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LETTER TO THE EDITOR

Random walks on ultrametric spaces: low temperature patterns

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Abstract. We present the numerically determined distribution of the number of sites visited by thermally activated walkers on ultrametric spaces, which mimic the energetic disorder found in amorphous materials. At high temperatures the results resemble those found for Sierpinski-type fractals. At low temperatures, the distributions are highly structured, showing discontinuities which *increase* with the number of steps, in contrast to an intuitive picture that would lead to smoothing. We apply the results to the energy transfer in disordered systems and study the decay due to trapping.

Ultrametric spaces (UMS) have seen an upsurge of interest in the last couple of years [1-7]. Though motivated by recent advances in the theories of spin glasses [1-3, 8, 9] and of computer architecture [10], the ideas behind UMS are based on classification [11] and are of a broad generality [11-15]. Topologically UMS are so simple as to be relegated to exercises in textbooks [13, 14]. The new physical aspects of the UMS are related to *dynamics*, the underlying structures being 'toy models' for anomalous behaviour [15].

In a recent review article on the reaction dynamics in glasses [16] we have pointed out relaxation aspects which may be related to a UMS picture. The main idea is with model transitions in real or phase space through activated jumps over a hierarchical system of energy barriers. For certain ranges of parameters the hierarchical structure leads to scaling behaviour so that UMS parallel in their dynamic features several aspects found for geometrical fractals; indeed one may associate at a given temperature with each regular (homogeneous) UMS an 'effective' spectral dimension [6, 7].

An advantage of the temperature dependence of the dynamical properties of UMS is that changes in temperature allow us to shift the dimension parameter smoothly through all positive values and to study the behaviour in regions *around and below unity*.

As model homogeneous fractal systems, the Sierpinski gaskets are in use [17]; they, however, display spectral dimensions $\tilde{d}$ between unity and two [18, 19] ($1 \leq \tilde{d} < 2$), where $\tilde{d} = 1$ holds for the trivial case of a linear chain (gasket in one-dimensional Euclidean space). Structures with $\tilde{d} < 1$ could possibly be envisaged for geometric fractals (*fractal* dimensions $\bar{d}$ lower than unity are well known, e.g. the Cantor dust [17]), but this would call for extensions of the definitions. In contrast, random walks on UMS at low temperatures correspond to effective spectral dimensions less than one [7].

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In this letter we present several properties of such walks. Interestingly, these walks show strikingly different behaviour from the properties found for Sierpinski gaskets and for regular lattices. For a large number of jumps the distribution of distinct sites visited by the walker attains a comb-like structure, which *sharpens* with increasing number of jumps n. Intuitively, one would in general expect a smoothing with increasing n (in the sense of convergence to a normal law); this is not the case on UMS at low temperatures, where a larger number of steps tends to better unveil the underlying hierarchical pattern. At higher temperatures, however, a smooth distribution is again recovered. These aspects carry over to the relaxation patterns, which show oscillatory behaviour in the effective decay rates. Here we present these findings using as an example the survival probability of a walker on a UMS on which traps are randomly distributed.

In realistic situations sites in a disordered material, such as a glass, are separated by energy barriers, whose height is, in general, random [16]. Taking for simplicity a non-quantal picture and identical ground states for all sites, a 'walker' (such as an impurity, a charge carrier or a localised excitation) needs thermal energy to surmount these barriers. A given activation energy allows a walker to vist only a subset (cluster) of sites around the starting point, the cluster being separated from the other sites by barriers higher than the prescribed activation energy. One may then classify the sites through the energy required to reach them [11]. To such a classification corresponds an ultrametric space (UMS) [11-14].

An example for a UMS is the set of *tips* of a finite Bethe lattice. Figure 1 shows the UMS Z_3; note that only the points on the baseline of the figure belong to the space and the structure above the baseline defines connections. A distance between two sites may now be defined as being the minimal number of branches one has to walk on the tree in order to get from one tip to the other. Such a distance has a physical meaning as being proportional to the energy required to overcome the intersite barrier. It is straightforward to verify that the distance $d(x, y)$ so defined satisfies the strong triangle inequality [13, 14]

$$d(x, y) \leq \max(d(x, z), d(y, z)) \qquad (1)$$

for all sites x, y, z of the UMS. Furthermore, specifying a value $\tilde{E}$ for the activation energy leads to the partition of the UMS into a set of disjoint clusters, where any two points of the *same* cluster are separated by barriers of energy lower than $\tilde{E}$ and any two points belonging to different clusters by barriers higher than $\tilde{E}$. Here we take the barrier heights to be hierarchically distributed for simplicity, so that all consecutive energy levels differ by Δ and assume that the branching ratio z is constant over the whole Bethe lattice (in figure 1 $z = 3$). The UMS considered here are thus homogeneous.

