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Biased Diffusion in Chainlike Fractal Structures: Universal Behaviour.

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Abstract. – We study diffusion on topologically linear fractal structures under the influence of a uniform external field. Due to the fractal nature of the chain, the uniform field acts on a random walker like random correlated (local) fields in a one-dimensional chain. We find that the mean square displacement of the walker is *universal* and depends logarithmically on time t as $\langle r^2 \rangle \sim \ln^2 t$, *independent* of the fractal dimension of the chain.

In recent years, the concept of fractal [1] has become an important tool in studying physical properties of disordered systems. In particular, the question how the laws of transport are changed when the system of interest exhibits fractal structure has recently attracted researchers in various scientific disciplines. The spectrum ranges from the intercalation fronts in solids and oil extraction from porous rocks to the physics of polymers, aggregates, and amorphous materials [2-7].

In this letter, we study random walks on topologically linear fractal structures, such as polymer chains, under the influence of a uniform external field $\boldsymbol{E}$. Without bias field, diffusion is anomalous and the mean square displacement of a walker on the chain *depends* on the fractal dimension d_f of the chain as $\langle r^2(t) \rangle \sim t^{1/d_f}$ (1). In contrast, we find here that under the influence of an external bias field $\langle r^2(t) \rangle$ behaves asymptotically as

$$\langle r^2(t) \rangle \sim \ln^2 t, \tag{1}$$

which is *universal* and independent of d_f.

To see this, consider a path as a sequence of N consecutive ordered segments (see fig. 1).

(1) To see this, consider the mean square displacement $\langle l^2 \rangle$ of a random walker along the fractal path, which is proportional to time t. Since l is also the mass of the path, it scales with r as $l \sim r^{d_f}$. Hence $\langle r^2 \rangle \sim \langle l^2 \rangle^{1/d_f} \sim t^{1/d_f}$.

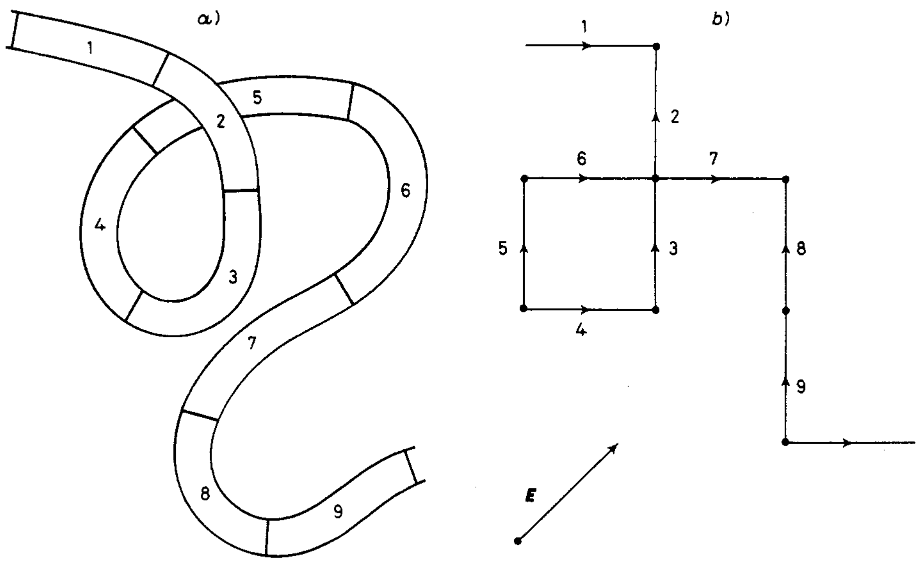

Fig. 1. – a) An illustration of a fractal path consisting of $N = 9$ consecutive ordered segments and b) the corresponding path on the square lattice. The arrows represent the direction of the local bias fields induced by the external field $\boldsymbol{E}$.

Although, when viewed geometrically, the path can intersect itself, it may still be defined uniquely as a linear chain of ordered segments. An example is an isolated metallic wire that may intersect geometrically, but the current sees only a linear conductor. The family of paths defined above is general and includes as special cases paths obtained by random walks and self-avoiding walks in d-dimensions.

For convenience let us assume that all segments have equal length and can be viewed as bonds connecting two nearest-neighbour sites. Now consider a random walker who steps between nearest-neighbour sites in the path, under the influence of a uniform bias field that we choose to have equal components in the directions of the positive axes. The field seen by the walker when moving along the path is random and depends on the direction of the given bond relative to the external field (see fig. 1). Accordingly, the probability $W_{i,i\pm1}$ to jump from site i to the nearest-neighbour site $i \pm 1$ can be either proportional to $1 - \varepsilon$ or $1 + \varepsilon$, where $0 \leqslant \varepsilon \leqslant 1$ is the local bias field induced by the external field; ε and E are related by $E \sim \ln((1+\varepsilon)/(1-\varepsilon))$. We denote the mean square displacement of the walker along the path by $\langle l^2 \rangle$. If the path is generated by an uncorrelated random walk, the local random fields along the path are distributed symmetrically and are uncorrelated. This case can be mapped exactly to the Sinai problem [8] and $\langle l^2 \rangle$ behaves asymptotically as

$$\langle l^2 \rangle \sim \ln^4 t . \tag{2}$$

The mean square displacement along the path, $\langle l^2 \rangle$, is related to the mean square displacement in the Euclidean space by (see ([1]))

$$\langle l^2 \rangle^{1/2} \sim \langle r^2 \rangle \sim \ln^2 t . \tag{3}$$

In the following we show that this relation between $\langle r^2 \rangle$ and t is general and holds for any fractal path where long-range correlations exist between its segments.

