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Corrections to scaling for diffusion in disordered media

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Abstract. We study the diffusion of a particle in a d-dimensional lattice where disorder arises from a random distribution of waiting times associated with each site of the lattice. Using scaling arguments we derive, in addition to the leading asymptotic behaviour, the correction-to-scaling terms for the mean square displacement. We also perform detailed Monte Carlo simulations for one, two and three dimensions which give results in substantial agreement with the scaling argument predictions.

1. Introduction

Disordered materials have recently become a challenging field, both from the point of view of the practical applications [1-6], as well as the understanding of the physical phenomena involved [7-11]. Transport phenomena in general, and diffusion in particular, can present anomalous properties in these systems, even in some cases where we have a regular lattice. The disorder in the system, whether in amorphous materials, or in regular lattices with trappings or other kinds of site disorder, produces in many cases a slowing down of the diffusion. The first manifestation of this phenomenon is the vanishing of the diffusion coefficient [9, 12], as usually defined from Fick's law. A more detailed analysis [7] shows that the mean square displacement as a function of the elapsed time behaves as a power law, with an exponent smaller than one, rather than having the characteristic linear behaviour of the normal random walk. The slowing down of the diffusive process may be due to some bottleneck, or particle trapping, which appears in the disordered material.

In the present work we shall concentrate on the problem of the diffusion of a particle in a regular lattice, with the proviso that the particle remains trapped in each site for a certain amount of time before it can hop to a nearest neighbour. This has become known in the literature as the site disorder case. In our case, we have taken the hopping probability to be uniform in all directions, and the same for all sites. The waiting times, instead, depend on each site, but are fixed for each quench. The probability distribution for transition rates (taken as the inverse waiting times) is taken as a power law distribution [7, 9].

For the one-dimensional case, Alexander *et al* [7] found anomalous diffusion using this power law distribution and calculated the anomalous exponent for the dominant term in the time dependence of the square displacement. This result was generalised to many dimensions using scaling arguments [9], and a renormalisation group approach

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[8]. Similar results were obtained for the case of hierarchical distributions of disordered barriers on a one-dimensional regular lattice [11]. However, in none of these works have the corrections to scaling been studied.

In this work we analyse, using both scaling arguments and numerical simulations, the long-time behaviour of a random walk with site disorder, performed in one, two and three dimensions, using a power law distribution for the transition rates. Initially we extend the scaling arguments used previously to calculate the leading asymptotic behaviour of the mean square displacement, to calculate the dominant correction terms to the scaling behaviour. In the asymptotic regime we obtain the same exponents as those predicted by the scaling laws [9, 10]. For the correction to scaling, we have found two terms which compete depending on the value of the exponent for the power law distribution for the transition rates. Monte Carlo simulations confirm the leading asymptotic behaviour giving results for the exponent of the leading term in very good agreement with the scaling argument predictions. Using the form of the correction terms predicted by scaling arguments together with the results of the numerical simulations, we are able to provide a fitting to the mean square displacement, valid for a larger time interval, and obtain a value for the amplitude of the leading term in good agreement with the exact results in one dimension [12].

In § 2 we introduce the model and use scaling arguments to obtain the results for the power law behaviour and its corrections. In § 3 we present the results from the numerical simulation, and give a brief discussion of the main results of the work.

2. Corrections to scaling

Let us consider a random walk in a d-dimensional lattice with site disorder. Associated with each site in the lattice, there is a waiting time before the next hop takes place to a neighbouring site. We have considered the particular case of a hypercubic lattices, but the results are independent of the type of lattice. The inverse of the waiting time, the transition rate, is given by a quenched random variable w. The walker hops to any of the nearest neighbours with equal probability, and the system is assumed to be isotropic. Following the pioneering work of Alexander *et al* [7], we assume a power law distribution for the release rate:

$$P(w)\,\mathrm{d}w = (1-\alpha)w^{-\alpha}\,\mathrm{d}w \qquad 0<\alpha<1 \qquad 0\leqslant w\leqslant 1. \tag{1}$$

This can be interpreted [9] as a temperature-dependent rate process, with the exponent being related to the critical temperature as $\alpha = 1 - T/T_c$. For negative values of α, the distribution (1) is no longer singular and hence we obtain normal diffusion, while positive values give rise to anomalous diffusion.

