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# Characterization and quantification of the cluster hopping mechanism responsible for transport in two-component random networks

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**Abstract.** A cluster hopping mechanism for transport in two-component random networks below $p_c$ is proposed and shown to account for observed conductivity exponents. Key structures forming paths of least resistance are identified. A novel, computationally efficient method for determining exponents results.

## 1. Introduction

Consider a two-component random resistor network made of elements 'a' and 'b' with $\sigma_a \gg \sigma_b$. In what follows let $\sigma_b/\sigma_a = \alpha$ and $\sigma_a = 1$. When $\alpha = 0$, one has a standard percolation problem in which the network is conducting when the concentration $p$ of type-'a' elements exceeds a critical value, $p_c$. Below $p_c$ the network is insulating. One has, for the general case, $\sigma = \sigma(\Delta p, \alpha)$ where $\Delta p = p - p_c$. This problem has received much attention in the past. It is known that the parameter space near $p_c$ and for small $\alpha$ separates into three regions characterized by different asymptotic forms for the conductivity:

$$\begin{array}{lll} p > p_c & |\Delta p| > \alpha^{1/(s+t)} & \sigma = |\Delta p|^t \\ p \approx p_c & |\Delta p| < \alpha^{1/(s+t)} & \sigma = \alpha^u \\ p < p_c & |\Delta p| > \alpha^{1/(s+t)} & \sigma = \alpha|\Delta p|^{-s}. \end{array}$$

The critical behaviour of these random resistor networks was first discussed by Efros and Shklovskii (1976) and Straley (1976). They independently derived the forms for the asymptotic conductivities as well as a relationship between the exponents: $u = t/(s+t)$. For two-dimensional square bond lattices one expects $s = t$ and $u = \frac{1}{2}$ (Straley 1977). While various conjectures have been made, a relationship between these exponents and the geometric exponents of percolation theory has not yet been established.

This problem is isomorphic to that of diffusion in a two-component medium in which the diffusant has different mobilities on the two types of sites. The diffusion constant is equivalent to the conductivity by an Einstein relation. Such a system might be used to imitate transport in random media with intramolecular motion. The diffusing particle moves freely on empty sites (type 'a'). Occasionally an occupied site (type 'b') will become temporarily vacant due to intramolecular rotation. This allows steps to be taken on usually occupied sites. The transport is diffusive above and below $p_c$.

In terms of the diffusion problem one may understand the three regimes as arising from a competition between time scales. In general, $D = \langle r^2(\tau)\rangle/\tau$, where $\tau$ is the time scale over which the trajectory looks like a random walk. For conventional percolation problems, $\tau = \tau_p = \Delta p^{-1/x}$ with $1/x = 1/(t + 2\nu - \beta)$ in terms of the usual percolation exponents.

This is the time for a particle to travel a distance $\xi' = \Delta p^{-\nu+\beta/2}$. For times longer than $\tau_p$ the behaviour is diffusive when $p > p_c$. For $p < p_c$ and $t \gg \tau_p$ the average displacement approaches a constant value $\xi'$ which is the average size of the finite clusters. When $\alpha > 0$, diffusion is possible for $p < p_c$ because travel on type-'b' sites is permitted. Another time scale then enters into the problem. $\tau_\alpha$ is the time scale over which the trajectory looks like a random walk through transport that involves travel on some type-'b' sites.

Consider the case $p < p_c$ where type-'a' clusters are finite. In the language of the conductivity problem, one would expect the paths of least resistance to dominate the asymptotic behaviour. Such a path would involve travel on the finite type-'a' clusters and then a cluster hop involving travel on as few type-'b' sites as possible. Consider finite cluster surface sites that are only one 'b' site away form another finite cluster. These will be referred to as 'hotspots' in what follows. Let the time required to travel across a portion of a finite cluster from one hotspot to another be denoted by $\tau_{CH}$. It is proposed that $\tau_\alpha$ is equal to $(1/\alpha)\tau_{CH}$. $(1/\alpha)$ may be thought of as the number of attempted moves onto a type-'b' site before such a move is accepted. In this paper, $\tau_{CH}$ will be measured as a function of $|\Delta p|$. The results will then be used to calculate the transport coefficient $D = \langle r^2(\tau_\alpha)\rangle/\tau_\alpha = \alpha|\Delta p|^{-s}$. The values of s obtained will be compared with values obtained by other methods. Agreement supports the hypothesis that the relevant time scale for diffusion in the region where $p \langle p_c$ and $|\Delta p|^{s+t}\rangle\alpha$ is $\tau_\alpha = (1/\alpha)\tau_{CH}$.

