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Extrema Statistics of Wiener–Einstein Processes in One, Two, and Three Dimensions

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The maxima and first-passage-time statistics of Wiener–Einstein processes are evaluated analytically in one, two, and three dimensions. We show that the mean square maximum displacement has the same time dependence as the mean square displacement, i.e., it grows linearly with time. The ratio of the mean square maximum to the mean square displacement is shown to decrease with increasing dimensionality. We also calculate the mean first passage time for the process to attain a given absolute displacement and find that it grows as the square of the displacement *and is independent of the dimensionality of the process.* In addition, we evaluate the dispersion of maxima and of first passage times and discuss their dependence on dimensionality.

KEY WORDS: Maxima statistics; first-passage-time statistics; Wiener–Einstein processes; random walks.

1. INTRODUCTION

The theory of extremes is the study of the distribution of the extreme values (maxima or minima) of a random variable within a given time interval. The distribution of extreme values is closely related to the distribution of first passage times of the random variable to a prescribed boundary.

Most previous work on the theory of extremes deals with independent random variables.(1) The calculation of extreme value distributions and their moments is much more difficult for Markov dependent variables than for independent variables. Some aspects of the behavior of extreme value distributions for single-variable Markov processes described by a Fokker–Planck equation have been investigated and some asymptotic results have been obtained.(2,3)

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In this paper we examine the extrema statistics of a Wiener–Einstein (WE) process in one, two, and three dimensions. We chose this process for a variety of reasons. The WE process is one of the standard stochastic processes which have been studied extensively.[4] It finds application in problems such as heat conduction, diffusion, and polymer statistics. The simplicity of the WE process allows one to obtain analytic results for first-passage-time and maxima statistics without recourse to extensive numerical computations. Also, the discrete analog of the WE processes, i.e., the symmetric, nearest neighbor random walk, has been used to qualitatively and quantitatively model a variety of physical processes in crystals. Some examples include transport properties of crystalline[5] and amorphous[6] materials and quenching of elementary excitations in regular lattices.[6–9] The behavior of the extrema of a WE process can thus yield information about transport processes including diffusion and also about trapping behavior. It should be noted that most previous work on extrema of Markov processes is based on a separation of eigenvalues, which does not occur in the WE process, so that the results found there are not directly applicable here.[2,3],[2]

One of the quantities that we calculate in later sections is the mean square maximum excursion of the process from the point of origin as a function of time. Since the WE process does not include any systematic drift contributions, one might expect that this mean square maximum and the mean square displacement from the origin have the same time dependence. We will show that this is indeed the case, i.e., that the mean square maximum of a WE process grows linearly with time, and explicitly evaluate the constant of proportionality in one, two, and three dimensions. Our three-dimensional results agree with those of Hollingsworth and with those of Weidmann *et al.*[11] Our conclusion is crucially dependent on the absence of a restoring force toward a given point. We will show elsewhere that in the presence of such a restoring force, as, for example, in an Ornstein–Uhlenbeck process,[3] the time dependences of the mean square displacement and of the mean square maximum displacement are drastically different.[12]

Another quantity that we calculate for the WE process is the mean first passage time for the process to attain a given displacement from the origin. We will show that the mean first passage time grows as the square of the displacement, a result which is in accord with the linear growth of the mean square maximum displacement with time and is also a consequence of the absence of a drift term.[12]

To calculate the behavior of extrema we must first obtain expressions for the cumulative distribution function for the extrema. This distribution function is defined precisely in Section 2. It is there shown that properties

[2] See Ref. 10 for a different approach.

such as the mean first passage time for a stochastic process to attain a given value and the mean maximum of a process within a given time interval are respectively temporal and spatial moments of this cumulative distribution. In Section 3 we calculate the extrema distribution function and its moments for WE processes in one, two, and three dimensions. We conclude with a discussion of our results in Section 4.

2. REVIEW OF THE THEORY OF EXTREMA

Let the displacement of a process from the origin at time t be denoted by the random variable $X(t)$. We define $f(x, t)\,dx$ as the probability that $X(t)$ lies within $(x, x + dx)$ without ever having crossed $\pm\zeta$ in time $(0, t)$, given $X(0) = 0$. The maximum absolute displacement in the time interval $(0, t)$ is

$$Z(t) \equiv \max\{|X(\tau)|,\quad 0 \leqslant \tau \leqslant t\} \tag{2.1}$$

The cumulative distribution function $F(\zeta, t)$ is given by

$$F(\zeta, t) = \int_{-\zeta}^{\zeta} dx\, f(x, t) \tag{2.2}$$

and is the probability that $Z(t) < \zeta$. The first passage time $T(\zeta)$ is defined as the time at which the random variable $X(t)$ first crosses $\pm\zeta$, i.e.,