In order to find the asymptotic behaviour of the mean-square displacement and its leading correction, we extend the scaling arguments used by Havlin *et al* [9, 10]. We first realise that, irrespective of the distribution of waiting times, the mean square displacement as a function of the number of steps in a d-dimensional walk, is given by

$$R^2 \equiv \langle r^2(t)\rangle = N. \tag{2}$$

The elapsed time t after N steps is

$$t = \langle t\rangle N \tag{3}$$

where $\langle t\rangle$ is the average time for each step. For the distribution given by (1), we obtain

$$\langle t\rangle=\int_{w_{\min}}^{1} P(w)w^{-1}\,\mathrm{d}w\sim w_{\min}^{-\alpha}-1. \tag{4}$$

Here $w_{\min}$ is a cut-off corresponding to the smallest transition rate encountered by the particle when the number of distinct visited sites is N_{d}. In order to estimate $w_{\min}$ in terms of N_{d} we proceed in the following way. We choose a random variable x $(0\leqslant x\leqslant 1)$ distributed uniformly so that $P(w)\,\mathrm{d}w=\mathrm{d}x$, i.e. $x=w^{1-\alpha}$. From statistical analysis, the minimum of x is given by

$$x_{\min}\sim\frac{1}{N_{\mathrm{d}}}\left[1+\frac{\text{constant}}{N_{\mathrm{d}}}\right] \tag{5}$$

where, in addition to the leading term, we have also included a correction. Hence $w_{\min}$ behaves as

$$w_{\min}\sim N_{\mathrm{d}}^{-1/(1-\alpha)}\left[1+\frac{\text{constant}}{N_{\mathrm{d}}}\right]. \tag{6}$$

We now need to relate the number of steps with the number of distinct sites visited by the same walk. The first investigation of this question was made by Dvoretzky and Erdos [13] who showed that the number of distinct sites visited N_{d} on an N-step lattice walk is given for large N by

$$N_{\mathrm{d}}\sim N^{1/2}\qquad d=1 \tag{7a}$$

$$N_{\mathrm{d}}\sim N/\ln N\qquad d=2 \tag{7b}$$

$$N_{\mathrm{d}}\sim N\qquad d\geqslant 3. \tag{7c}$$

Let us for the moment restrict ourselves to the one-dimensional case. By using (2), (3), (4), (6) and (7*a*), we obtain the following relation between the mean square displacement and the elapsed time:

$$t\sim R^{(2-\alpha)/(1-\alpha)}+\text{constant}\times R^{1/(1-\alpha)}+\text{constant}\times R^{2}. \tag{8}$$

The solution of the above equation gives

$$R^2=At^{2(1-\alpha)/(2-\alpha)}[1+Bt^{-\alpha/(2-\alpha)}+Ct^{-(1-\alpha)/(2-\alpha)}]. \tag{9}$$

Similarly for two dimensions (apart from a logarithmic correction) and three dimensions we obtain

$$R^2=At^{1-\alpha}[1+Bt^{-\alpha}+Ct^{-(1-\alpha)}]. \tag{10}$$

The constants A, B and C are the amplitudes for the leading and correction-to-scaling terms. In (9) and (10), the first correction term dominates for values of $\alpha<\frac{1}{2}$ and the second term is dominant for $\alpha>\frac{1}{2}$. For values of α near $\frac{1}{2}$ both terms give relevant contributions for the correction to scaling. One should emphasise that, except for the extreme values of α, the numerical determination of the correction-to-scaling exponent is difficult due to the competing nature of the terms for $\alpha>\frac{1}{2}$ and $\alpha<\frac{1}{2}$.

Although the results presented in this section are particularly valid for the distribution given in (1), the above approach can be used to obtain the correction-to-scaling terms for other types of distribution and for diffusion problems which, for example, take into account the effects of hard-core interactions [14].

