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Random walks on percolating clusters with energetic disorder†

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Abstract. Single random walker simulations on energetically disordered percolation clusters (in two dimensions) are presented. Exponential, Gaussian and uniform site energy distributions are investigated. The superposition of spatial and energetic disorder leads to reduced random walk ranges with decreasing temperature. An analogue subordination rule is derived: random walk on an energetically disordered fractal is equivalent to that on a geometrical fractal with a lower spectral dimension. This rule is strictly followed for the exponential distribution but only approximately for the Gaussian and uniform distributions. The last two distributions, and especially the uniform one, show a crossover behaviour analogous to that of random walks on percolation clusters away from criticality.

1. Introduction

Random walks have been used extensively in the study of diffusion processes and diffusion-limited reactions. Recent interest has focused on disordered systems involving fractal-like geometries and/or fractal time [1-4]. Geometric (spatial) disorder is often introduced as a binary random lattice, i.e. the percolation problem [5, 6]. Temporal disorder is introduced [1, 2, 7] by using a random distribution of time intervals between events, $\psi(t)$. In the fractal approach the spatial disorder is characterised [1-6] via the fractal dimension d_f and the spectral dimension d_s. The temporal disorder characterised by the distribution $\psi(t)$ has a long-time tail of the form $\psi(t) \sim t^{-1-\beta}$. The superposition of fractal geometry and temporal disorder results in a reduced effective spectral dimension βd_s where $\beta < 1$. This has been called a subordination effect [1, 4].

It is well known that temporal disorder usually arises due to energetic disorder [1-4, 7]. The fractal-like aspects of random walks on energetically disordered Euclidean and fractal lattices have also been described recently [6, 8, 9]. Essentially this energetic disorder introduces a temperature-dependent fractal-like distribution of waiting times, obtained by a Boltzmann-weighted probability for moves to sites with higher energy [3, 6, 8, 9]. A major question of interest is whether an analogue subordination rule can be applied to random walks on such temperature-dependent fractal-like domains [9]. Specifically, it is interesting to investigate whether effective spectral dimensions can be assigned for each given temperature (resulting in an analogue subordination rule).

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In the current paper we introduce energetic disorder on a percolating cluster exactly at criticality (which has an exact fractal structure [5]). Each site of the percolating cluster is assigned a random energy and the particle random walk is monitored via a Boltzmann-weighted probability for transfer to a site with a higher energy, effectively bringing in a temperature-dependent distribution [3].

A particle moves from site i to one of its z nearest neighbours, site j, with probability:

$$P_{ij} = \begin{cases} z^{-1} \exp[-(\varepsilon_j - \varepsilon_i)/kT] & \varepsilon_j > \varepsilon_i \\ z^{-1} & \varepsilon_j < \varepsilon_i \end{cases} \tag{1}$$

or remains on site i with probability:

$$P_{ii} = 1 - \sum_{j=1}^{z} P_{ij}. \tag{2}$$

The assignment of the site energies is done using uniform, exponential and Gaussian distributions. The customary random walk properties, the mean-square displacement, $\langle R_N^2 \rangle$, and the mean number of sites visited, $\langle S_N \rangle$, are used to monitor these processes.

