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LETTER TO THE EDITOR

Relaxation behaviour in ultrametric spaces

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Abstract. We model transport in random media through random walks on ultrametric spaces, which allow us to account for energetic randomness. We monitor the relaxation patterns for the trapping and target annihilation problems and show that the relaxation depends qualitatively on temperature.

Relaxation in amorphous media, such as polymeric and glassy systems, often deviates from the exponential form. Relaxation patterns range from stretched exponentials [1, 2] to algebraic time dependences [3, 4]. As was recently pointed out, such behaviours appear naturally in hierarchical models [5-8]. Furthermore the topological realisation of such models are ultrametric spaces [7, 9-13].

In previous works [8, 14, 15] we have analysed several types of disorder and have pointed out the interconnections between different aspects of randomness. Thus, the transport properties of spatially random systems (mixed crystals, alloys) are determined by a distribution of microscopic (site-to-site) transfer rates (temporal disorder) and by different interactions with the surroundings (energetic disorder). Treating the full microscopic problem is an arduous task, which calls for extensive numerical simulations. More analytically minded ways have to invoke some decoupling and to model each disorder type separately. Thus spatial randomness may be modelled through fractals, whereas temporal disorder can be accounted for using waiting time distributions, as are familiar from continuous-time random walk [16] (CTRW) and multiple trapping [5] (MT) approaches. Evidently, one may eventually combine the models, as we have recently demonstrated by considering CTRW on fractals [15].

Ultrametric spaces (UMS) now provide an elegant way to model the *energy* randomness of the sample, and complement the previous approaches. In UMS models the temperature dependence of the transport enters naturally. As we will show, dynamics on UMS is an extension of the MT formalism and involves fractal time.

In this letter we will discuss processes associated with Brownian motion on UMS, such as relaxations related to random walks.

Ultrametric spaces (UMS) occur naturally when classification of objects into distinct clusters is involved [9]. A simple example of a UMS is the *baseline* of figure 1, the whole figure being reminiscent of a Bethe lattice. Only the baseline points belong to the UMS, and the structure above it serves to indicate connections. Cutting the structure above the baseline and parallel to it leads to a system of disjoint clusters. These clusters increase when the height of the cut increases and merge together to form larger clusters

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(nesting property). The height of the cut thus determines a generalised distance for the set of points on the baseline.

More formally, for each hierarchical arrangement as in figure 1 (dendogram) [9] there is a corresponding UMS. In this space $\boldsymbol{X}$ the distance $d(x, y)$ between sites satisfies the strong triangle inequality

$$d(x, y) \leqslant \max(d(x, z), d(y, z)) \tag{1}$$

for all $x, y, z \in \boldsymbol{X}$ [9, 10]. As a consequence of equation (1) all triangles in the UMS are isosceles, i.e., the largest and the second largest of the numbers $d(x, y)$, $d(x, z)$, $d(y, z)$ are equal. Now, if one defines $B_a(r)$ as the sphere with centre a and radius r

$$B_a(r) = [x \in \boldsymbol{X}: d(a, x) \leqslant r] \tag{2}$$

then two spheres $B_a(r)$, $B_b(r)$ with the same radius are either disjoint $B_a(r) \cap B_b(r) = \varnothing$, or identical $B_a(r) = B_b(r)$. It follows that all points of a sphere may be viewed as centres. Any two spheres in a UMS are either disjoint, or one is completely contained in the other. Furthermore, topologically all UMS spheres are both closed and open ('clopen', as formulated in [10]). Thus the terms 'spheres' and the previously discussed 'hierarchical clusters' are synonymous.

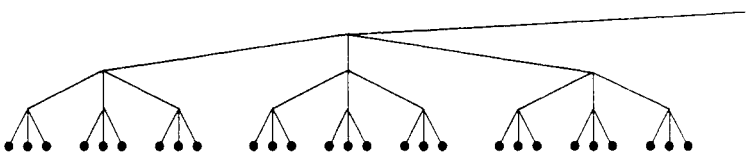

Figure 1. The ultrametric structure (UMS) $\boldsymbol{Z}_3$.

For physical applications we may specify further the term distance. As an example, one may envisage clusters of points in continuum percolation problems. Such clusters are defined by the requirement that the Euclidean distance between neighbouring points of the cluster C is less than a given value δ; then for each pair of points $(x, y) \in C^2$ one can find a path $(x, x_1, x_2, \ldots, x_n, y)$, so that all $x_i \in C$, and the Euclidean distance between successive points of the path is less than δ. If all points of the structure now interact via forces of range less than δ, then the percolation clusters defined above are non-interacting. One may then order the set of points according to the variable δ in a dendogram (UMS).

