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CONTINUUM PERCOLATION MODELS FOR THE ENERGY TRANSPORT IN DISORDERED SOLIDS

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Abstract We study energy transport in disordered media through random walks on continuum percolation models. The static (percolating) and dynamical (transport) aspects are monitored through their scaling properties with respect to distance and time. We compare our results with those for usual, discrete percolation. For the fractal exponent d we find good agreement, but the diffusion exponent D shows somewhat lower values, differing by about 10% from usual percolation. We discuss and analyze these observations.

I. INTRODUCTION

Transport in random media is an active area of research[1], whose applications range from the microscopic point of view (charge carriers and excitation transfer[2-6]) to the macroscopic one (diffusion through permeable rocks and patterns of river flow[7]). Organic crystals at low temperatures have been proven[2] to be very good test systems for such transport properties, since for them a wealth of experimental results exists. Thus for systems such as benzene, naphthalene, or anthracene mixed (chemically or isotopically) crystals one has adequate information for their interaction potentials,

and their first few electronic excited states, including lifetimes.

Because of simplicity basic theoretical models of disorder often start from an underlying discrete grid, on which sites or bonds are placed randomly, thus leading to site or bond percolation in the usual sense[1]. It is, however, evident, that the structure of amorphous systems is by far more complex than the structures attainable through this discrete approach. More flexible structures are obtainable through continuous models in which geometrical patterns are placed randomly in space[8-15]. In this work we focus on two-dimensional continuous percolation and study the transport of excitations through the continuous channels formed. As basic regular geometrical patterns former works have used both discs and squares[9-14]. Here we work with squares, because they are technically simpler to handle, and also because they do not impose an inherent curvature on the boundary separating the conducting from the non-conducting region. As in discrete percolation, one expects at the critical occupational probability, p_c, the infinite cluster to be fractal (i.e. to scale with distance)[11-14], and this is a criterion which we analyze in the following sections. We remind the reader that the critical probability p_c is that value of p at which an infinite cluster is formed for the first time. As regards the transport over the infinite cluster, we model it through a random walk in the continuum. Here we monitor the mean-square displacement, R^2, from the origin of the walk, and its time dependence. In Section II we describe the model in detail together with the new computational algorithm that generates percolating clusters exactly at their critical point, p_c. We feel that this is a superior method because then each computer realization percolates exactly. In Section

III we describe our results for $\bar{d}$, the fractal dimension, and D, the diffusion exponent. We compare these findings with the well known discrete lattice models, as well as with other recent related works.

II. DESCRIPTION OF THE MODEL

We use simulation methods that are based on a 2-dim model in which the continuum is introduced by eliminating all site symmetry. For this we use a number of squares N, whose centers are placed at random on a lattice of size LxL. The occupational probability p here is defined as $p=N/L^2$. A cluster is formed by two or more squares that have any amount of overlap. All particle motion is confined on such clusters. Thus, due to the random positioning of all squares, the perimeter of the incipient critical cluster loses all site symmetry characteristics and the diffusing particle moves inside a "continuous space" boundary.

For bookkeeping purposes only, we use a discrete underlying lattice made of LxL cells, each cell being exactly equal to the size of the square. We place n squares randomly in each cell. The number n is determined also at random by use of a Poisson distribution of the form[11-14]:

$$P(p,n) = e^{-p}p^n/n!$$

This process is equivalent to placing the total number of squares N directly in the LxL area, but has two advantages. First, we keep track of all square coordinates more easily, and secondly, when we investigate the squares' overlap to find the cluster formations we go cell by cell, and column by column, to scan the whole lattice in one sweep, from the upper left corner to the lower right. At every instance we check the eight neighboring cells, and two squares will be-

long to the same cluster if the x and y distance between their centers is less than one square unit away.

Our new model utilizes a technique that finds the critical cluster exactly for each random realization. This method is more time consuming when compared to the fast Cluster Growth Technique[16], but it is more accurate. We start at a p somewhat lower than the critical percolation threshold, p_c, and ensure that the critical cluster has not appeared yet. Then we add a certain number of squares, their exact number and location being recorded. Usually this number is a power of 2, say 2^{10}. If after this change there is still no infinite cluster a new additional set of squares is added and the process is repeated until the critical point is surpassed. At this point the last set of squares is removed; the set is partitioned into two equal sets and only the first half is now added; the lattice is tested again for criticality, but now with 2^9 squares being added. This process continues with the repeated division[21] of the original number (2^{10}), until it goes down to 2^0. At this point we are assured that we are exactly at the critical point, i.e. one single square has caused the appearance of the incipient percolating cluster. Testing for criticality is done using a new version of the Cluster-Multiple-Labelling-Technique (CMLT). The details have been reported elsewhere[6]. We only need to apply CMLT as many times as the power of 2, i.e. here we apply it 10 times, something not very time consuming. Using this technique we employ lattices of 100x100 or 150x150 in size.