2. Method of calculations

The following algorithm was used in this study. First a two-dimensional square lattice was constructed (size 300×300) made of open and closed sites with the probability of open sites p being specified equal to the square lattice critical percolation probability $p_c = 0.593$. The largest cluster was isolated using the well known CMLT (cluster multiple labelling technique), and all further work was confined to this cluster [5]. Each cluster site was assigned an energy value (in the range 0-30 000 arbitrary units) at random, according to one of three distributions: (*a*) uniform, (*b*) exponential, (*c*) Gaussian. The common random number generator RAN (by DEC) was used to generate the uniformly distributed random number R_i (in the interval $0 < R_i < 1.00$). The formula $X_i = -\log R_i$ was used for generating the exponential distribution by use of the previous R_i, and finally the known subroutine GRAND was used for the Gaussian distribution, also using the R_i. Thus, the energies were set as follows. In (*a*) $E_i = (30\,000)R_i$, and the average energy is $E = 15\,000$ arbitrary units. (*b*) If $X_i \leqslant 0.001$ then X_i was set equal to $X_i = 0.001$. If $X_i \geqslant 10$ then X_i was set equal to $X_i = 10$. Finally, $E_i = (3000)X_i$. (*c*) The mean of the distribution was set equal to 0.0; the standard deviation $\sigma = 1.0$. If $X_i < -3$ then X_i was set equal to $X_i = -3$. If $X_i > 3$ then X_i was set equal to $X = 3$. Finally $E_i = (X_i + 3)$ (5000), i.e. the mean energy value is $E = 15\,000$ arbitrary units. The jump probabilities were set as follows: $p = 0.25$ if the neighbour site has equal or lower energy; $p = 0.25 \exp(-\Delta E/kT)$ if the neighbour site has higher energy, with ΔE being the energy difference and T a reduced temperature (as the constant k was set equal to 30 000). All p (for the four-neighbour sites) are added up, with the remainder probability (difference from 1.000) taken to be the probability that the particle remains at its original site. Each run is followed for 10 000 time steps. The quantities we monitor are S_N, the number of distinct sites visited at least once in N steps, and R_N^2, the square of the displacement in N steps. We used reduced temperatures of $T = 1.0$, 0.5, 0.25, 0.15, 0.10 for the uniform distribution; $T = 1.0$, 0.10, 0.05, 0.03, 0.01 for the exponential and Gaussian distributions. Each calculated value is the average of 1000 realisations.

3. Results and discussion

In figure 1 we plot $\langle S_N \rangle$ against time in log-log form for several values of the reduced temperature T. The linearity of these curves immediately suggests a form:

$$\langle S_N \rangle \sim N^f \qquad N \to \infty \tag{3}$$

where f is the slope of the appropriate curve in this figure. At high temperatures

$$f \simeq 0.63 \simeq d_s/2 \tag{4}$$

where d_s is the spectral dimension, in parallel with the f values for normal random walk [5] on percolating clusters with no energetic disorder. For the latter, it has been found [5] that $f = 0.65 \pm 0.02$ for two-dimensional lattices (while $f = 0.666$ for $d \geqslant 3$). The lower temperatures illustrate the effects of subordination due to the superposition

