Journal of Statistcal Physics, Vol. 80, Nos. 5/6, 1995

Shape of the Clusters of a Percolative System in the Presence of Tunneling Bonds and a Finite Electric Field

Abhijit Kar Gupta[1] and Asok K. Sen[1]

Received February 14, 1995; final March 9, 1995

We consider a model correlated percolative system on a 2D square lattice with a finite electric field applied accross its two opposite sides. We study the shape of the clusters formed with the addition of a new kind of bond (we call them tunneling bonds) which respond only above a finite threshold voltage. As expected, the clusters do have an overall elongated shape in the direction of the applied field. Intuitively, one expects the elongation (with the aspect ratio >1) to increase indefinitely with the field. But, in a previous study, we found the model to belong to the same universality class in the limits of a zero and an infinite electric field. We explain this behavior by studying the change in these elongated shapes as a function of the applied voltage in finite size samples and find that actually the amount of elongation takes on a maximum value at a size (L)-dependent finite voltage $V_m(L)$ and that as $V \to \infty$ the overall deviation from isotropy in the field direction tends to zero (i.e., aspect ratio $\to 1$) again.

KEY WORDS: Ohmic bonds; tunneling bonds; correlated percolation, shape factor; random-resistor network; universality.

Percolation models[1] studied so far have been quite successful to explain the behavior of a variety of physical systems. We shall consider here a model correlated bond percolation problem on a 2D square lattice. This has already been introduced[2,3] to understand the essential features obtained from some recent studies of the nonlinearity associated with the response to electric field (see, e.g., ref. 2 and references therein) in some binary composites and seems to be applicable in similar situations to many other systems, e.g., amorphous semiconductors in high fields and biological systems such as lipid bilayers.

[1] Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Calcutta-700 064, India.

822/80/5-6-32

The model is as follows. We throw some conducting bonds (which are Ohmic and hence referred to as o-bonds from now on) randomly on a square lattice with a volume fraction p. The rest of the bonds with a fraction $(1-p)$ are insulating bonds. Let us call the horizontal direction the x direction and the vertical direction the y direction. Now we assume that with the application of appropriate electric fields (voltage) in the y direction, the electrons may tunnel through the gaps between two nearest neighbor (for simplicity) o-bonds. The bonds across these gaps are typically nonlinear (non-Ohmic). In this simple model we consider those bonds to be piecewise linear, i.e., they remain insulator up to some fixed threshold voltage (which is assumed, again for simplicity, to be the same for all such bonds) and then start conducting with some nonzero conductance which need not be equal to that of the o-bonds, but may be kept the same without changing the essential physics we are going to describe. We call such nonlinear bonds "tunneling bonds" ("t-bonds"). Once the conducting bonds are thrown, the positions for the t-bonds are fixed and they are correlated to the positions of the randomly thrown o-bonds. That is why one may view this model as a specific correlated bond percolation problem.

Clearly, in the absence of an electric field, none of the t-bonds would be conducting (i.e., be active) and the problem reduces to the usual geometrical percolation problem. Now as one switches on an external electric field (with a potential difference of V volts) across the two parallel electrodes on opposite sides of the system (in the y direction), some of the t-bonds may be able to overcome their threshold and start conducting. With increasing V, more and more t-bonds will join in this process. Finally, for $V \to \infty$ all the t-bonds would be conducting. Obviously, in the percolation picture, the system would now have a threshold at a much lower value of p (we call it p_{ct}) compared to the geometrical percolation threshold (p_c) in the absence of such "active" t-bonds (i.e., for $V=0$). But, more importantly, with the application of a finite voltage in the y direction, an additional number of current-carrying paths may be formed because of the active t-bonds which were previously absent. Let us consider a volume fraction p of the o-bonds, $p_{ct} < p < p_c$. The paths formed would be, as intuitively expected, *directed* from one electrode to the other. Since no electric field exists in the x direction, the spanning cluster would naturally be elongated towards the electrodes (i.e., in the y direction). Intuitively one expects this elongation to be more and more pronounced as the magnitude of V increases, and hence for large-length systems the conducting paths are expected to be quasi one dimensional as $|V| \to \infty$. This in turn should imply that the characteristic signature of the percolation (i.e., its universality class) for our model should change as V is turned on, and particularly as the applied field approaches infinity. But our previous studies[4]

indicate that in both of the limits of a vanishing electric field and of an infinite electric field, the system belongs to the same universality class.