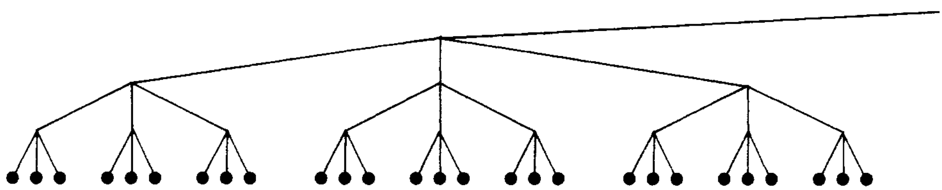

Figure 1. The ultrametric structure (UMS) Z_3.

An important quantity for describing dynamical aspects is the distribution of the number R_n of distinct sites visited by a walker in n steps. For instance the survival probability of the walker in the presence of randomly distributed traps is [20]

$$\Phi_n = \langle \exp[-\lambda (R_n - 1)] \rangle \tag{2}$$

where $\lambda \equiv -\ln(1-p)$, with p being the probability that a site is occpuied by a trap and where the average is to be taken over all realisations of random walks.

Even for regular lattices the knowledge of R_n is rudimentary and an analytical expression for Φ_n exists only in $d = 1$ [21]. Detailed knowledge is available for S_n, the mean number of distinct sites visited, i.e. for

$$S_n \equiv \langle R_n \rangle. \tag{3}$$

For S_n the marginal dimension is two. Thus, above $d = 2$ one has asymptotically $S_n \sim n$, whereas below it

$$S_n \sim n^{\tilde{d}/2} \tag{4}$$

holds, with $\tilde{d}$ being the spectral dimension for fractals [18, 19, 22] ($\tilde{d} = d$ for regular lattices). As we have discussed in [7], for UMS a similar picture emerges, with

$$\gamma = (kT/\Delta) \ln z = \ln z/(\Delta\beta) \tag{5}$$

being the parameter which determines the behaviour of S_n. Thus

$$S_n \sim \begin{cases} n & \text{for } \gamma > 1 \\ n^{\gamma} & \text{for } \gamma < 1. \end{cases} \tag{6}$$

It is therefore natural to view 2γ as being an 'effective' spectral dimension [6, 7], which, as indicated in (4), is temperature dependent.

Serious analytical efforts have revealed characteristics of the full R_n distribution for *regular* latices [23, 24]. Thus, it is known that for $d = 3$ the distribution of R_n tends to a Gaussian, whose normalised form sharpens towards a Dirac δ distribution for $n \to \infty$, and the same is expected for $d = 2$ whereas for $d = 1$ the normalised R_n distribution converges to a regular function (proper law). For a detailed picture in the full time regime both for regular lattices with $d \neq 1$ and also for fractals numerical simulations are necessary.

In previous works [20, 22, 25, 26] we have used simulation calculations to obtain via R_n the decay laws due to trapping (equation (1)). An analysis of the R_n distribution for fractals from numerical simulations has been presented by Angles d'Auriac *et al* [27]. For $\tilde{d} = 1.365$ (Sierpinski gasket embedded in $d = 2$) they find evidence for the convergence of R_n towards a proper law and conjecture that similar behaviour holds for all $\tilde{d} < 2$. The R_n distributions show an overall smooth shape with a broad maximum and a small superimposed structure (see figure 4 of [27]). The structures are reminiscent [21] of the findings in $d = 1$, which, for later convenience, we now recall.

In figure 2 we present the numerical findings for nearest-neighbour random walks on $d = 1$. The curves show the results of some 10 000 realisations of walks and the distributions after 10, 100 and 1000 steps. The normalised probability distributions $\rho_n(x)$ are given, where we set $x \equiv R_n/S_n$, and where the area under $\rho_n(x)$ equals unity. With increasing n one observes the emergence of an asymmetrically shaped form with a single broad peak.

