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1986 J. Phys. A: Math. Gen. 19 3925

(http://iopscience.iop.org/0305-4470/19/18/039)

J. Phys. A: Math. Gen. 19 (1986) 3925-3931. Printed in Great Britain

COMMENT

Disorder-induced transport: I. Simple cubic lattice

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Received 26 March 1986

Abstract. Using a VAX 11/780, a random walk motion is studied in a random-field disordered system. A non-monotonic transport behaviour is observed as a function of local field intensity. In contrast to the random walk motion in random percolating fractals, the root mean square displacement here increases as a function of time faster than that of diffusion. A crossover from diffusion to disorder-induced transport is discussed and its spectral dimensionality is estimated.

As a tool, the study of random walk motions has shown remarkable success in understanding the transport processes (Montroll and West 1979, Gefen *et al* 1983, Rammal and Toulouse 1982, Pandey *et al* 1984, Havlin and Ben-Avraham 1983, Zabolitzky 1984, Harris and Stinchcombe 1983) in random systems (particularly in fractals) and dynamics of various cooperative systems (Pandey *et al* 1984, Harris and Stinchcombe (1983). Basic mechanisms governing a variety of global properties in many of these systems have at least one common feature: the 'randomness' (static or dynamic, thermodynamic or geometric). For example, the stochastic motion of a particle and the correlation of the thermodynamic fluctuations seem to share this common feature via common description (Pandey *et al* 1984, Harris and Stinchcombe 1983): the dynamic scaling theory which described how the root mean square displacement of the particle in its random walk motion in the asymptotic regime develops in time. The RMS displacement R of a random walk particle on a random percolating system in time t shows (Gefen *et al* 1983, Pandey *et al* 1984) a power-law dependence $R \sim t^k$ with $2k = (2\nu - \beta)/(2\nu + \mu - \beta)$, where ν and β are the percolation exponents for the correlation length and percolation probability, respectively, and k is the conductivity exponent of the percolating network. The same exponent k relates (Pandey *et al* 1984, Harris and Stinchcombe 1983) the thermodynamic correlation length ξ_T with the relaxation time of spins in magnets (Hohenberg and Halperin 1977). A computer simulation study of the random walk motion of a particle in a random percolating system provides a simple way not only to evaluate this critical dynamic exponent k, but also to estimate the conductivity of the random system. Several such studies have been made in recent years in a variety of random systems (Pandey *et al* 1984, Havlin and Ben-Avraham 1983, Zabolitzky 1984). Here we present a simulation of the random walk motion of a particle in a random system which, to our knowledge, has not been studied so far. We also observe some interesting transport behaviour quite unexpected in view of the work mentioned above.

The disorder system considered here is a random-field cubic lattice. At each site there is a field of strength B pointing in one of the six directions chosen randomly. In the computer simulation we prepare a sample (called lattice realisation) by assigning one of the six directions chosen randomly to each site independently. A particular value is then set for the field intensity B, which determines the probability that a particle, once at a site, will hop from this site in its preset random direction. There are two extreme limits of B: in the limit $B = 0$ our system reduces to a homogeneous cubic lattice and a random walk motion of a particle will show a Fickian diffusion. On the other hand, in the limit $B = 1$, the diffuser is locked in randomly directed fields leading to complete trapping; it moves in a deterministic way in the field directions until it reaches a point where six neighbours favour motion to this point in conflicting directions (a frustrated state) where it is trapped forever. To begin a random walk transport in this random system, one of the sites is chosen randomly (called the local origin) and a particle (diffuser or 'ant') is then placed on it. To decide in which direction (to one of its six neighbouring sites) it will jump, a random number is selected and compared with the field B: if it is less than B then the diffuser is moved to the neighbouring site in the pre-assigned random direction to this site; otherwise it is moved to any of the six neighbouring sites chosen randomly as in simple random walk motion. Accordingly, the corresponding displacement is updated and time is increased by unity. The process of selecting a neighbouring hopping site using the above prescription, moving the particle to it and updating time and displacement, is repeated again and again for a preset (maximum) number of steps. For a reliable estimate of the average RMS displacement and its dependence on time, the whole procedure is repeated for several, randomly chosen, local origins and on many independent samples as well. The data presnted here are generated on sample sizes 30^3, 40^3 and 50^3. We use 25 local origins, each on 20 lattice realisations for each B. All the data are generated using a VAX 11/780; the whole study has taken about 100 h of CPU time.