In this short communication, our concern is to find out how such an interesting thing takes place. To do that, we consider a more general situation where only a fraction of the available t-bonds (out of all the possible tunneling positions) are active. This is the situation when the applied voltage V is finite. We always consider the system above p_{ct} ($\cong 0.181$ as estimated in ref. 4) so that the system may always have the possibility of conducting current with the addition of active t-bonds for some finite V. One may look at the problem in a different way. Let us note that each randomly thrown o-bond occupies two sites of the lattice. Once we identify these equivalent occupied sites, the problem reduces to an equivalent site-percolation problem and we check (for our computational purposes only) if there is any spanning cluster made of the occupied sites. From now on we refer to this cluster as the site-spanning cluster (SSC). It may be noted that in this equivalent site-percolation problem, we still cannot forget about the bonds, since we have to remember if the resistance between two nearest neighbor sites is infinite (insulating) or is finite (i.e., has an o- or an active t-bond). Thus the mere presence of an SSC does not imply that the system would percolate (again one sees the presence of correlation). The advantage in looking for an SSC lies in the fact that we need not spend time calculating the conductance when it is absent (it turns out that these are the configurations which spend most of the time iterating and yet not give any sensible results, for obvious reasons). Further, when an SSC exists, we may not be interested in all the other smaller clusters (disconnected from the SSC) for the calculation of the conductance because they would not contribute to the current-carrying network in our model system. Later, from the computer simulation also, we see that those isolated smaller clusters do not have active t-bonds which we would like to count. But for a finite voltage, there are smaller isolated clusters (in the original bond picture) within the SSC apart from a possible spanning cluster using only the o-bonds and the active t-bonds. The computer simulation finds that these smaller (nonspanning) clusters which are subsets of the SSC also possess active t-bonds. The possibility of having active t-bonds in these cases arises because for the purpose of facilitating the random-resistor network calculation we assigned the insulating bonds an extremely small conductance of 10^{-50}, and hence an extremely large resistance of 10^{+50}. The algorithm used here is of Hoshen–Kopelman type (see, e.g., ref. 1).

To have a quantitative estimate of the shape of the clusters, we may count the number of bonds parallel and perpendicular to the electrodes for all the clusters now formed. Each current-carrying path consists of vertical (y) and horizontal (x) bonds and naturally, the vertical bonds are larger

in number compared to the horizontal bonds. However, inside the SSC, the numbers of o-bonds in the x and the y directions are equal on average. So for our purpose it is just enough to count the active t-bonds at a particular V in all the clusters (within the SSC). The configurations which do not contain an SSC are assigned a conductance of zero without any further computation. In case an SSC exists for a certain configuration, we solve Kirchhoff's law at each node of the corresponding random-resistor network subject to a fixed V and use the standard Gauss–Seidel relaxation technique to identify the active t-bonds inside it. As described before, the computer simulation gives numerous active t-bonds (within the SSC, but not outside of it) which do not belong to the current-carrying network. We actually count all of them. Eventually (as we go on increasing the applied voltage) all the nearest neighbor t bonds become part of the current-carrying network. Let us suppose that $n_\perp$ is the number of the active t-bonds perpendicular to the electrodes and $n_{||}$ is the number of those in the parallel direction. We define a configuration-dependent shape factor $\chi = (n_\perp - n_{||})/(n_\perp + n_{||})$ and calculate χ at different V for various system sizes from $L = 10$ to 80 and take averages over 100–500 configurations each time. The plot of $\langle \chi \rangle$ against V is shown in Fig. 1 for different system sizes and for different values of p as indicated in the figure. For a fixed L the

