Sorting single events: Mean arrival times of N random walkers

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Using a scaling approach we investigate the first passage time $\langle \mu_{1,N}(r) \rangle$ for the first out of N identical independently diffusing particles in ordered and disordered structures. For Euclidean spaces we obtain $\langle \mu_{1,N}(r) \rangle$ in terms of a series in $(\ln N)^{-1}$, independent of dimension. In the case of disordered ramified fractals $\langle \mu_{1,N}(r) \rangle$ is expressed in terms of a series in $(\ln N)^{(1-d_w^{\ell})}$, where d_w^{ℓ} describes how the mean topological distance $\langle \ell(t) \rangle$ evolves with time t. We propose a scaling behavior for the related quantity $S_N(t)$, the number of distinct sites visited by N particles. We verify our predictions by numerical simulations. [S1063-651X(99)10612-3]

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Modern experimental techniques enable looking into single events in many, yet finite, particle systems [1–3]. Instead of considering ensemble averages over the participating particles, processes involving *single* particles or a *finite* number of particles have become of increasing interest. The possibility of sorting single particle events out of an ensemble allows a better understanding of particle dynamics at a level of detail which is usually burried under the statistical averaging.

Here we propose the applicability of the concept of mean first passage times to the observation of single particle events. The mean first passage time (MFPT) is the time that a particle needs, on average, to reach a given distance r for the *first* time. When considering a finite initial number of particles, N, one is led to the problem of the mean arrival time $\langle \mu_{j,N}(r) \rangle$ of j out of N particles. Of particular interest are the statistical properties of $\langle \mu_{1,N}(r) \rangle$ which describes the mean first passage time of the first out of N particles. Namely, instead of an ensemble average over N, we focus on a single particle out of the N participating particles, averaged over many configurations.

In the case of independent particles the MFPT $\langle \mu_{1,1}(r) \rangle$ is related to the average of the sorted events $\langle \mu_{j,N}(r) \rangle$, $\langle \mu_{1,1}(r) \rangle = (1/N) \Sigma_j \langle \mu_{j,N}(r) \rangle$. Therefore, obtaining information on the different $\langle \mu_{j,N}(r) \rangle$ provides insight into the independent contributions of the individual events to the MFPT [4].

Earlier studies of the properties of $\{\langle \mu_{j,N}(r) \rangle\}$, based on solving the diffusion equation with absorbing boundaries, were done for one-dimensional systems [5], and using renormalization approach for deterministic fractals [6]. In what follows we generalize the problem and provide a formulation which is independent of the underlying environement. We exemplify our approach by using random walk trails, self avoiding walk structures, and percolation clusters at criticality, the latter being characterized by complicated structures having loops and dangling ends. It has been shown that transport properties on percolation can be treated conveniently in terms of the topological distance [7,8]. The topological distance ℓ is defined as the length of the shortest path connecting two sites on a fractal that are separated by the Euclidean distance r. It scales with the Euclidean distance r as $\ell \sim r^{d_{\min}}$. The relevance of the topological metric ℓ for percolation clusters stems from the fact that the fluctuations of the probability density on sites at a fixed Euclidean distance r from the origin are large, but are negligible when considered at fixed topological distance ℓ [8]. For transport properties one applies the anomalous diffusion exponent d_w defined by the time dependence of the root mean square displacement, $\sqrt{\langle r^2(t) \rangle} \sim t^{1/d_w}$. When the topological distance is considered we expect the exponent $d_w^{\ell} = d_w / d_{\min}$, which characterizes how the mean topological distance $\langle \ell(t) \rangle \sim t^{1/d_w^{\ell}}$ evolves with time, to enter. Another quantity which is related to the mean arrival time of the first out of N walkers $\langle \mu_{1,N}(r) \rangle$ is $S_N(t)$, the number of distinct sites visited by the N random walkers during time t, a quantity that relates to a broad range of phenomena (see e.g. [9]). $S_N(t)$ is also expected to be characterized by the exponent d_w^{ℓ}.

