Nontrivial Exponent for Simple Diffusion

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The diffusion equation $\partial_t \phi = \nabla^2 \phi$ is considered, with initial condition $\phi(\mathbf{x}, 0)$, a Gaussian random variable with zero mean. Using a simple approximate theory we show that the probability $p_n(t_1, t_2)$ that $\phi(\mathbf{x}, t)$ (for a given space point $\mathbf{x}$) changes sign n times between t_1 and t_2 has the asymptotic form $p_n(t_1, t_2) \sim c_n[\ln(t_2/t_1)]^n (t_1/t_2)^{-\theta}$. The exponent θ has predicted values 0.1203, 0.1862, 0.2358 in dimensions $d = 1, 2, 3$, in remarkably good agreement with simulation results. [S0031-9007(96)01324-5]

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The diffusion equation $\partial_t \phi = \nabla^2 \phi$ is one of the fundamental equations of classical physics. The exact solution of this simple equation, for an arbitrary initial condition $\phi(\mathbf{x}, 0)$, can be written down explicitly: $\phi(\mathbf{x}, t) = \int d^d x\, G(\mathbf{x} - \mathbf{x}', t) \phi(\mathbf{x}', 0)$, where $G(\mathbf{x}, t) = (4\pi t)^{-d/2} \exp(-x^2/4t)$ is the Green's function (or "heat kernel") in d dimensions. The solution is characterized by a single growing length scale, the "diffusion length" $L(t) \sim t^{1/2}$. It may come as a surprise, therefore, to discover that there is a nontrivial exponent associated with this simple process.

It is the purpose of this Letter to point out that the solutions of the diffusion equation exhibit some remarkable and unexpected properties associated with their time evolution, and to present a simple theory which accounts for this behavior. We consider specifically a class of initial conditions where $\phi(\mathbf{x}, 0)$ is a Gaussian random variable with zero mean. Our basic question is the following. What is the probability $p_0(t)$ that the field ϕ at a particular point $\mathbf{x}$ has not changed sign up to time t? Precise numerical simulations in $d = 1$ and 2, discussed below, demonstrate a power-law decay of the form $p_0(t) \sim t^{-\theta}$, with $\theta = 0.1207 \pm 0.0005$ for $d = 1$ and 0.1875 ± 0.0010 for $d = 2$. We will present a simple analytic treatment which gives results in extraordinarily good agreement with the simulations. Furthermore, the analysis gives the more general result $p_n(t_1, t_2) \sim c_n[\ln(t_2/t_1)]^n (t_1/t_2)^{-\theta}$ for the probability that the field changes sign n times between t_1 and t_2, for $t_2 \gg t_1$. The key idea underlying these results is that the Gaussian process $\phi(\mathbf{x}, t)$ is a Gaussian *stationary* process in terms of a new time variable $T = \ln t$. The central assumption in the analysis is that the intervals between successive zeros of $\phi(\mathbf{x}, T)$ can be treated as independent.

Exponents θ analogous to that introduced above have recently excited much interest in other contexts [1–10]. The simplest such system is the $d = 1$ Ising model at temperature $T = 0$. For evolution under Glauber dynamics from a random initial state, the probability that a given spin has not flipped up to time t decays as $t^{-\theta}$, with $\theta = 3/8$, though the proof of this is surprisingly subtle [6]. This $d = 1$ method is difficult to extend to higher dimensions, although values for θ have been obtained numerically [1,3,4,7]. An approximate method for general dimensions has recently been developed [7], whose predictions are consistent with simulation results. In general, the nontriviality of $p_0(t)$ is a consequence of the fact that it probes the entire history of a non-Markovian process.

We begin by presenting the theoretical approach and the numerical simulation results. Experimental ramifications will be discussed briefly at the end of the Letter. Other contexts in which a nontrivial exponent θ might be expected will also be discussed.

The starting point for the discussion of the diffusion equation is the expression for the autocorrelation function of the variable $X(t) = \phi(\mathbf{x}, t)/\langle[\phi(\mathbf{x}, t)]^2\rangle^{1/2}$ for some fixed point $\mathbf{x}$. For "white noise" initial conditions, $\langle \phi(\mathbf{x}, 0) \phi(\mathbf{x}', 0) \rangle = \delta^d(\mathbf{x} - \mathbf{x}')$, this takes the form

$$a(t_1, t_2) \equiv \langle X(t_1) X(t_2) \rangle = [4 t_1 t_2/(t_1 + t_2)^2]^{d/4}. \quad (1)$$

More generally, this form is asymptotically correct provided the initial condition correlator is sufficiently short ranged (it must decrease faster than $|\mathbf{x} - \mathbf{x}'|^{-d}$).