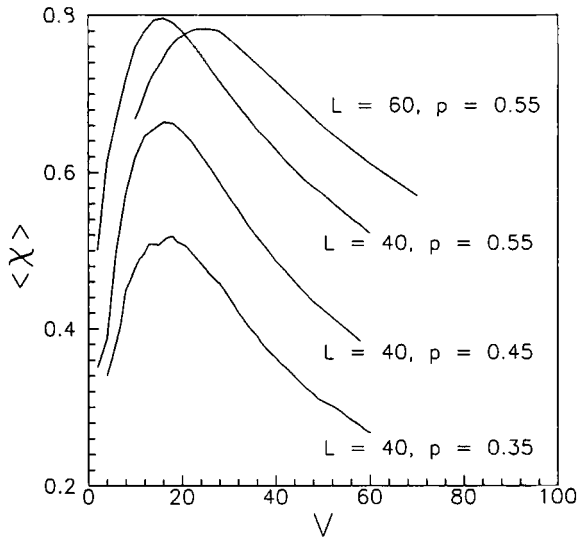

Fig. 1. Plot of the average "shape factor" $\langle \chi \rangle$ against applied voltage V. The curves are for different volume fractions p of the conducting bonds thrown and system sizes L as indicated in the figure.

peak in the curves appears at the same position (i.e., at the same V, which we call V_m) for any p. The shape factor $\langle \chi \rangle$ is always positive (i.e., $n_\perp > n_{||}$) which indicates that the effective spanning cluster actually has an elongated shape on average. The peak signifies that the clusters would be maximally elongated at that particular applied voltage V_m corresponding to that finite system size L. We observe that this peak position V_m increases linearly with the system size as may be expected intuitively. For example, we find that $V_m = 8$ V for $L = 20$, and that $V_m = 16$ V for $L = 40$.

As one increases V beyond V_m, more parallel than perpendicular t-bonds become active and finally for $V \to \infty$ all the t-bonds becomes active (in the sense that they can overcome their threshold). In that limit $\langle \chi \rangle \to 0$ as the t-bonds at any specified position (within the SSC) would be active, and hence $n_\perp = n_{||}$ on the assumption that the probability of parallel t-bonds is identical to that for perpendicular ones. Now one may ask at which fraction f defined as (no. of active t-bonds)/(no. of all possible t-bonds) in the SSC do the peaks in $\langle \chi \rangle$ appear. Again this fraction is configuration dependent. We call the peak in $\langle \chi \rangle$ as χ_m and the corresponding average fraction $\langle f \rangle$ as $\langle f_m \rangle$. In Fig. 2, we plot $\langle f_m \rangle$ against p for different system sizes as indicated in the figure. We find that the peak χ_m occurs around $\langle f_m \rangle = 0.50$, i.e., when 50% of the tunneling positions are filled up on average. This fraction $\langle f_m \rangle$ seems to be independent of system

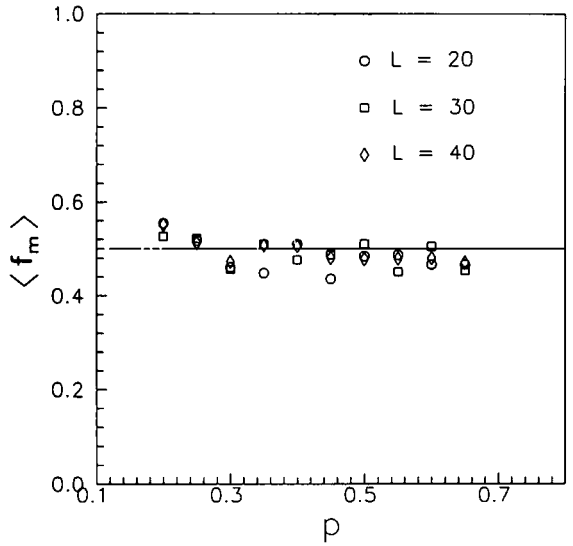

Fig. 2. Plot of $\langle f_m \rangle$ against p. Here f is the fraction of tunneling bonds which are above their threshold voltage (i.e., are active) out of all possible tunneling positions.