In figure 1, we present a plot of RMS displacement against time t on a logarithmic scale for various values of field intensity starting from $B = 0$. As expected, $B = 0$ gives a very good straight line fit with an exponent k equal to $\frac{1}{2}$ which verifies Einstein's diffusion law. For $B = 0.1$, we still obtain a good fit with the same diffusion exponent, although the values of R are smaller than its value without a field in the large time regime. Increasing the magnitude of B (from 0.1 to 0.5) we still observe similar diffusion behaviour in the initial time regime, but in the longer time regime, R develops faster with time t which leads to an asymptotic exponent k_e significantly larger than $\frac{1}{2}$ and presumably it ultimately approaches the drift value 1. Also, the magnitude of R is larger for higher values of B. The crossover behaviour from diffusion-like (in the small time regime) to effectively drift-like (in longer time) is more evident for higher values of B (0.4 and 0.5). Furthermore, one should note that the crossover time (t_{cr}) seems to decrease with increasing field intensity. Perhaps for the smaller values of B the relaxation time becomes much larger than the observation time, $t = 10^6$ taken to approach its faster (effectively drift-like) take-off limit. It is worth pointing out here that a similar crossover behaviour from diffusion to drift occurs in a homogeneous system with a global field (i.e. the same field at all sites in the same direction) (Pandey 1984a). This implies that the local random fields may induce the transport in the same way as the global homogeneous field. Nevertheless, the local fields govern the transport behaviour in dramatically different ways from that of the global field, as will be seen below.

On increasing the field intensity further, above a certain value B_{ch}, motion of the particle becomes slower (see figure 2 and compare it with figure 1): the RMS displacement R traversed in time t reduces on increasing the magnitude of B. The two types of motion, diffusive (in small time regime τ_D) and random-field-induced faster (in long

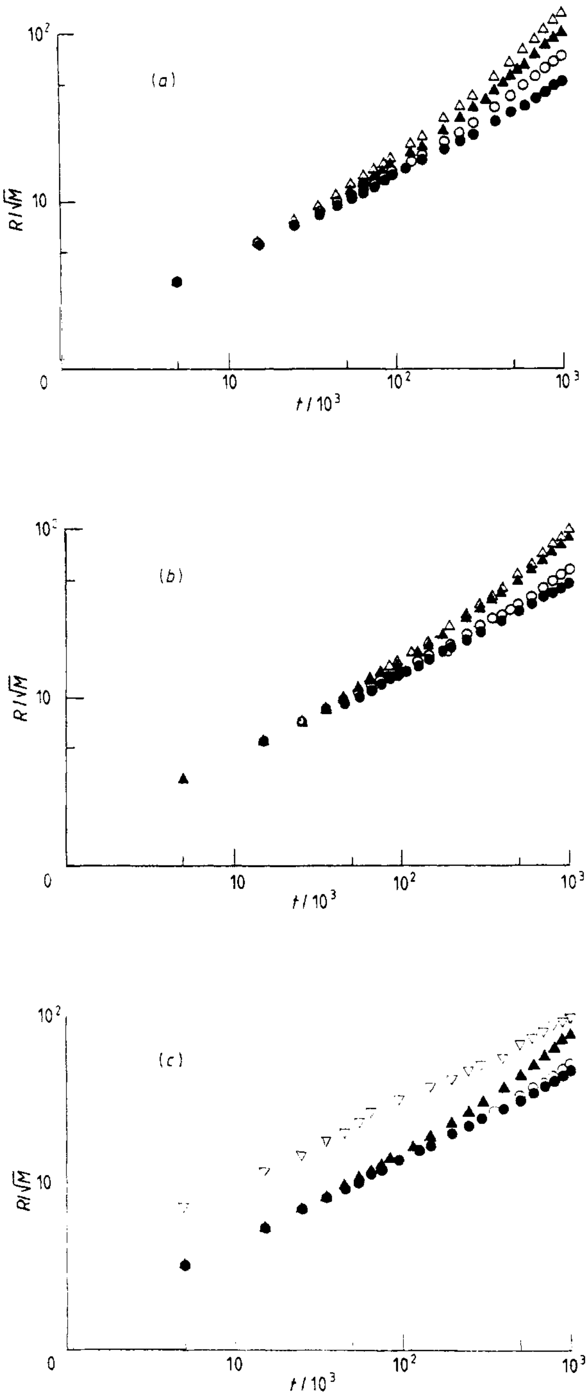

Figure 1. RMS displacement against time t on a log–log plot. Number of local origins $N = 25$, number of samples NRUN = 20 for all values of B, except for $B = 0$ which has $N = 20$, NRUN = 5. Symbols with corresponding values of field intensity: ∇, ($B = 0$); ●, ($B = 0.1$); ○, ($B = 0.2$); ▲, ($B = 0.4$); $\triangle$, ($B = 0.5$). (a), (b) and (c) are for samples of 30^3, 40^3 and 50^3, respectively.