Introducing the new time variable $T = \ln t$, one sees that the autocorrelation function becomes $a(T_1, T_2) = f(T_1 - T_2)$, where $f(T) = [\mathrm{sech}(T/2)]^{d/2}$. Thus the process $X(T)$ is *stationary* (the Gaussian nature of the process ensures that all higher-order correlators are also time-translation invariant). This is an important simplification. Note that the anticipated form of the probability of $X(t)$ having no zeros between t_1 and t_2, $p_0(t_1, t_2) \sim (t_1/t_2)^{\theta}$ for $t_2 \gg t_1$, becomes an exponential decay $p_0 \sim \exp[-\theta(T_2 - T_1)]$ in the new time variable. This reduces the calculation of an exponent to the calculation of a decay rate [7]. The only approximation we shall make is that the intervals between successive zeros of $X(T)$ are statistically independent. This "independent interval approximation" (IIA) was introduced in another context some forty years ago [11]. We shall find that it is an extraordinarily good approximation for the diffusion equation.

As a preliminary step, we introduce the "clipped" variable $\sigma = \mathrm{sgn}(X)$, which changes sign at the zeros of $X(t)$. Clearly, the correlator $A(T) = \langle \sigma(0)\sigma(T)\rangle$ is determined solely by the distribution $P(T)$ of the intervals between zeros. The strategy is to determine $P(T)$ from $A(T)$, and $p_0(T)$ from $P(T)$. To this end we note first that

$$A(T) = \frac{2}{\pi}\sin^{-1}[a(T)] = \frac{2}{\pi}\sin^{-1}\Big([\mathrm{sech}\,(T/2)]^{d/2}\Big), \tag{2}$$

where the first equality holds for any Gaussian process.

Next, one expresses $A(T)$ in terms of the interval-size distribution $P(T)$. Clearly,

$$A(T) = \sum_{n=0}^{\infty}(-1)^n p_n(T), \tag{3}$$

where $p_n(T)$ is the probability that the interval T contains n zeros of $X(T)$. We define $Q(T)$ to be the probability that an interval of size T to the right or left of a zero contains no further zeros. Then $P(T) = -Q'(T)$. For $n \geq 1$ one obtains immediately

$$\begin{aligned} p_n(T) = \langle T\rangle^{-1}\int_0^T dT_1\int_{T_1}^T dT_2\cdots\int_{T_{n-1}}^T \\ \times\, dT_n\, Q(T_1)P(T_2 - T_1)\cdots P(T_n - T_{n-1}) \\ \times\, Q(T - T_n), \end{aligned} \tag{4}$$

where $\langle T\rangle$ is the mean interval size. One has made the IIA by writing the joint distribution of n successive zero-crossing intervals as the product of the distribution of single intervals. Taking Laplace transforms gives $\tilde{p}_n(s) = [\tilde{Q}(s)]^2[\tilde{P}(s)]^{n-1}/\langle T\rangle$. But $P(T) = -Q'(T)$ implies $\tilde{P}(s) = 1 - s\tilde{Q}(s)$, where we have used $Q(0) = 1$. Using this to eliminate $\tilde{Q}(s)$ gives the final result

$$\tilde{p}_n(s) = \frac{1}{\langle T\rangle s^2}[1 - \tilde{P}(s)]^2[\tilde{P}(s)]^{n-1}, \quad n \geq 1, \tag{5}$$

$$= \frac{1}{\langle T\rangle s^2}[\langle T\rangle s - 1 + \tilde{P}(s)], \quad n = 0, \tag{6}$$

where the result for $\tilde{p}_0(s)$ follows from the normalization condition $\sum_{n=0}^{\infty} p_n(t) = 1$, which gives $\sum_{n=0}^{\infty}\tilde{p}_n(s) = 1/s$.

