparing this value to the analytically determined walk length $\langle n_T(s) \rangle_{th}$ of a walker, starting at s sites from the trap and moving to the right, { left }, with the probability $p \{ 1 - p \}$, one can assess the randomness of the sequence of numbers.

One can immediately see that this new test is a mixture of the « usual » statistical tests. In particular, the random walk experiment is very sensitive to non-Markovian effects as discussed extensively in § 4. Furthermore, we claim that the random walk test provides an efficient device for checking the existence for the pseudo-random generator, of an absolutely continuous measure with respect to the Lebesgue measure. When the map has sensitive dependence on initial conditions, a sequence of numbers x_i originating from a given seed x_0 will not follow the true orbit of x_0 since, at each iteration, a small but non-zero truncation error is made by the computer. For a given relative precision of about 10^{-16} , the *n*th number obtained by iterating the logistic map (1.2) will have lost completely the memory of its seed x_0 as soon as $n \gtrsim \log 10^{16}/\log 2 \sim 50$, where $\log 2$ is the upperbound of the Lyapunov characteristic exponent reached at R = 4 for which the map is surjective [1]. As a consequence, a sequence of numbers, generated by the iteration of (1.2), samples a different orbit roughly every 50 steps. Since the average random walk length is of the same order of magnitude (see tables I-IX), each walker will be directed by a different orbit. As a consequence, the comparison between the numerical experiment and analytical results provides a good test of the independence of the probability distribution (ρ -measure) on the choice of the seed x_0 .

Other relations between the random walk test and the usual statistical tests will be underlined in the presentation and discussion of the results in § 4.

3. Random walk with nearest neighbour transition on a 1-D periodic lattice.

To use the random-walk test requires knowledge of exact analytical results. The theoretical analysis of the symmetric case p = 1 - p = 1/2, has been investigated by Montroll [14] who proved in particular that the expected average walk length for a walker to be trapped starting from the site s is given by

$$\langle n_{\mathsf{T}}(s) \rangle_{\mathsf{th}} = s(N-s).$$
 (3.0)

However, it is important to realize that, in order to test the existence of an absolutely continuous invariant measure, investigations cannot be limited to the one particular cut-off yielding p=1-p=1/2 and must be extended to all values of p between 0 and 1. We derive in section § 3.1 the average walk length $\langle n_T(s) \rangle_{\text{th}}$ for arbitrary p. Furthermore, we give the expected walk length (§ 3b) for the special case of a weakly non-Markovian walker for which the memory effect extends over two steps: the probability at each step to go to the right or to the left becomes a conditional probability which depends on the preceding step. This result will be used in § 4 to discuss the short-range correlation effects inherent in the dynamics of deterministic processes.

3.1 Non-symmetric nearest-neighbour random walks. — We consider random walks on a N-periodic one-dimensional lattice where the walker jumps to nearest-neighbour lattice sites, with a probability p to go to the right and 1-p to go to the left.

Formally, the average walk length $\langle n(s) \rangle$ to reach the site $s_0 + s$ for the first time starting from the site s_0 is independent of s_0 and given by

$$\langle n(s) \rangle = \sum_{n=1}^{\infty} n F_n^{(N)}(s), \qquad (3.1)$$

where $F_n^{(N)}(s)$ is the probability that a random walker starting at the site s_0 reaches the site $s_0 + s$ for the first time at step n. We label the different sites counterclockwise.

One can relate $F_n^{(N)}(s)$ to the probability $P_n^{(N)}(s)$ of going from the starting site s_0 to the lattice site $s_0 + s$ after n steps through [14]

$$P_n^{(N)}(s) = \delta_{n,0} \cdot \delta_{s,0} + \sum_{j=1}^n F_j^{(N)}(s) P_{n-j}^{(N)}(0). \quad (3.2)$$

Introduction of the generating functions $F^{(N)}(s, z)$ and $P^{(N)}(s, z)$ given by

$$F^{(N)}(s,z) = \sum_{n=1}^{\infty} z^n F_n^{(N)}(s), \qquad (3.3)$$

and

$$P^{(N)}(s,z) = \sum_{n=0}^{\infty} z^n P_n^{(N)}(s), \qquad (3.4)$$

multiplication of (3.2) by z^n and summation over n yield

$$P^{(N)}(s, z) = F^{(N)}(s, z) P^{(N)}(0, z) + \delta_{s,0}.$$
 (3.5)

From (3.5) we obtain $F^{(N)}(s, z)$ in terms of $P^{(N)}(s, z)$:

$$F^{(N)}(s,z) = (P^{(N)}(s,z) - \delta_{s,0})/P^{(N)}(0,z). \quad (3.6)$$

Thus, the knowledge of $P^{(N)}(s, z)$ yields $F^{(N)}(s, z)$ which by differentiation at z = 1 leads to $\langle n(s) \rangle$:

$$\langle n(s) \rangle = \frac{\partial}{\partial z} F^{(N)}(s, z) \bigg|_{z=1}$$
 (3.7)

Now $P^{(N)}(s, z)$ is the generating function for random walks on a ring of N sites and satisfies the periodic condition:

$$P^{(N)}(s,z) = P^{(N)}(s+N,z).$$
 (3.8)

This generating function is equivalent to the sum of the generating functions $P^{\infty}(s, z)$ for all those walks on an infinite line which represent walks from s_0 to $s_0 + s$, s_0 to $s_0 + s + N$, ... as well as from s_0 to $s_0 + s - N$, s_0 to $s_0 + s - 2N$, ... Hence,

$$P^{(N)}(s,z) = P^{\infty}(s,z) + P^{\infty}(s+N,z) +$$

$$+ P^{\infty}(s+2N,z) + \dots + P^{\infty}(s-N,z)$$

$$+ P^{\infty}(s-2N,z) + \dots,$$
(3.9)

where $P^{\infty}(s, z)$ remains to be computed.