What is the situation on UMS? To obtain this information we have performed a series of calculations (mostly on Z_2, Z_3 and Z_5), in which we varied the temperature

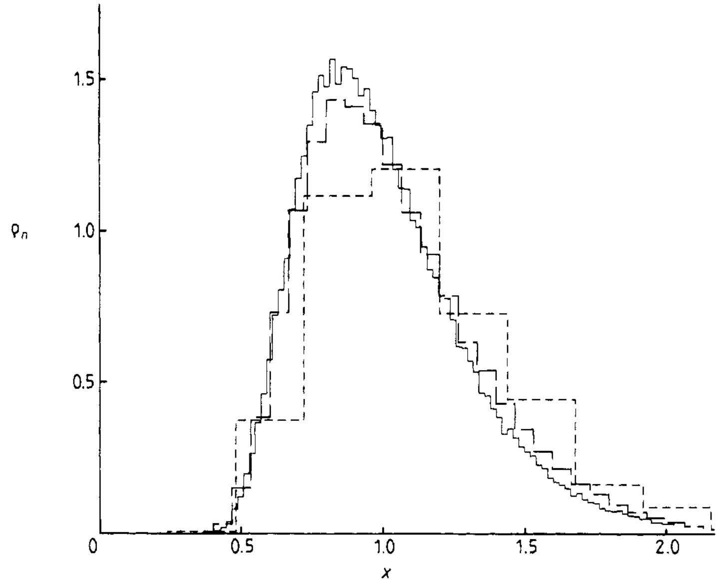

Figure 2. The normalised probability $\rho_n(x)$ of the number R_n of distinct sites visited after n steps plotted in units of $x \equiv R_n/\langle R_n \rangle$. The distributions depicted correspond to the situation after 10, 100 and 1000 steps for nearest-neighbour random walks on $d = 1$; $n = 10$ is designated by short, $n = 100$ by long dashes and $n = 1000$ by full lines.

parameter $\beta\Delta$, and hence γ (see (4)). In the simulations we let the random walker start at an arbitrary origin, all starting sites being equivalent for a homogeneous UMS. The walker attemps at fixed time intervals to perform a jump. The barrier heights a walker may reach are distributed according to the thermal activation. From an attained 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 100 hierarchical levels and thus z^{100} sites are included.

As a first example we consider in figure 3 a series of random walks on Z_3, where the parameter $\beta\Delta$ equals unity, $\beta\Delta = 1$ and hence one has $\gamma = 1.1$, which corresponds to an effective spectral dimension slightly larger than two, $\tilde{d} = 2.2$. Again the curves $\rho_n(x)$ for $n = 10$, 100 and 1000 are presented. With increasing n an almost symmetrical shape develops, much reminiscent of a normal distribution, the differences being a slightly steeper descent at higher x values (to be contrasted with figure 2, where the opposite is the case) and small oscillations in a threefold pattern, which stems from having walks on a UMS with $z = 3$.

A drastic change occurs for smaller temperatures. Figure 4 presents the change which comes about by doubling parameter $\beta\Delta$, and thus having $\beta\Delta = 2$. Here the curves for $n = 100$ and 1000 are presented. For $n = 1000$ practically no trace is left of a continuous curve and the distribution (for which an envelope may possibly be envisaged for $n = 100$) disintegrates into a series of spikes, most of which come in families of threes, and some of which may be 'genealogically' readily pursued up to the fourth generation. Again these threefold aspects are based on having $z = 3$ (and, of course, walks on Z_5 show a fivefold family structure). Note that for Z_3 $\beta\Delta = 2$ implies $\tilde{d} = 1.1$ and hence we are above the value $d = 1$ of figure 2. Thus, although $S_n = \langle R_n \rangle$ is well behaved and σ_n^2 is relatively well behaved (and thus they lend weight to the identification of 2γ with $\tilde{d}$) the R_n distributions are in no way well characterised

