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COMMENT

A conjecture on the Vogel–Fulcher law on hierarchical structures

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Abstract. We suggest modifying recent results on dyanmical phase transitions on systems with hierarchically distributed barriers. If we slightly change the transition rates, given by the barriers, we obtain a Vogel-Fucher law for the diffusion constant.

Ultrametric structures are of considerable interest in statistical mechanics of transport and relaxation phenomena. Ultrametricity is a simple topological concept [1], but the relevance for some physical problems was recognised very recently [2] on investigation of the mean-field theory of spin glasses. It was discovered that the distribution of the ground states in configurational space have ultrametric structure. A simple sketch of an example of an ultrametric space is given in figure 1, where the ultrametric space is represented by the baseline of the tree. These ultrametric structures are an excellent tool to model energetic disorder. Imagine a particle sitting at one of the points of the baseline. If the particle wants to jump to neighbouring sites it has to cross energy barriers which are hierarchically distributed. In the above figure the smallest energy barrier is given by Δ. The hierarchical distribution of the barriers is a weaker constraint than random barriers [3], but the results are similar. It is interesting to note that there are now three ways of modelling disordered structures. The ultrametric space is connected with energetic disorder as described above. Spatial disorder can be modelled by fractal objects [4], while temporal disorder can be treated by the continuous time random walk [5].

All these models are discussed in connection with special features shown by disordered systems. For example, non-exponential relaxation in dielectric and mechanical response in a wide range of materials like glasses [6] or polymers [7] can be explained by using constrained dynamics [8]. Recent investigations on spin dynamics [9] and experiments on physical aging in spin glasses obtain similar results. In the context of chemical reactions in disordered systems fractals and ultrametic

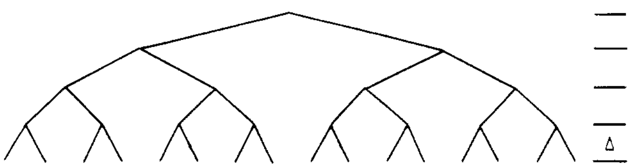

Figure 1. A simple sketch of an ultrametric structure with branching index 2 and barrier height Δ between each level of generation.

spaces have been treated [11] where it was found that the number of particles undergoing the reaction is non-exponential in time. On the other hand, if one tries to model disordered systems with these kinds of considerations the discussion on the behaviour transport coefficients should be taken into account. Considering the particle on an ultrametric space like in figure 1 it is easy to imagine that at high temperatures compared to the barrier height the particle can jump on every site of the ultrametric space. The particle does not 'feel' the hierarchical barriers. At low temperatures compared to the barrier height the mobility of the particle should be reduced drastically. This has an effect on the transport properties such as the diffusion constant. We expect therefore strong dependence of temperature in the diffusion coefficient. It was already pointed out by Teitel and Domany [12] that there is a phase transition from normal to anomalous diffusion. Normal diffusion states the mean square displacement following the classical $R^2 \sim t$ dependence, while the term anomalous diffusion stands for all other laws for the mean square displacement of the particle. Apparently there are two possibilities of $R^2 \sim t^\alpha$ with $\alpha > 1$ (fast anomalous diffusion occurring in turbulence [13]) or $\alpha < 1$ as well as $R^2 \sim (\log t)^\alpha$ (slow anomalous diffusion) found in all sorts of irregular systems (ant/termite problem) [14].

In this comment we want to look at the dynamics on the ultrametric problems under the detailed consideration of the temperature dependence for the diffusion coefficient D. General aspects on the dynamics have been studied previously [15, 16]. It was shown that the relevant quantity for relaxation patterns is the autocorrelation function $P_0(t)$ being the probability of a particle to return to the origin, where it started at $t=0$. $P_0(t)$ is given by

$$P_0(t) \sim t^{-\log z/\beta\Delta}$$

where z is the branching index of the ultrametric space. From the general theory on self-similar lattices it was shown that $P_0(t) \sim t^{d_s/2}$ [17, 18] and by comparison $d_s = 2(\log z)/\beta\Delta$. d_s is the spectral dimension of the structure [17, 18] (see also [11]). The above result is only true if the barriers at each level (see figure 1) are the same.

Here we choose a one-dimensional model studied by Teitel and Domany [11]. These authors found a transition from normal to anomalous diffusion. In their model the transition was ruled by a critical value of the barrier height (or the transition probabilty which is the inverse of the barrier height).