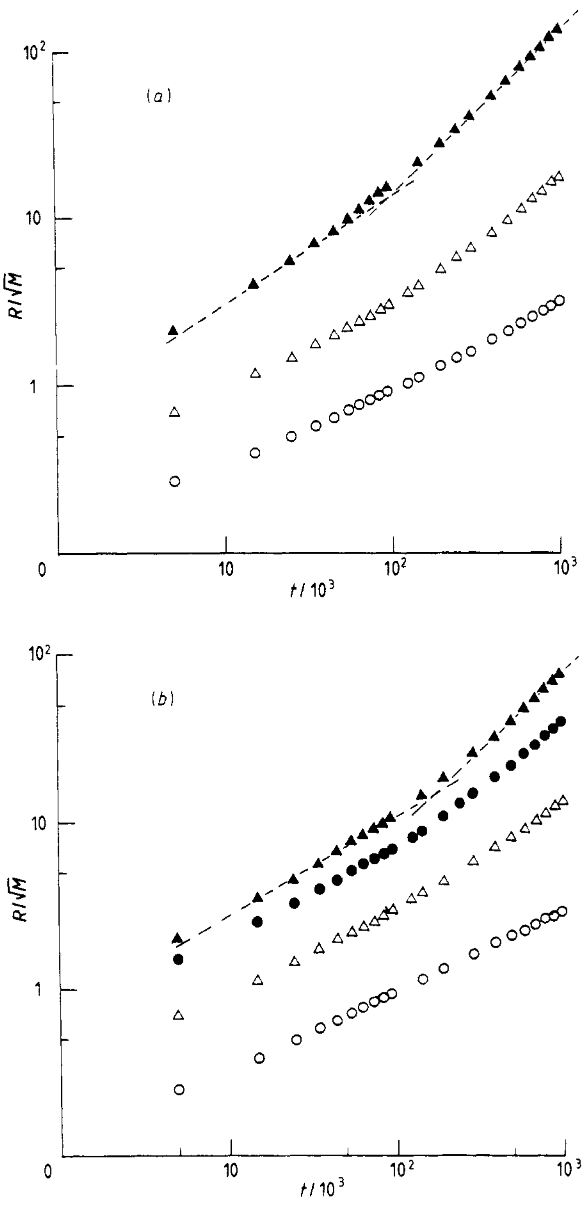

Figure 2. Same as figure 1 but for higher values of field intensity. Symbols with their field intensities are: ▲, ($B = 0.9$); ■, ($B = 0.95$); △, ($B = 0.99$); ○, ($B = 0.999$).

time regime τ_t), still persist, but now in an opposite way to the behaviour described above. The crossover regime t_{cr} in which the field-induced motion takes over from diffusion motion becomes larger at higher field values. Finally, at the extreme value of $B = 1$, the motion completely ceases due to the random field (i.e. the particle is localised).

Non-monotonic properties of the transport as a function of field intensity B, described above, are caused by the disorder (i.e. the random fields). Similar behaviour

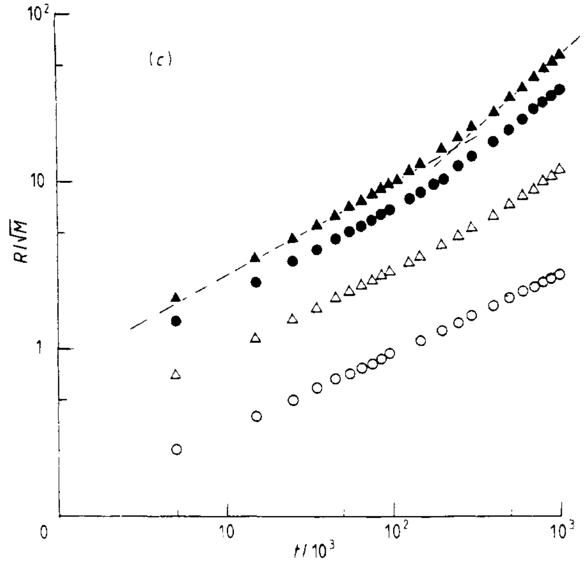

Figure 2. Continued.

has already been observed in a random percolating system in the presence of a global bias field (Barma and Dhar 1983, White and Barma 1984, Dhar 1984, Pandey 1984a, Stauffer 1985, Gefen and Goldhirsch 1985), where the competition between bias field and ramified geometry (the barriers due to dangling ends and deep valleys in the direction of bias) lead to non-monotonic behaviour. However, the two disordered systems, random field (studied here) and random percolating systems (in the presence of a global bias), are quite different as far as the transport of the diffuser is concerned. The random percolating systems are very well studied and most of their self-similar properties (like fractal dimensionality, spectral dimensionality and their relation to transport indices) are reasonably well understood. On the other hand, for the transport properties of the random-field systems, this is to our knowledge the first attempt to illustrate their behaviour using computer simulations.

