Order statistics for *d*-dimensional diffusion processes

S. B. Yuste* and L. Acedo†
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

Katja Lindenberg‡
Department of Chemistry and Biochemistry and Institute for Nonlinear Science, University of California San Diego, La Jolla, California 92093-0340

(Received 15 May 2001; published 26 October 2001)

We present results for the ordered sequence of first-passage times of arrival of N random walkers at a boundary in Euclidean spaces of d dimensions.

DOI: 10.1103/PhysRevE.64.052102 PACS number(s): 05.40.Fb, 66.30.Dn, 02.50.Ey

It is customary to assume that the important behaviors of a group of *independent* events can all be characterized by studying the behavior of one such event. For instance, one focuses on the mean time that it takes a single random walker to arrive somewhere even when there are many such random walkers in the system provided the walkers are independent. However, it is clear that there are situations in which one might be interested, for example, in the mean time for the *first* of the walkers to arrive somewhere or, more generally, in the ordered sequence of a particular outcome. The statistics of ordered outcomes clearly depends on the number N of events even when these are independent. For example, the mean time for the *first* of N walkers to arrive somewhere must clearly decrease with increasing N. The interest in so-called order statistics has grown with the development of experimental techniques that make it possible to follow single events on the microscopic scale. An example can be found in experiments in which fluorescent molecules in solution diffuse into a laser light cavity and individually emit quanta when leaving the cavity [1]. Another occurs in the study of the opening times of knots in vertically vibrated granular chains. A recent model of this process involves three (excluded volume but otherwise independent) random walkers, and the knot survival probability is related to the probability that all three walkers remain confined to a finite domain [2].

One way to characterize the behavior of N random walkers is to focus on the order statistics for the arrival at a boundary, and, in particular, on the mean and variance for the first arrival of the first, second, third, etc. walker out of a set of N. Most of the early literature dealt with mean arrival times in one dimension [3–5]. More recent literature has extended these concepts to fractal lattices [6–8] and has attempted to include higher-dimensional Euclidean lattices as well [8,9]. Some of these recent efforts [9] have relied on a parallel literature about another quantity of interest in these problems, namely, the distinct number of sites visited by N walkers [10]. In this approach the first arrival time statistics are obtained through a conjectured relation between arrival times and distinct number of sites visited. Yet another approach [8] relies on scaling arguments that are said to be independent of the underlying environment and can be applied in any dimension to both ordered and disordered structures. However, the results obtained in that work do not agree with any of the other published results (nor with those obtained herein), even in the well-established one-dimensional problem. This difference is apparent in the leading term of the result and also in the form of the series that follows the leading term. In addition to the order statistics and distinct number of sites visited, the behavior of N random walkers has also been characterized in terms of the maximal excursion [11–13].

In order to complete the N-independent-walker panorama, in this report we present results for the ordered sequence of first-passage times of arrival at a boundary in Euclidean spaces of d dimensions. This completion is made possible by a result reported in the maximal excursion literature [11]. The leading terms obtained here agree with those obtained earlier [9] and therefore confirm the conjecture made in that work (at least to leading order).

The calculation of ordered sequences of first-passage time moments is rather elaborate but has been laid out in detail in a number of previous papers [4–7]. These steps are easy to state but complex to carry out. The mth moment of the jth-passage time, that is, of the first arrival of the jth particle out of N at a (hyper-) spherical boundary at a distance r from the origin, is

$$\langle t_{j,N}^m(r)\rangle = \int_0^\infty t^m \psi_{j,N}(r,t)\,dt. \tag{1}$$

Here $\psi_{j,N}(r,t)$ is the probability density of the time it takes the jth particle to first reach the given distance r. The relationship between the probability distribution $\psi_{j,N}(r,t)$ and the first-passage time density of a single particle to this distance, $\psi(r,t)\equiv\psi_{1,1}(r,t)$, is standard in extreme-value theory [4,14,15],

$$\psi_{j,N}(r,t) = \frac{N!}{(N-j)!(j-1)!}\,\psi(r,t)h^{j-1}(r,t) \times[1-h(r,t)]^{N-j}. \tag{2}$$

Here $h(r,t)=\int_0^t \psi(r,\tau)\,d\tau$ is the mortality function, i.e., the probability that a single diffusing particle has reached the

