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Monte Carlo simulation of long-time percolation diffusion on $d = 2$ lattices above the threshold

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Abstract. Monte Carlo simulations of percolation diffusion at and below the percolation threshold give results in accordance with theory. Above the percolation threshold, however, this is not the case. It was thought that above the threshold a well-defined crossover point separated the anomalous and classical diffusion regimes, with the classical diffusion coefficient having the same critical exponent as the lattice conductivity, but Monte Carlo simulations failed to confirm this expected behaviour. Analysis of new Monte Carlo results presented here for the square lattice shows that percolation diffusion is classical only strictly asymptotically. Instead of a crossover, the approach to classical behaviour is better described as a very slow relaxation. Accounting for this relaxation enables the critical behaviour of percolation diffusion to be confirmed with a corresponding critical exponent $\mu = 1.291 \pm 0.024$.

1. Introduction

There has been a great deal of interest in the dynamic properties of the percolation lattice such as conduction and diffusion which, historically, provided the initial motivation for the development of percolation theory [1]. The percolation lattice is infinite in extent and lattice sites or bonds are occupied with a probability p. Nearest neighbour sites or bonds form clusters and for all $p > p_c$ there exists an infinite cluster which spans the lattice. Conduction on the lattice takes place via percolation clusters only. On the infinite lattice the conductivity, Σ, is zero for all $p < p_c$ and increases to a maximum value as $p \to 1$. Similarly, diffusion is also confined to percolation clusters. Progress of a diffusing particle on the lattice is measured by the mean square distance travelled, $\langle R^2 \rangle$, in N discrete steps, as discussed by De Gennes [2].

Below the threshold the trajectory of a diffusing particle is ultimately restricted by the cluster perimeter but above the threshold diffusion is unbounded. When $p = 1$, the correlation length of the lattice, ξ, equals zero and the percolation lattice is uniform on all length scales. Diffusing particles are free to behave classically and the mean square distance $\langle R^2 \rangle$ diffused in N steps obeys the law

$$\langle R^2 \rangle = DN \tag{1}$$

where D is the classical diffusion coefficient, in this case equal to unity.

When $p_c < p < 1$, $\xi \neq 0$ and the fractal cluster structure [3] influences diffusion on the lattice. It was conjectured by Gefen *et al* [4] that initially the particle would undergo anomalous diffusion, obeying the law

$$\tilde{R} = \langle R^2 \rangle^{1/2} \propto N^k \tag{2}$$

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with $k \cong \frac{1}{3}$. The particle was thought to behave classically, with $k = \frac{1}{2}$ but $D < 1$, only after some characteristic crossover time, $\tau_>$, which diverged at the percolation threshold; there, it is known that percolation diffusion is anomalous for all N.

Static cluster properties such as P_∞, the strength of the infinite cluster, and ξ are known to scale with $(p - p_c)$ as $P_\infty \propto (p - p_c)^\beta$ as $p \to p_c+$ and $\xi \propto |p - p_c|^\nu$. The values of the exponents β and ν are known exactly in two dimensions, $\beta = \frac{5}{36}$, $\nu = \frac{4}{3}$, and to a high degree of certainty in three, $\beta = 0.41$, $\nu = 0.88$ [5]. In common with these static scaling laws it is assumed that D and Σ also have a critical dependence on the distance $(p - p_c)$. According to the Einstein relation, D is proportional to Σ [6] implying that both dynamic properties share the same dynamic critical exponent, μ,

$$\Sigma \propto D \propto (p - p_c)^\mu \tag{3}$$

as $p \to p_c+$.

There is no exact analytical determination of μ. Neither, aside from the disputed Alexander–Orbach conjecture [7] from which $\mu = \frac{1}{2}[\nu(3d - 4) - \beta]$ may be deduced, is there an exponent relation which defines μ solely in terms of static exponents such as β or ν. In the absence of such a theory, percolation diffusion is often studied by Monte Carlo simulations using the labyrinth ant [2].

Although results of such simulations agree with theory [8, 9] below the threshold, above the threshold this is not the case. Here, according to the crossover conjecture of Gefen *et al*, graphs of $\langle R^2 \rangle$ versus N should show initial curvature followed by clear linearity and according to (1) the slope of the linear region should be equal to the coefficient D allowing the scaling behaviour of D to be determined. Following this method, Mitescu *et al* [10] found that $\mu = 0.98 \pm 0.02$ for the square lattice and that $\mu = 1.72 \pm 0.03$ for the cubic latice. This latter estimate was then revised to $\mu = 1.70 \pm 0.05$ [9], but it was still at odds with the value $\mu \cong 2.06$ which they obtained from exponent relations given in earlier work below the threshold [11]. This led Mitescu *et al* [9] to postulate the existence of two dynamic exponents, one for D and one for Σ.