$$T(\zeta) \equiv \min\{\tau | X(\tau) = \pm\zeta\} \tag{2.3}$$

The first passage time and the cumulative distribution function are related by

$$F(\zeta, t) = \operatorname{Prob}\{T(\zeta) > t | X(0) = 0\} \tag{2.4}$$

The kth moments of the distributions of $Z(t)$ and $T(\zeta)$ are then respectively given by

$$Z_k(t) = k\int_0^\infty d\zeta\, \zeta^{k-1}[1 - F(\zeta, t)] \tag{2.5}$$

and

$$T_k(\zeta) = k\int_0^\infty dt\, t^{k-1} F(\zeta, t) \tag{2.6}$$

3. MAXIMA AND FIRST-PASSAGE-TIME STATISTICS

3.1. One Dimension

The one-dimensional WE process is defined by the equation

$$\partial p(x, t)/\partial t = D\, \partial^2 p(x, t)/\partial x^2 \tag{3.1}$$

where $p(x, t)\,dx$ is the probability that $X(t)$ lies within $(x, x + dx)$ given $X(0) = 0$. The distribution $f(x, t)$ for the probability that $X(t)$ lies within $(x, x + dx)$ without ever having crossed $\pm\zeta$ satisfies Eq. (3.1) with absorbing boundaries at $x = \pm\zeta$.[3] The solution for $f(x, t)$ with the initial condition $f(x, 0) = \delta(x)$ is easily obtained to be[10]

$$f(x, t) = \frac{1}{\zeta}\sum_{n=0}^{\infty}\cos\left[\frac{(2n + 1)\pi x}{2\zeta}\right]\exp\left[-\frac{D(2n + 1)^2\pi^2 t}{4\zeta^2}\right] \tag{3.2}$$

The cumulative distribution function $F(\zeta, t)$ of (2.2) is given by

$$F(\zeta, t) = \int_{-\zeta}^{\zeta} f(x, t)\,dx = 2\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n + 1)\pi/2}\exp\left[-\frac{D(2n + 1)^2\pi^2 t}{4\zeta^2}\right] \tag{3.3}$$

We first Laplace-transform Eq. (3.3), and sum the resulting series by contour integration to obtain

$$\tilde{F}(\zeta, \epsilon) = (1/\epsilon)\{1 - \operatorname{sech}[\zeta(\epsilon/D)^{1/2}]\} \tag{3.4}$$

Using Eqs. (2.5) and (3.4) gives $\tilde{Z}_2(\epsilon) = 4DG/\epsilon^2$, where $G = 0.915965594...$ is the Catalan number.[13] The inverse Laplace transform of $\tilde{Z}_2(\epsilon)$ yields

$$Z_2(t) = 4DGt = 3.6638...Dt \tag{3.5}$$

A similar calculation for the maximum displacement yields $Z_1(t) = (\pi Dt)^{1/2}$, which leads to the dispersion $\gamma \equiv \{[Z_2(t) - Z_1^2(t)]/Z_1^2(t)\}^{1/2} = 0.4077....$

Let us examine the first-passage-time moments. After some algebra, Eqs. (2.6) and (3.4) yield

$$T_1(\zeta) = \zeta^2/2D \tag{3.6}$$

and

$$T_2(\zeta) = \tfrac{5}{12}\zeta^4/D^2 \tag{3.7}$$

The dispersion is $\sigma \equiv \{[T_2(\zeta) - T_1^2(\zeta)]/T_1^2(\zeta)\}^{1/2} = (2/3)^{1/2}$.

In Appendix A we obtain the corresponding results for a discrete, one-dimensional, symmetric random walk.

3.2. Two Dimensions

The WE process in two dimensions is

$$\frac{\partial p(x, y, t)}{\partial t} = \frac{D}{2}\left[\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right] \tag{3.8}$$