*Email address: santos@unex.es
†Email address: acedo@unex.es
‡Email address: klindenberg@ucsd.edu

distance r during the time interval $(0,t)$. Asymptotic extreme-value theory for large N provides useful results directly for the distribution $\psi_{j,N}(r,t)$ [15]. For example, for $j \ll N$ Eq. (2) simplifies to

$$\psi_{j,N}(r,t) \approx \frac{N!}{(N-j)!(j-1)!}\psi(r,t)h^{j-1}(r,t) \times \exp[-(N-j)h(r,t)] \tag{3}$$

where now $h(r,t)$ stands for its short-time approximation [see Eq. (9) below]. On the other hand, knowledge of the function $\psi(r,t)$ [or $h(r,t)$] in principle also allows the full evaluation of first-passage time moments—provided one can carry out the integral in Eq. (1). Alternatively, one can calculate the generating function of the moments,

$$\mathcal{U}_{N,m}(z) = \sum_{j=1}^{N} \langle t_{j,N}^m \rangle z^{j-1}, \tag{4}$$

and from this obtain the moments via a Taylor series expansion in z.

Herein, of course, lies the difficulty of the problem: neither can the integral in Eq. (1) be done easily, nor can the generating function be calculated easily. Indeed, the literature is based on rather elaborate expansions to obtain the generating function, methods that rely on there being a very large number of walkers (N large), and on the walker of interest being one of the first few ($j \ll N$) so that short times dominate the moments. The formal results are similar from one system to another (Euclidean, fractal), the differences arising because of the differences in the mortality function and, specifically, in the short-time behavior of this function.

The mortality function (and particularly its short-time behavior) for one-dimensional systems was calculated in the early work on order statistics [4,5]. For certain deterministic fractal geometries this function was considered in more recent work [6,7]. In all of these, the short-time behavior of $h(r,t)$ has a ''universal'' form. It depends only on the combination t/r^2 (which we denote simply as τ, understanding that it is the distance-scaled time) and is given by

$$\tilde{h}(\tau) \approx A\tau^{\mu} e^{-\beta/\tau^{\gamma}}(1 + h_1\tau^{\delta}) \tag{5}$$

where the tilde just stresses the fact that this is an asymptotic result for $\tau \to 0$. The constants A, μ, β, γ, and δ vary from one system to another.

Although the mortality function for Euclidean systems has long been known and used in the random walk literature for a variety of problems [11,13,16], its short-time behavior for systems of dimension $d > 1$ has not been incorporated into the order statistics context. Perhaps not surprisingly, it turns out to fit the pattern Eq. (5) and therefore the existing theories can directly be applied to these systems. In particular, the time Laplace transform of the mortality function $h(r,s) = \mathcal{L}h(r,t)$ (indicated by the same symbol as the function but with the argument t replaced with the Laplace variable s) is [11]

$$sh(r,s) = \frac{2^{1-d/2}}{\Gamma(d/2)} \frac{(2dr^2 s)^{(d-2)/4}}{I_{d/2-1}(\sqrt{2dr^2 s})}, \tag{6}$$

where I_ν is a modified Bessel function of order ν, and

$$I_{d/2-1}(z) = \frac{e^z}{\sqrt{2\pi z}}\left[1 - \frac{(d-1)(d-3)}{8z} + O(z^{-2})\right] \tag{7}$$

for $z \gg 1$. In writing Eq. (6) an implicit choice of the diffusion coefficient D in the standard mean squared displacement relation $\langle r^2 \rangle = 2dDt$ has been made, namely, $D = 1/2d$, so that $\langle r^2 \rangle = t$ in each Euclidean dimension. The inverse Laplace transform of $s^\nu \exp(-as^{1/2})$ is [17]

$$\mathcal{L}^{-1}(s^\nu e^{-as^{1/2}}) = \frac{1}{2^{\nu+1/2}\pi^{1/2}t^{\nu+1}} e^{-a^2/(8t)} D_{2\nu+1}\left(\frac{a}{\sqrt{2t}}\right), \tag{8}$$

where $D_n(x)$ is a parabolic cylinder function (or Whitaker's function). Asymptotic expansion of this function for $x \gg |n|$ [18] leads for $r^2/t \gg 1$ to

$$h(r,t) = \frac{2}{\Gamma(d/2)}\left(\frac{dr^2}{2t}\right)^{-1+d/2} e^{-(dr^2/2t)}\left[1 + \frac{(d-3)}{2d}\frac{t}{r^2} + O\left(\frac{t^2}{r^4}\right)\right], \tag{9}$$

which is precisely of the form (5) with

$$A = \frac{2}{\Gamma(d/2)}\left(\frac{d}{2}\right)^{-1+d/2}, \tag{10}$$

$$\mu = 1 - \frac{d}{2}, \tag{11}$$

$$h_1 = \frac{d-3}{2d}. \tag{12}$$

Since the steps leading to the moment expansions are well documented in the literature once the form (5) has been established [4–7], we only present the results. For the mth moment of the first-passage time of the first of $N \gg 1$ particles we find