In this paper we derive the dependence of $\langle \mu_{1,N}(r) \rangle$ and of $S_N(t)$ on N and show that they are characterized by the exponent d_w^{ℓ}. Our results are relevant to those cases where single events can be observed, especially if the particles trigger some process when arriving at a trap or a sensor. In addition, the dependence of the observables $S_N(t)$ and $\langle \mu_{1,N}(r) \rangle$ on d_w^{ℓ} emphasizes the importance of the concept of topological space in investigating transport properties on percolation.

Let us assume N independent diffusing particles in a Euclidean space. Then a length scale $r_c(N)$ is imposed on the system. For $r \ll r_c(N)$ the mean arrival time $\langle \mu_{1,N}(r) \rangle$ should scale according to [10]

$$\langle \mu_{1,N}(r) \rangle = r/v, \tag{1}$$

where in a discrete system v is the ratio of a length given in terms of the lattice constant and the corresponding elementary step time unit. Equation (1) follows from the assumption that among a sufficiently large number of random walkers one can find on average one walker which reaches the distance r unscattered [10]. In the continuum description v enters by assuming a finite velocity which is given by ratio of mean free path and the averaged scattering time. For $r \gg r_c(N)$,

$$\langle \mu_{1,N}(r) \rangle = g(N) r^2, \tag{2}$$

which follows from the general solution of the diffusion equation where r plays the role of distance between the (absorbing) boundaries [5]. The critical distance $r_c(N)$ for d-dimensional Euclidean space is obtained in a straightforward way from calculating the probability of finding *one* random walker that travels the distance $r_c(N)$ in time $t = r_c(N)/v$,

$$\frac{1}{N} = (k/\beta c) P(r,t)\big|_{r=r_c(N),t=r_c(N)/v} = \frac{\lambda_0}{(\beta r_c(N))^{(1-d/2)}} \exp[-\beta r_c(N)], \tag{3}$$

where $P(r,t)$ is the probability density to be at distance r at time t and $\beta = v/D$. The factor $k/\beta c$ is the unit length of the system expressed by the diffusion constant D, the velocity v, and a numerical constant k of order 1. The normalization condition $\int P(r,t)dr = 1$ for a fixed t yields $\lambda_0 = 2k/\Gamma(d/2)$. In order to derive the critical distance $r_c(N)$, we now define in Eq. (3),

$$\rho \equiv (\lambda_0 N)^{-1} = \tau^{\alpha} e^{-1/\tau}, \tag{4}$$

with $\alpha = 1 - d/2$ and $\tau = (\beta r_c(N))^{-1}$. Since ρ increases monotonically with τ and $\rho(\tau \to 0) \to 0$, we obtain, by taking the logarithm of Eq. (4),

$$\tau(\rho) = [\ln(1/\rho) + \xi(\rho)]^{-1}, \tag{5}$$

where $\xi(\rho)$, to be discussed below, obeys $\lim_{\rho \to 0} \xi(\rho)/\ln(1/\rho) = 0$. Being interested in the behavior of $\xi(\rho)$ for $\rho \sim 0$ (corresponding to $N \gg 1$), we can expand $\xi(\rho)$ in a series, by substituting Eq. (5) in Eq. (4). This leads, in second order, to

$$\xi(\rho) \simeq -\alpha \ln[\ln(1/\rho)] \left\{ 1 - \frac{\alpha}{\ln(1/\rho)} \right\}. \tag{6}$$

Substituting Eq. (6) into Eq. (5) yields

$$r_c(N) = (\beta \tau(\rho))^{-1} \simeq \beta^{-1} \left(\ln(1/\rho) - \alpha \ln[\ln(1/\rho)] \times \left\{ 1 - \frac{\alpha}{\ln(1/\rho)} \right\} \right). \tag{7}$$

In order to satisfy both scaling regimes in Eqs. (1) and (2) we assume that $\langle \mu_{1,N}(r) \rangle = (r_c(N)/v) f(r/r_c(N))$ with $f(x) = x$ for $x \ll 1$, and $f(x) = x^2$ for $x \gg 1$. Accordingly, for $r \gg r_c(N)$,

$$\langle \mu_{1,N}(r) \rangle = (r_c(N) v)^{-1} r^2. \tag{8}$$

Inserting Eq. (7) into Eq. (8), expanding the result into a series and taking into account Eq. (4) yields