In polar coordinates (r, θ), the distribution function is independent of θ for θ-independent initial conditions. Thus, Eq. (3.8) reduces to

$$\frac{\partial P(r, t)}{\partial t} = \frac{D}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right]P(r, t) \tag{3.9}$$

where $p(x, y, t)\, dx\, dy = 2\pi P(r, t) r\, dr$. The distribution function $f(r, t)$, which represents the probability density that the process is within dr of r at time t without ever having crossed $r = \zeta$, satisfies Eq. (3.9) with a circular absorbing boundary at $r = \zeta$. A solution that satisfies these conditions and obeys the initial condition $f(r, 0) = \delta(r)/r$ can easily be shown to be

$$f(r, t) = \sum_{m=0}^{\infty} \frac{2}{\zeta^2[J_1(x_{0m})]^2} J_0\left(\frac{x_{0m} r}{\zeta}\right) \exp -\frac{D x_{0m}^2 t}{2\zeta^2} \tag{3.10}$$

where J_0 and J_1 are the zeroth and first Bessel functions and x_{0m} is the mth root of the Bessel function J_0. The cumulative distribution function is given by[14]

$$F(\zeta, t) = \int_0^{\zeta} r f(r, t)\, dr$$

$$= \sum_{m=0}^{\infty} \frac{2}{x_{0m} J_1(x_{0m})} \exp -\frac{D x_{0m}^2 t}{2\zeta^2} \tag{3.11}$$

We Laplace-transform (3.11) and sum the resulting series using contour integration to obtain

$$\tilde{F}(\zeta, \epsilon) = \frac{1}{\epsilon} - \frac{1}{\epsilon I_0(\zeta(2\epsilon/D)^{1/2})} \tag{3.12}$$

where I_0 is the zeroth Bessel function of imaginary argument. We now proceed to calculate the moments of the distribution of maxima. Using Eq. (3.12) in the Laplace transform of (2.5) and inverse-transforming, we obtain

$$Z_2(t) = \left[D \int_0^{\infty} \frac{x\, dx}{I_0(x)}\right] t \tag{3.13}$$

We have evaluated the integral in (3.13) numerically. The result is

$$Z_2(t) = 3.0688... Dt \tag{3.14}$$

We similarly find for the first moment of the maximum displacement $Z_1(t) = 1.6622...(Dt)^{1/2}$. The dispersion in this case is $\gamma = 0.3327...$.

To obtain the first-passage-time moments we proceed as in one dimension. From Eqs. (3.12) and (2.6) we obtain

$$T_1(\zeta) = \zeta^2/2D \tag{3.15}$$

and

$$T_2(\zeta) = 3\zeta^4/8D^2 \tag{3.16}$$

Hence the dispersion in two dimensions is $\sigma = 1/\sqrt{2}$.

3.3. Three Dimensions

A WE process in three dimensions is given by the equation

$$\frac{\partial p}{\partial t} = \frac{D}{3}\left[\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2}\right] \tag{3.17}$$

The equation of evolution of the probability distribution in spherical polar coordinates (r, θ, ϕ) is

$$\frac{\partial P}{\partial t} = \frac{D}{3r}\frac{\partial^2 (rP)}{\partial r^2} \tag{3.18}$$

where we have exploited the symmetry of the problem to set the derivatives with respect to θ and ϕ equal to zero. Once again the distribution function $f(r, t)$ defined earlier is the solution to a boundary value problem for Eq. (3.18) with an absorbing boundary at $r = \xi$. The solution for the initial condition $f(r, 0) = \delta(r)/r^2$ is

$$f(r, t) = \sum_{m=1}^{\infty} \frac{2m\pi}{\zeta^2}\frac{\sin(m\pi r/\zeta)}{r}\exp\frac{-Dm^2\pi^2 t}{3\zeta^2} \tag{3.19}$$

as also found by Weidmann *et al.*[11] The Laplace transform of the cumulative distribution function corresponding to (3.19) can be summed exactly and used in Eq. (2.5) to yield[11]

$$Z_2(t) = 2.8048...Dt \tag{3.20}$$

For the first moment we find $Z_1(t) = (\pi^3 Dt/12)^{1/2}$, so that the dispersion is $\gamma = 0.2924....$

The moments of the first-passage-time distribution are given by

$$T_1(\zeta) = \zeta^2/2D \tag{3.21}$$

and

$$T_2(\zeta) = 7\zeta^4/20D^2 \tag{3.22}$$

The dispersion in three dimensions is thus $\sigma = (2/5)^{1/2}$.

4. DISCUSSION

Our main results are summarized in Table I. The trends that can be seen from the table are the following:

(a) The mean square maximum displacement $Z_2(t)$ approaches the mean square displacement $X_2(t) = 2Dt$ as the dimensionality of the system increases. To further confirm this statement, we have computed the ratio $Z_2(t)/X_2(t)$ in four dimensions and find that it is equal to 1.33.... The reason

Table I. Extrema for the Wiener–Einstein Process[a]

Dimension	Z_2/X_2	$[(Z_2 - Z_1^2)/Z_1^2]^{1/2}$	T_1	$[(T_2 - T_1^2)/T_1^2]^{1/2}$
1	1.8319	0.4077	$\zeta^2/2D$	$(2/3)^{1/2}$
2	1.5344	0.3327	$\zeta^2/2D$	$(2/4)^{1/2}$
3	1.4024	0.2924	$\zeta^2/2D$	$(2/5)^{1/2}$

[a] $X_2(t)$ is the mean square displacement and is equal to $2Dt$.

for this monotonic behavior is that as dimensionality increases, a WE process is less likely to return to a previously covered spatial region, so that the displacement and the maximum displacement are more likely to coincide.