Another example is provided by the hopping conductivity. Here temporarily localised charge carriers are thermally activated over random energy barriers E_i. In this example the distance which defines the clusters of sites depends on the activation energies via the corresponding Boltzmann factor $e^{-\beta E_i}$. If, after being thermally activated, the charge carriers relax (get trapped) at any site of the system, this example leads to the MT model. To wit, we recover MT expressions by taking the allowed barrier heights to be equidistant, $E_i \in \{j\Delta: j \in N\}$ and to be exponentially distributed $P(E)\,dE \sim e^{-\rho E}\,dE$. The probability of remaining on a site during time t is, averaged over all sites,

$$\Psi(t) = A \sum_{j=1}^{\infty} e^{-\rho j \Delta} \exp(-t\, e^{-\beta j \Delta}) \tag{3}$$

with $A = e^{\rho\Delta} - 1$. The waiting-time distribution $\psi(t)\,dt$ follows from equation (3) by

differentiation, $\psi(t) = -(\mathrm{d}/\mathrm{d}t)\Psi(t)$. Differentiating equation (3) and setting $b = \mathrm{e}^{-\beta\Delta}$ and $N = \mathrm{e}^{-\rho\Delta}$ one obtains

$$\psi(t) = (N^{-1} - 1) \sum_{j=1}^{\infty} N^j b^j \exp(-tb^j). \tag{4}$$

This expression is identical to the one put forward by Montroll and Shlesinger [17, equation (2.122)], in discussing MT. At longer times $\psi(t)$ scales, since $b < 1$ and

$$\psi(bt) = \psi(t)/Nb - (N^{-1} - 1)\exp(-tb) \sim \psi(t)/Nb \tag{5}$$

and thus $\psi(t) \sim t^{-1-\gamma}$, with

$$\gamma = \ln N/\ln b = \rho/\beta. \tag{6}$$

Dispersive transport obtains $b < N$ for $\gamma < 1$.

This picture can now be generalised by considering UMS. The idea is that after an activation by the energy E the charge carrier may reach only sites which belong to the sphere centred on the original site, the sphere radius depending, of course, on E. Using figure 1, and again equidistant energy barriers, a particle activated by E with $\Delta \leqslant E < 2\Delta$ may reach 3 sites (including the original one) and generally for $j\Delta \leqslant E < (j+1)\Delta$ may reach 3^j sites. Here the number 3 appears because of the specific geometry of figure 1, which depicts the UMS $\boldsymbol{Z}_3$. To a general space, say in which the clusters are nested hierarchically, in groups of z objects corresponds the UMS $\boldsymbol{Z}_z$, and an activation energy of $j\Delta \leqslant E < (j+1)\Delta$ allows it to reach z^j sites.

We now consider a simple qualitative argument for random walks on UMS. Basic quantities for such random walks are the distribution $R(t)$ of distinct sites visited in time t, its mean $S(t) = \langle R(t) \rangle$ over all realisations, and the probability $P_0(t)$ of being at the origin.

Consider the time intervals $\mathrm{e}^{k\beta\Delta} \leqslant t_k < \mathrm{e}^{(k+1)\beta\Delta}$. During these intervals the z^k points of the sphere $B_k(\mathbf{0})$ are accessible to the walker, and one has

$$z^k \sim z^{(\beta\Delta)^{-1}\ln(t_k)} = \mathrm{e}^{\gamma \ln(t_k)} = t_k^{\gamma} \tag{7}$$

where we set

$$\gamma = \ln z/(\beta\Delta). \tag{8}$$

For $\gamma < 1$, i.e. $\beta\Delta > 1$, z^k increases more slowly than t_k, and the walker explores practically all points in $B_k(\mathbf{0})$ (compact exploration). Therefore $S(t_k) \sim z^k \sim t_k^{\gamma}$, i.e.

$$S(t) \sim t^{\gamma}. \tag{9}$$

Furthermore, assuming an equipartition of probabilities

$$P_0(t_k) \sim z^{-k} \sim t_k^{-\gamma} \tag{10}$$

i.e. $P_0(t) \sim t^{-\gamma} \sim [S(t)]^{-1}$. The last relation is reminiscent of random walk results in fractal spaces under compact exploration [18].

On the other hand, for $\gamma > 1$ (i.e. $\beta\Delta < 1$), z^k increases more rapidly than t_k and the mean number of distinct sites visited stays proportional to t_k, i.e. $S(t) \sim t$. Here the exploration is non-compact. We note that here one still has $P_0(t) \sim t^{-\gamma}$, as obtained analytically in [13] for walks on the UMS $\boldsymbol{Z}_2$ and in [12] for walks over the *whole* hierarchical lattice.