In light of this discrepancy, Pandey *et al* [8] evaluated D above the threshold on cubic lattices of various sizes and found that μ appeared to increase with the edge length, L, of the lattice, i.e. $\mu = 1.71$, 1.80 and 1.85 for $L = 30$, 60 and 180 respectively. If one plots μ versus L^{-1} it can be seen that $\lim_{L\to\infty} \mu \cong 1.88$. On the other hand, simulations carried out by Pandey *et al* [8] at the threshold yielded estimates for k which from the exponent relation $2k = (2\nu - \beta)/(2\nu - \beta + \mu)$ gave $\mu = 1.28 \pm 0.02$ for $d = 2$ and $\mu = 2.0 \pm 0.2$ for $d = 3$.

The cited results for the scaling behaviour of D above the threshold fail to agree with that of Σ. Recent values of μ obtained from conductivity simulations are $\mu = 1.299 \pm 0.002$ on the two-dimensional lattice [12] and $\mu = 2.003 \pm 0.047$ in three dimensions [13]. This discrepancy fails to satisfy the condition implied by the Einstein relation that D and Σ share the same critical exponent.

The discrepancy between the expected behaviour of percolation diffusion and that observed from simulations above the threshold has thus far remained unresolved. The inconsistency lies with the predicted time-dependent behaviour of percolation diffusion and is due to the absence of a well-defined crossover time. To investigate this hypothesis, ant-in-the-labyrinth (AIL) simulations were carried out on the square lattice above the threshold for N far larger than in previously reported simulations. Analysis of these results, discussed in the next section, shows that instead of clear crossover behaviour there is in fact a very slow relaxation to strictly asymptotic classical behaviour.

2. Results

All simulations were carried out on percolation lattices of size $L = 1000$. Simulations [14] have shown that only a very small proportion of walks exceed a distance L^2 when $N = L^2$ and $p \ll 1$. The blind AIL algorithm was used and walks were permitted to take place on all clusters as in [8]. Simulations were carried out for a range of p, $0.61 < p < 0.7$. For each value of p, 200 walks were carried out on each of 100 lattice configurations and the distance R^2 was evaluated after every hundredth step.

For the analysis of the results it was assumed that diffusion, whether anomalous or classical, may be described by equation (2); recall that $k < \frac{1}{2}$ implies anomalous behaviour and $k = \frac{1}{2}$ implies classical. The local value of k was estimated for different N, where $3 \leqslant \log(N) \leqslant 6$, from the slope of the graph $\log \tilde{R}$ versus $\log(N)$. Plotting the local value of k versus $\log(N)$ suggests a relaxation to classical behaviour as N increases, with the progression toward classical behaviour being slower as $p \to p_c+$. This is shown in figure 1 for for $p = 0.65$ (circles), $p = 0.62$ (squares) and $p = 0.61$ (triangles). There is no indication of a well-defined crossover from anomalous diffusion with $k \cong \frac{1}{3}$ to classical diffusion with $k = \frac{1}{2}$ as proposed by Gefen *et al* [4]. In view of this behaviour, one is faced with the difficulty of determining D since due to the absence of a clear region of classical diffusion graphs of $\langle R^2 \rangle$ versus N are nowhere linear. By plotting the results in the form $\tilde{R}/N^{1/2}$ versus $1/N^{1/2}$, however, linear plots were yielded for sufficiently large N, emphasising the slow relaxation to classical behaviour where $k = \frac{1}{2}$. Were there a sharp crossover to $k = \frac{1}{2}$ after some time $\tau_>$ then such graphs would show $\tilde{R}/N^{1/2}$ equal to a constant for some range of $1/N^{1/2}$ in a well-defined classical region. Figure 2 shows the graph of $\tilde{R}/N^{1/2}$ versus $1/N^{1/2}$ for $p = 0.65$ (circles), $p = 0.62$ (squares) and $p = 0.61$ (triangles). The tendency to linear behaviour is clearly evident. One can inspect the linear