Since the random walk is Markovian, $P_n^{\infty}(s)$ (which is the probability equivalent to $P_n^{(N)}(s)$ but for an infinite line) satisfies the usual recursion formula (master equation):

$$P_{n+1}^{\infty}(s) = pP_{n}^{\infty}(s-1) + (1-p)P_{n}^{\infty}(s+1)$$
. (3.10)

By multiplying (3.10) by z^n , summing over all n and with the initial condition $P_0^{\infty}(s) = \delta_{s,0}$, one obtains:

$$P^{\infty}(s, z) - P_0^{\infty}(s) = z [pP^{\infty}(s - 1, z) + (1 - p) P^{\infty}(s + 1, z)]. \quad (3.11)$$

Introducing the Fourier transform of $P^{\infty}(s, z)$

$$u(\phi, z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} P^{\infty}(s, z) e^{i\phi s} ds$$
, (3.12)

in equation (3.11) and inverting equation (3.12) yields

$$P^{\infty}(s,z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\phi s} d\phi}{1 - z(p e^{i\phi} + (1-p) e^{-i\phi})},$$
(3.13)

which reduces to the result of reference [14] in the symmetric case p = 1 - p = 1/2.

We now define the constant α such that

ch
$$\alpha = 1/\sqrt{4 p(1-p)}$$
,
sh $\alpha = (2 p - 1)/\sqrt{4 p(1-p)}$, (3.14)

which allows one to transform (3.13) into

$$P^{\infty}(s,z) = \frac{1}{2\pi} e^{\alpha s} \int_{-\pi}^{\pi} \frac{e^{-i(\phi - i\alpha)s} d\phi}{1 - z\sqrt{4p(1-p)}\cos(\phi - i\alpha)}.$$
(3.15)

With the change of variables, $\varphi = \phi - i\alpha$ and $Z = z\sqrt{4 p(1-p)}$, equation (3.15) involves an integral along the linear contour parallel to the real axis but displaced from it by the amount $-\alpha$. Then, it is straightforward (2) to show that $P^{\infty}(s, z)$ is equal to

$$P^{\infty}(s,z) = \frac{1}{2\pi} e^{\alpha s} \int_{-\pi}^{\pi} \frac{e^{-i\varphi s} d\varphi}{1 - Z\cos\varphi}, \quad (3.16)$$

which can be explicitely calculated [15]

$$P^{\infty}(s,z) = e^{as} \frac{X^{|s|}}{(1-Z^2)^{1/2}},$$
 (3.17)

with

$$X = \frac{1 - (1 - Z^2)^{1/2}}{Z}; \qquad Z = \sqrt{4 \, p(1 - p)} \, z.$$
(3.18)

Substitution of expression (3.17) for $P^{\infty}(s, z)$ into equation (3.9) yields after summation

$$P^{(N)}(s,z) = \frac{e^{\alpha s}}{(1-Z^2)^{1/2}} \left[\frac{X^s}{1-(e^{\alpha}X)^N} + \frac{X^{N-s}e^{-\alpha N}}{1-(e^{-\alpha}X)^N} \right]. \quad (3.19)$$

Then from (3.6) and (3.7) we finally get

$$\langle n(s) \rangle = \frac{1}{1 - 2p} \left[-s + N \frac{1 - \left(\frac{p}{1 - p}\right)^s}{1 - \left(\frac{p}{1 - p}\right)^N} \right].$$
(3.20)

The average walk length for a walker starting at the site s to reach the site 0 which is supposed to be the trapping site is obtained by changing the labelling of

⁽²⁾ Equation (3.16) results from the integration on a contour in a complex plane lying on the two horizontal segments at $\text{Im } \varphi = 0$ and $-i\alpha$ respectively, closed by two vertical segments (Re $\varphi = \pm \pi$), and which does not contain any pole of the integrand.

the sites from counter clockwise to clockwise that is p into 1 - p in (3.20)

$$\langle n_{\rm T}(s) \rangle = \frac{1}{2p-1} \left[-s + N \frac{1 - \left(\frac{1-p}{p}\right)^s}{1 - \left(\frac{1-p}{p}\right)^N} \right].$$
(3.21)

This formula reduces to (3.0) in the limit $p \to 1/2$.

3.2 Non-Markovian random walk with a two-step memory. — We now extend the anisotropic random walk model by allowing for a short-range correlation. The probability for the walker to go to the right { left } now depends on the direction of its previous step. This requires the definition of four conditional probabilities namely $p_{\rm RR}$ the probability to have two successive steps to the right, $p_{\rm LL}$ the probability to have two successive steps to the left, $p_{\rm RL}$ the probability that a step to the right is followed by a step to the right. This problem reduces to the previous case when the four probabilities we have introduced obey the relation:

$$p = p_{RR} + p_{LR}, \quad 1 - p = p_{LL} + p_{RL},$$

$$p_{RR} = p^2, \quad p_{LL} = (1 - p)^2, \quad p_{RL} = p_{LR} = p(1 - p).$$
(3.22)

A similar problem has been studied by other authors, who give, for the continuous case, the asymptotic behaviour of the diffusion coefficient [16] and the variance of the probability distribution [17]. In addition to being a model of anisotropic neutron pseudo-diffusion, this picture may be useful to describe several physical systems such as dielectric relaxation anomalous transients and noise phenomena. As we will see in § 4, this situation also occurs when using the logistic map (1.2) to generate pseudo-random numbers for R = 4 and with the particular cut-off value $x_c = f^{-1}(1/2)$.

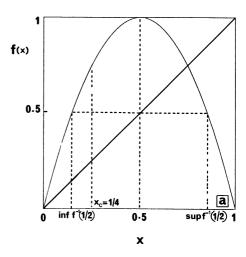
The expected average walk length is computed as follows. A straightforward generalization of equation (3.10) reads

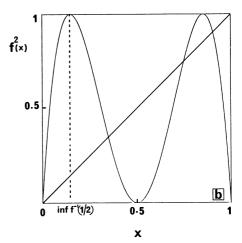
$$P_n^{\infty}(s) = p_{RR} P_{n-2}^{\infty}(s-2) + (1-p) P_{n-2}^{\infty}(s) + + p_{LL} P_{n-2}^{\infty}(s+2). \quad (3.23)$$

The general method for calculating $P^{\infty}(s, z)$ being slightly more involved than in § 3.1, is presented in Appendix A. Knowing $P^{\infty}(s, z)$ yields $P^{(N)}(s, z)$ by equation (3.9). Then differentiating $F^{(N)}(s, z)$ obtained with equation (3.6) with respect to z at z = 1 yields $\langle n(s) \rangle$ (Eq. (A.15)).