Finally the Laplace transform of (3) gives $\tilde{A}(s) = \sum_{n=0}^{\infty}(-1)^n\tilde{p}_n(s)$. Performing the sum employing (5) and (6), and using the result to express $\tilde{P}(s)$ in terms of $\tilde{A}(s)$, gives the desired result

$$\tilde{P}(s) = [2 - F(s)]/F(s), \tag{7}$$

where

$$F(s) = 1 + (\langle T\rangle/2)\, s[1 - s\tilde{A}(s)]. \tag{8}$$

Equations (5)–(8) are a general consequence of the independent interval approximation. The function $F(s)$, defined by (8), is completely determined by the autocorrelation function $A(T)$, and contains all the information needed to compute the probabilities $p_n(T)$. We have in mind, of course, to apply this approach to the diffusion equation, where $A(T)$ is given by (2). For this case the mean interval size $\langle T\rangle$, required in (8), can be simply evaluated. For $T \to 0$, the probability to find a zero in the interval T is just $T/\langle T\rangle$, so $A(T) \to 1 - 2T/\langle T\rangle$. This gives $\langle T\rangle = -2/A'(0) = \pi\sqrt{8/d}$, using (2) in the final step.

We note a very important point at this stage. The fact that $A'(0)$ is finite [i.e., $f'(0) = 0$ and $f''(0) \neq 0$] is special to the diffusion equation, which allows us to use the IIA. Physically, this means that the density of zeros is a finite number. However, for many Gaussian stationary processes, such as the one that arises in an approximate treatment of the Ising model [7], $f'(0) \neq 0$, implying that $A'(0)$ diverges. In this case, the IIA cannot be used. For such processes, the variational and perturbative methods developed in Ref. [7] give reasonably accurate results.

The asymptotics of $p_0(T)$ are controlled by the singularity of $\tilde{p}_0(s)$ with the largest real part, i.e. [from (6)], by the corresponding singularity of $\tilde{P}(s)$. The expectation that $p_0(T) \sim \exp(-\theta T)$ suggests that this singularity is a simple pole, i.e., that $F(s)$ has a simple zero at $s = -\theta$. Using (2) in (8), and inserting $\langle T\rangle = \pi\sqrt{8/d}$, gives

$$F(s) = 1 + \pi\left(\frac{2}{d}\right)^{1/2} s\left\{1 - \frac{2s}{\pi}\int_0^{\infty} dT\, \exp(-sT)\sin^{-1}\left[\mathrm{sech}^{d/2}\left(\frac{T}{2}\right)\right]\right\}. \tag{9}$$

Clearly, $F(0) = 1$, while $F(s)$ diverges to $-\infty$ for $s \to -d/4$. Between these two points $F(s)$ is monotonic, implying a single zero in the interval $(-d/4, 0)$. Solving (9) numerically for this zero, and identifying the result with $-\theta$, gives the values of θ shown in Table I. For future reference, we note from (7) that the residue R of the corresponding pole of $\tilde{P}(s)$ is $R = 2/F'(-\theta)$. The values of R, which control the amplitude of the asymptotic decay of $p_n(T)$, are also given in Table I. Recall that the behavior $p_0(T) \sim \exp(-\theta T)$ translates in "real" time to a decay law $p_0(t) \sim t^{-\theta}$ for the probability that ϕ at a given point has not changed sign. It is also easy to extract the large-d behavior of θ from Eq. (9): We find, to leading order in d, $\theta \approx 0.145\,486\sqrt{d}$.

TABLE I. Exponents θ from theory (θ_{th}) and simulations (θ_{sim}), and the value of the residue R (see text), for various spatial dimensions d.

d	θ_{th}	θ_{sim}	R
1	0.1203	0.1207 ± 0.0005	0.1277
2	0.1862	0.1875 ± 0.0010	0.2226
3	0.2358	0.2380 ± 0.0015[a]	0.2940
4	0.2769	⋯	0.3527
5	0.3128	⋯	0.4033

[a]The "$d = 3$" simulation result refers to a $d = 1$ simulation with correlated initial conditions (see text).

The predicted values of θ were tested in $d = 1$ and 2 by numerical simulations. The diffusion equation was discretized in space and time in the form

$$\phi_i(t+1) = \phi_i(t) + a\sum_j[\phi_j(t) - \phi_i(t)], \qquad (10)$$

where j runs over the nearest neighbors of i on a linear ($d = 1$) or square ($d = 2$) lattice. A stability analysis shows that the solution is unstable for $a \geq a_c = 1/(2d)$. Preliminary studies showed that the asymptotic exponent is independent of a for $a < a_c$, but that a value $a = a_c/2$ seems to give the quickest onset of the asymptotic behavior. This value was therefore used in all simulations reported here. Systems of 2^{20} (2^{22}) sites were studied in $d = 1$ ($d = 2$), for times up to 2^{17} (2^{12}). Data for longer times in $d = 2$ suffer from noticeable finite-size effects. The initial values of ϕ_i were chosen independently from a Gaussian distribution of zero mean. Using a rectangular distribution gave the same asymptotic exponent within the errors. Several random number generators were tried: All gave consistent results (within the errors).

