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LETTER TO THE EDITOR

Exact renormalisation group approach to ultradiffusion in a hierarchical structure

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Abstract. A model of diffusion in one dimension, with a hierarchical pattern of hopping rates, is studied by an exact renormalisation method. Non-universal time scaling exponents are obtained for autocorrelation function, range and average diffusion distance.

In a recent paper, Huberman and Kerszberg (1985) propose a model for relaxation in hierarchical structures, which they expect to display an anomalous decay process, termed ultradiffusion. As these authors remark, systems having a whole hierarchy of time scales appear in several fields, ranging from molecular diffusion on complex macromolecules (Austin *et al* 1975), to spin glasses (Sompolinsky 1981), or computing structures (Huberman and Hogg 1984).

In the present letter, we show that the model of Huberman and Kerszberg (1985) actually allows for an exact dynamical renormalisation group treatment. The approach presented here provides a complete description of the scaling properties associated with ultradiffusion at long times, and thus a rigorous check of previous approximate and numerical predictions (Huberman and Kerszberg 1985); this approach should also stimulate additional interest in the model itself, in view of the wide range of physical situations which its mathematics is expected to exemplify.

Following Huberman and Kerszberg (1985), let us consider the diffusion of a particle in the one-dimensional environment schematically represented in figure 1. The vertical segments in the figure represent energy barriers, which obstruct the hopping of the particle from a given cell to its nearest neighbours. The length of each segment is inversely proportional to the probability, ε_i, that the barrier is crossed in unit time (i.e. the taller the energy barrier, the smaller ε_i).

Diffusion on such a hierarchical structure has been termed ultradiffusion by Huberman and Kerszberg (1985), with emphasis on the fact that hierarchical systems possess an ultrametric topology (Bourbaki 1966).

Denoting by $P_m(t)$ the probability that the particle occupies cell m at time t, and by $\tilde{P}_m(\omega)$ its Laplace transform, a system of equations of the form

$$\omega\tilde{P}_m = \alpha_{m+1,m}(\tilde{P}_{m+1} - \tilde{P}_m) + \alpha_{m-1,m}(\tilde{P}_{m-1} - \tilde{P}_m) + \delta_{m,0} \tag{1}$$

describes the diffusion. In equation (1) the term $\delta_{m,0}$ specifies the initial condition: the particle is assumed to be in cell 0 at the initial time, i.e. $P_m(t=0) = \delta_{m,0}$. For each couple of nearest-neighbour cells, m and $m+1$, $\alpha(m, m+1)$ takes the appropriate

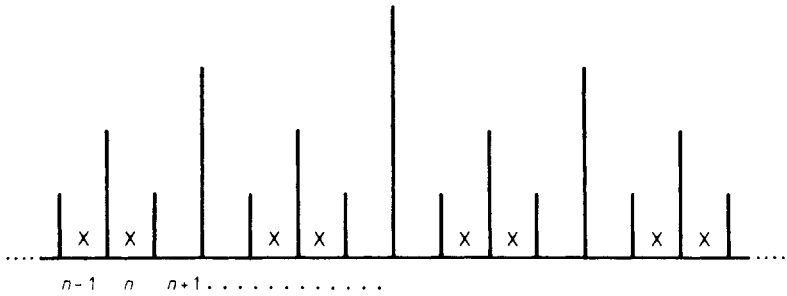

Figure 1. Cells with crosses are decimated in the present renormalisation scheme.

value, ε_i, of the hopping rate associated with the corresponding barrier (to avoid confusion we will use labels i or j exclusively to specify hopping rates across barriers in our hierarchy; for simplicity we will also put $\varepsilon_0 = 1$, for the lowest barrier, which amounts to fixing the unit of time).

The renormalisation group approach we propose amounts to a dynamical decimation of (1), carried out in such a way as to leave its basic structure invariant. With reference to figure 1, imagine that we eliminate from the linear system (1) all the values of P corresponding to cells marked by crosses. With such an elimination, the 'surviving' P values, after a proper rescaling and redefinition of ω, satisfy a system of the same form as (1), with modified, frequency-dependent, values of ε.

The new system describes a problem spatially rescaled by a factor $l = 2$, with respect to the original one. The actual computation yields

$$\omega' = (\omega+1)^2 \frac{(\omega+1+2\varepsilon_1)}{\varepsilon_1} - \frac{(\omega+1)}{\varepsilon_1} - 2 \tag{2}$$

$$\varepsilon_i' = \frac{(\omega+1+\varepsilon_1)^2 - \varepsilon_1^2}{\varepsilon_1} \varepsilon_{i+1} \qquad i = 1, 2, \ldots \tag{3}$$

$$\tilde{P}'_{n'} = \frac{\varepsilon_1}{(\omega+1+\varepsilon_1)^2 - \varepsilon_1^2} \tilde{P}_n. \tag{4}$$

The value of ε_0' stays equal to 1, by construction. The surviving cells are properly relabelled by an integer n'. Moreover it will be assumed that cell 0, at which diffusion starts, survives decimation ($n' = 0$ for $n = 0$) in such a way that the inhomogeneous equation for $\tilde{P}_0'$ remains of the same form as the one for $\tilde{P}_0$.