Our criterion for percolation here is that squares belonging to the critical cluster must appear on all four sides of the lattice and must touch in at least one point in both directions. This is because we want to ensure (using periodic

boundary conditions) the possibility of unlimited motion. A particle is placed at random on the largest cluster at time t=0. The direction of its motion is also chosen at random. If an attempted move leads to a point outside the critical cluster this move is not permitted. But the move "consumes" one time unit, i.e. we are in the so-called "blind ant"[17] model. At the lattice boundaries, for random walk purposes, we use periodic conditions, i.e. the particle is allowed to move from one end of the lattice to the other if it remains on the largest cluster. We keep track of its position at all times by monitoring its coordinates, which due to the boundary conditions may span a distance much larger than the lattice itself. This happens only if squares of the largest cluster touch the lattice boundaries. The critical cluster structure is now based on its form in the LxL region. Thus small clusters that coalesce with the largest cluster only under periodic boundary conditions are not assumed to be part of the largest cluster, the latter being the largest cluster of the LxL region, indefinitely repeated via periodic boundary conditions. We monitor R^2, the mean-square displacement as a function of time. We use two step lengths, one equal to the side of the component squares, and one equal to one-tenth this length.

III. RESULTS AND DISCUSSION

The p derived in our model is:

$$p_c = 1.127 \pm 0.003$$

where the uncertainty is obtained by averaging two sets of calculations containing 100 realizations each. One set uses lattice sizes of 100x100 and one set sizes 150x150. This p_c value is in good agreement with previously reported[9,10,13]

values of $p_c = 1.1 \pm 0.1$. Ref. 13 gives for a slightly different condition $p_c = 1.11 \pm 0.04$. It should also be remembered that the criterion used here for percolation is that the critical cluster must touch at all four sides of the square lattice and have at least one common point under periodic boundary conditions in both coordinates. We checked that somewhat different criteria result in slightly different p_c values, but again with small uncertainty bounds.

We now verify that the largest cluster we use is indeed characterized by a fractal exponent, by calculating its size at different scales of magnification. We do this by choosing from the original lattice several square sublattices of different size, and centered on the origin of the whole lattice. We then calculate the number N(L) of squares belonging to the largest cluster, that are present within each sublattice of length L. The results are given in Figure 1, where we plot N as a function of the sublattice side length, L. We see that in logarithmic scales the relationship is linear and obeys the form:

$$N \sim L^{\bar{d}}$$

Here $\bar{d}$ is the fractal exponent and it is given by the slope of this curve. Its value is $\bar{d} = 1.95 \pm 0.02$. We remark that the last few points in each curve deviate slightly from linearity. This is most probably due to boundary effects, especially since this deviation is always around the new boundaries when the lattice size increases. The value $\bar{d} = 1.95$ is about 2.5% higher than the usual $\bar{d} = 1.90$ for discrete lattices, also derived from $\bar{d} = d - \beta/\nu$, where d is the usual Euclidean dimensionality, in our case d=2, and β and ν are the static percolation exponents. However, this difference may also be due to the criterion used for defining the critical percolating cluster. The customary definition is to require that

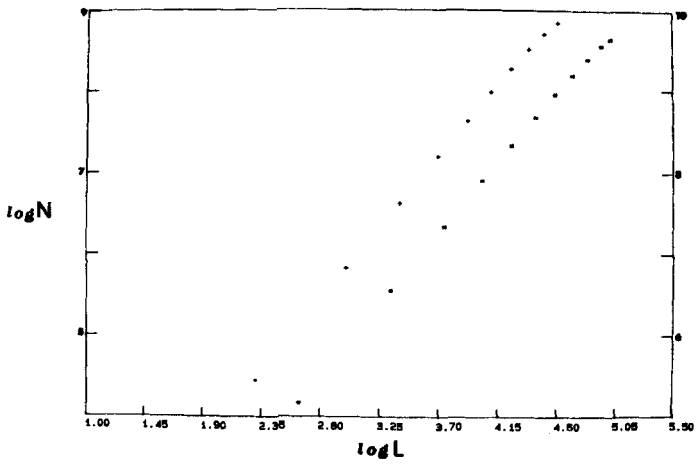

FIGURE 1. Plot of LogL (L=sublattice side length) vs. logN (N=number of squares belonging to the largest percolating cluster exactly at criticality). Left y-axis is for lattice size 100x100, whereas the right y-axis is for size 150x150. All averages are taken after 100 realizations. All logarithms are natural.

the largest cluster at p_c must touch either the up-down or the left-right sides of the lattice and not both as we require here (see previous section). The difference in the $\bar{d}$ value may well be due to this fact, since under our condition the structure is denser. This is also borne out in Fig. 1, in which, by shifting the y-axes to equality, the 150x150 curve lies slightly above the one for the 100x100 case.