(b) The dispersion in the maximum displacement of WE processes is finite for all dimensions. This behavior is quite different from that of a process with a restoring force toward a point, e.g., an Ornstein–Uhlenbeck process, since in the latter this dispersion vanishes at long times.[3] The decrease in the dispersion of the maximum displacement with increasing dimensionality is again due to the fact that the WE process is less likely to revisit previously visited regions.

(c) The mean first passage time to a distance ζ from the origin is the same in one, two, and three dimensions. In Appendix B we use a hierarchy of differential equations obeyed by the first-passage-time moments to arrive at the remarkable result that *the mean first passage time is in fact the same in all dimensions*. It should be noted that the first passage times considered here are different from those of Montroll and Weiss.[9] They calculate first passage times to one or more lattice sites that do not enclose the origin, while we consider first passage to a surface that completely surrounds the origin of the WE process.

(d) The dispersion in the first passage time to a prescribed boundary is finite in all dimensions, as shown in Table I for one, two, and three dimensions and in the Appendix for all dimensions. The dispersion decreases slowly with dimensionality. We note that this result persists even when there is a restoring force toward a point.[3]

APPENDIX A

The discrete, one-dimensional, symmetric random walk problem is defined by the difference equation[8]

$$P_{n+1}(l) = \tfrac{1}{2}[P_n(l-1) + P_n(l+1)] \tag{A1}$$

where $P_n(l)$ is the probability of occupation of site l at the nth step. The distribution $f_n(l)$, which is the probability that the walker is at site l on the

nth step without ever having crossed $\pm s$, is obtained by solving this difference equation with absorbing boundaries at $l = \pm s$.[3] The cumulative distribution function is the sum of $f_n(l)$ over all sites within the boundaries, i.e.,

$$F_n(s) = \sum_{l=-s+1}^{s-1} f_n(l) \tag{A2}$$

Let $Q(s, z)$ be the generating function for $F_n(s)$, i.e.,

$$Q(s, z) = \sum_{n=0}^{\infty} z^n F_n(s) \tag{A3}$$

This generating function can be related to that of a perfect ring of $2s$ sites,[8,10] with the result

$$Q(s, z) = \frac{1}{1 - z}\left(1 - \frac{2x^s}{1 + x^{2s}}\right) \tag{A4}$$

where $x = [1 - (1 - z^2)^{1/2}]/z$.

The moments of the distribution of absolute maxima can be obtained from the generating function (A4) via the relation

$$Z_{k,n} = k \sum_{s=0}^{\infty} s^{k-1}[1 - F_n(s)] \tag{A5}$$

Consider $Z_{2,n}$, the mean of the square of the maximum displacement within $(0, n)$. For this purpose we define a generating function $Z_{2,z}$ as

$$Z_{2,z} = \sum_{n=0}^{\infty} z^n Z_{2,n} \tag{A6}$$

Substituting Eq. (A4) in (A5) with $k = 2$ gives

$$Z_{2,z} = \frac{1}{1 - z} \sum_{s=0}^{\infty} s \frac{2x^s}{1 + x^{2s}} \tag{A7}$$

A straightforward application of the Euler–McLaurin formula[15] to Eq. (A7) yields

$$Z_{2,z} = \frac{2}{1 - z}\left[\frac{2G}{(\log x)^2} - \frac{1}{12} + \cdots\right] \tag{A8}$$

where G is the Catalan number. By construction, the quantity $Z_{2,n}$ is the coefficient of z^n in the expansion of $Z_{2,z}$ in a power series in z. An expansion of the right-hand side of (A8) in powers of z valid for all n is very cumbersome, but an elegant asymptotic expansion can be obtained for large n by using a Tauberian theorem.[16] The result is

$$Z_{2,n} \sim 2Gn \tag{A9}$$

A completely analogous calculation can be done to obtain $Z_{1,n}$, the mean of the maximum displacement. The asymptotic result is $Z_{1,n} \sim (\pi n/2)^{1/2}$. The dispersion in the maximum displacement is then $\gamma = 0.4077\ldots$.

