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LETTER TO THE EDITOR

Superuniversality of acceleration correlations for random walks on fractals

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Abstract. The acceleration-acceleration correlation function, $K(t)=\langle \boldsymbol{a}(t)\cdot\boldsymbol{a}(0)\rangle$ ($\boldsymbol{a}=\mathrm{d}^2\boldsymbol{r}/\mathrm{d}t^2$, where $\boldsymbol{r}$ is the displacement), of a random walker on a fractal lattice is studied analytically and numerically on percolation clusters and on diffusion-limited aggregates at dimensions $d=2, 3$. After $t(\gg 1)$ discrete time steps, we find $K(t)=A(t)/\langle r^2(t)\rangle$, with $A(t)\sim(-1)^t$. At a fixed distance R from the origin we find the superuniversal law $K(R)\sim R^{-2}$ on all fractals and for all d.

Many macroscopically inhomogeneous systems are characterised by the existence of self-similar structures on certain scales. These include metal-insulator mixtures near the percolation threshold, diffusion-limited aggregates, polymer solutions, etc. The progress made in understanding transport in such systems reveals unusual behaviour of various transport coefficients [1-4]. Naturally, much effort has been devoted to characterising the underlying *universal* properties of the relevant quantities (e.g. evaluating the critical exponents) [5]. The aim of the present letter is to propose a 'superuniversal' exponent, characterising diffusion on fractals.

Consider a random walker on a discrete fractal network. If the probability to hop from site $\boldsymbol{r}'$ to its nearest-neighbour site $\boldsymbol{r}$ is $W(\boldsymbol{r},\boldsymbol{r}')$, then the occupation probability at site $\boldsymbol{r}$ at time t, $P(\boldsymbol{r},t)$, obeys the master equation

$$P(\boldsymbol{r},t+1)-P(\boldsymbol{r},t)=\sum_{\boldsymbol{r}'}[W(\boldsymbol{r},\boldsymbol{r}')P(\boldsymbol{r}',t)-W(\boldsymbol{r}',\boldsymbol{r})P(\boldsymbol{r},t)]. \tag{1}$$

If a particular walk went through sites $\boldsymbol{r}(t-1)$, $\boldsymbol{r}(t)$ and $\boldsymbol{r}(t+1)$ at the corresponding discrete time steps, the local acceleration is defined as $\boldsymbol{a}(t)=[\boldsymbol{r}(t+1)+\boldsymbol{r}(t-1)-2\boldsymbol{r}(t)]$. We can now consider the acceleration correlation function $K(t)=\langle\boldsymbol{a}(0)\cdot\boldsymbol{a}(t)\rangle$, where the average is performed over all possible walks of t time step, starting at all possible origins. We find that the function $K(t)$ performs a regular oscillation with time, $K(t)=|K(t)|(-1)^t$ (figure 1). The envelope $|K(t)|$ is found to be inversely proportional

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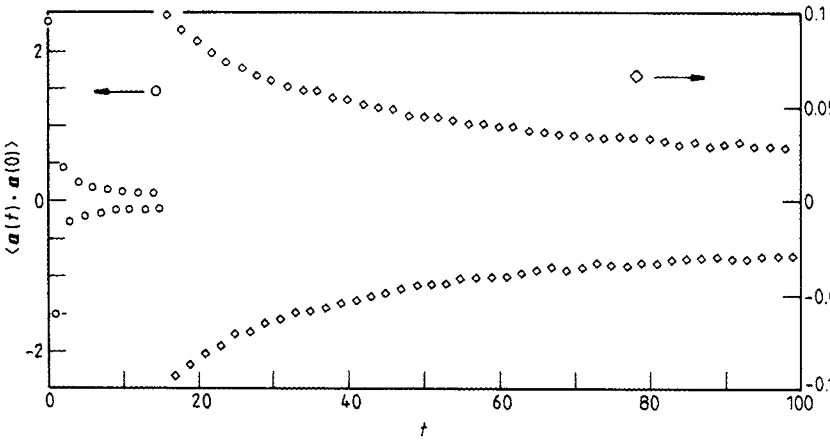

Figure 1. Raw average values of the correlation function for 100 steps of random walk on a percolation cluster at P_c (same data as in figure 2(a)). All 100 points are plotted and the sign changes at every step. The standard errors, as determined by batch standard deviation (see text) are always smaller than the size of the symbol and very close to it toward the 100th step.

to the mean square distance travelled by the walker, $\langle r^2(t)\rangle$, which is known [2] to have the anomalous time dependence $t^{2/(2+\theta)}$. The law

$$K(t) = \langle \boldsymbol{a}(0) \cdot \boldsymbol{a}(t)\rangle \propto (-1)^t / \langle \boldsymbol{r}^2(t)\rangle \tag{2}$$

is found to superuniversal, i.e. true for *all* random walks on *all* fractals, independent of their fractal dimensionalities or any other individual characteristics.