Now, applying this result to the random walk experiment, performed with the logistic map with R = 4,

 $x_c = \inf f^{-1}(1/2)$, as the random number generator, requires the determination of p_{LL} , p_{RR} , p_{RL} and p_{LR} defined above. As shown in figure 2, the interval [0, 1]





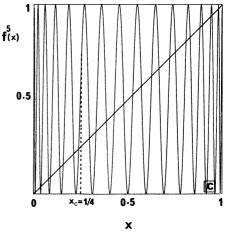


Fig. 2. — (a) The logistic map f(x) given by equation (1.2) for R=4; three cut off values used in the Monte-Carlo experiment are shown. (b) The second iterate $f^2(x)$ of the logistic map for R=4; the subinterval $[0, \inf f^{-1}(1/2)]$ is mapped onto the whole definition interval [0, 1]. (c) Fifth iterate $f^5(x)$ of the logistic map for R=4; the subinterval $[0, x_c=1/4]$ is mapped several times onto [0, 1]; the relative importance of the mismatch shown by the dashed line becomes negligible for such high iterates of (1.2).

can be partitioned into four disjoint intervals:

$$\begin{bmatrix} 0, f_{\inf}^{-1}(x_{c}) \end{bmatrix}, \quad]f_{\inf}^{-1}(x_{c}), x_{c}], \quad]x_{c}, f_{\sup}^{-1}(x_{c})]$$
 and
$$]f_{\sup}^{-1}(x_{c}), 1].$$

At each step, the iteration of (1.2) lies in one of these subintervals. If $x_n \in [0, f_{\inf}^{-1}(x_c)]$ then x_n is less than x_c and the walker goes to the left at the *n*th step. At the next step, $x_{n+1} = f(x_n)$ still belongs to $[0, x_c]$ and again the walker will go to the left. Therefore

$$p_{\rm LL} = \int_0^{f_{\rm inf}^{-1}(x_c)} \rho(x) \, dx \,, \qquad (3.24a)$$

where $\rho(x)$ is the absolutely continuous invariant measure defined in (1.1). The same analysis carried on the other three subintervals leads to:

$$p_{RR} = \int_{x_c}^{f_{su}_b(x_c)} \rho(x) dx = p - p_{LL}, \quad (3.24b)$$

$$p_{\rm RL} = \int_{f_{\rm sup}(x_{\rm c})}^{1} \rho(x) \, dx = p_{\rm LL},$$
 (3.24c)

$$p_{LR} = \int_{f_{in}^{-1}(x_c)}^{x_c} \rho(x) dx = 1 - p - p_{LL}.$$
 (3.24d)

With the cut-off value $x_c = \inf f^{-1}(1/2)$ the logistic map yields p = 3/4, $p_{LL} = 1/8$ and $Y = e^{2\alpha} = 5$; owing to the large value of Y, $\langle n_T(s) \rangle$ is then given to leading order by

$$\langle n_{\rm T}(s) \rangle = 2 N \left(1 - \frac{1}{5^{1/2}} - \frac{s}{N} + O\left(\frac{1}{5^{\frac{N-1}{2}}}\right) \right).$$

(3.25)

Equation (3.25) has been used to compute the theoretical values of $\langle n_T(s) \rangle_{th}^*$ which are compared with the experimental values in table III.

4. Numerical results of the Monte-Carlo random walk experiment.

In this section, we present numerical results obtained when using the logistic map (1.2) or one of its iterates $f^n = f \circ f \circ \cdots \circ f$, $n = 2, \ldots$ as the random number generator for different values of the control parameter spanning the interval bounded by the chaotic threshold $R_c = 3.5699$ and R = 4. The procedure chosen for the Monte-Carlo experiment has been described in § 2 (see also Appendix B). In order to examine in what sense the Monte Carlo random walk experiment tests the existence of such a measure, we first study the case R = 4 for which the map is surjective and possesses an absolutely continuous inva-

riant measure [18] with density $\rho(x) = \frac{1}{\pi} [x(1-x)]^{-1/2}$ (see Fig. 1).

4.1 R = 4. — In table I, we report numerical experiments carried with a symmetric cut-off $x_c = 1/2$ corresponding to a probability p = 1/2. We obtain results similar to those described in reference [11]. Experiment and theory (see § 3.1) are in agreement within statistical error; the mean standard deviation is of the order of one percent for $\mathcal{N}=20~000$. However, considering the monotonous behaviour of the map (1.2) on each subinterval, (see Fig. 2) one could expect a systematic discrepancy due to the existence of short-range correlations. By direct numerical computation, we find that two-point correlation functions (see Eq. (2.0)) (with the condition that the first point belongs to one of the two subintervals) show exponential decay with a correlation length equal to the Liapunov characteristic exponent, $\lambda = \log 2$. Although such correlation effects are always experimentally present, they are buried in the statistical error, because of their low amplitude. In order to make them observable in the random walk experiment, fairly prohibitive statistics would be required. Runs up to $\mathcal{N} \sim 10^6$ have not permitted us to detect these effects. Therefore the random walk test is much less sensitive to this type of correlation than the serial correlation test (see § 2). However, we now show that it is very sensitive to another type of correlation, namely the ill-definition of the probability p at each step which occurs for non-symmetric cut-offs $(p \neq 1/2)$. Indeed, as soon as one of the boundaries of either subinterval $\left\lceil \frac{R^2}{4} \left(1 - \frac{R}{4} \right), x_c \right\rceil$ and $[x_c, R/4]$ is not mapped onto one of the boun-

Table I. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual sites on a N=13 periodic lattice for R=4 and p=1/2 ($x_c=1/2$) and using $f. \langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).

S	$\langle n_{\rm T}(s) \rangle_{{\rm exp},f}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	11.90	12.00
2	22.24	22.00
3	30.24	30.00
4	36.27	36.00
5	39.58	40.00
6	41.71	42.00
7	42.03	42.00
8	39.93	40.00
9	36.29	36.00
10	29.89	30.00
11	22.22	22.00
12	12.30	12.00

daries of the whole invariant subinterval $\left[\frac{R^2}{4}\left(1-\frac{R}{4}\right)\right]$, p becomes a conditional probability which

depends on the preceding step. This non-Markovian effect can lead to a strong discrepancy between theory and experiment as illustrated in table II. In this case, failing to get a fixed p for each step arises from partial overlap of the invariant interval with the iterate of one of the two subintervals (see Fig. 2a). Further experiments performed with a higher iterate f^n of the logistic map lead to considerably better agreement with theory. Numerical computation of the probability p for each step shows indeed convergence to the mean value of p as n is increased. Then each subinterval is mapped several times onto the inva-

riant interval with the result that the relative importance of the mismatch diminishes with the number of mappings as shown in figures 2b, c.