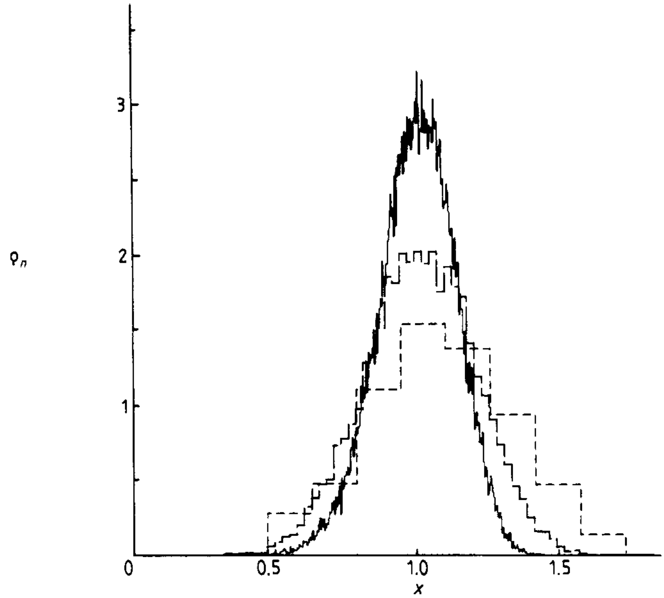

Figure 3. Same as in figure 2, where the random walk takes place over the UMS Z_3 and the temperature parameter $\beta\Delta = 1$ ($\gamma = 1.1$, $\tilde{d} = 2.2$).

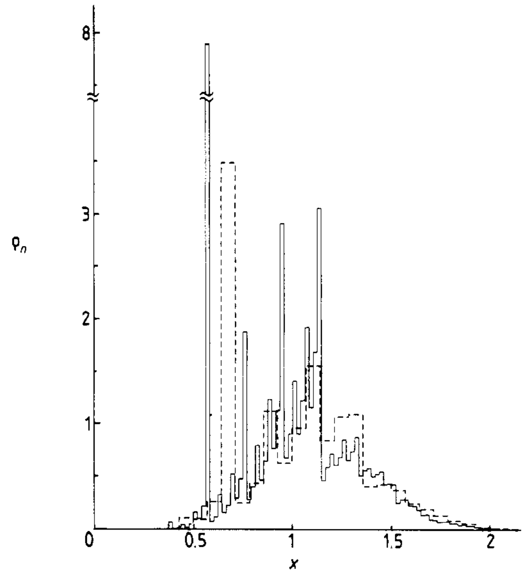

Figure 4. Same as in figure 2, where the random walk takes place over the UMS Z_3 and $\beta\Delta = 2$ ($\gamma = 0.55$, $\tilde{d} = 1.1$). For clarity only the situation after 100 and 1000 steps is presented.

by their first moments for large $\beta\Delta$ (small T). The fascinating aspect of the matter (at least to us) is the emergence of the structured picture at $n = 1000$ from a quite shapeless form at $n = 10$; the increase in the number of steps *sharpens* our possibility of observation and unveils the underlying UMS, while in general, under usual conditions, on regular lattices a global *smoothing* is observed with increasing n.

For smaller values of γ (we have also used $\beta\Delta=3$ and 4) and hence $\gamma=0.37$ ($\tilde{d}=0.74$) and $\gamma=0.27$ ($\tilde{d}=0.54$) the main peaks increase at the cost of the background, so that for $n=1000$ and $\tilde{d}=0.54$ one is left in practice with only the equidistant four main peaks of figure 4, where the leftmost one is considerably increased compared to the other three.

Let us now follow the consequences of these R_n distributions in the case of trapping (equation (2)). As we have discussed in the context of regular lattices [20], there one could, at least in the short-time regime, use a cumulant expansion and approximate Φ_n through

$$\Phi_n \simeq e^{\lambda} \exp\left(\sum_{j=1}^{N} (-\lambda)^j K_{j,n}/j!\right) \equiv \Phi_{N,n} \tag{7}$$

where $K_{j,n}$ are the cumulants (semi-invariants) of the R_n distribution and are related to its moments. It is known that for regular lattices (7) is poor at extremely long times, since asymptotically a non-analytical dependence on λ obtains in general in the exponent. Indeed, for UMS the corresponding analysis leads to the form

$$\Phi_n \sim \exp(-C\lambda^{\gamma/(\gamma+1)} n^{1/(\gamma+1)}) \tag{8}$$

akin to a simlar form for fractals [25, 29]. Equation (7) is quite useful at small and moderately large n in the three-dimensional case [20]. The domain of validity of (7) is very restricted, however, for $d=1$ [21]. The same also holds, as we have observed, for UMS, when the parameter 2γ approaches unity [7] due to the poor representation of the R_n distribution through its first moments. Hence an expansion in terms of cumulants is quite ineffective as an approximation method when γ approaches even lower values, $\gamma<0.5$.