$$\langle t_{1,N}^m(r) \rangle = \left(\frac{dr^2}{2\ln\lambda_0 N}\right)^m \left\{1 + \frac{m}{\ln\lambda_0 N}(\mu \ln\ln\lambda_0 N - \gamma) + \frac{m}{2\ln^2\lambda_0 N}\left[(1+m)\left(\frac{\pi^2}{6} + \gamma^2\right) + 2\mu\gamma - h_1 d - 2\mu[\mu + (1+m)\gamma]\ln\ln\lambda_0 N + \mu^2(1+m)\ln^2\ln\lambda_0 N\right] + O\left(\frac{\ln^3\ln\lambda_0 N}{\ln^3\lambda_0 N}\right)\right\}, \tag{13}$$

where

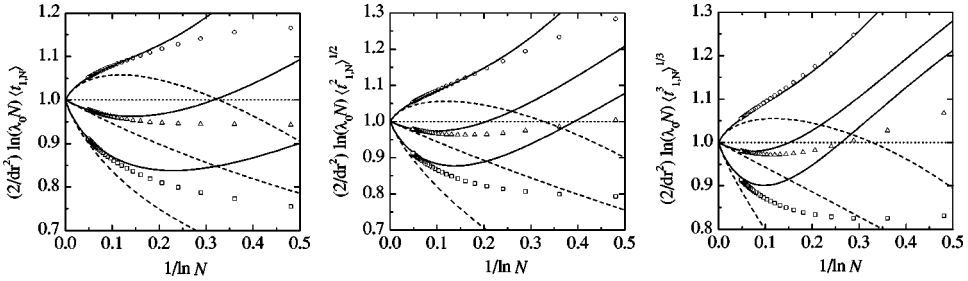

FIG. 1. Scaled moments for first arrival of the first of N particles at a prescribed boundary as a function of $1/\ln N$. First panel: first moment (i.e., mean first-passage time); second panel: second moment; third panel: third moment. Numerical results are indicated by circles ($d=1$), triangles ($d=2$), and squares ($d=3$). Asymptotic results [cf. Eq. (13)] to zeroth order, first order, and second order are shown by dotted curves, dashed curves, and solid curves, respectively.

$$\lambda_0=\frac{2}{\Gamma(d/2)}. \tag{14}$$

The mth moment of the first-passage time of the jth particle with $j\ll N$ is

$$\langle t_{j,N}^m(r)\rangle\approx\langle t_{1,N}^m(r)\rangle+\frac{(dr^2)^m m}{2^m\ln^{m+1}\lambda_0 N}\sum_{n=1}^{j-1}\frac{\mathbf{\Delta}_n(m)}{n}, \tag{15}$$

where

$$\mathbf{\Delta}_n(m)=1+\frac{m+1}{\ln\lambda_0 N}\left[(-1)^n\frac{S_n(2)}{(n-1)!}+\mu\ln\ln(\lambda_0 N)-\frac{\mu}{m+1}-\gamma\right]+O\left(\frac{\ln^2\ln\lambda_0 N}{\ln^2\lambda_0 N}\right), \tag{16}$$

and $S_i(n)$ is a Stirling number of the second kind [18]. In particular, the variance $\sigma_{j,N}^2(r)\equiv\langle t_{j,N}^2(r)\rangle-\langle t_{j,N}(r)\rangle^2$ can be obtained from Eqs. (15) and (13):

$$\sigma_{j,N}^2(r)=\left(\frac{dr^2}{2\ln^2\lambda_0 N}\right)^2\left[\frac{\pi^2}{6}-\left(\sum_{n=1}^{j-1}\frac{1}{n}\right)^2+\sum_{n=1}^{j-1}(-1)^n\frac{2S_n(2)}{n!}\right]\left[1+O\left(\frac{\ln^3\ln\lambda_0 N}{\ln\lambda_0 N}\right)\right]. \tag{17}$$

To check on the range of validity of these results it would be desirable to carry out direct computer simulations involving a very large number of walkers, an exercise that is costly. Another approach is to integrate numerically the exact Eq. (1) with Eq. (2) and the exact mortality function in the integrand for values of t beyond the range of validity of the short-time expansions. The survival probability, related to the mortality function of Eq. (2) by $S(r,t)\equiv 1-h(r,t)$, is known exactly in Euclidean geometries. In one dimension it is [13]

$$S(r,t)=\frac{4}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\exp\left[-\frac{(2n+1)^2\pi^2 t}{8r^2}\right]. \tag{18}$$