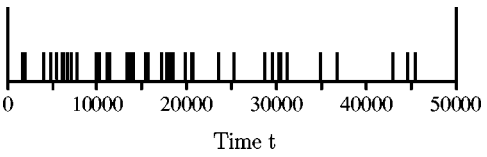

FIG. 1. Time series of the arrival times $\langle \mu_{j,N}(r) \rangle$, $j = 1, \ldots, 50$, of $N = 50$ particles from a starting point on a three-dimensional percolation cluster at criticality to distance $r = 15$.

$$\langle \mu_{1,N}(r) \rangle = \frac{D^{-1} r^2}{\ln(\lambda_0 N)} \left(1 + \frac{\alpha \ln\ln(\lambda_0 N)}{\ln(\lambda_0 N)} + \frac{\alpha^2 (\ln\ln(\lambda_0 N) - \ln^2 \ln(\lambda_0 N))}{\ln^2(\lambda_0 N)} + \cdots \right). \tag{9}$$

To zeroth order the arrival time $\langle \mu_{1,N}(r) \rangle$ becomes

$$\langle \mu_{1,N}(r) \rangle \simeq \frac{D^{-1} r^2}{\ln(\lambda_0 N)}, \tag{10}$$

which in the one-dimensional case reproduces earlier results [5].

We now extend the approach to the case where the movement of the random walker is constrained to geometrically disordered structures such as random walk trails, self avoiding walk structures, and percolation clusters at criticality. Figure 1 presents a series of the arrival times of $N = 50$ particles diffusing on a percolation cluster at criticality from an origin to a distance r. Averaging a set of such time series for a given j leads to the observable $\langle \mu_{j,N}(r) \rangle$. Since our derivation is based on the concept of the topological space, in addition to percolation we consider, as examples for the relevance of the topological distance ℓ, topologically linear fractals such as trails of a random walk, where only sequentially created sites on the trail are considered connected, and self avoiding walk structures. The fractal dimension of the shortest path is $d_{\min} = 1/2$ for random work trails, $d_{\min} = 3/4$ for self avoiding walk structures, and $d_{\min} \simeq 1.35$ for percolation in $d = 3$ [7]. The probability density for a particle to be located at time t at a topological distance ℓ from its starting point is asymptotically given by [7,8]

$$P(\ell, t) = P(0,t) \ell^{d_\ell - 1} \exp[-(\ell / L(t))^{\delta_\ell}]. \tag{11}$$

Here d_ℓ is the topological distance exponent, $\delta_\ell = d_{\mathrm{w}}^{\ell}/(d_{\mathrm{w}}^{\ell} - 1)$, and $L(t) = (D_\ell t)^{1/d_{\mathrm{w}}^{\ell}}$ is proportional to the mean chemical distance $\langle \ell(t) \rangle$ [7]. For the linear case $d_\ell = 1$, $d_{\mathrm{w}}^{\ell} = 2$ so that Eq. (11) reduces to a Gaussian. Following our earlier argument we now derive the mean arrival time $\langle \mu_{1,N}(\ell) \rangle$ in topological space. We first obtain the critical topological distance $\ell_{\mathrm{c}}(N)$ that divides the scaling behavior of $\langle \mu_{1,N}(\ell) \rangle$ into two scaling regimes. We calculate the probability of finding one out of the set of N random walkers that arrives at the topological distance $\ell_{\mathrm{c}}(N)$ during time $t = \ell_{\mathrm{c}}(N)/v_\ell$,

$$\frac{1}{N}=(k_p/\beta_p)P(\ell,t)|_{\ell=\ell_c(N),t=\ell_c(N)/v_\ell}$$

$$=\frac{\lambda_p}{(\beta_p\ell_c(N))^{(1-d_\ell/\delta_\ell)}}\exp[-\beta_p\ell_c(N)], \qquad (12)$$