The central role played by $\gamma = \ln z/(\Delta\beta)$ may also be inferred from an analogy to MT, where b^j is the activation barrier $b^j = \mathrm{e}^{-\beta j\Delta}$ and the level density in the hierarchy

decreases with increasing level as z^{-j}, i.e. $N \sim 1/z$. Then

$$\gamma = \ln(z^{-1})/\ln(e^{-\beta\Delta}) = (\ln z)/(\beta\Delta). \tag{11}$$

From this picture we obtain $\psi(t) \sim t^{-1-\gamma}$ and the relaxation pattern is algebraic.

Returning to random walks we note that the first moments $S(t) = \langle R(t) \rangle$, $\sigma^2(t) = \langle R^2(t) \rangle - \langle R(t) \rangle^2$ of the distribution $R(t)$ of distinct sites visited in t, are analytically difficult to obtain even for walks on regular lattices [19] and an exact expression for $R(t)$ is known only in $d = 1$. On the other hand the knowledge of $R(t)$ is fundamental in the trapping problem, and we obtain this information through simulations.

We have performed a series of simulations on UMS (mostly $\boldsymbol{Z}_2$ and $\boldsymbol{Z}_3$), in which we varied the temperature parameter $\Delta\beta$ and hence γ, equation (8). From the foregoing discussion, $\gamma = 1$ is marginal, and 2γ plays an analogous role [12] to the spectral dimension $\tilde{d}$. We have thus chosen γ values both above and below $\gamma = 1$.

In the simulation calculation we let the random walker start at an arbitrary site of the UMS. The walker attempts at a fixed time interval to perform a step. The level height a walker may reach is distributed according to the activation energies. From this level the walker is directed randomly to one of the points of the corresponding cluster and may therefore land also on the original site. In the simulation we account for 1000 hierarchical levels and thus z^{1000} sites are included.

Consider first the mean number of distinct sites visited in n steps, $S_n = \langle R_n \rangle$. This quantity offers both a check on the accuracy of our simulation procedure, and also allows us to monitor apparent deviations from the leading n^{γ} behaviour, due to logarithmic corrections for γ around 1. The results are presented in figure 2, where

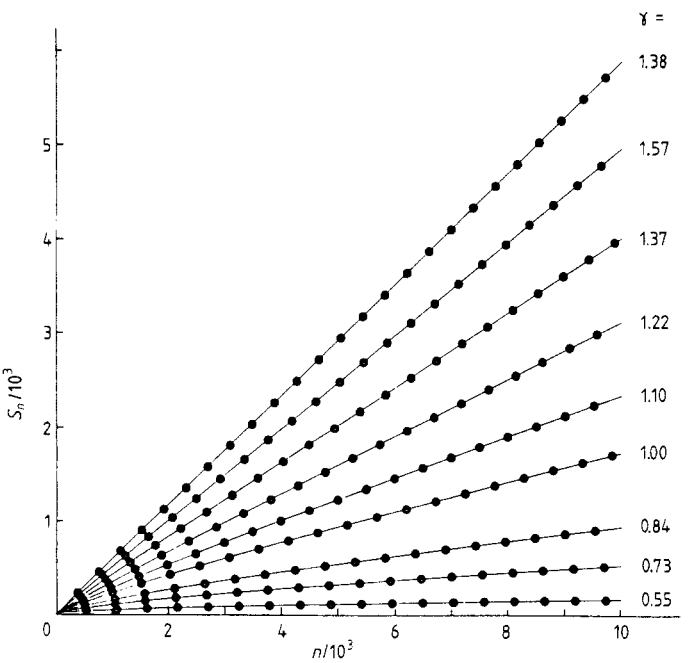

Figure 2. Mean number S_n of distinct sites visited in n steps. The simulation results are given as dots, and the curves are fitted according to equation (12). The values of γ are as indicated.

for each curve 10^4 distinct random walk realisations were averaged. The dots represent the numerical findings, whereas the lines are the best fit ($n \leqslant 10^4$) to the trial function

$$S_n = An^{\alpha}. \tag{12}$$

We summarise the A and α values in table 1. From this table it seems that for $\gamma \leqslant 0.5$, α and γ practically coincide, whereas for $\gamma > 1.5$, α is practically unity. For γ around 1, α is systematically lower, as could be expected from the analogy between 2γ and $\tilde{d}$, since for random walks on two-dimensional lattices $S_n \sim An/\ln n$ holds.