In two dimensions [13]

$$S(r,t)=\sum_{n=0}^{\infty}\frac{2}{x_{0n}J_1(x_{0n})}\exp\left[-\frac{x_{0n}^2 t}{4r^2}\right], \tag{19}$$

where J_1 is the first Bessel function and x_{0n} is the nth root of the Bessel function J_0. For $d=3$ one obtains the Hollingsworth distribution [16]

$$S(r,t)=1-\left(\frac{6r^2}{\pi t}\right)^{1/2}\sum_{n=-\infty}^{\infty}\exp\left[-\frac{3(2n+1)^2r^2}{2t}\right]. \tag{20}$$

To carry out the integration in Eq. (1) it is convenient to integrate by parts so that

$$\langle t_{j+1,N}^m(r)\rangle=\langle t_{j,N}^m(r)\rangle+m\frac{N!}{(N-j)!\,j!}\times\int_0^\infty t^{m-1}[1-S(r,t)]^j S(r,t)^{N-j}dt, \tag{21}$$

where

$$\langle t_{1,N}^m(r)\rangle=m\int_0^\infty t^{m-1}S(r,t)^N dt \tag{22}$$

and where Eq. (2) has been used. Note that these integrations become rather awkward for large values of N.

The numerical results and comparisons with asymptotic expressions are presented graphically in a set of figures. In Fig. 1 we present scaled results for the N dependence of $\langle t_{1,N}^m(r)\rangle^{1/m}$, that is, the $(1/m)$th power of the mth moment of the first-passage time of the first of N particles. The exact results obtained from the integration (22) are indicated by symbols and the theoretical results of various orders by lines. Circles denote exact results for $d=1$, triangles for $d=2$, and squares for $d=3$. The first panel shows results for $m=1$, that is, for the mean first-passage time of the first particle to the desired boundary; the second panel presents the second moment ($m=2$), and the third panel the third moment. The moments on the ordinates are scaled so that the scaled moment approaches 1 as $1/\ln N\to 0$. The integrations were performed for $N=2^3,2^4,\ldots,2^{30}$. The dotted curves correspond to the asymptotic results Eq. (13), to zeroth order, that is, only the first term in the series. The dashed lines include two terms, the solid lines three. Clearly the convergence to the exact results improves with order retained, but more slowly

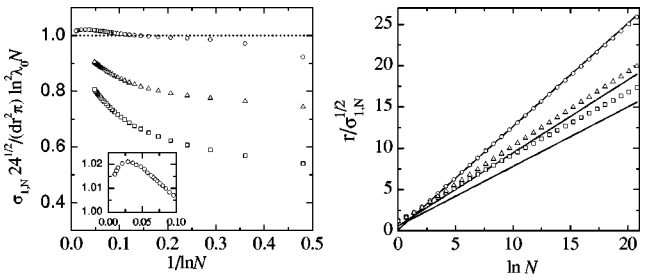

FIG. 2. N dependence of the variance for first arrival of first of N walkers at a prescribed boundary. Symbols and lines are as in Fig. 1. First panel: variance scaled so that the zeroth order asymptotic result is unity in all dimensions (indicated by the dotted line). Inset: detail of the $d=1$ numerical results. Second panel: same results, unscaled.

with increasing dimension. In any case, the deviations even at order 2 are clear on the scale of the figure at around $N=100$.

The two panels shown in Fig. 2 deal with the variance $\sigma_{1,N}^2(r)\equiv\langle t_{1,N}^2(r)\rangle-\langle t_{1,N}(r)\rangle^2$. The leading term in the large-N analysis of the variance is given in Eq. (17); for the variance we have only calculated this leading (zeroth order) term. In the first panel we present the $(1/\ln N)$-dependent behavior of the variance scaled in such a way that the leading term in the theoretical expression gives unity for all the dimensions $d=1,2,3$ (indicated by the dotted line in the figure). The circles ($d=1$), triangles ($d=2$), and squares ($d=3$) are the numerical results obtained from explicit integration. A number of interesting observations are apparent from this panel. First, we see that the leading term in the expansion of the variance leads to adequate results for some range of N only in one dimension. In two and three dimensions even for extremely large N it is necessary to go beyond zeroth order to obtain adequate analytic results. It is thus clear that the correction terms for the variance are much more important than for the first-passage time moments. This can be seen from our asymptotic expansions since the ratio of first-to-zeroth order terms goes as $\ln(\ln N)/\ln N$ for the moments but as $[\ln(\ln N)]^3/\ln N$ for the variance. In fact, the second actually *grows* with increasing N at first, becoming larger than unity, and only begins to decrease for extremely large values of N (of order $2^{30}\sim 10^9$). This in turn leads to the ''anomaly'' observed in the first panel and enlarged in the inset, namely, that the exact variance actually crosses and becomes *larger* than the zeroth order theoretical one before settling down to the asymptotic value at extremely large N. (We only carried the numerical calculations to these very large N values for one-dimensional systems and in fact reach the limit of numerical reliability in that region.)