In such cases we found an analytic lower limit to Φ_n to be the appropriate tool. As we will show elsewhere

$$\Phi_n \geqslant \sum_{m=0}^{\infty} (\omega_m^n - \omega_{m-1}^n)(1-p)^{z^m-1} \tag{9}$$

where $\omega_m = 1 - R^m(z-1)/(z-R)$ and $R=\exp(-\beta\Delta)$. We use the right-hand side of (9) as an approximation to Φ_n. This approximation depends on how well a walker visits *all* sites on a UMS level before proceeding to the next level (compact exploration [25, 26, 29]) and works better for low γ values.

To display our findings we present in figure 5 the decay due to trapping on the UMS $\boldsymbol{Z}_3$, when the parameter $\beta\Delta=4$ and where one hence has $\gamma=0.27$ ($\tilde{d}=0.54$). The results of simulations which are obtained when the concentrations of traps in (2) are $p=0.03$, 0.1, 0.3 and 0.5 are shown. Indicated are both the decay forms which follow from the use of the cumulant expansion (equation (7)) with $N=1$ and $N=2$ as well as the expressions giving the lower limit (equation (9)). While in the initial decay region, where $0.1 \leqslant \varphi_n \leqslant 1$, the short-time cumulant expression $\Phi_{2,n}$ works well, at longer times the cumulant expressions become inadequate, whereas the approximating quality of the lower bound, equation (9), increases. A similar finding also holds for the relaxation forms for $\beta\Delta=2$, as presented in figure 5 of [7]; there $\Phi_{2,n}$ approximates well only for the first order of magnitude of the decay. On the other hand, an analysis of the data shows the lower limit to become a reasonable approximation at longer times (although not so good as in figure 5 here). An interesting feature evident from figure 5 is the appearance of piecewise quasi-exponential regions, due to large differences in the microscopic decay rates. The situation is reminiscent of the

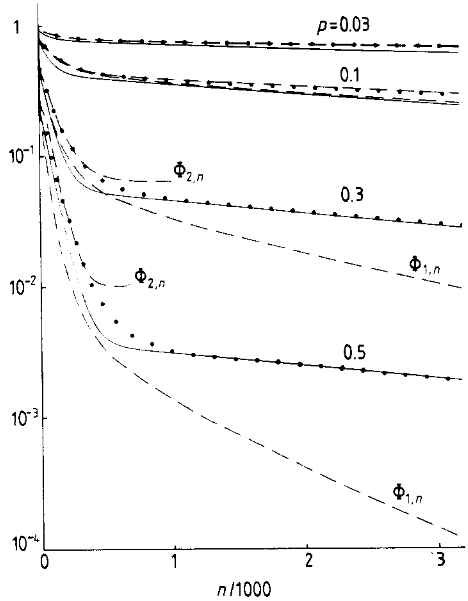

Figure 5. Survival probability of a random walker on the UMS Z_3 in the presence of randomly distributed traps. The probability that UMS sites are traps is given by p and equals 0.03, 0.1, 0.3 and 0.5, respectively. The results of the simulations (dots), the cumulant expansions $\Phi_{1,n}$ and $\Phi_{2,n}$ (equation (7)) (full curves) and the lower bound expression (equation (9)) (broken curve) are displayed.

findings in relaxation patterns based on direct transfer processes in low-dimensional spaces [30] but we postpone an extended discussion of this feature here.

Summarising, random walks on fractals and UMS show, besides remarkable parallels, interesting differences in their behaviour related to reactions. We thus reiterate our conviction that such aspects may show up in experiments which study relaxation in disordered systems, when monitored in an extended range of temperatures. At low temperatures the underlying UMS structure (when present) will become visible and multiple step processes will not smooth out but enhance the observable structured pattern.

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