Consider a *one-dimensional* chain with z^n sites where a particle can hop. The transtion rates from one site to another are assumed to be symmetric, say $W_{k,k\pm1} = W_{k\pm1,k}$. The dynamics of the particle is given by the master equation

$$\partial P_k/\partial t = W_{k,k+1}(P_{k+1} - P_k) - W_{k-1,k}(P_k - P_{k-1}). \tag{1}$$

The simplest model of equally distributed barriers [12, 16] is

$$W_{k,k+1} = R^m \qquad \forall l \leq m,\ k(\mathrm{mod}\ 2^l) = 0 \tag{2}$$

where R is the transition rate on the ultrametric scheme. The result for $P_0(t)$ is given by [12]

$$P_0(t) \sim \begin{cases} (D(R)t)^{-1/2} & R_c < R < 1 \\ t^{-x} & 0 < R < R_c \end{cases} \tag{3}$$

where

$$x = \frac{\log z}{\log z + \beta\Delta}. \tag{4}$$

Note that this exponent is different from the first equation in this paper coming from the one-dimensional character of the model here. $D(R)$ is the diffusion constant depending on the rate. Interpretation of (3) is as follows: as long as $D(R)>0$ one has normal diffusion $\langle R^2(t)\rangle = D(R)t$. If R approaches the critical value R_c the diffusion turns out to be (slow) anomalous.

$D(R)$ can be calculated by using [19]

$$\frac{1}{D}=\frac{1}{N}\sum_{k=1}^{N}\frac{1}{W_{k,k+1}}. \tag{5}$$

Zwanzig [19] has shown that for a one-dimensional chain with random barriers D exhibits a 'long time tail', but for our considerations these corrections are not of interest. Applying (5) to the ultrametric problem D is found to be (in the limit of $N\to\infty$)

$$\frac{1}{D}=\frac{1}{z}\sum_{m=0}^{\infty}\left(\frac{1}{zR}\right)^m=\frac{1}{z}\frac{1}{1-(zR)^{-1}} \tag{6}$$

and

$$D\sim(1-1/zR) \tag{6a}$$

so that $R_c=z^{-1}$.

If we assume temperature induced hopping we put

$$R=\mathrm{e}^{-\beta\Delta} \tag{7}$$

and we find for the diffusion constant

$$D\sim\{1-\exp[\beta\Delta(1-\gamma)]\} \tag{8}$$

where $\gamma=(\log z)/\beta\Delta$. As γ approaches 1 the exponential may be expanded and we find

$$D\sim(1-T_0/T). \tag{9}$$

The transition temperature is given by

$$T_0=\Delta/\log z. \tag{10}$$

T_0 now depends purely on structural parameters of the ultrametric space, a result which is expected.

It is quite common, however, to use the hierarchical structures as a model for disordered or glass-like systems. The glass transition in amorphous materials shows similar behaviour to the transition discussed above. At higher temperature the particles are mobile and the long-time behaviour of a particle in a fluid is $R^2(t)\sim t$ following the Einstein law. Decreasing the temperature and approaching the glass transition temperature the particles become more and more immobile and one can expect anomalous diffusion at extremely long times. Clearly the glass transition itself is a highly non-equilibrium phenomenon and depends on the kinetics of the system [20].

Nevertheless we will try to find common features of the glass transition and the mobility transition on the ultrametric space. One universal fact of the glass transition seems to be the Vogel-Fulcher law which has an unusual essential singularity in temperature. For the diffusion constant it becomes [20]

$$D\sim\exp\left(-\frac{A}{T-T_0}\right) \tag{11}$$

where A and T_0 are fit parameters. T_0 is not the glass temperature T_g, but a temperature below: $T_0 \approx T_g - 50°$. Edwards and Vilgis have calculated the Vogel-Fulcher law directly for a system of dense hard rods [21, 22]. There the Vogel-Fulcher law was the consequence of cooperative motion of some rods, while a law of the type of (9) was a result of a mean-field theory (see [21] for details).

As a consequence the next step would be to find a modification of the ultrametric structure so that the Vogel-Fulcher law appears. To do this we define a new rate

$$\left(\frac{1}{R}\right)^m := \left(\frac{1}{R_0} - \frac{1}{R_1} + \frac{1}{R_1}\frac{1}{\sqrt{m}}\right)^n \tag{12}$$

where R_1 is assumed to be a small perturbation of the original rate R_0. Defining

$$\frac{1}{R_0} - \frac{1}{R_1} = \exp[\beta(\Delta - \varepsilon)] \tag{13}$$

as a formal identity where ε is, according to $1/R_1$, a small quantity. Equation (12) would mean in the context of [16]

$$\begin{aligned}\Delta(m) &= (\Delta - \varepsilon)m + \frac{1}{\beta} m \log\left[1 + \frac{1}{\sqrt{m}}(e^{\beta\varepsilon} - 1)\right] \\ &\underset{\substack{\varepsilon \to 0 \\ m \to \infty}}{\approx} (\Delta - \varepsilon)m + \varepsilon\sqrt{m}.\end{aligned} \tag{14}$$

$\Delta(m)$ is then the distance between each level of generation (see figure 1) which reduces to equidistant energy barriers by $\varepsilon \to 0$.

