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COMMENT

Monte Carlo study of random walks on a 2D gasket fractal in an external field

Gi Ok Kim, Jong Hoon Oh† and Jong-Jean Kim

Department of Physics, Korea Advanced Institute of Science and Technology, PO Box 150, Chongyangni, Seoul, Korea

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Abstract. Using Monte Carlo simulation, random walks on a two-dimensional Sierpinski gasket in the presence of an external field were studied. It was observed that the random walk motion of a particle displayed a crossover from anomalous diffusion to drift for a non-zero bias field, and the crossover time t_{cr} was a decreasing function of the external bias field. The associated dynamic exponents obtained in our computer simulation agree with the predictions of Stinchcombe's scaling treatment.

Diffusion in fractal structures (de Gennes 1976, Mandelbrot 1983) has been of great interest to many research workers. Fractals can, in general, be divided into two classes: regular fractals which are geometrically self-similar, such as the family of the Sierpinski gaskets, and random fractals which are statistically self-similar, such as the percolation clusters (see Stauffer 1979 for a review), even though the former has been proposed as a model for the latter (infinite cluster backbones) at the percolation threshold.

Most investigations of the random walk problem have been devoted to percolation clusters (Gefen *et al* 1983, Gould and Kohin 1984, Rammal and Toulouse 1983) and self-avoiding walks (Helman *et al* 1984, Ball and Cates 1984, Chowdhury and Chakrabarti 1985), where it was found that systems close to the percolation threshold exhibited an anomalous diffusion regime with the mean-square displacement of the particle following a non-integral power law for distances less than the percolation correlation length.

Random walks on regular fractals (Rammal and Toulouse 1983, Angles d'Auriac *et al* 1983) have also shown the same non-classical behaviour as those on percolation clusters at the percolation threshold.

Recently, many authors have studied random walks on random fractals, e.g., percolation clusters (Barma and Dhar 1983, Dhar 1984, Pandey 1984) and self-avoiding walks (Chowdhury 1985) in the presence of an external field, using scaling treatments or computer simulation methods. They predicted that under the external bias field the random walk motion would exhibit a crossover from diffusion to drift-like behaviour at a time t_{cr} after switching the field on, and t_{cr} should be a decreasing function of the bias field. This is known to be true in the case of dispersive hopping transport in amorphous materials in the presence of a strong electric field (Böttger and Bryskin 1980, Adler and Silver 1982) and in the case of diffusion of ions in chromatographic columns.

† Permanent address: Pohang Institute of Technology, Pohang, Korea.

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Random walks on regular fractals in an external field were first discussed by Stinchcombe (1985) on the basis of the scaling argument for the two-dimensional triangular Sierpinski gasket. Important results of Stinchcombe's work include (i) the anomalous dynamic critical exponent $k = 1/z = \log_5 2 \simeq 0.431$ for the isotropic case, (ii) bias field-induced crossover from diffusion to drift with exponent $k = \log_2 2 = 1$, and (iii) the irrelevance of the rotational anisotropy operator.

In this comment we report our computer simulation work on the random walk in the two-dimensional triangular Sierpinski gasket under external fields of various strength and direction using the Monte Carlo method to examine the crossover behaviour and the power laws.

We used a ten-stage two-dimensional Sierpinski gasket, which has 88 575 sites. The labelling procedure for the sites follows that of Angles d'Auriac *et al* (1983).

Using the Monte Carlo method we simulated the diffusive motion of a particle on the Sierpinski gasket in the presence of an external field.

In the Sierpinski gasket structure there are six directions for the random walker to jump on, but any site in the Sierpinski gasket lattice has only four nearest-neighbour sites, corresponding to four directions out of six possible ones. Thus in the case of unbiased diffusion, i.e. in the isotropic case, the probability for the particle to move from a site to any of its four possible nearest-neighbour sites is just $\frac{1}{4}$. On the other hand, when a bias field with intensity $B(0 < B < 1)$ is switched on along a specified direction, the hopping probability for each of six possible directions would be distributed as shown in figure 1. At each step from any site the probabilities for all the possible nearest-neighbour sites should be normalised.