Since different ω are not coupled in (1), in order to study the leading singular behaviour associated with scaling at long times, we can simply consider the $\omega \to 0$ limit of (2)-(4) and perform a renormalisation group analysis on them. Thus the memory effects associated with the sub-leading dependences in (2), (3) and (4) do not need to be considered†, and we simply obtain

$$\omega' = 2 \frac{2\varepsilon_1 + 1}{\varepsilon_1} \omega \tag{5}$$

$$\varepsilon_j' = \frac{1+2\varepsilon_1}{\varepsilon_1} \varepsilon_{j+1} \qquad j = 1, 2, \ldots \tag{6}$$

† For a discussion of corrections to the leading dynamical scaling behaviour, these effects should be taken into account. This would imply working with a functional equation, which transforms a general function of ω, instead of simply ω, as well as with functional recursions for ω-dependent ε.

and

$$\tilde{P}_{n'}(\omega', \{\varepsilon'\}) = \frac{\varepsilon_1}{1+2\varepsilon_1} \tilde{P}_n(\omega, \{\varepsilon\}). \tag{7}$$

On the basis of (5)-(7) the dominant singular behaviour for $\omega \to 0$ of the $\tilde{P}$, or related quantities, can be discussed: we only need to analyse the possible fixed points of (6) and their stability.

The mapping (6) actually turns out to allow for a whole line of fixed points $\{\varepsilon^*\}$, with

$$\varepsilon_i^* = \varepsilon_1^* \left(\frac{\varepsilon_1^*}{1+2\varepsilon_1^*} \right)^{i-1} \qquad i = 1, 2, \ldots \tag{8}$$

and ε_1^* ranging from 0 to $+\infty$. The fixed point with $\varepsilon_1^* = 0$ corresponds to a situation in which the particle is trapped, because of the presence of infinite barriers. The fixed point with $\varepsilon_1^* \to \infty$, on the contrary, corresponds to zero height barriers, at all levels, except for the zeroth one ($\varepsilon_0 = 1$). In this case we should expect normal diffusion to take place. One can easily verify that the $\varepsilon_1^* = 0$ fixed point, under iteration of (6), attracts all initial $\{\varepsilon\}$ for which ε_i becomes 0 for $i \geqslant i_0 \geqslant 1$ or $\varepsilon_{j+1}/\varepsilon_j \to 0$ for $j \to \infty$. On the other hand, a fixed point with $\varepsilon_1^* > 0$ attracts all those initial $\{\varepsilon\}$ for which ε_j approaches 0 for $j \to \infty$, with

$$\lim_{j\to\infty} \frac{\varepsilon_{j+1}}{\varepsilon_j} = \frac{\varepsilon_1^*}{1+2\varepsilon_1^*}.$$

One can also show that when

$$\lim_{j\to\infty} \frac{\varepsilon_{j+1}}{\varepsilon_j} = C \geqslant \tfrac{1}{2}$$

the iteration of (6) leads to $\varepsilon_j^* = \infty$ and $\varepsilon_{j+1}^*/\varepsilon_j^* = C$ $(j = 1, 2, \ldots)$.

On the basis of (5) and (7) it is easy to discuss the diffusion exponent pertaining, e.g., to the autocorrelation function, i.e. the probability $P_0(t)$ of being back at cell 0, where diffusion started, after a long time t. We expect a scaling behaviour of the form $P_0(t) \sim t^{-x/2}$, for $t \to \infty$. The exponent x takes the value 1 for normal diffusion. Another interesting quantity describing diffusion is the range $S(t)$, i.e. the average number of distinct cells visited up to time t. In the case of one-dimensional normal diffusion this quantity scales simply as the reciprocal of $P_0(t)$. Taking into account (7) for the case $n = 0$, $n' = 0$ and the above discussion of fixed points and stability, we easily conclude that the exponent x, describing the $t \to \infty$ behaviour of $P_0(t)$, is given, for our model, by

$$x = 2 \ln 2 / \ln[2(2\varepsilon_1^* + 1)/\varepsilon_1^*] \tag{9}$$

where ε_1^* characterises the fixed point to which the initial $\{\varepsilon\}$ is attracted under iteration of (6)†. In deriving (9), the fact has been taken into account that, after n iterations of the transformation, the resulting rescaling factor for P approaches $[\varepsilon_1^*/(1+2\varepsilon_1^*)]^n$, for large n. When $\varepsilon_1^* = 0$, i.e. the case of trapping, x becomes zero, and increases up to the limit value 1, for $\varepsilon_1^* \to \infty$, as it should. It is easy to see that $x = 1$ if $\varepsilon_{j+1}/\varepsilon_j = C > \frac{1}{2}$ for $j \to \infty$. In particular if $\varepsilon_j = R^j$ our recursion equations (5)-(7) lead to the fixed