3. Numerical results

In order to compare the results given in (9) and (10), we have performed Monte Carlo simulations of the random walk with waiting times in one, two, and three dimensions, for several values of α. In order to avoid finite-size effects in the simulations, we have taken a lattice of sufficiently large size such that no walk ever reached its boundary. The Monte Carlo calculation was averaged over 50 000–100 000 trajectories. On each trajectory, we measured the square displacement as a function of time, with up to 30 000 time steps. This allows us to look at the asymptotic behaviour, and compare the anomalous exponents for various values of α plotting $\langle r^2 \rangle$ as a function of t in a logarithmic scale.

The numerical results for the mean square displacement for one, two and three dimensions are shown in figures 1 and 2. We notice immediately from these figures that the slope tends to 1 as α goes to 0. The exponent we compute from the Monte Carlo simulation agrees with the leading term in (9) and (10) in the asymptotic region, for all the dimensionalities we calculated.

Let us now look at the correction terms. The first point to notice is the fact that its contribution is minimum for $\alpha = \frac{1}{2}$. This implies that the asymptotic regime is attained at later times, both for larger and smaller values. Numerical simulations actually give better results for the exponent of the leading term for values of α near

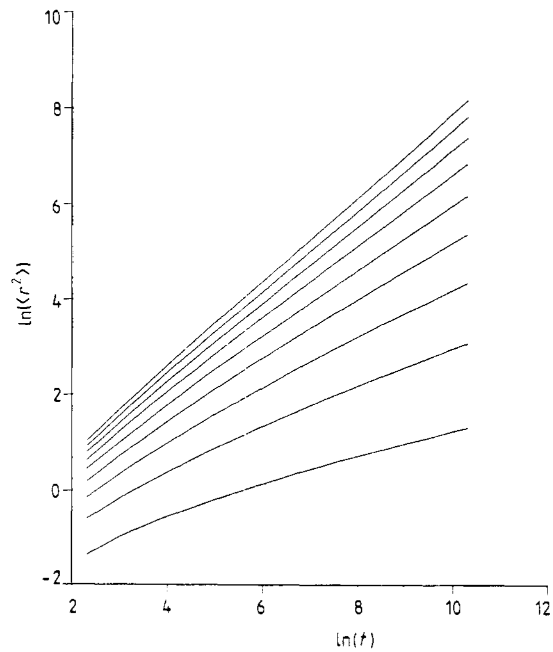

Figure 1. Mean square displacement against time for a one-dimensional lattice. Averages were taken over 50 000–100 000 samples. The curves corresponds to values of α between 0.1 (uppermost curve) and 0.9 (lowermost curve).

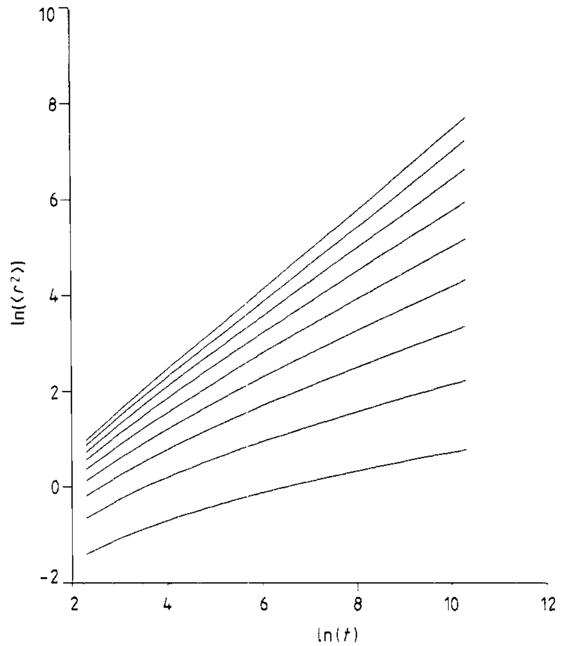

Figure 2. Same as figure 1 for a two-dimensional lattice.