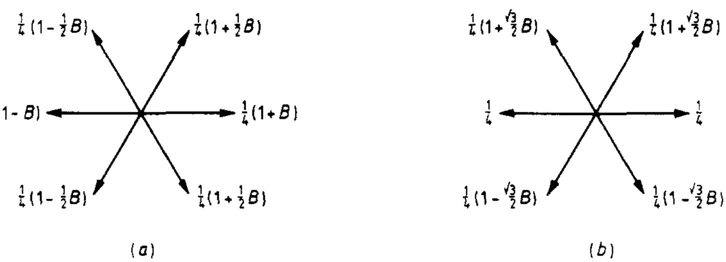

Figure 1. Probability distribution for each of six possible directions (*a*) in the presence of a horizontally rightward bias field and (*b*) in the presence of a vertically upward bias field.

Given the probabilities, we performed the routine random walk calculations and a large number of configurations for each value of t and B were generated by varying the initial position of the particle. The square of the end-to-end distance of a t-step random walk for a given B was averaged over all these configurations to obtain $\langle R_t^2 \rangle$. The procedure was repeated for various values of t and B.

An MV-10000 computer was used in the present work, where the statistical error bars were estimated to be less than 0.5%.

We have examined the variation of the mean-square displacement of the particle with time for various intensities and directions of the bias field.

In figure 2, the log-log plot of R against t for the isotropic case exhibits the power law $R(t) \propto t^k$ with the exponent $k \simeq 0.436$, and the random walk motion of the particle for the rotationally anisotropic case also shows the same behaviour as for the isotropic

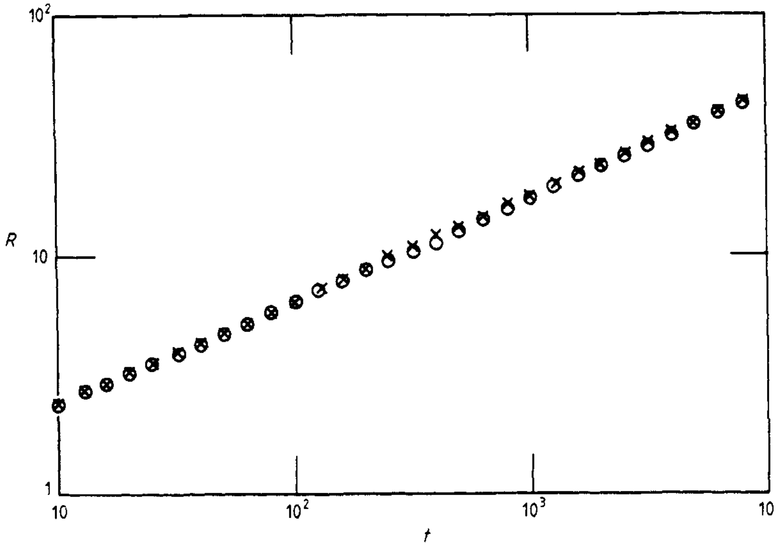

Figure 2. Log-log plots of the RMS distance R with time t (○, isotropic case; ×, rotationally anisotropic case).

case, i.e. the dynamic exponents for the two cases are obtained to be the same. According to Stinchcombe (1985) the operator of the rotationally anisotropic diffusion is irrelevant. Therefore the rotational anisotropy has no effect on diffusion, and only the isotropic diffusion effect is exhibited.

In the uniaxially anisotropic case (figures 3 and 4) the diffusive motion of a particle is changed into drift-like motion ($k = 1$) at a time t_{cr}. For shorter times ($t < t_{cr}$) the

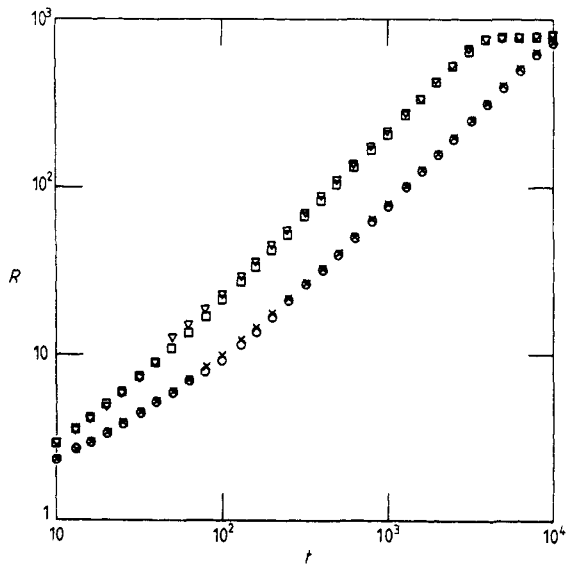

Figure 3. Log-log plots of the RMS distance R with time t in an external bias field along one axis of the Sierpinski gasket: along one of the axial directions (○, $B = 0.11$; □, $B = 0.22$) and with the direction reversed (×, $B = 0.11$; ▽, $B = 0.22$).