Note that the ill-definition of p at each step is related to the occurrence of monotonic subsequences of numbers when iterating f. The sensitivity of the random walk test to such correlation effects indicates that it supports the comparison with the statistical run-test briefly described in § 2.

Whatever the cut-off value x_c , one can always compensate numerically for the ill-definition of p at each step by using a sufficiently high iterate of f. However for R=4 and particular cut-off values — that is the nth inverse iterates of the critical point 1/2 of the logistic map for all n — this ill-definition of p strictly disappears when considering f^{n+1} as the random-number generator, as illustrated in table III

Table II. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=4, p=2/3 ($x_c=1/4$) and using f, f^2 and f^{10} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).

S	$\langle n_{\rm T}(s) \rangle_{{\rm exp};f}$	$\langle n_{T}(s) \rangle_{\exp;f^2}$	$\langle n_{\mathrm{T}}(s) \rangle_{\exp;f^{10}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	2.911	2.992	2.941	2.991
2	5.964	6.000	5.930	5.976
3	8.770	9.033	8.962	8.953
4	11.65	11.92	11.87	11.91
5	14.28	15.06	14.86	14.83
6	16.90	17.79	17.66	17.67
7	19.22	20.84	20.36	20.37
8	20.98	23.46	22.75	22.76
9	22.06	25.74	24.75	24.54
10	21.88	27.00	25.10	25.11
11	19.43	25.41	23.35	23.24
12	13.41	18.03	16.59	16.50

Table III. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=4, $p=3/4\left(x_c=\frac{1}{2}-\frac{1}{2\sqrt{2}}\right)$ and using f and f^2 respectively. $\langle n(s) \rangle_{th}$ is derived from equation (3.21). Exact results obtained for a non-Markovian two-step effect random walk (Eq. (3.25)) are shown in the first column and compare well with experimental results when using f.

S	$\langle n_{\rm T}(s) \rangle_{\rm th}^*$	$\langle n_{\mathbf{T}}(s) \rangle_{\exp;f}$	$\langle n_{\rm T}(s) \rangle_{\exp;f^2}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	1.998	1.960	1.992	2.000
2	3.996	3.997	3.984	4.000
3	5.992	5.942	6.010	6.000
4	7.981	7.925	7.957	7.999
5	9.958	9.863	10.00	9.996
6	11.91	11.66	11.98	11.99
7	13.79	13.50	13.94	13.96
8	15.53	15.12	15.84	15.89
9	16.96	16.28	17.63	17.68
10	17.67	16.88	19.00	19.04
11	16.80	16.20	19.19	19.11
12	12.37	12.40	15.39	15.33

Table IV. — Average length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=4, p=0.96883 ($x_c=\inf f^{-4}(1/2)$) using f, f^5, f^{10} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21). The comparison between $\langle n_T(s) \rangle_{exp}$ and $\langle n_T(s) \rangle_{th}$ is more direct when tabulating and comparing the deviation $|\langle n_T(s) \rangle_{exp} - \langle n_T(s) \rangle_{th}|$ with the predicted mean standard deviation (Eq. (B.24)): see table V.

S	$\langle n_{T}(s) \rangle_{exp,f}$	$\langle n_{T}(s) \rangle_{exp,f^5}$	$\langle n_{\rm T}(s) \rangle_{\exp,f^{10}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	1.065	1.065	1.068	1.067
2	2.136	2.132	2.131	2.133
3	3.194	3.196	3.203	3.200
4	4.262	4.269	4.266	4.266
5	5.329	5.331	5.337	5.333
6	6.392	6.395	6.403	6.400
7	7.456	7.472	7.464	7.466
8	8.509	8.535	8.533	8.533
9	9.533	9.600	9.598	9.600
10	10.54	10.67	10.67	10.67
11	11.44	11.72	11.71	11.72
12	11.94	12.34	12.35	12.35

for $x_c = \inf f^{-1}(1/2)$. For this simple case we obtain, as expected, good numerical results when using f^2 , which reflects a two-step correlation effect. This simple non-Markovian behaviour has been analysed in § 3.2. Good agreement is found betwen the theoretical prediction equation (3.25) and the numerical simulations performed with f (see Table III).

In tables IV and V, we also present results obtained for large p=0.96883 corresponding to $x_c=\inf f^{-4}(1/2)$, for which we have theoretically estimated the mean standard deviation $\Lambda_{T,\mathcal{N}}(s)$ of $\langle n_T(s) \rangle_{\exp}$ in Appendix B. As expected the numerical deviations fall within $2 \Lambda_{T,\mathcal{N}}(s)$ when using f^n with $n \ge 5$.

Let us remark that the use of some iterate f^n , with $n \ge 2$, amounts to extracting a subsequence out of the original sequence. Our numerical results thus show that when combining the random walk test with the subsequence test (see § 2) one is able to select a «truly» random sequence of numbers from the initial deterministic sequence.

4.2 $R_c < R < 4$. — We now investigate the general case $R \ne 4$. For the set of Misiurewicz's R values [8], one can easily convince oneself that the problem simply reduces to the case R = 4, when using f^k instead of f as a random generator. These R values correspond to the different stages of the reverse cascade [1] for which the 2^{k+1} -band chaotic attractor merges to 2^k -bands. Indeed in each of the 2^k -bands, f^k is surjective as is f on [0, 1] for R = 4.

We first concentrate on values of R in the last step of the reverse cascade, R = 3.67857... to R = 4. For R = 3.8, and a bisecting cut-off such that p=1/2, we obtain the same poor results as those presented in reference [11] when using f. However with f^{20} considerable improvement is obtained as shown in

Table V. — Normalized deviations

$$\delta_n = \left| \left\langle n_{\rm T}(s) \right\rangle_{\rm exp} - \left\langle n_{\rm T}(s) \right\rangle_{\rm th} \right| / \Lambda_{\rm T, \mathcal{N}}(s)$$

of the average length for trapping from individual site on a N=13 periodic lattice for R=4, p=0.96883 $(x_c=\inf f^{-4}(1/2))$ using f^n , n=1, 5, 6, 8, 10 where $\Lambda_{T,\mathcal{N}}(s)$ is the mean standard deviation estimated in Appendix B (Eq. (B.24)). When using f, we obtain deviations up to ~ 90 r.m.s. while for f^n , $n \geq 5$, the deviation always lies within 2 r.m.s. This confirms that with high iterates of f, we get rid of non-Markovian effects inherent in iterations of deterministic process.