Alternatively, one may average the acceleration correlation function for a fixed distance $\boldsymbol{R}$ between the two ends of the walk, $K(\boldsymbol{R}) = \langle \boldsymbol{a}(0) \cdot \boldsymbol{a}(\boldsymbol{R})\rangle$. We find the superuniversal law $|K(\boldsymbol{R})| \propto |\boldsymbol{R}|^{-2}$.

Figures 2 and 3 exhibit examples of our computer simulation results of random walks on large percolation clusters (at the percolation threshold) and on diffusion-limited aggregates (DLA) on both square and simple cubic lattices (see [6] for a preliminary account of these simulations). The simulations used the 'myopic ant' model [7] for which the walker *must move* at each time step, and thus $W(\boldsymbol{r}, \boldsymbol{r}') = 1/z(\boldsymbol{r}')$, $z(\boldsymbol{r}')$ being the number of occupied nearest neighbours of site $\boldsymbol{r}'$. We averaged $\boldsymbol{a}(0) \cdot \boldsymbol{a}(t)$ and $\boldsymbol{r}^2(t)$ and the figures show the envelope $|K(t)|$. Convergence is faster for percolation in $d = 2$ and DLA in $d = 3$. The statistical error of the averages of $K(t)$ was calculated by first subdividing the data into several subsets (typically five) and then computing the standard deviations among the batch averages. For example, for the percolation clusters in $d = 2$ for each of the two clusters simulated, five batches of 10^6 walks of 100 steps each were used. The standard deviation for $K(t)$ varied from 0.1% for the first few steps to ~5% at the 100th step. In $d = 3$ the error was ~10% at the 500th step. Similar errors were obtained for DLA. Within the standard error bars (figures 2 and 3) our data are consistent with the straight lines $|K(t)| \sim 1/\langle r^2(t)\rangle$ (also shown in the figures). The numerical results presented should be taken only as an indication of the universal behaviour predicted here. Although we have averaged over a relatively large number of walks, these walks are rather short. We now present several analytical arguments supporting and explaining our predictions.

The following scaling argument explains the result $|K(\boldsymbol{R})| \propto |\boldsymbol{R}|^{-2}$. Consider a particular walk that went via the sequence of sites $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, $\boldsymbol{r}_3$ at $t = 0$, and then went

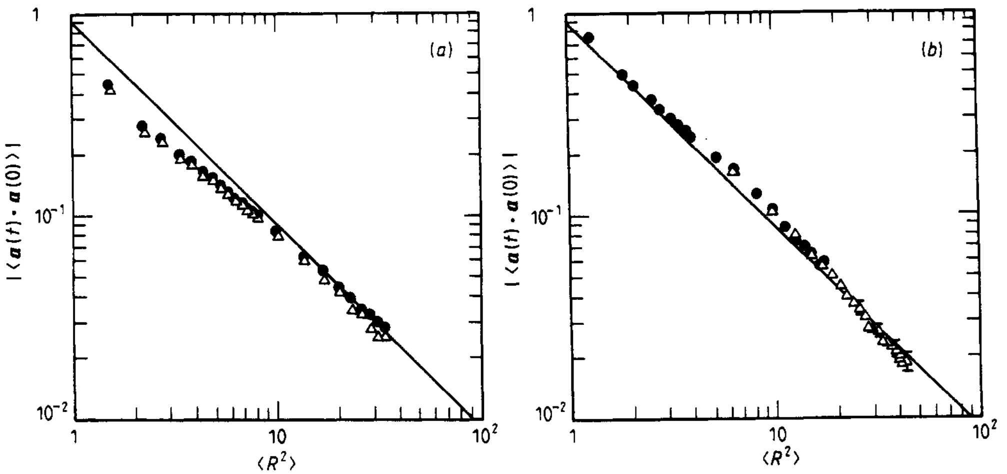

Figure 2. Acceleration-acceleration correlations for diffusion on percolation clusters plotted against $\langle r^2\rangle$. A line with slope -1 is drawn to guide the eye. The two symbols represent averages over two different 2500 site clusters. (*a*) Square lattice; 5×10^6 walks of 100 steps on each cluster. All standard errors are smaller than the symbol size. (*b*) Simple cubic lattice; 5×10^6 walks of 100 steps on one cluster and 2.5×10^6 walks of 500 steps on the other. Only a few selected error bars (at the 200th, 300th, 400th and 500th steps) are drawn. The errors for steps up to 100 are smaller than the symbol size.