where $\lambda_p=k_p\delta_\ell/\Gamma(d_\ell/\delta_\ell)$, $\beta_p=(v_\ell/D_\ell)^{\delta_\ell/d_w^\ell}$, and k_p/β_p is the unit length in the system expressed by the diffusion constant D_ℓ, the velocity v_ℓ, and a numerical constant k_p of order 1. As for the Euclidean case the velocity v_ℓ is defined by the ratio of the mean free path and the mean time between collisions. If we introduce new variables $\tau_p=(\beta_p\ell_c(N))^{-1}$ and $\alpha_p=1-d_\ell/\delta_\ell$, Eq. (12) can be rewritten as $\rho_p\equiv(\lambda_pN)^{-1}=\tau_p^{\alpha_p}e^{-1/\tau_p}$. In an analogous way to Eqs. (4)–(7) we obtain

$$\ell_c(N)=\beta_p^{-1}\left(\ln(1/\rho_p)-\alpha_p\ln[\ln(1/\rho_p)]\left\{1-\frac{\alpha_p}{\ln(1/\rho_p)}\right\}\right). \qquad (13)$$

Since we expect $\langle\mu_{1,N}(\ell)\rangle=\ell/v_\ell$ for $\ell\ll\ell_c(N)$ and $\langle\mu_{1,N}(\ell)\rangle=g_p(N)\ell^{d_w^\ell}$ for $\ell\gg\ell_c(N)$ we require $\langle\mu_{1,N}(\ell)\rangle=(\ell_c(N)/v_\ell)f_p(\ell/\ell_c(N))$ with $f_p(x)=x$ for $x\ll1$ and $f_p(x)=x^{d_w^\ell}$ for $x\gg1$. For $\ell\gg\ell_c(N)$ this yields the scaling relation

$$\langle\mu_{1,N}(\ell)\rangle\simeq(\ell_c(N)^{1-d_w^\ell}/v_\ell)\ell^{d_w^\ell}. \qquad (14)$$

From Eq. (13) the arrival time $\langle\mu_{1,N}(\ell)\rangle$, to order zero and for fixed topological distance, becomes

$$\langle\mu_{1,N}(\ell)\rangle\simeq\frac{D_\ell^{-1}\ell^{d_w^\ell}}{(\ln(\lambda_pN))^{d_w^\ell-1}}. \qquad (15)$$

For linear fractals Eq. (15) is the same as Eq. (10) with $d=1$ and with r replaced by ℓ. In order to derive the arrival time in Euclidean space we denote by $\phi(\ell|r)$ the probability that two sites on the fractal that are apart by a Euclidean distance r are separated by the topological distance ℓ. The mean arrival time $\langle\mu_{1,N}(r)\rangle$ for a fixed Euclidean distance r can now be calculated by the convolution

$$\langle\mu_{1,N}(r)\rangle=\int\langle\mu_{1,N}(\ell)\rangle\phi(\ell|r)d\ell. \qquad (16)$$

The distribution function $\phi(\ell|r)$ of ℓ for fixed r is given by

$$\phi(\ell|r)=\frac{C_1}{\ell}F\left(\frac{r}{\ell^{1/d_{\min}}}\right)\quad\text{with}\quad F(x)=x^g\exp[-C_2x^\delta], \qquad (17)$$

with $\delta=d_{\min}/(d_{\min}-1)$, $g\simeq1.35$ and $C_2\simeq0.8$ for percolation in $d=3$ [11]. The constant C_1 is given by the normalization condition $\int\phi(\ell|r)d\ell=1$ yielding $C_1=[(d_{\min}-1)C_2^{g/\delta}\Gamma(g/\delta)]^{-1}$. Inserting Eqs. (15) and (17) into Eq. (16) and performing the substitution $d\ell\to dx$ with $x=r/\ell^{1/d_{\min}}$ yields

$$\langle\mu_{1,N}(r)\rangle=(\ell_c(N)^{1-d_w^\ell}/v_\ell)Kr^{d_w}, \qquad (18)$$