S	δ_1	δ_5	δ_6	δ_8	δ_{10}
1	0.85	0.85	0.85	0.09	0.77
2	1.6	0.63	0.22	0.41	1.1
3	2.1	1.5	0.63	0.46	1.21
4	1.6	1.84	0.03	2.1	0.26
5	1.23	0.71	0.82	0.12	1.18
6	2.2	1.3	1.1	0.59	1.1
7	2.8	1.6	1.3	1.0	0.57
8	6.1	0.48	0.55	0.57	0.10
9	16	0.33	0.98	0.26	0.29
10	31	0.28	0.28	0.25	0.13
11	63	0.13	0.50	0.63	1.1
12	92	1.9	0.67	0.02	0.31

table VI. A numerical estimate of the short-range correlation effects shows unambiguously that the ill-definition of p at each step is responsible for the misleading claim of Kozak $et\ al$. Our conclusion is corroborated by simulations with different cut-off values, for which the correlation effects are less dramatic and easier to handle with lower iterates of

Table VI. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a $N=13$ periodic lattice for $R=3.8$,
$p = 1/2$ ($x_c = 0.690258$) and using f, f^5 and f^{20} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).	

S	$\langle n_{\mathbf{T}}(s) \rangle_{\exp,f}$	$\langle n_{T}(s) \rangle_{exp,f^5}$	$\langle n_{\rm T}(s) \rangle_{\exp,f^{20}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	31.24	8.584	11.44	12.00
2	55.50	15.85	21.63	22.00
3	76.31	21.29	29.14	30.00
4	90.52	25.55	35.13	36.00
5	99.82	28.60	39.06	40.00
6	106.6	30.26	40.76	42.00
7	109.3	30.13	41.12	42.00
8	103.6	29.44	38.91	40.00
9	91.51	25.88	34.97	36.00
10	76.68	22.02	29.55	30.00
11	58.17	15.59	21.58	22.00
12	30.71	8.643	12.08	12.00

Table VII. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=3.8, p=0.7222 ($x_c=1/2$) and using f, f^5 , and f^{14} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).

S	$\langle n_{T}(s) \rangle_{exp,f}$	$\langle n_{T}(s) \rangle_{exp,f^5}$	$\langle n_{\rm T}(s) \rangle_{\exp,f^{14}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	2.241	2.274	2.259	2.251
2	4.510	4.493	4.504	4.501
3	6.732	6.675	6.787	6.750
4	8.974	8.964	8.974	8.998
5	11.23	11.20	11.28	11.24
6	13.49	13.33	13.51	13.47
7	15.77	15.45	15.67	15.66
8	17.98	17.49	17.85	17.76
9	20.25	18.90	19.61	19.62
10	22.53	19.87	20.93	20.84
11	24.76	19.30	20.59	20.43
12	18.49	14.66	16.00	15.75

the logistic map (see Table VII). In fact, cut-off values such that $p \sim 1/2$ lead to short-range oscillating behaviour reminiscent of the systematic periodicity 2 superimposed to chaotic behaviour as it occurs in the previous stage of the reverse cascade.

The results for R=3.8275 are presented in table VIII. For this value of the parameter, the logistic map shows intermittent [19] behaviour preceding the occurrence of a stable period-three cycle. This characteristic short-range order in chaotic dynamics is reflected in the random walk experiment by the necessary use of rather high iterates of f. The bias increases drastically when R approaches the bifurcation value $R=1+\sqrt{8}=3.828427...$ Avoiding this intermittent regularity could be attempted by selecting those points in the dynamics which are not in the resonant channels; but even for such points, memory of the periodicity persists.

We have also extended our numerical study to the different stages of the reverse cascade, and we obtain similar results when the non-connexity of the chaotic attractor is taken into account. In particular the disconnected structure of the attractor reflects into a back and forth walk, when using f as the random number generator in the symmetric case p = 1/2. For a 2^{k-1} -band attractor, the general procedure requires at least the kth iterate of f. This restricts the analysis to one of the bands of the attractor which is invariant under f^k . Next by choosing an arbitrary cut-off in this band, we face again a situation similar to that one encountered in the last stage of the reverse cascade discussed above. In table IX, we present experimental results for R=3.62 in the 2-band chaotic region. For f^{20} as the random number generator, good agreement is obtained between theory and experiment. Many additional numerical experi-

Table VIII. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=3.8275, p=0.725404 ($x_c=0.4$) and using f and f^{20} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).

S	$\langle n_{T}(s) \rangle_{exp,f}$	$\langle n_{\rm T}(s) \rangle_{\exp,f^{20}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	2.075	2.212	2.218
2	4.182	4.433	4.436
3	6.247	6.669	6.653
4	8.334	8.884	8.868
5	10.39	11.07	11.08
6	12.48	13.29	13.28
7	14.55	15.52	15.44
8	16.64	17.62	17.52
9	18.75	19.58	19.37
10	20.82	21.05	20.62
11	22.90	21.09	20.27
12	16.01	16.35	15.70

Table IX. — Average walk length $\langle n_T(s) \rangle$ for trapping from individual site on a N=13 periodic lattice for R=3.62, p=0.2919 ($x_c=1/2$) and using f^2 and f^{20} respectively. $\langle n_T(s) \rangle_{th}$ is obtained from equation (3.21).

s	$\langle n_{T}(s) \rangle_{\exp,f^2}$	$\langle n_{\mathrm{T}}(s) \rangle_{\mathrm{exp},f^{20}}$	$\langle n_{\rm T}(s) \rangle_{\rm th}$
1	18.95	16.27	15.96
2	26.39	21.36	21.12
3	24.09	22.12	21.84
4	21.68	20.81	20.72
5	19.21	19.00	18.85
6	16.84	16.63	16.66
7	14.42	14.44	14.35
8	12.03	12.10	11.99
9	9.581	9.582	9.600
10	7.247	7.226	7.203
11	4.790	4.733	4.803
12	2.400	2.397	2.402

ments were performed for other arbitrary values of R. They all confirm the results presented above: when the Liapunov characteristic exponent is computed positive, the logistic map can be used as a pseudorandom number generator provided its deterministic nature is taken into account.