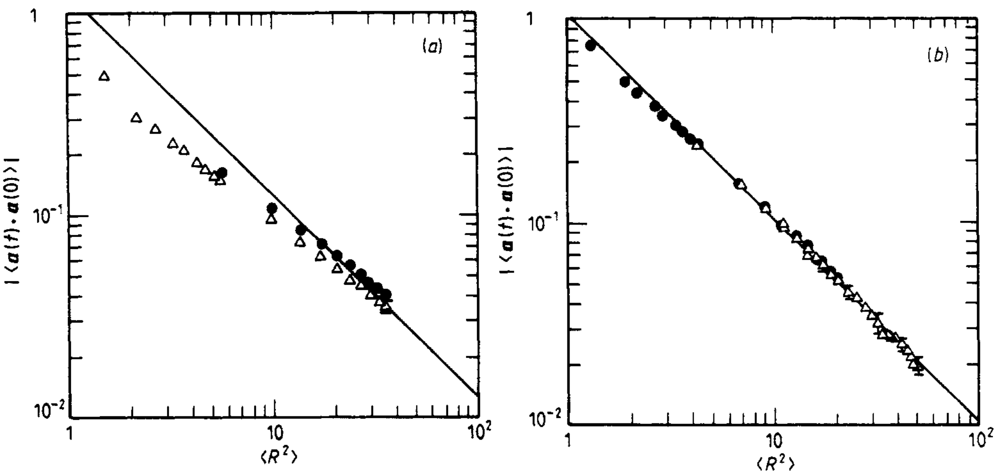

Figure 3. Acceleration-acceleration correlations for diffusion on DLA. (*a*) Square lattice; 5×10^6 walks on 100 steps on each cluster (cluster sizes: 6000 and 5910 sites). Only the error at the 100th step for one cluster is drawn, all other errors being smaller than the symbol size. (*b*) Simple cubic; 0.5×10^6 walks of 100 steps on a 1706 site cluster and 1.5×10^6 walks of 400 steps on a 4310 site cluster. Error bars are drawn at selected steps (80th, 120th, 200th, 300th and 400th steps), errors for steps up to the 60th being within the size of the symbol.

via $\boldsymbol{r}_1'$, $\boldsymbol{r}_2'$, $\boldsymbol{r}_3'$ at some later time, with $\boldsymbol{r}_3'-\boldsymbol{r}_2=\boldsymbol{R}$. Considering all possible walks, the probability of this particular walk is

$$\omega = W(\boldsymbol{r}_3', \boldsymbol{r}_2')\,W(\boldsymbol{r}_2', \boldsymbol{r}_1')\,W(\boldsymbol{r}_3, \boldsymbol{r}_2)\,W(\boldsymbol{r}_2, \boldsymbol{r}_1)\rho(\boldsymbol{r}_2)\rho(\boldsymbol{r}_2')\delta(\boldsymbol{r}_2'-\boldsymbol{r}_2-\boldsymbol{R}) \tag{3}$$

where $\delta(\boldsymbol{r})=1$ if $\boldsymbol{r}=0$ and zero otherwise, while $\rho(\boldsymbol{r})$ is the average probability (per step on a specific walk) to pass through $\boldsymbol{r}$. For very long walks, the $\rho(\boldsymbol{r})$ become independent of each other. The average acceleration correlation function is therefore

$$K(\boldsymbol{R}) = \sum_{\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3}\ \sum_{\boldsymbol{r}_1',\boldsymbol{r}_2',\boldsymbol{r}_3'} (\boldsymbol{r}_1+\boldsymbol{r}_3-2\boldsymbol{r}_2)\cdot(\boldsymbol{r}_1'+\boldsymbol{r}_3'-2\boldsymbol{r}_2')w\left(\textstyle\sum\sum w\right)^{-1}. \tag{4}$$