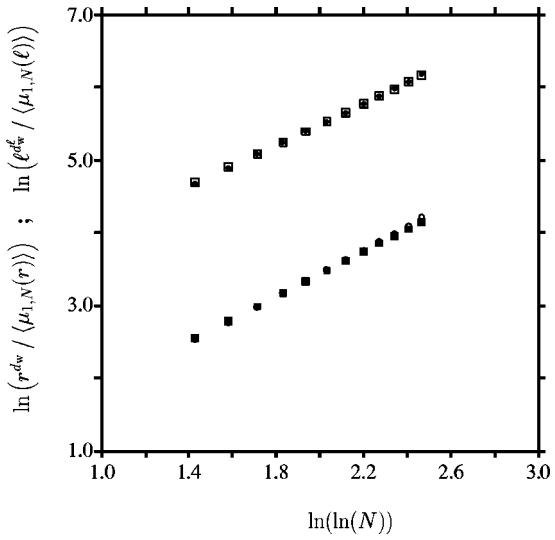

FIG. 2. Double logarithmic scaling plot of the mean first passage time for the first out of N diffusing particles, $\langle\mu_{1,N}(r)\rangle$, on a three-dimensional infinite percolation cluster at criticality. Shown are $\langle\mu_{1,N}(r)\rangle$ for Euclidean distances $r=15$ (squares) and $r=20$ (filled circles) with $d_w\simeq3.55$, and $\langle\mu_{1,N}(\ell)\rangle$ for chemical distances $\ell=40$ (filled squares) and $\ell=60$ (circles) with $d_w^\ell\simeq2.67$. The slope $\simeq1.62$ is in good agreement with Eqs. (15) and (18). The data for the fixed chemical distances have been shifted up.

with $K=C_2^{d_w/\delta}\Gamma((g-d_w)/\delta)/\Gamma(g/\delta)$ which is numerically of order 1. The comparison of Eqs. (14) and (18) reveals that the arrival times for fixed ℓ and for fixed r show the same N dependence. This is demonstrated in Fig. 2 where the numerical results of our simulation of $\langle\mu_{1,N}(\ell)\rangle$ and $\langle\mu_{1,N}(r)\rangle$ are plotted logarithmically versus $\ln N$ and show the same slope. The explicit N dependence of the mean arrival times is therefore determined by the anomalous diffusion exponent d_w^ℓ in topological space and not by the exponent d_w [6]. The latter result does hold for the Sierpinski gasket where $d_{\min}=1$ and therefore $d_w^\ell=d_w$.

Finally, we use Eq. (14) to derive an asymptotic expression for the number $S_N(t)$ of distinct sites visited by N independent diffusing particles on a random self similiar structure. We argue that the mean longest Euclidean distance $R_N(t)$ reached by any of the N independent random walkers during time t should be proportional to the distance r at which the first out of the N walkers arrives at time $t=\langle\mu_{1,N}(r)\rangle$ [6]. According to Eq. (18) this leads to $R_N^{d_w}(t)\sim t\ell_c(N)^{(d_w^\ell-1)}\simeq t\ln^{d_w^\ell-1}(\lambda_pN)$. Since the trail of a random walk is compact for media with spectral dimension $d_s=2d_\ell/d_w^\ell<2$ [12], as it is the case for percolation in $d=2$ and $d=3$, the number of distinct visited sites, $S_N(t)$, scales as $S_N(t)=R_N^{d_f}(t)$, so that

$$S_N(t)\sim(\ln\lambda_pN)^{(d_s/2)(d_w^\ell-1)}t^{d_s/2}. \qquad (19)$$

The numerical results of our simulation for $S_N(t)$ on three-dimensional percolation clusters are shown in Figs. 3 and 4. While Fig. 3 shows the data in an unscaled form for different values of N, the data collapse in Fig. 4 strongly supports the scaling behavior given by Eq. (19).