The second panel in Fig. 2 shows the same information as the first but plotted in a different way to stress other features. It is simply a plot of $r\sigma_{1,N}^{-1/2}$ vs $\ln N$ comparing numerical (symbols) and zeroth order asymptotic (lines) results in one, two, and three dimensions. Again, it is clear that for $d=1$ the zeroth order asymptotic result is quite good but for higher dimensions it is not adequate.

In conclusion, we have filled some missing pieces in the mosaic of results for the order statistics of N independent random walkers in d-dimensional lattices. These results complement and confirm previous conjectures, indicate that large-N asymptotic expansions converge more rapidly in lower dimensions, and that convergence of higher cumulants such as variances is more problematic than that of first-passage time moments.

This work was supported in part by the Ministerio de Ciencia y Tecnología (Spain) through Grant No. BFM2001-0718 and by the Engineering Research Program of the Office of Basic Energy Sciences at the U.S. Department of Energy under Grant No. DE-FG03-86ER13606. S.B.Y. is also grateful to the DGES (Spain) for a sabbatical Grant No. PR2000-0116 and to the Department of Chemistry and Biochemistry of the University of California, San Diego for its hospitality.

[1] S. Nie, D. T. Chiu, and R. N. Zare, Science **266**, 1018 (1994).
[2] E. Ben-Naim, Z. A. Daya, P. Vorobieff, and R. E. Ecke, Phys. Rev. Lett. **86**, 1414 (2001).
[3] K. Lindenberg, V. Seshadri, K. E. Shuler, and G. H. Weiss, J. Stat. Phys. **23**, 11 (1980).
[4] G. H. Weiss, K. E. Shuler, and K. Lindenberg, J. Stat. Phys. **31**, 255 (1983).
[5] S. B. Yuste and K. Lindenberg, J. Stat. Phys. **85**, 501 (1996).
[6] S. B. Yuste, Phys. Rev. Lett. **79**, 3565 (1997).
[7] S. B. Yuste, Phys. Rev. E **57**, 6327 (1998).
[8] J. Dräger and J. Klafter, Phys. Rev. E **60**, 6503 (1999).
[9] S. B. Yuste and L. Acedo, J. Phys. A **33**, 507 (2000).
[10] H. E. Larralde, P. Trunfio, S. Havlin, H. E. Stanley, and G. H. Weiss, Nature (London) **355**, 423 (1992); Phys. Rev. A **45**, 7128 (1992); G. M. Sastry and N. Agmon, J. Chem. Phys. **104**, 3022 (1996); P. L. Krapivsky and S. Redner, J. Phys. A **29**, 5347 (1996); S. Redner and P. L. Krapivsky, Am. J. Phys. **67**, 1277 (1999); S. B. Yuste and L. Acedo, Phys. Rev. E **60**, R3459-62 (1999); **63**, 011105 (2001).
[11] R. Bidaux, J. Chave, and R. Vocka, J. Phys. A **32**, 5009 (1999).
[12] P. Erdös and M. Kac, Bull. Am. Math. Soc. **52**, 292 (1946); R. J. Rubin and G. H. Weiss, Macromolecules **11**, 1046 (1978); J. Koplik, S. Redner, and E. J. Hinch, Phys. Rev. E **50**, 4650 (1994).
[13] V. Seshadri and K. Lindenberg, J. Stat. Phys. **22**, 69 (1980).
[14] W. Feller, *An Introduction to Probability Theory and its Applications*, 2nd ed. (Wiley, New York, 1973), Vol. I; *An Introduction to Probability Theory and its Applications*, 3rd ed. (Wiley, New York, 1971), Vol. II.
[15] H. A. David, *Order Statistics* (Wiley, New York, 1970); J. Galambos, *The Asymptotic Theory of Extreme Order Statistics* (Wiley, New York, 1978).
[16] C. A. Hollingsworth, J. Chem. Phys. **16**, 544 (1948).
[17] *Table of Laplace Transforms*, edited by G. E. Roberts and H. Kaufman (Saunders, Philadelphia, 1966).
[18] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1972).