For the 'blind' ant, $W(\boldsymbol{r}, \boldsymbol{r}')=W(\boldsymbol{r}', \boldsymbol{r})=1/z$, z being the coordination number of the underlying uniform (undilute) lattice. In this case, for $t\to\infty$, all initial and final points are equally probable, $\rho(\boldsymbol{r})=\text{constant}$. Using the symmetry in W we can now write

$$\sum_{\boldsymbol{r}_2,\boldsymbol{r}_3}(\boldsymbol{r}_3-\boldsymbol{r}_2)\,W(\boldsymbol{r}_3, \boldsymbol{r}_2)\delta(\boldsymbol{r}_2'-\boldsymbol{r}_2-\boldsymbol{R}) = \sum(\boldsymbol{r}_2-\boldsymbol{r}_3)\,W(\boldsymbol{r}_3, \boldsymbol{r}_2)\delta(\boldsymbol{r}_2'-\boldsymbol{r}_3-\boldsymbol{R})$$

$$= -\tfrac{1}{2}\sum(\boldsymbol{r}_3-\boldsymbol{r}_2)\,W(\boldsymbol{r}_3, \boldsymbol{r}_2)\boldsymbol{\nabla}_{\boldsymbol{R}}\delta(\boldsymbol{r}_2'-\boldsymbol{r}_2-\boldsymbol{R})\cdot(\boldsymbol{r}_3-\boldsymbol{r}_2).$$

For a homogeneous translationally invariant lattice the final sums in (4) vanish by symmetry. In the more general case, we can use $\Sigma_{\boldsymbol{r}}\ W(\boldsymbol{r}, \boldsymbol{r}')=1$ and $\Sigma_{\boldsymbol{r}}(\boldsymbol{r}-\boldsymbol{r}')^2\,W(\boldsymbol{r}, \boldsymbol{r}')\propto a^2$ (a is the nearest-neighbour distance) to reduce (4) to

$$K(\boldsymbol{R})\propto\sum\nabla_{\boldsymbol{R}}^2\delta(\boldsymbol{r}_2'-\boldsymbol{r}_2-\boldsymbol{R})\left(\sum\delta(\boldsymbol{r}_2'-\boldsymbol{r}_2-\boldsymbol{R})\right)^{-1}. \tag{5}$$

On a fractal, the average density $(\Sigma\delta)$ of occupied sites at a distance $\boldsymbol{R}$ scales as $|\boldsymbol{R}|^{D-d}$, where D and d are the fractal and Euclidean dimensionalities. Thus, $K(\boldsymbol{R})\propto|\boldsymbol{R}|^{-2}$, as claimed above.

For the 'myopic' ant we expect that $\rho(\boldsymbol{r})\propto z(\boldsymbol{r})$. Thus, $W(\boldsymbol{r}, \boldsymbol{r}')\rho(\boldsymbol{r}')=W(\boldsymbol{r}', \boldsymbol{r})\rho(\boldsymbol{r})$ and the above symmetry arguments yield the same result (5).

If the average is performed at fixed t instead of fixed R, then the delta function in (3) must be replaced by $\bar{P}(\boldsymbol{r}_2'-\boldsymbol{r}_2, t)$, the average probability to travel a distance $(\boldsymbol{r}_2'-\boldsymbol{r}_2)$ in t time steps. Expecting a scaling form [2, 5] $\bar{P}(\boldsymbol{R}, t)=t^{-d_s/2}g(|\boldsymbol{R}|^{2+\theta/t})$, (4) will be replaced by

$$\sum_{\boldsymbol{r}}\nabla_{\boldsymbol{R}}^2\bar{P}(\boldsymbol{R}, t)\left(\sum_{\boldsymbol{R}}\bar{P}(\boldsymbol{R}, t)\right)\propto t^{-2/(2+\theta)}\propto\langle r^2\rangle^{-1}$$

as we found for the envelope $|K(t)|$.

To understand the regular oscillation in the sign of $K(t)$, as observed in figure 1, we next calculated $K(t)$ exactly on various structures. On a regular hypercubic d-dimensional lattice, $K(t)$ exhibits one oscillation $[K(1)<0]$ before it vanishes for $t>1$. On a 'comb' lattice (a one-dimensional chain with dangling ends of one bond from each site), the solution for the myopic ant is $K(1)=\frac{8}{3}$, $K(t)=16(-3)^{-t}/3(t>1)$. Although the envelope decays exponentially, since this is not a self-similar fractal, the sign oscillations persist at all t. The oscillations arise because of the anticorrelation between consecutive steps, dominated by the ends of the dangling bonds (at which the ant *must* turn back). Qualitatively, a similar effect arises in all dilute structures, since the bond for stepping back is always there, unlike some of the bonds for stepping forward.