The diffusion exponent, D, is derived by monitoring the mean-square displacement, R^2. Here the relationship is:

$$R^2 \sim t^{2/D}$$

where t is time. Again we notice that this should be a

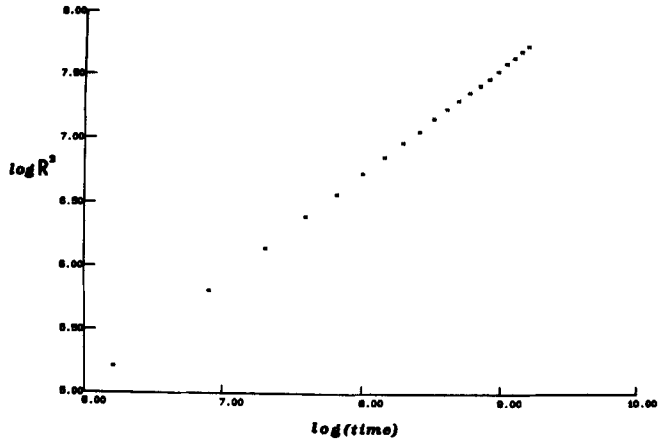

FIGURE 2. Plot of $\log R^2$ as a function of log(time) for step length of one (1). The average is taken after 5000 realizations of random walks performed on 100 different random lattices (i.e. 50 walks per each lattice).

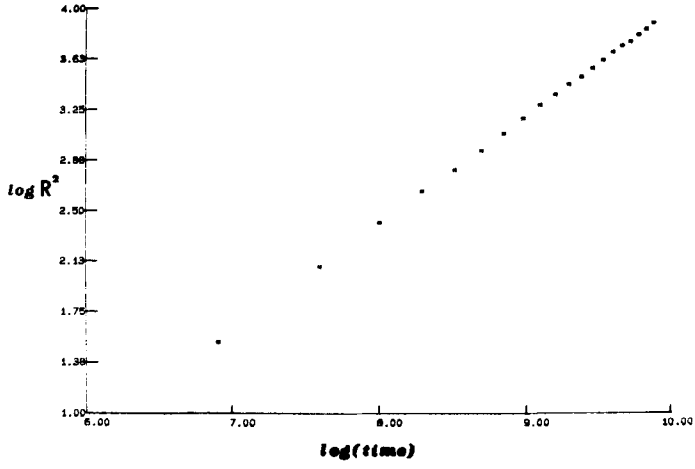

FIGURE 3. Plot similar to that in Fig. 2, but for step length of 0.1 units.

linear plot in logarithmic form. This is shown in Figures 2 and 3 for step lengths equal to 1 and 0.1, respectively. We see clearly that the exponential relationship holds, producing $D=2.42\pm0.05$ (step length of 1) and $D=2.55\pm0.05$ (step length of 0.1). The second result (for 0.1) is trustworthier, since small steps are less prone to occur crossing empty regions, and thus they probe the cluster more accurately. We notice that both values are somewhat lower than the D exponents reported in the discrete lattice case, which have been reported[6,18] around D=2.70, and also[19] D=2.80, for 2-dim lattices. It is worth noting that in a recent study[20] of the critical exponents in transport properties it was found that the elasticity and permeability exponents in the continuum model differ from those in the discrete model by 3/2 while no difference was observed in the conductivity exponents, for 2-dim lattices. In that model, however, continuity was brought in by employing a continuous distribution of bond strengths, unlike our spatial continuity.

In summary, we reported here a preliminary study of a model for dynamics in continuous percolation systems. We presented an efficient algorithm that generates critical percolation clusters exactly at criticality. We found that the fractal exponents of these clusters are in fair agreement with the discrete lattice case. We then monitored random particle diffusion via the mean-square displacement and we found that this phenomenon is governed by the same form of critical exponents as in the discrete lattice case. Our results show that here D is somewhat lower than its value for the discrete lattice, and furthermore, that different step lengths result in variations of the D value.

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