Another quantity which is readily evaluated from the distribution R_n is the variance $\sigma_n^2 = \langle R_n^2 \rangle - \langle R_n \rangle^2$. The results are given in figure 3, and are fitted to

$$\sigma_n^2 = Dn^{\delta} \tag{13}$$

where the D and δ values are again summarised in table 1. For small γ values δ is practically 2γ, whereas for γ larger than 1, δ tends to one. Again this result parallels the behaviour for regular lattices, for which the dependence of the variance on d is largest for $d = 2$; one has $\sigma_n^2 \sim n$ ($d = 1$), $\sigma_n^2 \sim n^2/\ln^4 n$ ($d = 2$) and $\sigma_n^2 \sim n \ln n$ ($d = 3$). Interestingly, for $\gamma < 1$, $2\alpha \simeq \delta$, which seems to imply $\sigma_n^2 \sim S_n^2$, an expression which is exact in $d = 1$, and which holds well [18] for random walks over compact spaces, $\tilde{d} < 2$. It is tempting to conjecture that for the higher cumulants $K_{j,n}$ of the distribution R_n one also has $K_{j,n} \sim n^{\gamma j}$, for $\gamma \ll 1$.

We are now in a position to investigate relaxation phenomena on the UMS. Two interesting problems are the trapping of walkers and the target annihilation.

In the trapping problem mobile walkers are annihilated when hitting immobile traps, randomly distributed on the UMS [19, 20]. As we have often discussed [14, 20, 21], the decay law of the walkers due to a trap density p is

$$\Phi_n = e^{\gamma} \langle e^{-\lambda R_n} \rangle \tag{14}$$

where $\lambda = -\ln(1-p)$ and where the average runs over all realisations of the walk. Equation (14) may be expressed as a cumulant expansion for small n

$$\Phi_n \sim e^{\lambda} \exp\left(\sum_{j=1}^{\infty} (-\lambda)^j K_{j,n}/j! \right). \tag{15}$$

Table 1. Mean $S(t)$, equation (12), and variance $\sigma^2(t)$, equation (13), of the number of distinct sites visited by walkers on the UMS Z_3. For the fit the first 10^4 steps are used.

$\Delta\beta$	γ	A	α	D	δ
4	0.275	1.351	0.288	0.249	0.(57)
2	0.549	1.071	0.548	0.094	1.11
1.5	0.732	0.775	0.708	0.037	1.41
1.3	0.845	0.632	0.793	0.018	1.56
1.2	0.915	0.563	0.839	0.017	1.60
1.1	0.999	0.517	0.882	0.017	1.62
1.0	1.099	0.489	0.921	0.012	1.66
0.9	1.221	0.470	0.956	0.035	1.52
0.8	1.373	0.490	0.979	0.120	1.33
0.7	1.569	0.537	0.992	0.319	1.15
0.6	1.831	0.604	0.997	0.454	1.04
0.5	2.197	0.681	0.999	0.407	0.99
0.1	10.986	0.948	1.000	0.048	1.01

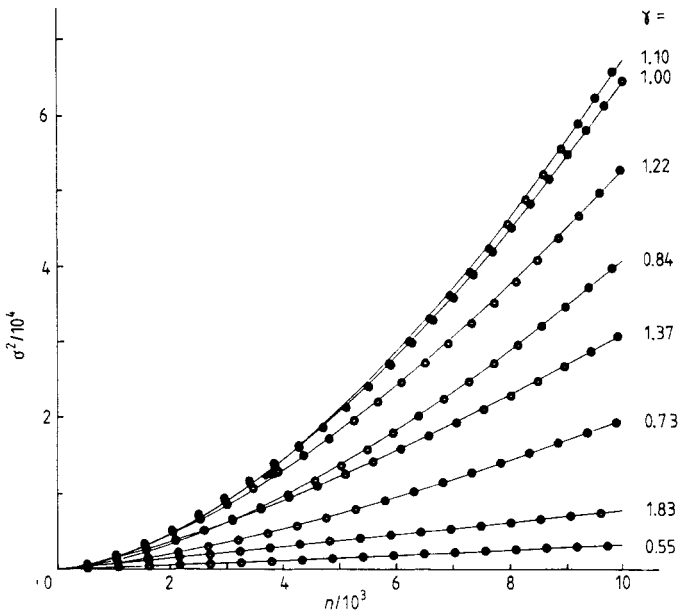

Figure 3. The variance σ_n^2 of the number of distinct sites visited. The notation is as in figure 2, and the fit corresponds to equation (13).