The simulation results are presented in Fig. 1. The data are an average of 17 ($d = 1$) and 22 ($d = 2$) runs with independent initial conditions. An effective exponent $\theta(t)$ is extracted from a least-squares fit of $\log_2 p_0$ against $\log_2 t$ over five consecutive values of $\log_2 t$. The error bars shown in the figure were obtained from the fits. The resulting exponent $\theta(t)$ is then plotted against $1/\log_2 t$, where here $\log_2 t$ is the midpoint of the five values. The best estimates of θ, shown in Table I, were obtained by plotting $t^\theta p_0(t)$ against $\log_2 t$ and choosing θ such that, after an initial transient, the data show no systematic upward or downward trend with increasing t. The agreement with the theoretical predictions (Table I) is quite remarkable, showing that the IIA is an extraordinarily good approximation in this context.

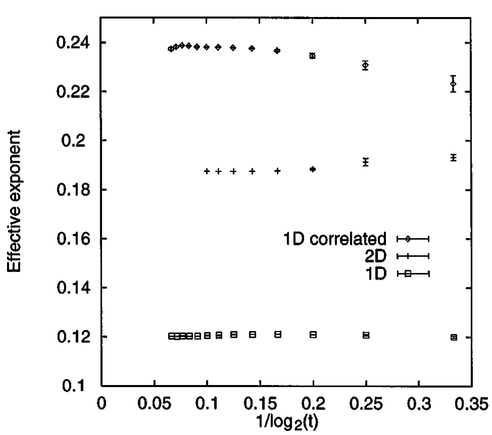

FIG. 1. Effective exponents $\theta(t)$ plotted against $1/\log_2 t$ for the diffusion equation in $d = 1$ (lower data set), $d = 2$ (middle set), and $d = 1$ with correlated initial conditions (upper set). The downturn in the upper set at late times is not statistically significant (note the larger errors on the last two points). The best estimates of θ are given in Table I.

The case of correlated initial conditions is also of interest. If the Fourier-space correlations are $\langle\phi_{\mathbf{k}}(0)\phi_{-\mathbf{k}}(0)\rangle \sim k^\sigma$ for $k \to 0$ ($\sigma > -d$), the autocorrelation function of $X(t)$ still has the form (1), but with d replaced by $d + \sigma$. Since any Gaussian process is completely specified by its autocorrelation function, it follows that θ depends only on the combination $d + \sigma$. To obtain results for $d = 3$ with uncorrelated initial conditions, therefore, we can simulate the case $d = 1$, $\sigma = 2$, noting that $\sigma = 2$ corresponds in real space to differentiating uncorrelated initial conditions (or taking finite differences on a lattice). The result from 12 runs (Fig. 1) is $\theta = 0.2380 \pm 0.0015$, close to the predicted result 0.2358.

The asymptotics of the probability $p_n(t_1, t_2)$ for having n zeros between times t_1 and t_2 are also readily calculable within the IIA. From (5) and (6), the singularity in $\tilde{p}_n(s)$ as $s = -\theta$ is an $(n+1)$th-order pole of strength $R^{n+1}/\langle T\rangle\theta^2$, where R is the strength of the simple pole in $\tilde{P}(s)$. Inverting the Laplace transform, and retaining only the leading large-T behavior, gives (for all n)

$$p_n(T) \to \frac{R}{\langle T\rangle\theta^2}\frac{(RT)^n}{n!}\exp(-\theta T). \qquad (11)$$

With $T = \ln(t_2/t_1)$, one obtains

$$p_n(t_1, t_2) \to (R^{n+1}/\langle T\rangle\theta^2 n!)[\ln(t_2/t_1)]^n (t_1/t_2)^\theta. \quad (12)$$

When the time t_1 corresponds to the initial condition, one has to set t_1 equal to a constant of order unity, as was implicit in the earlier treatment of $p_0(t)$. Setting $t_2 = t$ one then gets $p_n(t) \sim c_n(\ln t)^n t^{-\theta}$. This rather strange-looking result does not have the scaling form found in the voter model and in Ising systems in $d = 1$ and 2, where one finds [5,12] $p_n(t) \sim \langle n\rangle^{-1} f(n/\langle n\rangle)$, with $\langle n\rangle \sim \sqrt{t}$. [The exponent θ in those systems emerges from a singular behavior of the scaling function $f(x)$ as $x \to 0$. Note that in the present work $\langle n\rangle \sim T \sim \ln t$.]