An alternative way to solve for $K(t)$ is to note that, on any finite cluster of N sites, one has

$$P(\boldsymbol{r}, t) = \sum_{\Lambda} u_{\Lambda}(\boldsymbol{r}, 0)\Lambda^{t} \tag{6}$$

where the Λ are the N eigenvalues of the matrix $W(\boldsymbol{r}, \boldsymbol{r}')$ and where the walk started at site $\boldsymbol{r}=0$. For the myopic ant on a bipartite lattice, the eigenvalues appear in pairs, $+|\Lambda|$ and $-|\Lambda|$. Therefore, $P(\boldsymbol{r}, t)$ splits into two parts:

$$\sum_{|\Lambda|} [u_{|\Lambda|}(\boldsymbol{r}, 0) + (-1)^{t} u_{-|\Lambda|}(\boldsymbol{r}, 0)]|\Lambda|^{t}.$$

Fixing the acceleration at $t=0$, $\boldsymbol{a}(0)$, we can now use $P(\boldsymbol{r}, t)$ to calculate the average acceleration at time t:

$$\boldsymbol{a}(t) = \sum_{\boldsymbol{r}} \boldsymbol{r}[P(\boldsymbol{r}, t+1) + P(\boldsymbol{r}, t-1) - 2P(\boldsymbol{r}, t)].$$

Also averaging over the initial steps and the origin we end up with $K(t) = \Sigma_{\Lambda} k_{\Lambda}\Lambda^{t}$ and k_{Λ} is proportional to $\Lambda + \Lambda^{-1} - 2$ (and to some average projections of the initial state on the corresponding eigenvectors). For long times, the sum over Λ will be dominated by $|\Lambda|$ near 1, and the ratios $k_{|\Lambda|}/k_{-|\Lambda|}$ become very small, so that $K(t)$ is *dominated by the negative eigenvalues*, hence practically pure oscillations. We calculated these ratios explicitly for several percolation clusters and confirmed this result numerically. For one percolating square lattice cluster of 192 sites, the ratio $|k_{-|\Lambda|}/k_{|\Lambda|}|$ remains larger than 2520 for the largest seven eigenvalues, with $|\Lambda| > 0.98$, and has values smaller than 1 only for 26 eigenvalues, all in the range $|\Lambda| < 0.743$. Indeed, the *calculated* function $K(t) = \Sigma\, k_{\Lambda}\Lambda^{t}$ shows no observable deviations from the pure oscillation $(-1)^{t}|K(t)|$.

For very large clusters, the sum over Λ may be turned into an integral, $K(t) = (-1)^{t}\int \mathrm{d}|\Lambda| n(|\Lambda|)k(|\Lambda|)|\Lambda|^{t}$. Our numerical finding that $|K(t)| \sim t^{-x}$, with $x = 2/(2+\theta)$, implies that $n(|\Lambda|)k(|\Lambda|)$ should scale as $\ln|\Lambda|)^{x}$. Our exact evaluation of $n(|\Lambda|)(|\Lambda|)$, for relatively small clusters on a square lattice, indeed seems to fluctuate about $(-\ln|\Lambda|)^{x}$, with $x = 0.69$.

For the myopic ant on a bipartite lattice, $\Lambda = -1$ is always one of the eigenvalues. Therefore, at $t \gg 1$, $K(t)$ will always approach a non-zero oscillating value, $k_{-1}(-1)^{t}$. This term will be absent on non-bipartite (e.g. triangular) lattices. Our other results all apply to all lattices and to all kinds of (e.g. blind) ants. In fact, very similar pure oscillations, whose magnitude decays as r^{-2}, are also expected for the velocity-velocity correlation function†.

Finally, we mention an interesting possible relation between our results and the Langevin equation. If the equation of motion of a particle is $m\ddot{\boldsymbol{r}} + \gamma\dot{\boldsymbol{r}} = \boldsymbol{F}(t)$, and if the random force has zero average and power law correlations, $\langle \boldsymbol{F}(0)\cdot\boldsymbol{F}(t)\rangle \sim |t|^{-x}$, then the time-dependent diffusion coefficient is given by [11] $D(t) = Ct/I(t)$, where $I(t) = \int_{-t}^{0} \mathrm{d}s(t+s)\langle \boldsymbol{F}(0)\cdot\boldsymbol{F}(s)\rangle \sim t^{2-x}$, so that $D(t) \sim t^{x-1} \sim \langle \boldsymbol{r}^2(t)\rangle^{-\theta/2}$, as expected for anomalous diffusion [2]. Indeed, for timescales of order m/γ the Langevin equation yields $\boldsymbol{a} = \ddot{\boldsymbol{r}} \propto \boldsymbol{F}$ and everything is consistent.

In conclusion, we have demonstrated that oscillations play an intrinsic role in acceleration and velocity correlation functions and that the magnitude of these correlations decays with a superuniversal exponent.

† Oscillations in $P(r, t)$ on one-dimensional structures were previously discussed in [8]. Also, see a discussion on discontinuities in P in fractals [9]. Power law velocity-velocity correlations were previously discussed in the context of the Lorentz gas [10].

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