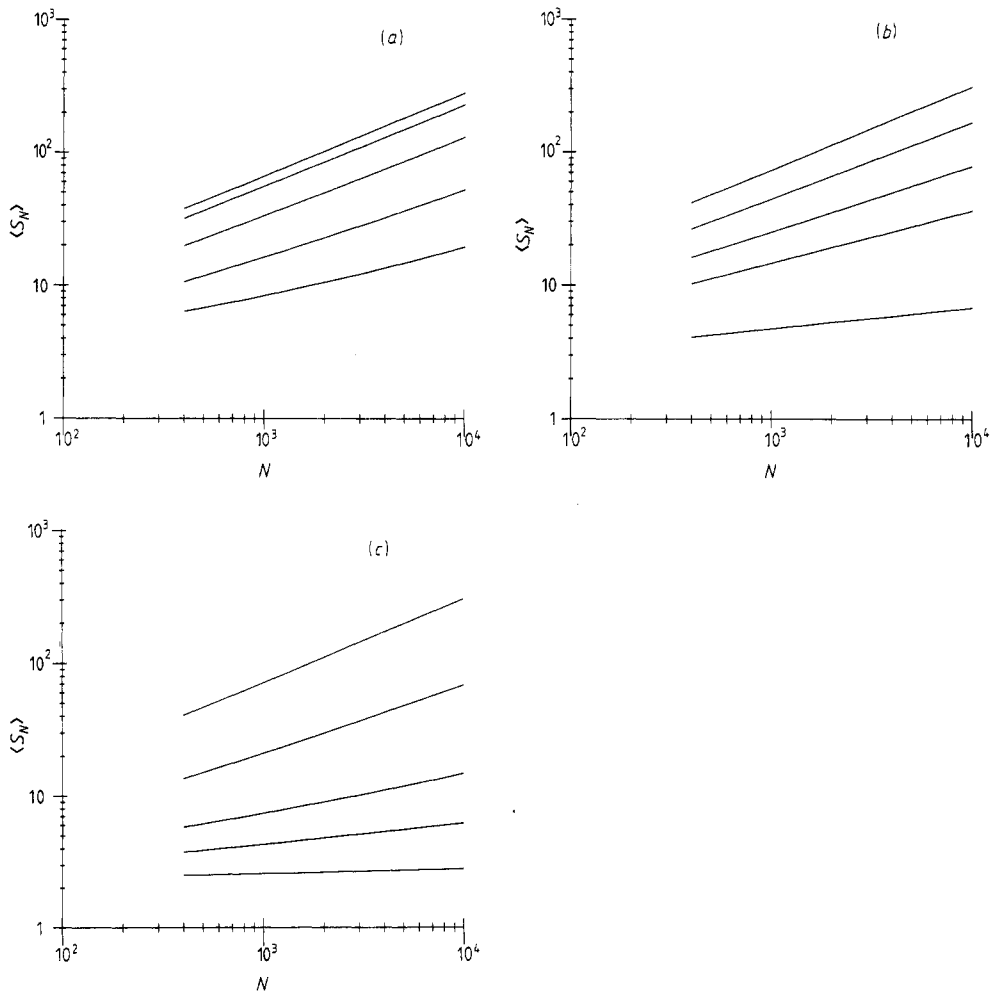

Figure 1. Mean number of distinct sites visited, $\langle S_N \rangle$, by a single particle, as a function of time, for a series of reduced temperatures T as follows, reading from top to bottom: (*a*) uniform, $T = 1.0$, 0.5, 0.25, 0.15, 0.10; (*b*) exponential, $T = 1.0$, 0.1, 0.05, 0.03, 0.01; (*c*) Gaussian distributions of energies, $T = 1.0$, 0.1, 0.05, 0.03, 0.01.

of energetic disorder on a fractal, which is analogous to the superposition of temporal disorder on a fractal [1, 3]. Thus, we observe in table 1 that in (*a*) f goes down to about 0.37 while in (*b*) and (*c*) it goes down to about 0.16 and 0.04, respectively. Also, it is interesting to observe in figure 1 that at the lowest temperatures, $T = 0.01$, the linearity of the curves is preserved in cases (*b*) and (*c*) while this is not so in case (*a*), where a curvature appears. This behaviour resembles the crossover behaviour in percolation clusters *away* from criticality [5]. It has also been observed for random walk on *energy disordered* Sierpinski gaskets [9]. Thus, energetic disorder at the critical point preserves the fractal character and, for high temperatures, gives numerically the same fractal exponent (spectral dimension) as the underlying spatial structure.

Similar behaviour is observed in figure 2, which is a plot of R_N^2 against time, also in log-log form. The resulting curves also suggest the known relation [10]

$$\langle R_N^2 \rangle \sim N^{2/D} \qquad N \to \infty \tag{5}$$

where D is derived as the slope of the straight lines at high temperatures. Here, for $T = 1$, $D \simeq 2.81$ (uniform), $D \simeq 2.88$ (exponential) and $D \simeq 2.83$ (Gaussian) in these various energy disorder cases, as compared to $D \simeq 2.80$ for the pure spatial disorder [10]. The lower T curves give slopes that lead to progressively increasing D values, illustrating again the subordination effect (see table 1).

In figure 3 we plot the value of f (left y axis) and the value of β (right y axis) as a function of the reduced temperature T for all three energy distributions. Table 1 describes the exponents f and D as a function of T for all three energy distributions. The f exponents in table 1 can be written as $f = \beta d_s/2$ where $d_s/2 = 0.63$ and β is a function of temperature, with $\beta \to 1$ as $T \to 1$. Obviously, here β does not describe a time distribution but a hopping probability distribution, which is determined by the temperature and the energy distribution. Within the above context of β we obtain a

Table 1. Exponents f and D.

		f			
Uniform		Exponential		Gaussian	
T	f	T	f	T	f
1.0	0.63	1.0	0.63	1.0	0.63
0.5	0.62	0.1	0.58	0.1	0.51
0.25	0.59	0.05	0.49	0.05	0.29
0.15	0.50	0.03	0.40	0.03	0.16
0.10	0.37	0.01	0.16	0.01	0.04