We turn to a brief discussion of the experimental relevance of our results. The ubiquity of the diffusion equation in physics implies that applications will be many and varied. As a concrete example, however, consider the reaction-diffusion process $A + B \to C$, where C is inert and immobile. The corresponding rate equations for the concentrations are $dn_A/dt = \nabla^2 n_A - R$, $dn_B/dt = \nabla^2 n_B - R$, and $dn_C/dt = R$, where R is the reaction rate per unit volume ($R \propto n_A n_B$ for $d > 2$ [13]). The concentration difference, $\Delta n \equiv n_A - n_B$, obeys the simple diffusion equation. If the A and B species are randomly mixed at $t = 0$ the system evolves, for $d < d_c = 4$, to a coarsening state in which the two species segregate into domains [14], separated by domain walls whose locations are defined by $\Delta n = 0$. Subsequent production of the inert species C is slaved to the motion of the domain walls, which are zeros of the diffusion field Δn. The fraction of space not infected by the C species will therefore decay asymptotically as $t^{-\theta}$.

We conclude with other examples of nontrivial exponents θ which have not been addressed in the literature.

The first is associated with the dynamics of the *global* order parameter $M(t)$ (e.g., the total magnetization of an Ising ferromagnet) at a critical point T_c, following a quench to T_c from the high-temperature phase. The quench prepares the system in a state with random initial conditions. In the subsequent evolution (now stochastic, rather than deterministic), the probability that $M(t)$ has not changed sign since $t = 0$ decays as $t^{-\theta_c}$, where θ_c is a *new critical exponent* [15]. For reasons similar to those given for the diffusion problem, we expect θ_c to be an independent exponent, i.e., not related by any scaling law to the usual static and dynamic exponents. As a second example, one can consider $M(t)$ for a quench to $T = 0$ from high temperature. In this case, $p_0(t) \sim t^{-\theta_0}$, where θ_0 differs from the corresponding exponent for single spins. For the $d = 1$ Glauber model, for example, the probability that $M(t)$ has not changed sign decays with an exponent $\theta_0 = 1/4$ [15], which differs from the exponent $3/8$ obtained for the zero-flip probability of a given spin [6].

As a final example, consider the generalized one-dimensional random-walk equation $d^n x/dt^n = \xi(t)$, where ξ is Gaussian white noise. The cases $n = 1, 2, \ldots$ correspond to a random velocity (the usual random walk), random acceleration, etc. The first two θ_n are $\theta_1 = 1/2$ and $\theta_2 = 1/4$ [16], but larger n have not been considered before to our knowledge. Application of the independent interval approximation [17] gives equations of the same structure as for the diffusion process, but with $\mathrm{sech}^d(T/2)$ in (2) and (9) replaced by $(2 - 1/n)\exp(-T/2)\,{}_2F_1[1, 1 - n; 1 + n; \exp(-T)]$, where ${}_2F_1$ is the hypergeometric function. This approach gives $\theta_2 = 0.2647$ (instead of $1/4$) while, for larger n, θ_n approaches a limiting value $\theta_\infty = 0.1862\ldots$, i.e., the same exponent as the $d = 2$ diffusion equation. In fact, the equality of the exponents for the $n = \infty$ process and $d = 2$ diffusion can be proved exactly [17], implying a limiting exponent 0.1875 ± 0.0010 (from Table I) for the former.

To summarize, we have calculated the probability for n zero crossings, between times t_1 and t_2, of a diffusion field at a given point in space, by assuming that the intervals between crossings, measured in the variable $T = \ln t$, are independent. The time dependence of these probabilities is characterized by a single nontrivial exponent θ, the predicted values of which are in excellent agreement with precise simulation results in $d = 1, 2$, and 3. These ideas are relevant to any system where the diffusion equation (or "heat equation") plays a role, ranging from physical and chemical systems to fluctuations in financial markets, and can be extended to other Gaussian processes.

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