In this region approximations to Φ_n are

$$\Phi_{N,n} = e^{\lambda} \exp\left(\sum_{j=1}^{N} (-\lambda)^j K_{j,n}/j! \right). \tag{16}$$

In figure 4 we present the decay due to trapping on Z_3 for $\Delta\beta = 3/4$, i.e. $\gamma = 1.465$, for several values of p, and compare it to the approximate forms $\Phi_{1,n}$ and $\Phi_{2,n}$. We note that over four orders of magnitude in the decay Φ_n is practically exponential, and that $\Phi_{1,n}$ approximates very well, whereas the agreement with $\Phi_{2,n}$ is excellent. This situation is very reminiscent of the decay for $d = 3$ (see figure 4 of [20]).

A decrease in temperature has a very drastic effect on Φ_n. In figure 5 we present the decay at $\Delta\beta = 2$, i.e. $\gamma = 0.549$. The decay is clearly non-exponential. Furthermore here neither $\Phi_{1,n}$ nor $\Phi_{2,n}$ describe the decay well, and one has to go to a higher order in N to obtain a somehow reasonable approximation. The situation is similar to the one encountered for trapping on the linear chain, $d = 1$ (figure 2 of [20]) and for trapping on the planar Sierpinski gasket, $\tilde{d} = 1.365$ (see figure 3 of [14]). As discussed by us in [21], in the short and in the long time domains Φ_n displays Williams-Watts stretched exponential forms [1, 2]. Of interest here is that a change from exponential to stretched exponential behaviour occurs due to a change in temperature.

To conclude this discussion, we would like to point out that on UMS the target problem, in which immobile targets are annihilated by mobile walkers, admits an exact solution. As in the case for regular lattices [22], for non-interacting walkers, randomly placed on the UMS following a Poisson distribution, we obtain as the decay law

$$\tilde{\Phi}_n = \exp[-\tilde{p}S_n] \tag{17}$$

where now $\tilde{p}$ is the density of the walkers. The derivation of equation (17) follows the lines of our work [22] and our numerical simulations support the above form.

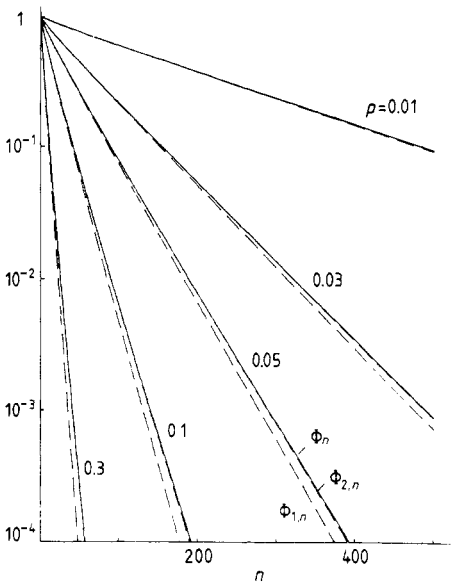

Figure 4. Decay law Φ_n due to trapping on Z_3, where $\gamma = 1.465$ and the trap density p is as indicated. Also given as broken lines are $\Phi_{1,n}$ and $\Phi_{2,n}$, equation (16).

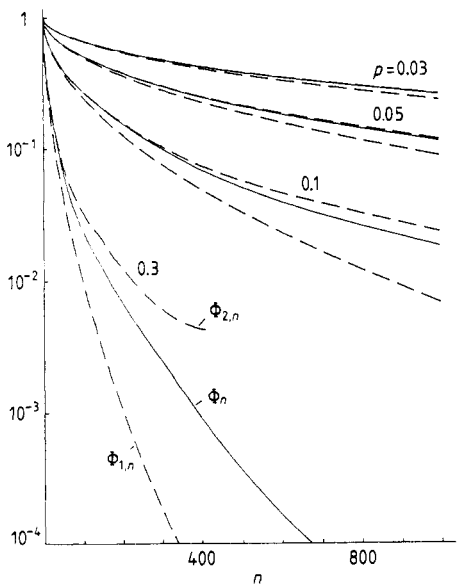

Figure 5. Same as figure 4, for $\gamma = 0.549$.

We remark that for $\gamma < 1$, equation (17) again corresponds to a Williams-Watts type decay [1, 2].

In this work we have analysed dynamical relaxation behaviours on UMS, and have pointed out the analogies to our previous results for random walks on regular lattices and on fractals. All aspects suggest that random walks on UMS with a parameter

$\gamma = \ln z/\Delta\beta$ parallel findings for lattices with a spectral dimension $\tilde{d} = 2\gamma$. Interestingly, one may therefore switch through the marginal behaviour at $\gamma = 1$ ($\tilde{d} = 2$) through a simple temperature change. Such a phase transition should then be clearly visible already in the qualitative pattern (exponential against stretched exponential) of the corresponding decay laws.

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