According to (6) we have to sum a series of the type

$$S = \sum_n \left(\alpha + \frac{\alpha_1}{\sqrt{n}}\right)^n.$$

This can be done by parametrisation [21]

$$S \cong \int_0^\infty dn \exp[-(1-\alpha)n + \alpha_1\sqrt{n}] \tag{15}$$

and the diffusion constant becomes

$$\frac{1}{D} \sim \int_0^\infty dn \exp\left[-\left(1 - \frac{1}{R_0} + \frac{1}{R_1}\right)n + \frac{1}{R_1}\sqrt{n}\right]. \tag{16}$$

The integral contains an error function, but the main contribution is given by the steepest descent approximation

$$D \sim \exp\left(-\frac{\frac{1}{4}(1/R_1)^2}{1 - \frac{1}{2}(1/R_0 - 1/R_1)}\right). \tag{17}$$

By use of the definition (13) we find for R_1

$$\frac{1}{R_1} = e^{\beta\Delta}(1 - e^{-\beta\varepsilon}). \tag{18}$$

Inserting the definition (13) and (18) in (17) we find the final result (ε small)

$$D \approx \exp\left(-\frac{\frac{1}{4}e^{2\Delta/T}(\varepsilon/T)^2}{1 - \theta/T}\right) \tag{19}$$

where the transition temperature is now given by

$$\theta = \frac{\Delta - \varepsilon}{\log z} = T_0 - \frac{\varepsilon}{\log z}. \tag{20}$$

At $T \approx \theta$ (19) can expressed by

$$D \sim \exp\left(-\frac{\frac{1}{4}e^{2\Delta/\theta}(\varepsilon/\theta)^2}{T-\theta}\right) \tag{21}$$

which is now in the form of the Vogel-Fulcher law (11). We want to stress that the corrections we used show similar behaviour on the Vogel-Fulcher law and hence the same features as given in [21].

The last remark would be to see if there is a significant change in the dynamical quantity $P_0(t)$. In order to do a crude estimate of this one can take a modification of (9) of [16] and use (14) of this paper. $P_0(t)$ is then given by

$$P_0(t) \sim \int_0^\infty \mathrm{d}x \exp[-x \log z - \alpha(\beta\Delta)t \exp(-\rho\Delta(m) - m \log z)]. \tag{22}$$

$\alpha(\beta\Delta)$ is a slow varying function of temperature. In the limit of $\varepsilon \to 0$ the result given in [12] is recovered. There is no simple way of expressing the integral in (22) by elementary methods but we expect no significant change of $P_0(t)$ in the limit of small ε. A more detailed analysis will be given elsewhere.

In summary we have presented a simple modification of a one-dimensional ultrametric space which produces a Vogel-Fulcher law for the diffusion coefficient. This modification does not change the dynamical quantity $P_0(t)$ significantly. The modifications leading to the Vogel-Fulcher law here are different kinds as in [21, 22]. The physical picture in these references is that cooperative motion produces the Vogel-Fucher law, while here a modification of the ultrametric structure produced this behaviour for the diffusion constant. Cooperativity means that more and more particles are involved in the motion as the transition temperature is approached.

Nevertheless the modification does not change the dynamical behaviour. The same result was found in [22], where it was stated that cooperativity does not change the relaxation behaviour significantly.

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References

[1] Schikhof W H 1984 *Ultrametric Calcules* (Cambridge: Cambridge University Press)
[2] Mézard M, Parisi G, Sourlas N, Toulouse G and Virasoro M 1984 *Phys. Rev. Lett.* **52** 1156
[3] Alexander S, Bernasconi J, Schneider W R and Orbach R 1981 *Rev. Mod. Phys.* **53** 175
[4] Mandelbrot B B 1982 *The Fractal Geometry of Nature* (San Francisco: Freeman)
[5] Montroll E W and Scher H 1973 *J. Stat. Phys.* **9** 101
[6] Ngai K L and Wright G B (ed) 1985 *Relaxation in Complex Systems* (Washington: NRL)
[7] Williams G and Watts D C 1970 *Trans. Faraday Soc.* **66** 80
[8] Palmer R G, Stein D L, Abrahams E and Anderson P W 1984 *Phys. Rev. Lett.* **53** 958

[9] Rammal R 1985 *J. Physique* **46** 1837
[10] Ocio M, Alba M and Hamman J 1985 *J. Physique Lett.* **46** L1101
[11] Zumofen G, Blumen A and Klafter J 1986 *Preprint*
[12] Teitel S and Domany E 1985 *Phys. Rev. Lett.* **55** 2176
[13] Grossmann S, Wegner F and Hoffmann K H 1985 *J. Physique Lett.* **46** L575
[14] Hughes D 1984 *Mathematics and Physics of Disordered Media* (*Lecture Notes in Mathematics*) (Heidelberg: Springer)
[15] Paladin G, Mézard M and de Dominicis C 1985 *J. Physique Lett.* **46** L985
[16] Ogielski A T and Stein D L 1985 *Phys. Rev. Lett.* **55** 1634
[17] Rammal R and Toulouse G 1983 *J. Physique Lett.* **44** L13
[18] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625
[19] Zwanzig R 1982 *J. Stat. Phys.* **28** 127
[20] Jäckle J 1986 *Rep. Prog. Phys.* **49** 171
[21] Edwards S F and Vilgis T 1985 *Physics of Disordered Materials* ed D Adler, H Fritsche and S Ovshinsky (New York: Plenum)
[22] Edwards S F and Vilgis T *Preprint*