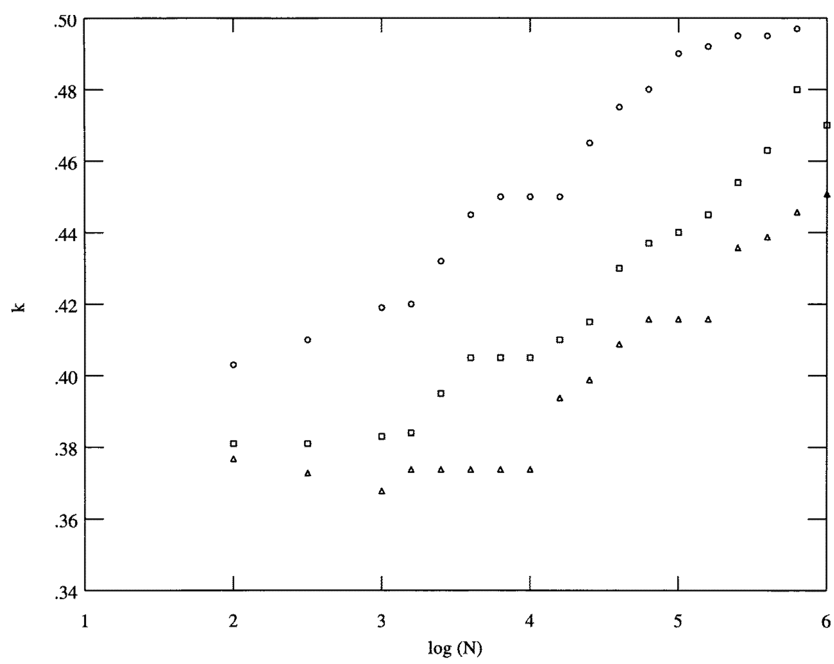

Figure 1. The behaviour of k with $\log(N)$ for various p.

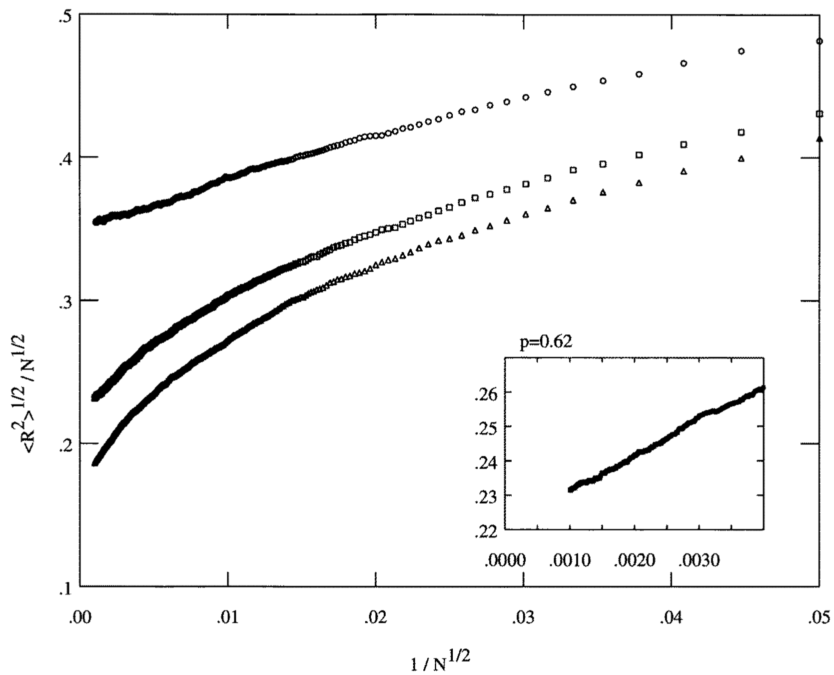

Figure 2. The relaxation to classical diffusion for various p; the inset shows the leftmost region for $p = 0.62$.

behaviour at first glance for $p = 0.65$. Although the region of linearity is reduced as the threshold is approached, for example that for $p = 0.62$ is shown in the inset, linear behaviour was always observed for some range of $1/N^{1/2}$ when the results were plotted in this fashion. The intercept on the vertical axis of $\tilde{R}/N^{1/2}$ versus $1/N^{1/2}$ is $D^{1/2}$. Thus D can be simply estimated from such graphs.

Then, recalling the dynamic scaling law $D \propto (p - p_c)^{\mu}$ as $p \to p_c+$, the estimates of D were plotted as $\ln(D)$ versus $\ln(p - p_c)$ where $p_c = 0.5927$. The slope of the linear region of this graph shown in figure 3 gives $\mu = 1.291 \pm 0.024$ where the error quoted is the standard error. This is in good agreement with other recent Monte Carlo estimates of μ for $d = 2$ percolation systems as shown in table 1, but excludes the value of $\mu = \frac{91}{72}$ deduced from the Alexander–Orbach conjecture.