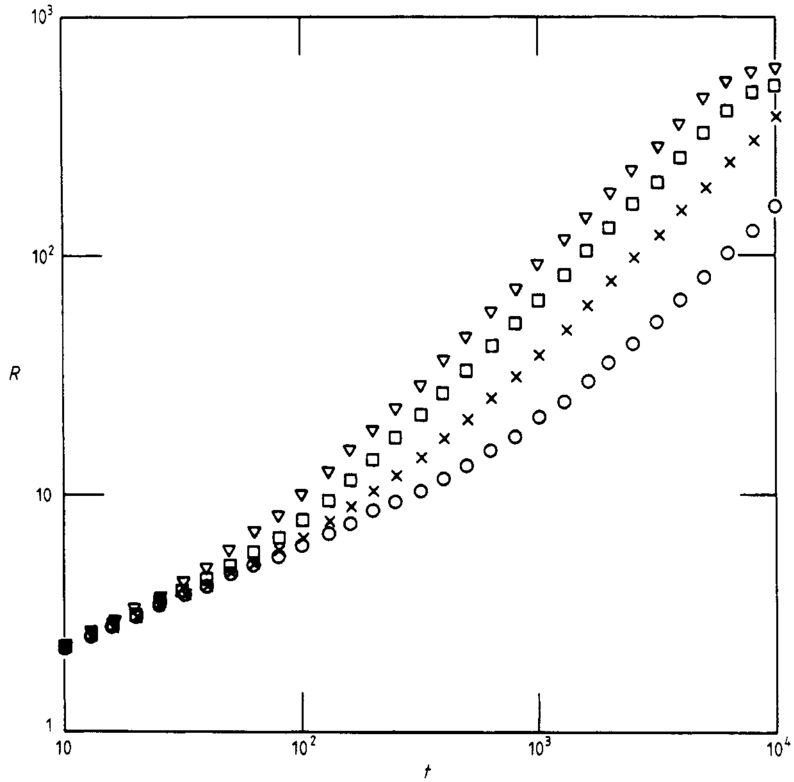

Figure 4. Log-log plots of the RMS distance R with time t for various values of the bias field B along the upward direction of the Sierpinski gasket: ○, $B = 0.13$; ×, $B = 0.26$; □, $B = 0.39$; ▽, $B = 0.52$.

particle diffuses in the same way as for the isotropic case ($k \simeq 0.436$), but for longer times ($t > t_{cr}$) the motion of the particle shows a new behaviour ($k = 1$) which represents the drift motion of the particle. This crossover behaviour is irrespective of the bias field directions, as shown in figure 3.

Trapping effects arise frequently in percolation clusters due to cages or dead-end branches, but in our Sierpinski gasket we found no trapping and therefore no characteristic value of the field strength at which the drift velocity became zero (Barma and Dhar 1983). In figures 3 and 4 the slope of each curve tends to be flattened after long time t, but in this case the flattening of the curves occurs, not due to trapping of the particle, but due to the boundary effect of our finite Sierpinski gasket. However, it did not prevent us from observing the crossover behaviour of a particle.

In figure 4 the RMS displacement of a particle with time t for various values of the bias field B is displayed, where the external field is applied along the upward direction of the Sierpinski gasket. The crossover time t_{cr} decreases with the strength of the field B. This feature is similar to that in the case of the random walk on percolation clusters (Pandey 1984, Barma and Dhar 1983) and the self-avoiding walk (Chowdhury 1985).

To summarise, we have observed the crossover behaviour from anomalous diffusion to drift for a particle on a regular fractal (Sierpinski gasket) in the presence of an external field. Our observations of the anomalous critical exponent $k \simeq 0.436$ for isotropic diffusion dynamics, bias field-induced crossover to drift dynamics of the exponent $k = 1$ and the irrelevant operator characteristics of rotational anisotropy agree very well with the values of Stinchcombe (1985). It seems to be advantageous to simulate diffusion studies of a particle on fractal structures in an external field on a regular fractal so long as we are not specifically interested in the trapping effect.

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