† It should be noticed that the expression for the autocorrelation function, approximately derived by Huberman and Kerszberg (1985), turns out to be consistent with the exact exponent obtained here.

point $\varepsilon_1^* = R/(1-2R)$ and $\varepsilon_{j+1}^*/\varepsilon_j^* = R$ with $x = 2/(1-\log_2 R)$ for $R < \frac{1}{2}$ while for $R > \frac{1}{2}$ $\varepsilon_j^* = \infty$ and $\varepsilon_{j+1}^*/\varepsilon_j^* = R$ $(j = 1, 2, \dots)$ with $x = 1$†. It is this dependence of x on ε_1^* which leads to the expected temperature-dependent exponent (Huberman and Kerszberg 1985) if a thermal activation mechanism is assumed for hopping across the barriers, i.e. if one puts $\varepsilon_{i+1}/\varepsilon_i \sim \exp(-\text{constant}/T)$.

Values of x obtained by numerical simulations (Huberman and Kerszberg 1985) compare rather well with the exact result (9). Indeed, for $\varepsilon_{i+1}/\varepsilon_i = e^{-2}$ and $e^{-2.7}$, these authors find $x = 0.48$ and 0.38, respectively. On the basis of (9), putting $\varepsilon_1^*/(1+2\varepsilon_1^*) = e^{-2}$ and $e^{-2.7}$, we obtain $x = 0.515$ and 0.409, respectively.

We can also investigate the scaling of $S(t)$. Indicating by $Q_i(t)\,dt$ the probability that the particle, starting from cell 0 at time 0, will reach cell i between times t and $t+dt$, without having been there before, we obviously have

$$P_i(t) = \int_0^t dt'\, Q_i(t') P_{0i}(t-t') \tag{10}$$

where P_{0i} is the autocorrelation function for a diffusion starting at cell i. Obviously $S(t)$ will be given by

$$S(t) = \sum_i \int_0^t dt'\, Q_i(t'). \tag{11}$$

On the basis of (10) and (11) and the previous results for P, we can conclude that, for small ω

$$\sum_{i'} \tilde{Q}_{i'}(\omega')/\omega' = \tilde{S}(\omega', \{\varepsilon'\}) = \{\varepsilon_1/[4(1+2\varepsilon_1)]\}\tilde{S}(\omega, \{\varepsilon\}) = \sum_i \tilde{Q}_i(\omega)/\omega \tag{12}$$

with $\tilde{Q}_{i'}(\omega', \{\varepsilon'\}) = Q_i(\omega, \{\varepsilon\})$. The result (12) is consistent with $\tilde{S}(\omega) \sim \omega^{-1-x/2}$ for $\omega \to 0$, i.e. with $S(t) \sim t^{x/2}$ for $t \to \infty$. Thus, in general $S(t) \propto P_0(t)^{-1}$, for $t \to \infty$, as in the case of normal diffusion.

We can also obtain the asymptotic behaviour of the average square distance travelled by the particle $R^2(t) = \Sigma_i P_i(t) i^2$ in terms of x. By considerations similar to those above one finds $R^2(t) \sim t^x$ for $t \to \infty$.

In summary, we have presented an exact and complete renormalisation group analysis of the leading scaling properties of a one-dimensional model of ultradiffusion. An important physical feature of the model, namely the possibility of leading to temperature-dependent exponents, has been explained in terms of the existence of a line of fixed points. Implications of the above results for directly related problems, such as those concerning properties of electronic (tight-binding Schrödinger equation) or vibrational(phonon) states, can be easily derived.

In particular, for a vibrational eigenmode problem with a hierarchical interaction structure, like the one presented by the above hopping rates, x can be seen to coincide with the spectral dimension, i.e. with the exponent characterising the behaviour of the density of modes at low frequency (Rammal and Toulouse 1983). Ultradiffusion can actually be seen as a problem of diffusion on a fractal. In this case the geometrical fractal dimension (Mandelbrot 1982) of the cell lattice is trivially 1, i.e. coincides with the dimension of the embedding Euclidean space; the spectral dimension, on the other hand, is lower than 1, because of the presence of the infinite hierarchy of time scales.

‡ After the submission of this letter we became aware of the fact that Teitel and Domany (1985) were able to conjecture this result following approximate methods. However, their renormalisation group picture is not consistent with the exact one produced here (Maritan and Stella 1985).

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