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FRACTAL ENERGY TRANSPORT: RANDOM WALK SIMULATIONS ON LONG-RANGE PERCOLATION CLUSTERS

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Luminescence from naphthalene alloys is quenched by long-range exciton hops. These are modeled by long-range random walks on long-range percolation clusters with a range-dependent hopping time. Both linear and exponential range dependencies are simulated, over nearest to fifth nearest neighbor hops. At critical percolation thresholds the random walk properties obey the super-universality hypothesis (spectral or fracton dimension of about 4/3). However this asymptotic limit is approached at different rates for different functional forms of the hopping time (constant, r, e^r, 10^r).

Recent luminescence experiments on isotopic mixed naphthalene crystals were interpreted in terms of fractal energy transport.[1-4] Basically this involves random walks on percolation clusters (defined by the $C_{10}H_8$ in the $C_{10}D_8$ host). However, these clusters are defined via long-range bonds and the long-range random walks were assumed to be in the same universality class (spectral dimension) as nearest neighbor walks on ordinary percolation clusters. The question is not only whether the asymptotic (long time) behavior is the same but also how soon such asymptotic behavior is approached (considering the finite experimental time-scale).

The static properties of long-range percolation are well-studied.[5,6] The thresholds for different interaction ranges have been derived via Monte-Carlo methods by Hoshen et al.[5] and via a position space renormalization group method by Gouker and Family.[6] The percolation exponents (β, γ, ν, etc.), and therefore fractal dimensions, are the same as for nearest-neighbor interactions. We perform random walk simulations at these thresholds and monitor the number of distinct sites visited at least once $\langle S_N \rangle$, and the mean-squared distance $\langle R^2_N \rangle$, as a function of time (number of steps N), for different concentrations (p).

The relationship for nearest-neighbor walks is

$$S_N \sim N^f \qquad N \to \infty$$

where $f = d_s/2$ and the spectral dimension d_s is expected to equal about 4/3.[7] Above the threshold (critical concentration p_c) the behavior of Eqn(1) is

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expected to "crossover"[8] to a classical behavior, where f = 1 for 3-dimensional perfect lattices, but f $\lesssim$ 1 for 2-dimensional perfect lattices. Below the threshold we expect an effective exponent f, where 0 < f < 2/3.

The jump probability depends on the distance between sites. For each walk a maximum range of interaction is defined and jumps are allowed to take place only to sites within this range. We vary this range from R = 2 to R = 5 lattice distances. The hopping frequency $\nu(r)$ is a function of the distance r. In this work we treat four functional forms: (a) constant, (b) r^{-1}, (c) e^{-r}, (d) 10^{-r} (the last two are closely related to excitation exchange interactions and differ little from each other). The details of the particular random walk techniques were reported elsewhere.[9,10]

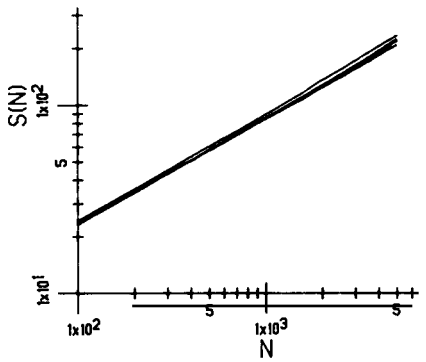

FIGURE 1
S_N vs N as a function of the cutoff range R, for R = 5, 2, 3, 4 (top to bottom, for threshold concentration p_c = 0.07, 0.29, 0.16 and 0.10, respectively). Here $\nu(r)$ = constant. Notice that in this case of $\nu(r)$ = constant all ranges produce practically the same S_N, so that the lines are indistinguishable.

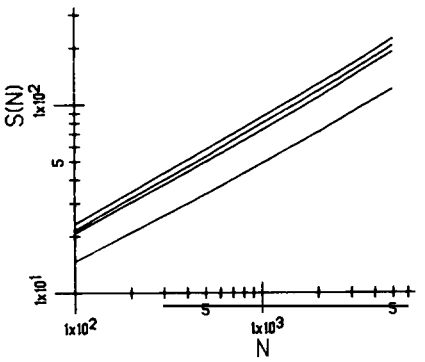

FIGURE 2
S_N vs N, as a function of $\nu(r)$, for R = 2 at p_c = 0.29. Top to bottom: $\nu(r)$ = constant, r^{-1}, e^{-r} and 10^{-r}, respectively.

Our results are summarized in two figures. Figure 1 shows S_N vs N as a function of the interaction range R (R = 2 to 5) for a distance independent jump frequency: $\nu(r)$ = const(r). It is interesting to see that one gets a similar and nearly constant slope f for all R > 1, but this slope f is somewhat smaller than the ordinary (R = 1) slope, i.e., it is below 2/3. However, the general behavior for this family of curves (for all values of R) is similar to the nearest-neighbor random walk results[10] we recently reported. Figure 2

shows the effects of the distance dependence (of the jump frequency) for R = 2. The main effect is the non-linearity for all non-flat $\nu(r)$, i.e., $\nu(r) = r^{-1}$, e^{-r}, 10^{-r}. This curvature may reflect a slower approach to the asymptotic value. Specifically, for a case of a steeply falling-off function $\nu(r)$, the walk, at short times, performs nearest neighbor jumps only. Thus the effective short time percolation threshold is about $p_c = 0.59$ and hence an effective $f << 2/3$ is expected at early times. For longer times, longer range jumps become probable and f approaches 2/3 as the effective threshold (p_c) approaches the nominal values.[5,6] We plan to pursue the long-time limit in another study. Similar behavior to that of R = 2 (Figures 1,2) was also obtained for R = 3 to R = 5.

In summary, we have performed simulation calculations at the critical percolation threshold for binary lattices with long-range interactions. Our results show that scaling and universality of the fractal behavior are largely intact. In the short-time limit that we investigated (up to 5000 steps) the qualitative results showed an effective exponent f somewhat smaller than expected. This is also in agreement with recent experimental observations[2,3,11] and simulations.[12]

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