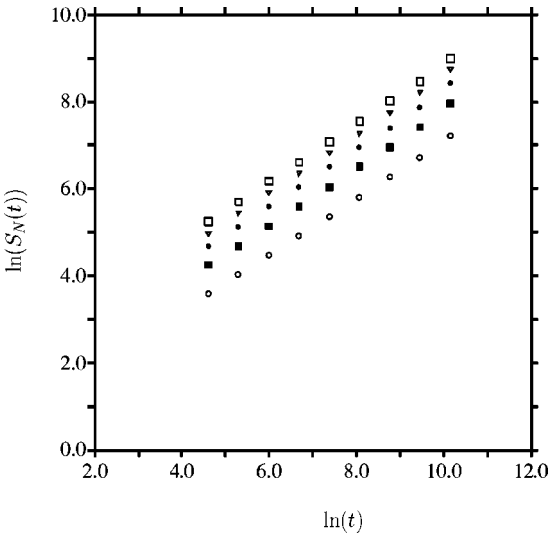

FIG. 3. Number of distinct sites $S_N(t)$ visited by N random walkers on a three-dimensional infinite percolation cluster at criticality. Plotted is $\ln(S_N(t))$ versus $\ln(t)$ for $N=16$ (circles), $N=2^7$ (filled squares), $N=2^{10}$ (filled circles), $N=2^{13}$ (triangles), and $N=2^{16}$ (squares).

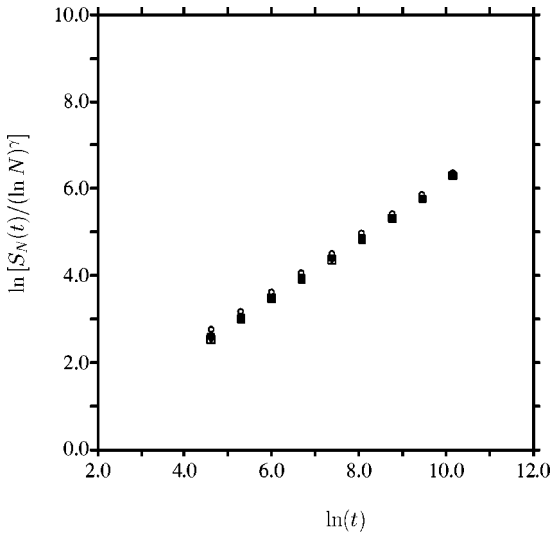

FIG. 4. The same data as in Fig. 3 but in a scaling form according to Eq. (19) with $\gamma \equiv (d_s/2)(d_w'-1)$. The data collapse and the slope $\simeq 0.68$ support Eq. (19), since $d_s \simeq 1.38$ for the critical percolation in $d=3$ [7].

In summary, we have introduced expressions for the mean arrival time of the first out of N independent random walkers $\langle \mu_{1,N}(r) \rangle$ in ordered and in disordered systems. This quantity should be closely related to experiments which are able to follow single events in many particle systems. We have also derived the mean number $S_N(t)$ of new sites visited in such systems. Both $\langle \mu_{1,N}(r) \rangle$ and $S_N(t)$ are characterized by the anomalous diffusion exponent d_w' in topological space.

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[1] S. Nie, D. T. Chiu, and R. N. Zare, Science **266**, 1018 (1994).
[2] T. Zambelli, J. Trost, J. Wintterlin, and G. Ertl, Phys. Rev. Lett. **76**, 795 (1996).
[3] M. Eigen and R. Rigler, Proc. Natl. Acad. Sci. USA **91**, 570 (1994).
[4] A. Bar-Haim, J. Dräger and J. Klafter (unpublished).
[5] G. H. Weiss, K. E. Shuler, and K. Lindenberg, J. Stat. Phys. **31**, 255 (1983); S. B. Yuste and K. Lindenberg, *ibid.* **85**, 501 (1996).
[6] S. B. Yuste, Phys. Rev. Lett. **79**, 3565 (1997).
[7] S. Havlin and D. ben-Avraham, Adv. Phys. **36**, 695 (1987).
[8] A. Bunde, S. Havlin, and H. E. Roman, Phys. Rev. A **42**, 6274 (1990); J. Dräger and A. Bunde, Phys. Rev. E **54**, 4596 (1996).
[9] H. Larralde, P. Trunfio, S. Havlin, H. E. Stanley, and G. H. Weiss, Nature (London) **355**, 423 (1992).
[10] A. Bunde and J. Dräger, Physica A **202**, 371 (1994).
[11] A. Bunde and J. Dräger, Philos. Mag. B **71**, 721 (1995); N. Dokholyan, Y. Lee, S. Buldyrev, S. Havlin, P. King, and H. Stanley, J. Stat. Phys. **93**, 603 (1998).
[12] P.-G. de Gennes, J. Chem. Phys. **76**, 3316 (1982).