$\frac{1}{2}$ and become increasingly less accurate for values of α away from $\frac{1}{2}$. In order to compare the theoretical results for the correction to scaling with the numerical results from the Monte Carlo simulation, we have plotted the mean square displacement divided by the appropriate power of time against an inverse power of time, as follows from (9) and (10) in figures 3 and 4. If only one of the correction terms appeared in (9) and (10), the plot should be a straight line. Asymptotically we find this to be true, and we can extract the correct A, B and C coefficients from the numerical results. Two comments are in order at this point: in the one-dimensional case the numerical fluctuations are larger than in higher dimensions, but the asymptotic behaviour is also linear and, secondly, the two-dimensional case shows a larger deviation from the scaling behaviour plus corrections, due to the fact that there are additional logarithmic terms, as clearly seen in (7), which have not been included in our calculations in § 2. The values for the coefficients in (9) and (10) are α-dependent and can be found by a linear best fit using the appropriate scaled variables. In one dimension, for $\alpha = 0.9$ (figure 3) we obtain $A = 0.98$ and $C = 1.05$. The value of the leading amplitude A is in reasonable agreement with the exact value $A = 1.10$ found by Nieuwenhuizen and Ernst [12].

In summary, we have studied a random walk model in a d-dimensional lattice with site disorder using scaling arguments and Monte Carlo simulations. Using a power law distribution for the transition rates ($w^{-\alpha}$) the mean square displacement was measured as a function of time for various values of α. In addition to the leading asymptotic behaviour we have found two correction-to-scaling terms. These terms compete for values of α around $\frac{1}{2}$. The numerical simulations confirm these theoretical predictions and allow us to obtain the amplitudes of the leading and correction to scaling terms for different values of α.

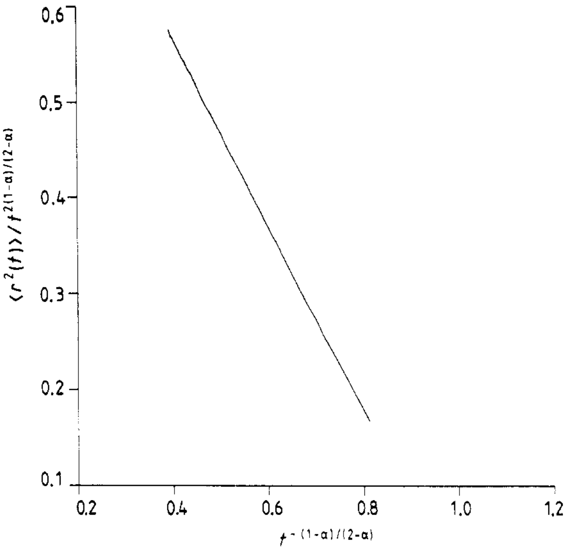

Figure 3. Plot of $\langle r^2(t)\rangle / t^{2(1-\alpha)/(2-\alpha)}$ against $t^{-(1-\alpha)/(2-\alpha)}$ for a one-dimensional lattice and for $\alpha = 0.9$. Averages were taken over 100 000 samples.

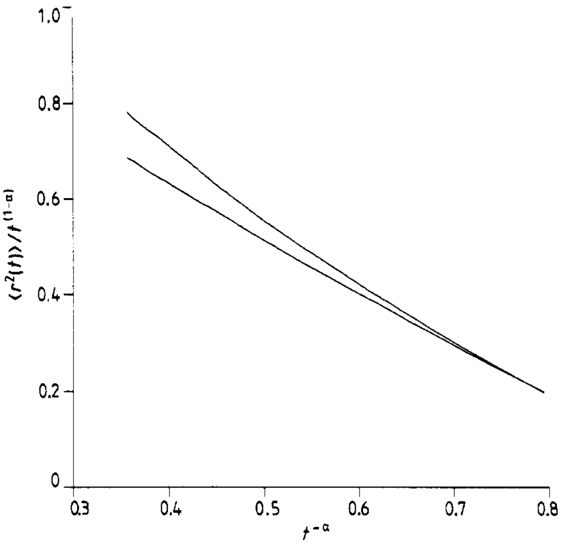

Figure 4. Plot of $\langle r^2(t)\rangle / t^{(1-\alpha)}$ against $t^{-\alpha}$ for a two-dimensional (upper curve) and three-dimensional (lower curve) lattices and for $\alpha = 0.9$. Averages were taken over 100 000 samples.

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