In conclusion, we hope that the present work has shown the relevance of the random walk test as an easily tractable and powerful statistical test. Its use has helped in clarifying the nature of the chaos exhibited by discrete dynamical systems and lent strong experimental support to Ruelle's conjecture.

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Appendix A.

We start from the recursion relation (3.23)

$$P_n^{\infty}(s) = p_{RR} P_{n-2}^{\infty}(s-2) + (1-p) P_{n-2}^{\infty}(s) + p_{LL} P_{n-2}^{\infty}(s+2). \tag{A.1}$$

Multiplication of (A.1) by z^n summation over all n and use of the initial conditions

$$\begin{cases} P_{n=0}^{\infty}(s) = \delta_{s,0} \\ P_{n=1}^{\infty}(s) = p\delta_{s,1} + (1-p)\delta_{s,-1} \end{cases}$$
(A.2)

vield

$$(1 - (1 - p) z^{2}) P^{\infty}(s, z) = p_{RR} z^{2} P^{\infty}(s - 2, z) + p_{LL} z^{2} P^{\infty}(s + 2, z) + z[p\delta_{s,1} + (1 - p) \delta_{s,-1}] + \delta_{s,0}.$$
(A.3)

This equation can be solved like equation (3.11); using the Fourier expansion of $P^{\infty}(s, z)$, we obtain

$$P^{\infty}(s,z) = \frac{1}{1 - (1-p)z^2} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1 + z(p e^{i\phi} + (1-p) e^{-i\phi})}{1 - \frac{z^2}{1 - (1-p)z^2} (p_{RR} e^{2i\phi} + p_{LL} e^{-2i\phi})} e^{-i\phi s} d\phi.$$
 (A.4)

With the new variables r, φ, Z defined by :

$$p_{\rm LL} = r \, \mathrm{e}^{-\alpha} \,, \qquad p_{\rm RR} = r \, \mathrm{e}^{\alpha} \,, \tag{A.5}$$

and

$$Z = 2 r \frac{z^2}{1 - (1 - p) z^2},$$
(A.6)

Equation (A.4) transforms into

$$P^{\infty}(s,z) = \frac{1}{1 - (1 - p)z^{2}} \left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\phi s} d\phi}{1 - Z\cos(2\phi - i\alpha)} + zp \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\phi(s-1)} d\phi}{1 - Z\cos(2\phi - i\alpha)} + z(1 - p) \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\phi(s+1)} d\phi}{1 - Z\cos(2\phi - i\alpha)} \right\}.$$
 (A.7)

Each integral in (A.7) reduces to an integral evaluated on the real line when introducing, as in § 3.1, the new variable $\varphi = \phi - i\frac{\alpha}{2}$.

Then $P^{\infty}(s, z)$ can be reexpressed as

$$P^{\infty}(s,z) = \frac{1}{1 - (1 - p)z^{2}} \left\{ e^{i\alpha \frac{s}{2}} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\varphi s} d\varphi}{1 - Z\cos 2\varphi} + z + zp e^{\frac{\alpha(s-1)}{2}} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\varphi(s-1)} d\varphi}{1 - Z\cos\varphi} + z + z(1 - p) e^{\frac{\alpha(s+1)}{2}} \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\varphi(s+1)} d\varphi}{1 - Z\cos 2\varphi} \right\}.$$
 (A.8)

Explicit integration of the integrals involved in (A.8) can be found in tables of definite integrals [15]

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{e^{-i\varphi s} d\varphi}{1 - Z\cos 2\varphi} = 0 \quad \text{if } s \text{ is odd };$$

$$= \frac{X^{|s/2|}}{(1 - Z^2)^{1/2}} \quad \text{if } s \text{ is even };$$
(A.9)

where Z is given by equation (A.6) and

$$X = \frac{1 - (1 - Z^2)^{1/2}}{Z} \; ; \tag{A.10}$$

then we get

$$P^{\infty}(s,z) = \frac{X^{\left|\frac{s}{2}\right|} e^{\alpha \frac{s}{2}}}{(1 - (1 - p)z^{2})(1 - Z^{2})^{1/2}} \quad \text{if s is even};$$

$$= zp \frac{X^{\left|\frac{s-1}{2}\right|} e^{\alpha \frac{s-1}{2}}}{(1 - (1 - p)z^{2})(1 - Z^{2})^{1/2}}$$

$$+ z(1 - p) \frac{X^{\left|\frac{s+1}{2}\right|} e^{\alpha \frac{s+1}{2}}}{(1 - (1 - p)z^{2})(1 - Z^{2})^{1/2}} \quad \text{if s is odd.}$$
(A.11)

Substituting (A.11) into (3.9) yields after summation of the two series :

$$P^{(N)}(s,z) = \frac{1}{(1-(1-p)z^2)(1-Z^2)^{1/2}} \left\{ \frac{Y^{\frac{8}{2}}}{1-Y^N} + \frac{T^{N-\frac{3}{2}}}{1-T^N} + \frac{1}{1-T^N} + zp \left[\frac{Y^{\frac{N+s-1}{2}}}{1-Y^N} + \frac{T^{\frac{N-s-1}{2}}}{1-T^N} \right] + z(1-p) \left[\frac{Y^{\frac{N+s+1}{2}}}{1-Y^N} + \frac{T^{\frac{N-s-1}{2}}}{1-T^N} \right] \right\}, \quad (A.13)$$

where

$$Y = e^{\alpha} X$$
, $T = e^{-\alpha} X$. (A.14)

Equation (A.13) only holds for s even. For s odd, $P^{(N)}(s, z)$ is easily obtained by remarking that since N is odd (which is our choice in our numerical experiments), s and N - s are of different parities. If s is odd, then N - s is even and $P^{(N)}(s, z)$ is obtained from (A.13) by replacing s by N - s and p by 1 - p.