The above treatment of the asymptotic nature of percolation diffusion leads to far more accurate estimates of D than can possibly be obtained by simply assuming linearity [10] in graphs of $\langle R^2 \rangle$ versus N, for finite N or by the use of various types of *ad hoc* correction terms [9]. Estimates from the results above reveal that to measure D to within 5% of the value obtained here by such methods would require $N \cong 9 \times 10^4$ time steps at $p = 0.65$ increasing to $N \cong 1.2 \times 10^7$ time steps for $p = 0.61$, much larger than have previously been used. It is for this reason that previous estimates of μ from the scaling behaviour of D on $d = 2$ and $d = 3$ percolation lattices have failed to agree with μ obtained from the scaling behaviour of Σ. The very slow relaxation behaviour cannot be attributed to the fractal cluster structure as for large length scales the lattice can be considered to be essentially uniform. Instead it may be argued [14] that the relaxation is due to the continual impedance and reflection of the particle's motion by site vacancies, a time-dependent effect which cannot be anticipated when discussing percolation diffusion in terms of time-independent

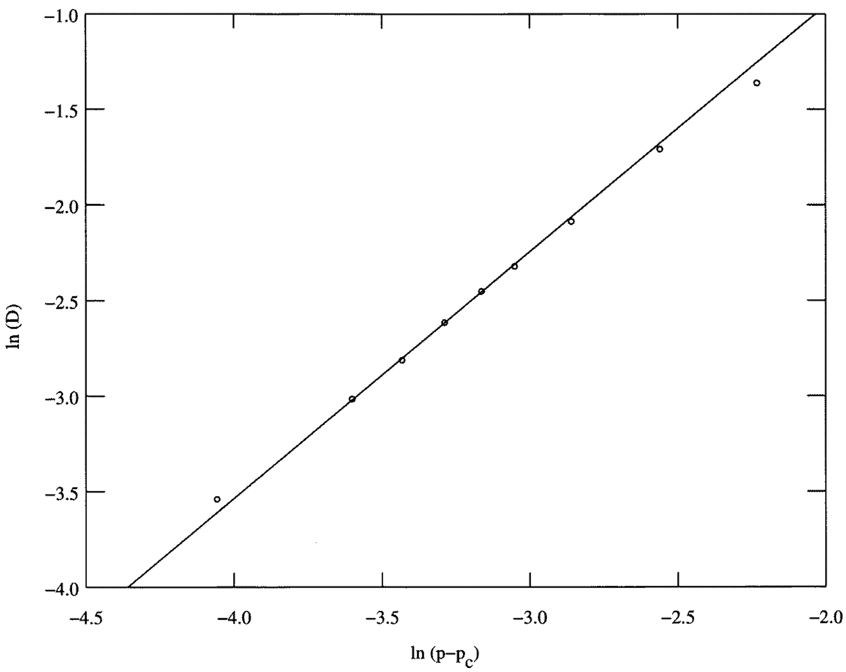

Figure 3. The scaling behaviour of D with $(p - p_c)$.

Table 1. Values of μ from various sources.

Value of μ	Method	Reference
1.291 ± 0.024	Estimate of D as $N \to \infty$	Reported here
1.299 ± 0.002	Bond lattice conductivity	[12]
1.297 ± 0.005	Bond lattice conductivity	[15]
1.31 ± 0.04	Bond lattice conductivity	[16]
1.28 ± 0.02	Diffusion on site lattice; $p = p_c$	[8]
1.26 ± 0.03	Site lattice conductivity	[17]
91/72	Alexander–Orbach conjecture	[7]
$1.0 \leqslant \mu \leqslant 1.3$	Bond lattice conductivity	[18]
1.10 ± 0.05	Bond lattice conductivity	[19]
1.25 ± 0.05	Site lattice conductivity	[19]
0.98 ± 0.02	Diffusion on site lattice; $p > p_c$	[10]

properties such as conductivity. The relaxation is a real effect that must be accounted for when studying the asymptotic classical behaviour—neglecting it leads to inaccurate estimates of the dynamic exponent.

3. Conclusion

It has been shown that percolation diffusion above the critical percolation threshold is best described in terms of a very slow relaxation towards strict asymptotic classical behaviour.

For sufficiently large N this relaxation is expressed as

$$\frac{\tilde{R}}{N^{1/2}} - \lim_{N\to\infty} \frac{\tilde{R}}{N^{1/2}} = \frac{C}{N^{1/2}}$$

where C is a constant. The critical exponent μ where $D \propto (p - p_c)^{\mu}$ as $p \to p_c+$, for $d = 2$ percolation diffusion was found to be $\mu = 1.291 \pm 0.024$. This is the first accurate estimate of the critical exponent from the scaling behaviour of D above the percolation threshold.

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