		D			
Uniform		Exponential		Gaussian	
T	D	T	D	T	D
1.0	2.81	1.0	2.88	1.0	2.83
0.5	2.86	0.1	3.02	0.1	3.38
0.25	2.93	0.05	3.51	0.05	5.61
0.15	3.76	0.03	4.23	0.03	9.63
0.10	4.46	0.01	10.90	0.01	36.91

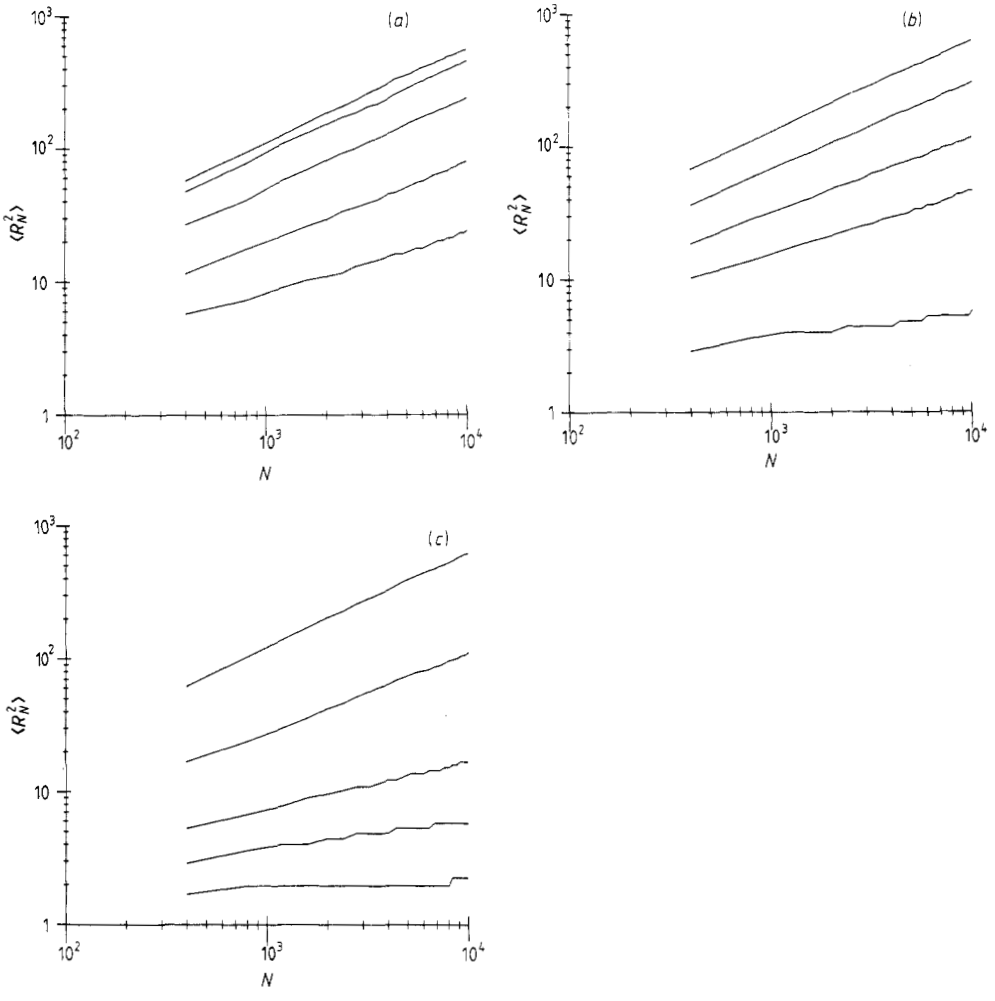

Figure 2. Mean-square displacement, $\langle R_N^2 \rangle$ as a function of time, for a single-particle random walk, for a series of reduced temperatures, T, the same as in figure 1: (*a*) uniform; (*b*) exponential; (*c*) Gaussian distributions of energies.