In a general fractal path, the effect of the field is to provide large random delays on the

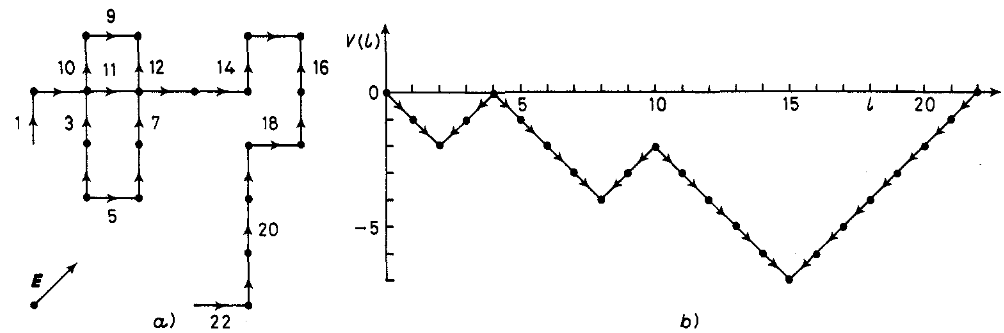

Fig. 2. – Illustration of the mapping of a fractal path with ordered segments and local bias fields (*a*)) to a one-dimensional potential landscape experienced by a random walker (*b*)). The average potential depth $\langle V(l)\rangle$ is given by eq. (5).

motion of a random walker, which can get easily stuck in compensated regions of the chain where fields of opposite directions point to the same site. These compensated regions can be considered as deep potential valleys (see fig. 2). The time t' to escape a valley of depth V follows Arrhenius law, $t' \sim \exp[V]$, and we expect that the *typical* time t which is required to travel a distance l along the chain scales with l as

$$t \sim \exp[\langle V(l)\rangle], \tag{4}$$

where $\langle V(l)\rangle$ is the mean depth of the valleys in the fractal chain of length l; $\langle V(l)\rangle$ scales with the field E as

$$\langle V(l)\rangle \sim \left\langle\left(\sum_1^l \boldsymbol{E}\cdot\boldsymbol{u}_i\right)^2\right\rangle^{1/2}, \tag{5}$$

where $\boldsymbol{u}_i$ is the unit vector of the i-th ordered segment of the path. Since all components of the field are equal, we obtain

$$\sum_{i,j=1}^{l} \langle(\boldsymbol{E}\cdot\boldsymbol{u}_i)(\boldsymbol{E}\cdot\boldsymbol{u}_j)\rangle = E^2 \sum_{i,j=1}^{l} \langle\tau_i\tau_j\rangle, \tag{6}$$

where the τ_i's attain the values ± 1; $+1$, if $\boldsymbol{E}\cdot\boldsymbol{u}_i$ is positive and -1, if it is negative. Thus we have

$$\sum_{i,j=1}^{l} \langle\tau_i\tau_j\rangle = d\sum_{i,j}^{l} \langle\boldsymbol{u}_i\cdot\boldsymbol{u}_j\rangle = d\langle r^2\rangle. \tag{7}$$

Using eqs. (4)-(7) we obtain the universal result, eq. (1), which is independent of the fractal dimension or the correlations of the chain. Equation (1) was derived, for simplicity, on a discrete hypercubic lattice, where the field has equal components in the direction of the positive axes; but the derivation can be extended to the more general case where the field points in arbitrary direction and to continuous systems as well. Since for a linear structure the path length l scales with r as $l \sim r^{d_t}$, we obtain for the mean square displacement of the walker along the path

$$\langle l^2\rangle \sim \langle r^2\rangle^{d_t} \sim \ln^{2d_t} t. \tag{8}$$

As an example consider the case that the path is a self-avoiding walk in d-dimensions. In this case one has the Flory result $d_f = (d+2)/3$ (see, *e.g.*, [9]). Thus for diffusion on a SAW in $d=2$ in the presence of uniform external fields we expect