In order to explore the spectral properties of the underlying random system, it would be interesting to study its spectral (fracton) dimensionality (Alexander and Orbach 1982) which we define using the relation (Rammal and Toulouse 1983, Pandey *et al* 1984) $s \sim t^{d_s/2}$, where s is the number of distinct visited sites in time t and d_s is the spectral dimensionality. Now if we evaluate the number of distinct visited sites in time t, then the slope of a log-log plot of s against t may give an estimate for d_s. Some typical plots are shown in figure 3(a) Clearly, the data in the initial time regime (t up to 6×10^4) suggest $d_s \simeq 1.8(\sim 2)$, but in the long time regime it decreases systematically. Figure 3(b) shows the variation of the effective fracton dimensionality d_s^e with t. It would be interesting to extend this simulation at least an order of magnitude more to see where it settles in time but obviously such resources are out of reach to us at the present. One must also note that stretching the observation time alone is not sufficient to understand the asymptotic behaviour well, as the finite-size effects start playing an important role in determining the long time behaviour.

Obviously, to gain more precise data, as in most of the computer experiments, one has to work with larger samples for longer time. Nevertheless, a deviation in the

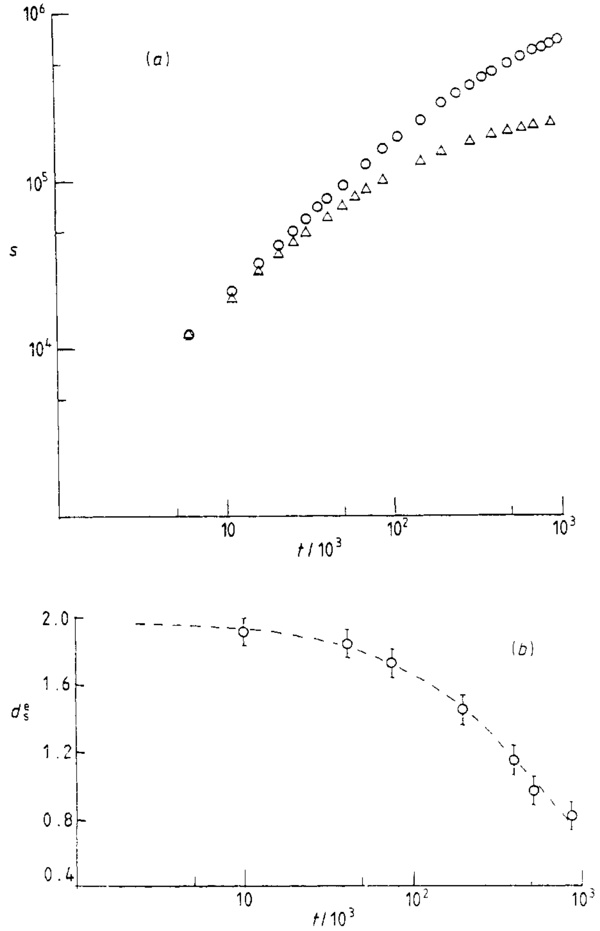

Figure 3. (*a*) Number of distinct visited sites against time plotted on a log-log scale. Statistics: $N = 25$, NRUN = 20. Samples: 50^3, ○, ($B = 0.9$); 30^3, △, ($B = 0.9$). (*b*) Plot of effective spectral dimensionality d_s against time on a semi-log scale.

magnitude of d_s^e from about two in the small time regime to about 0.8 in the long time regime seems to suggest that there is more than one power law regime in which the simple diffusive motion is followed by a rapid transport in the long time regime. As a note of caution, although we have presented data on different sample sizes, it would be worth testing them on much bigger samples.

In conclusion, our simple study suggests that in a random-field disordered system, the variation of the RMS displacement with t is quite different from that in the usual random fractals (i.e. percolating systems). Contrary to a slow anomalous motion in random percolating systems (Gefen *et al* 1983, Pandey *et al* 1984), the random walk motion is enhanced here in random-field systems leading to disorder-induced transport. A similar disorder-induced transport was predicted by Heinrichs and Kumar (1984), but in a different context (i.e. in a one-dimensional system in the presence of random fields) (Pandey 1984b). We observe a non-monotonic behaviour in transport on increasing the local field intensity. Clearly, different power laws on a different time scale and the non-monotonic variation in the RMS displacement with time t may give a variation in the effective diffusion constant D_e defined by $R = 2D_e t^k$. Such behaviour may be related to the recent theoretical observation of the classical transport in modulated structures (Golden *et al* 1985). Vibrational properties of the random-field system seem to suggest more than one mode, leading to a variation in effective spectral dimensionality. A similar study in two dimensions (part II of this series, in preparation) also shares some of these findings.

The author would like to thank A Kerstein, S D Mahanti and D Stauffer for useful discussions. Computer time was supported by the Academic Research Computer Center at Jackson State University.

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