behaviour that is completely analogous to the Blumen-Klafter-Zumofen (BKZ) subordination rule [1, 4]. The BKZ work addresses the combined effect of disorder, derived from two different contributions: (1) the fractal structure and (2) the CTRW mechanism. The two processes combine asymptotically in a multiplicative manner. The present work has disorder incorporated from: (i) the fractal structure and (ii) the site-energy distribution, producing a random walk with jumps that are temperature dependent. Thus, here, we speak of an analogy between the BKZ work and ours, but not of an exact parameter-for-parameter comparison. In a recent work Tamor [11] has also treated thermally activated random walks in energetically disordered lattices. However, his work is restricted to geometrically ordered lattices, as opposed to the present work on energetically disordered fractal structures (percolation cluster). Tamor also emphasises both the analogy and the difference between the traditional CTRW approach [7] and the energy-disorder-based variable range hopping [6]; comparing parameters

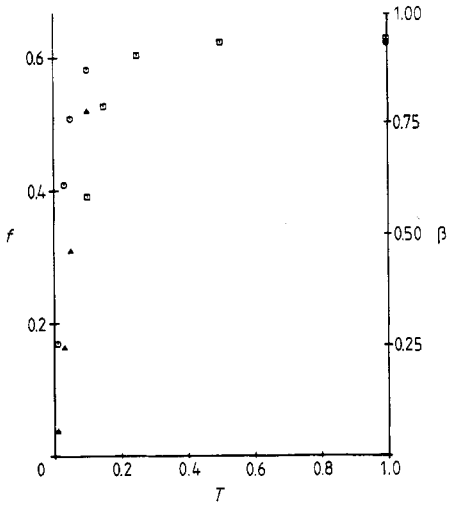

Figure 3. Exponent f, as a function of the reduced temperature, for the uniform (squares), exponential (triangles) and Gaussian (circles) distribution of site energies.

directly leads to puzzling results regarding the role of the temperature. This dilemma should be solved for the cubic (or square) lattice before it is addressed for the more complicated fractal media (percolation cluster).

Using the calculated f (or β) values we now form the waiting-time distribution functions $\psi(t)$ for all three cases of the energy distribution. The result is given in figure 4, where we have plotted $\psi(t)$ against time for $T=1.0$ and $T=0.1$. We notice that, since all three distributions (uniform, exponential, Gaussian) have the same effective dimension ($f=0.63$), for $T=1.0$, $\psi(t)$ is identically the same function. However, for $T=0.1$, we find three different curves (shown in figure 4), i.e. for any

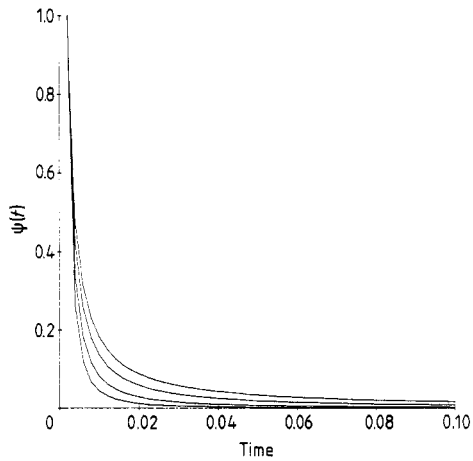

Figure 4. Waiting-time distribution $\psi(t)$ against time. This $\psi(t)$ is derived from the equation $\psi(t)=t^{-(1+\beta)}$ using the proper β values from table 1. Shown are the cases (top to bottom): $T=1.0$ (all three distributions), $T=0.1$ (uniform), $T=0.1$ (exponential), $T=0.1$ (Gaussian).

given waiting time, $\psi(t)$ decreases as one goes from the uniform to the exponential to the Gaussian distribution.

4. Conclusions

The basic power law relation for the number of distinct sites visited, equation [3], is a good approximation for energetically disordered fractals (percolating clusters) with temperature-dependent Boltzmann weighting factors. This relationship works well over a wide range of temperatures. The differences between the exponential, Gaussian and uniform site-energy distributions are small. However, the uniform and Gaussian distributions show some kind of crossover behaviour at low temperatures. On the other hand, the exponential distribution gives a genuine fractal-like behaviour, i.e. it closely follows equation (3). The exponential distribution provides a clear-cut analogue of the subordination rule. Even the Gaussian and uniform distributions follow such an analogue subordination rule to a good approximation.

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