We now examine the first-passage-time moments. From the relation

$$T_k(s) = k \sum_{n=0}^{\infty} n^{k-1} F_n(s) \tag{A10}$$

and Eq. (A3) we obtain

$$T_1(s) = \lim_{z \to 1} Q(s, z) \tag{A11}$$

$$T_2(s) = \lim_{z \to 1} \frac{\partial Q(s, z)}{\partial z} \tag{A12}$$

Using the formulas in Eq. (15) of Ref. (8), we can expand $Q(s, z)$ in a power series in $(1 - z)$. Substituting this series into (A11) and (A12) results in

$$T_1(s) = s^2 \tag{A13}$$

and

$$T_2(s) = \tfrac{5}{3} s^2 (s^2 - 1) \tag{A14}$$

The dispersion in one dimension is $\sigma \sim (2/3)^{1/2}$ for large s.

The continuum results (3.5)–(3.7) for the temporal and spatial moments are identical to the corresponding discrete results obtained above if one uses the relation $D = \lim_{a,\tau \to 0} a^2/2\tau$, where a is the step size and τ is the time between steps.

We note that formulas for the cumulative distribution function (A2) and for the first-passage-time moments (A10) have been given by Spitzer[17] for a general one-dimensional random walk with finite variance.

In two and three dimensions the extrema for a discrete random walk problem are difficult to obtain, for two reasons. First, no closed, analytic expressions exist for the lattice Green's functions that one needs to solve the extrema problem. Second, the boundary value problem obtained by defining an appropriate lattice analog of a sphere leads to absurdly difficult mathematics. On the other hand, we expect the extrema statistics of the discrete problem to be well represented by those of the corresponding continuum process for long times and large distances.

APPENDIX B

For spherically symmetric initial conditions the WE process in d dimensions is

$$\frac{\partial P(r, t|r_0)}{\partial t} = \frac{D}{d} \frac{1}{r^{d-1}} \frac{\partial}{\partial r} r^{d-1} \frac{\partial}{\partial r} P(r, t|r_0) \tag{B1}$$

[cf. Eqs. (3.1), (3.9), and (3.18) for $d = 1$, 2, and 3, respectively], where we have indicated the initial position r_0 explicitly. Since the solution of (B1) is a function only of $(r - r_0)$, we can write (B1) as a "backward equation,"[4] i.e.,

$$\frac{\partial P(r, t|r_0)}{\partial t} = \frac{D}{d} \frac{1}{r_0^{d-1}} \frac{\partial}{\partial r_0} r_0^{d-1} \frac{\partial}{\partial r_0} P(r, t|r_0) \tag{B2}$$

From this equation we can obtain a hierarchy of equations for the first-passage-time moments by multiplying by t^n and by r^{d-1} and integrating over t and over the position coordinate r.[18,19] The result is

$$\frac{D}{d} \frac{1}{r_0^{d-1}} \frac{\partial}{\partial r_0} r_0^{d-1} \frac{\partial}{\partial r_0} T_n(\zeta|r_0) = -nT_{n-1}(\zeta|r_0) \tag{B3}$$

where $T_0(\zeta|r_0) \equiv 1$ and where we have explicitly indicated the initial position r_0 in the first-passage-time moments. The boundary conditions for (B3) with $n \geqslant 1$ are

$$T_n(\zeta|\pm\zeta) = 0 \qquad \text{for} \quad d = 1 \tag{B4a}$$

$$\left.\begin{aligned} T_n(\zeta|\zeta) &= 0 \\ T_n(\zeta|0) &= \text{finite} \end{aligned}\right\} \quad \text{for} \quad d \geqslant 2 \tag{B4b}$$

The integration of (B3) with $n = 1$ and with the boundary conditions (B4) is straightforward and yields

$$T_1(\zeta|r_0) = \frac{\zeta^2}{2D} - \frac{r_0^2}{2D} \tag{B5}$$

for all dimensions. This reduces to the results in the text when $r_0 = 0$. Inserting (B5) into the right side of (B3) for $n = 2$ and integrating gives

$$T_2(\zeta|0) = \frac{\zeta^4}{4D^2} \left(\frac{d + 4}{d + 2}\right) \tag{B6}$$

which reduces to the results in the text when $d = 1$, 2, and 3. The dispersion obtained from (B6) and (B5) is

$$\sigma = \left(\frac{T_2 - T_1^2}{T_1^2}\right)^{1/2} = \left(\frac{2}{d + 2}\right)^{1/2} \tag{B7}$$

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