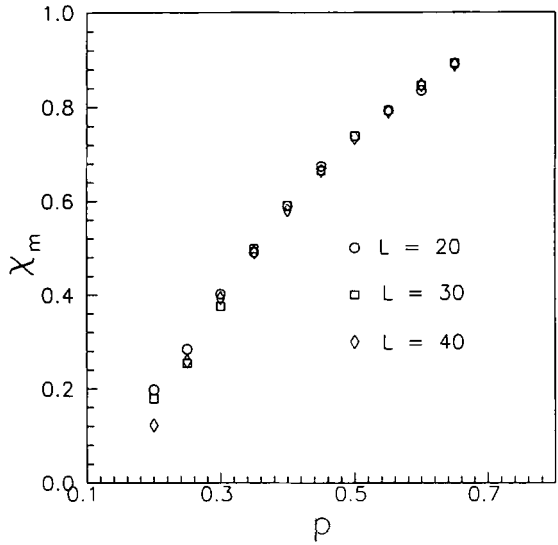

Fig. 3. Plot of maximum value of $\langle \chi \rangle$ (indicated in the figure as χ_m) against p. The curves for three different system sizes fall on each other.

size L but weakly dependent on p. Finally, we find that the maximum value of the shape factor on average is also independent of the size, but depends on the volume fraction p. We have show this in Fig. 3 by plotting χ_m against p for three different system sizes. The curves for different sizes seem to fall on each other for $p > 0.4$. Mismatch at lower p's seems to be due to stronger finite-size effects.

In conclusion, then, we find that the overall orientation of the clusters formed at any finite voltage for our model percolation system is always directed along the applied field, i.e., the clusters have aspect ratios greater than unity. A finite voltage here implies that not all the tunneling bonds (at the correlated positions) are active. We find that the elongation as defined above through the parameter $\langle \chi \rangle$ is maximum for finite-size systems at a finite voltage V_m, and that it tends to zero (i.e., the aspect ratios tend to unity) both for vanishing and infinite voltages. This is consistent with our universality class studies[4] in these two limits. The maximum elongated clusters along the applied field occur when on average approximately half of all the possible tunneling positions are active. The elongation in a finite field raises the interesting possibility that the system may not be in the same universality class as that for pure geometric percolation in the absence of any tunneling bonds. Work in this direction is in progress. In passing, we note that this problem has some similarity to the electric breakdown problem in the

sense that it is somewhat the reverse of what we are doing here. For details the reader is referred to Benguigui and Ron,[5] who identify the breakdown paths and also the other broken elements (not belonging to the breakdown paths) in a network of resistors and light-emitting diodes (LED) which can mimic an insulating element having a property similar to that of the t-bonds we consider. Several figures obtained by computer simulation given in ref. 5 are very instructive in this respect.

REFERENCES

1. D. Stauffer and A. Aharony, *Introduction to Percolation Theory* (Taylor and Francis, London, 1992).
2. A. K. Sen and A. Kar Gupta, in *Non-Linearity and Breakdown in Soft Condensed Matter*, K. K. Bardhan, B. K. Chakrabarti, and A. Hansen, eds. (Springers-Verlag, Berlin, 1994); A. K. Sen, *Phys. Rev. Lett.* **74**:1693 (1995).
3. Y. Gefen, W.-H. Shih, R. B. Laibowitz, and J. M. Viggiano, *Phys. Rev. Lett.* **57**:3097 (1986).
4. A. Kar Gupta and Asok K. Sen, *Physica A* **215**:1 (1995).
5. L. Benguigui and P. Ron, in *Non-Linearity and Breakdown in Soft Condensed Matter*, K. K. Bardhan, B. K. Chakrabarti, and A. Hansen, eds. (Springer-Verlag, Berlin, 1994).

Communicated by D. Stauffer