Now from (3.6) and (3.7) we find

$$\langle n(s) \rangle = \frac{N}{(p^2 - 4r^2)^{1/2}} (\beta(0) - \beta(s)),$$
 (A.15)

where

$$\beta(s) = \frac{Y^{\frac{s}{2}} + pY^{\frac{N+s-1}{2}} + (1-p)Y^{\frac{N+s+1}{2}}}{1-Y^{N}} - \frac{1}{N} \left[N - \frac{s}{2} + p \frac{N-s+1}{2} + (1-p) \frac{N-s-1}{2} \right]. \tag{A.16}$$

The average walk length $\langle n_T(s) \rangle$ to be trapped starting from the site s is thus deduced from (A.15) and (A.16) by replacing p by 1 - p which by (A.14) and (A.10) amounts to replace Y by Y^{-1} in (A.16).

Appendix B.

In this Appendix, we estimate theoretically the mean standard deviation between the exact average walk length for a walker to go from the site s_0 to the site $s_0 + s$ and its numerical estimate obtained by averaging over \mathcal{N} walkers. The probability $\mathcal{L}_{\mathcal{N}}(\mathcal{N}_n)$ that among \mathcal{N} walkers, \mathcal{N}_n walkers reach the site $s_0 + s$ for the first time after n steps, is given by:

$$\mathfrak{I}_{\mathcal{N}}(\mathcal{N}_n) = \mathcal{C}_{\mathcal{N}}^{\mathcal{N}_n} [F_n^{(N)}(s)]^{\mathcal{N}_n} [1 - F_n^{(N)}(s)]^{\mathcal{N} - \mathcal{N}_n}, \tag{B.1}$$

where $F_n^{(N)}(s)$ is defined in § 3.1. For large \mathcal{N} and \mathcal{N}_n , the binomial law (B.1) becomes Gaussian:

$$\mathfrak{I}_{\mathcal{N}}(\mathcal{N}_n) \to \frac{1}{[2 \pi \widetilde{F}_N^{(N)}(s) \mathcal{N}]^{1/2}} \exp\left\{-\frac{(\mathcal{N}_n - F_n^{(N)}(s) \mathcal{N})^2}{2 \widetilde{F}_n^{(N)}(s) \mathcal{N}}\right\},\tag{B.2}$$

where $\tilde{F}_{n}^{(N)}(s)$ is expressed in terms of $F_{n}^{(N)}(s)$ as:

$$\frac{1}{2\,\widetilde{F}_n^{(N)}(s)} = \frac{1}{F_n^{(N)}(s)} + \frac{1}{1 - F_n^{(N)}(s)}.\tag{B.3}$$

A typical numerical experiment will yield \mathcal{N}_{n_1} walkers making n_1 steps, ..., $\mathcal{N}_{n_{\infty}}$ walkers making n_{∞} steps. The \mathcal{N}_{n_j} , $j=1,...,\infty$ are not independent but satisfy the relation

$$\sum_{j=1}^{\infty} \mathcal{N}_{n_j} = \mathcal{N} . \tag{B.4}$$

From this realization, a numerical estimate of the average walk length $\langle n(s) \rangle$ is given by :

$$\langle n(s) \rangle_{\mathcal{N}} = \frac{1}{\mathcal{N}} \sum_{j=1}^{\infty} \mathcal{N}_{n_j} n_j.$$
 (B.5)

To obtain the mean standard deviation $\langle (\langle n \rangle_{\mathcal{N}} - \langle n(s) \rangle)^2 \rangle$, one has first to compute the law of probability of $\langle n \rangle_{\mathcal{N}}$ which reads:

$$\mathfrak{I}(\langle n \rangle_{\mathcal{N}}) = \sum_{\mathcal{N}_{1}} \cdots \sum_{\mathcal{N}_{m}} \left[\prod_{j=1}^{\infty} \mathfrak{I}_{\mathcal{N}}(\mathcal{N}_{n_{j}}) \right] \cdot \delta \left(\sum_{j=1}^{\infty} \mathcal{N}_{n_{j}} - \mathcal{N} \right) \cdot \delta \left(\langle n \rangle_{\mathcal{N}} - \frac{1}{\mathcal{N}} \sum_{j=1}^{\infty} \mathcal{N}_{n_{j}} \cdot n_{j} \right), \quad (B.6)$$

where the summation runs over all configurations of \mathcal{N} walkers such that (B.4) and (B.5) are fulfilled, each configuration being weighted by its corresponding probability. For large \mathcal{N} and $\mathcal{N}_{n_j}(j=1,...,\infty)$, the discrete sums in (B.6) can be replaced by continuous integrals over new variables x_i defined by:

$$x_i = \mathcal{N}_{n_i} - F_{n_i}^{(N)}(s) \,\mathcal{N} \,. \tag{B.7}$$

Equation (B.6) thus becomes:

$$\Im(\langle n \rangle_{\mathcal{N}}) = \int \cdots \int \left[\prod_{j=1}^{\infty} dx_{j} \frac{\exp\left(-\frac{x_{j}^{2}}{2 \tilde{F}_{n}^{(N)}(s) \mathcal{N}}\right)}{(2 \pi \tilde{F}_{n_{j}}^{(N)}(s) \mathcal{N})^{1/2}} \right] . \delta\left(\sum_{j=1}^{\infty} x_{j}\right) . \delta\left(\langle n \rangle_{\mathcal{N}} - \langle n(s) \rangle - \frac{1}{\mathcal{N}} \sum_{j=1}^{\infty} n_{j} . x_{j}\right).$$
(B.8)

The second δ -function cancels out by Fourier transforming $\mathfrak{I}(\langle n \rangle_{\mathcal{N}})$ with respect to $\langle n \rangle_{\mathcal{N}} - \langle n(s) \rangle$, whereas the first δ -function can be removed by integration over a chosen x_m . We thus obtain:

$$\widetilde{\mathcal{J}}(k) = \frac{1}{\left[2 \pi \widetilde{F}_{n_{m}}^{(N)}(s) \mathcal{N}\right]^{1/2}} \int \cdots \int \left[\prod_{\substack{j=1\\j \neq m}}^{\infty} \frac{\mathrm{d}x_{j}}{\left(2 \pi \widetilde{F}_{n_{j}}^{(N)}(s) \mathcal{N}\right)^{1/2}} \right] \times \\
\times \exp \left\{ -\frac{1}{2 \mathcal{N}} \sum_{\substack{j=1\\j \neq m}}^{\infty} \frac{x_{j}^{2}}{\widetilde{F}_{n_{j}}^{(N)}(s)} - \frac{1}{2 \mathcal{N} \widetilde{F}_{n_{m}}^{(N)}(s)} \left(\sum_{\substack{j=1\\j \neq m}}^{\infty} x_{j} \right)^{2} + \frac{ik}{\mathcal{N}} \sum_{\substack{j=1\\j \neq m}}^{\infty} (n_{j} - n_{m}) x_{j} \right\}. \tag{B.9}$$