$$\langle l^2 \rangle \sim \ln^{8/3} t / A^{8/3}, \tag{9a}$$

where A depends on the bias field,

$$A(\varepsilon) = \ln((1+\varepsilon)/(1-\varepsilon)). \tag{9b}$$

To put our prediction to a direct test, we have studied numerically $\langle l^2 \rangle$ in SAWs on a square lattice. First we generated a long SAW using the enrichment method [10] and checked the fractal dimension of the chain. Typically we considered chains of 1000 sites. We have chosen the middle of the chain as origin where the random walker starts and used the exact enumeration method (see, *e.g.*, [6]) to calculate the distribution function and its second moment $\langle l^2 \rangle$. The result was averaged over 1000 configurations. In order to obtain fast convergency to the asymptotic regime, we studied the effect of large fields, $\varepsilon = 0.8$ and $\varepsilon = 0.9$. Since $\langle l^2 \rangle^{1/2}$ was below 50 in the considered time regime, boundary effects are negligible. The results for $\langle l^2 \rangle$, plotted *vs.* $(\ln t)^{8/3}$, are shown in fig. 3. For large times, both curves approach straight lines; the ratio of their slopes is in good agreement with our prediction, eq. (8).

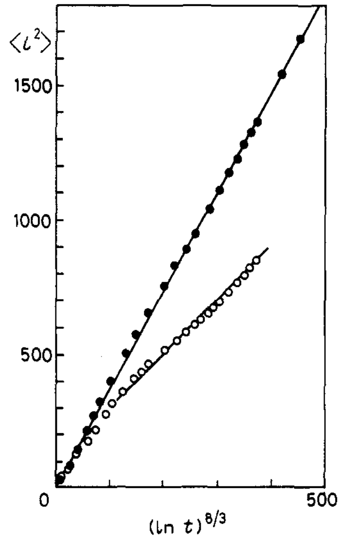

Fig. 3. – Plot of the mean square displacement along the path, $\langle l^2 \rangle$, as a function of $\ln^{8/3} t$ for two values of the bias field ε: ● 0.8, ○ 0.9. The straight lines support the prediction (8) and the field dependence is in agreement with (9*a*) and (9*b*).

In summary, we have discussed diffusion in topologically linear fractal structures in the presence of an external homogeneous bias field. We have found that diffusion was logarithmically slow, and the asymptotic behaviour of the mean square displacement was universal. We expect a similar *asymptotic* behaviour in quasi-linear structures where «bridges» between nearest-neighbour sites are present or for structures which are compact on a short length scale but show chainlike structures on larger length scales. Those structures occur, *e.g.*, in models for branched polymers [11] or in models for epidemics when the growth sites have a finite lifetime [12]. For *short* times, the walker is not affected by the presence of the chainlike fractal structures at large length scales and we expect power law behaviour, in agreement with numerical results on SAWs with bridges [13]. It is interesting to note that the *same logarithmic* time dependence was found numerically (within the error bars of the numerical calculation) also in diffusion on percolation clusters at criticality, when an external bias field is applied [14]. This suggests that our result is possibly more general and may also hold for percolation clusters.

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REFERENCES

[1] MANDELBROT B. B., *Fractals: Forms, Chance, and Dimension* (Freeman, San Francisco, Cal.) 1977; *The Fractal Geometry of Nature* (Freeman, San Francisco, Cal.) 1983.
[2] FAMILY F. and LANDAU D. P. (Editors), *Kinetics of Aggregation and Gelation* (North-Holland, Amsterdam) 1984.
[3] STANLEY H. E. and OSTROWSKY N. (Editors), *On Growth and Form* (Martinus Nijhoff Publishers, Boston, Dordrecht, Lancaster) 1986.
[4] BLUMEN A., KLAFTER J. and ZUMOFEN G., in *Optical Spectroscopy of Glasses*, edited by I. ZSCHOKKE (Reidel, Dordrecht) 1986, p. 199.
[5] BUNDE A., *Adv. Solid State Phys.*, **26** (1986) 113.
[6] HAVLIN S. and BEN-AVRAHAM D., *Adv. Phys.*, **36** (1987) 695.
[7] SAPOVAL B., ROSSO M. and GOUYET J. F., in *Superionic Conductors and Solid Electrolytes*, edited by A. LASKAR and S. CHANDRA (Academic Press, London) 1988.
[8] SINAI Y., *Theor. Prob. Appl.*, **27** (1982) 256.
[9] DE GENNES P. G., *Scaling Concepts in Polymer Physics* (Cornell University Press, Ithaka, N. Y.) 1979.
[10] BRENDER C., BEN-AVRAHAM D. and HAVLIN S., *J. Stat. Phys.*, **31** (1983) 661 and references cited therein.
[11] HAVLIN S., TRUS B. and STANLEY H. E., *Phys. Rev. Lett.*, **53** (1984) 1288.
[12] BUNDE A., MIYAZIMA S. and STANLEY H. E., *J. Stat. Phys.*, **47** (1987) 1; BUNDE A. and MIYAZIMA S., *J. Phys. A*, **21** (1988) L-345.
[13] CHOWDHURY D., *J. Phys. A*, **18** (1985) L-761.
[14] HAVLIN S., BUNDE A., GLASER A. and STANLEY H. E., *Phys. Rev. A*, **34** (1986) 3492; BUNDE A., HARDER H., HAVLIN S. and ROMAN H. E., *J. Phys. A*, **20** (1987) L-865.