The argument A of the exponential in (B.9) can be expressed in matricial form:

$$\mathbf{A} = -{}^{t}XAX - ik{}^{t}BX, \tag{B.10}$$

where the elements of A and B are given by :

$$A_{ij} = \frac{1}{2 \mathcal{N}} \left(\frac{1}{\tilde{F}_{n_i}^{(N)}(s)} + \frac{1}{\tilde{F}_{n_m}^{(N)}(s)} \right) \delta_{ij} + \frac{1}{2 \mathcal{N} \tilde{F}_{n_m}^{(N)}(s)},$$
 (B.11a)

$$B_{j} = -\frac{1}{N}(n_{j} - n_{m}). \tag{B.11b}$$

Introducing the change of variables

$$Y = X + \frac{ik}{2} A^{-1} B, (B.12)$$

we find

$$\mathbf{A} = -{}^{t}YAY + \frac{k^{2}}{4}{}^{t}BA^{-1}B, \qquad (B.13)$$

where we have used the fact that the matrix A^{-1} is symmetric. Hence, equation (B.9) reads

$$\widetilde{\mathcal{J}}(k) = \frac{\exp\left(-\frac{k^2}{4} {}^t B A^{-1} B\right)}{(2 \pi \widetilde{F}_{n_m}^{(N)}(s) \mathcal{N})^{1/2}} \int \cdots \int \left[\prod_{\substack{j=1 \ j \neq m}}^{\infty} \frac{\mathrm{d} y_j}{(2 \pi \widetilde{F}_{n_j}^{(N)}(s) \mathcal{N})^{1/2}} \right] \mathrm{e}^{-\iota Y_{AY}}.$$
(B.14)

Integration over the y_j 's gives a number independent of k. Taking the inverse Fourier transform of (B.14) leads back to

$$\Im(\langle n \rangle_{\mathcal{N}} - \langle n(s) \rangle) \sim \exp\left[-\frac{(\langle n \rangle_{\mathcal{N}} - \langle n(s) \rangle)^2}{2 \Lambda_{\mathcal{N}}^2(s)}\right]$$
 (B.15)

with

$$\Lambda_{\mathcal{N}}(s) = (\frac{1}{2} {}^{t}BA^{-1} B)^{1/2}. \tag{B.16}$$

Therefore, as one expects for large \mathcal{N} , the $\langle n \rangle_{\mathcal{N}}$ are normally distributed around $\langle n(s) \rangle$ with a mean standard deviation $\Lambda_{\mathcal{N}}(s)$ given by equation (B.16). Using expressions (B.11) $\Lambda_{\mathcal{N}}(s)$ becomes:

$$\Lambda_{\mathcal{N}}(s) = \left[\left(\frac{1}{2} \, {}^{t}ba^{-1} \, b \right) \, \tilde{F}_{n_{\text{inv}}}^{(N)}(s) \right]^{1/2} / \mathcal{N}^{1/2} \,, \tag{B.17}$$

in which the numerator does not depend anymore on \mathcal{N} , but only on the probabilities $F_{n_i}^{(N)}(s)$.

The matrices a and b are defined by :

$$a_{ij} = \frac{1}{2} \left(1 + \frac{\tilde{F}_{n_m}^{(N)}(s)}{\tilde{F}_{n_i}^{(N)}(s)} \right) \delta_{ij} + 1, \qquad (B.18a)$$

$$b_j = n_j - n_m. ag{B.18b}$$

The quadratic form ${}^tba^{-1}b$ is not analytically computable in general, except when the probability $F_n^{(N)}(s)$ is sharply peaked around the average walk length $\langle n(s) \rangle$. This occurs when the probability p for the walker to go to the right is small (or conversely 1-p is small). Let us notice that $F_n^{(N)}(s)$ is a delta function in the limit $p \to 0$. By choosing n_m as the nearest integer value to $\langle n(s) \rangle$ one can write:

$$a_{ij}^{-1} \approx 2 \frac{\tilde{F}_{n_j}^{(N)}(s)}{\tilde{F}_{-}^{(N)}(s)} \delta_{ij},$$
 (B.19)

since $\tilde{F}_{n_m}^{(N)}(s)$ is much greater than $\tilde{F}_{n_j}^{(N)}(s)$ for all $j \neq m$. Substituting (B.19) in (B.17) yields:

$$\Lambda_{\mathcal{N}}(s) \approx \sigma/\mathcal{N}^{1/2}$$
, (B.20)

where $\sigma^2 = \langle (n - \langle n \rangle)^2 \rangle$ is the variance of the first passage walk length. σ can be exactly computed using the methods exposed in section 3. In terms of the generating function $F^{(N)}(s, z)$, σ^2 reads:

$$\sigma^{2} = \frac{\partial^{2} F^{(N)}(s, z)}{\partial z^{2}} \bigg|_{z=1} + \frac{\partial F^{(N)}(s, z)}{\partial z} \bigg|_{z=1} - \left(\frac{\partial F^{(N)}(s, z)}{\partial z} \bigg|_{z=1}\right)^{2}. \tag{B.21}$$

From equations (3.6) and (3.19) we obtain:

$$\sigma^2 \approx 4 p(N-s)$$
 for $s \neq 1$ (B.22)

which yields through equation (B.20)

$$\Lambda_{\mathcal{N}}(s) = 2 p^{1/2} (N - s)^{1/2} / \mathcal{N}^{1/2}. \tag{B.23}$$

Now since the average walk length $\langle n_T(s) \rangle$ for a walker starting from the site s to be trapped at the origin can be deduced from $\langle n(s) \rangle$ by replacing either p by 1 - p or s by N - s in (3.20), we end with the following estimate of the mean standard deviation of $\langle n_T(s) \rangle$:

$$\Lambda_{T_{w}}(s) = 2(ps)^{1/2}/\mathcal{N}^{1/2}$$
 (B.24)

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