## 2. Dimension of hotspots at $p_c$

Although not central to the results of this paper, I also present results for the dimension of the hotspots at $p_c$. The number of these sites on the incipient infinite cluster at $p_c$ was counted on square lattices of lengths 10 to 100. A plot of $\ln N_{HS}$ against $\ln L$ gave $d_{HS} = 1.75 \pm .02$. The total number of sites on the incipient infinte cluster was also measured as a function of $L$ for comparison. This gave a value of $1.86 \pm .03$ for the dimension of the incipient infinite cluster at $p_c$. Data was obtained using 200 realizations at each value of $L$. It appears that the hotspots scale as the surface. Measurements of the incipient infinite cluster surface dimension give $d_s = 1.751 \pm .002$ (Ziff 1986).

## 3. $\tau_{CH}$ Measurement

To measure $\tau_{CH}$ for $p < p_c$ an ant is put on a randomly chosen type-'a' site. A neighbouring site is chosen at random. If the site is type-'a', the move is accepted. When the ant hits a hotspot, the time is recorded and a new walk is started. If the initial spot was a hotspot, the time is recorded as zero. $\tau_{CH}$ was measured on two-dimensional square lattices of length $L = 100$, 200, and 400 for values of $|\Delta p|$ ranging from 0.02 to 0.12. Thirty realizations of the lattice were used at each $p$ value for $L = 100$ and $L = 200$. For $L = 400$ only 10 realizations were used. The time-consuming part of this investigation is the cluster identification. Consequently it is desirable to have many walks on a given realization while avoiding redundancy. Near $p_c = 0.59725$, $L^2/2$ walks per realization allows nearly each occupied site to be the starting point for a walk without oversampling. In all cases, $L^2/2$ walks were performed on each realization.

$\ln \tau_\alpha$ was plotted against $\ln|\Delta p|$ to give slopes of $-1.159 \pm 0.044$, $-1.262 \pm 0.033$ and $-1.266 \pm 0.030$ for the $L = 100$, 200, and 400 lattices respectively. The range of $|\Delta p|$ used here was 0.04 to 0.12. Figure 1 shows a plot of $\ln \tau_{CH}$ versus $\ln|\Delta p|$ for $L = 400$. The distance traveled in $\tau_{CH}$ was also measured. It was found that $l^2_{\tau_{CH}} \approx \tau_{CH}^{0.45}$.

In three dimensions a cubic lattice of length $L = 30$ was used to determine $\tau_{CH}$. $p_c$ was taken to be 0.3115. With 10 realizations and $L^2/3$ walks per realization, $\tau_{CH} \propto |\Delta p|^{-0.63\pm0.05}$.

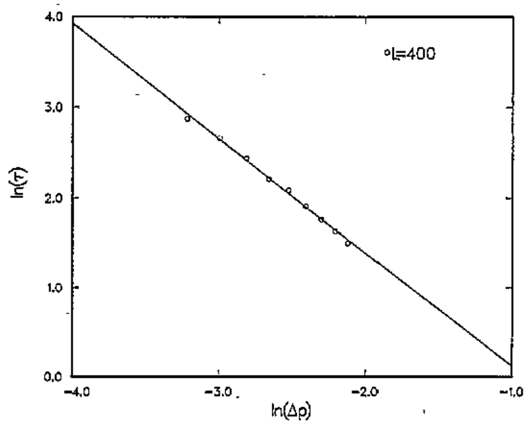


**Figure 1.** A plot of $\ln \tau_{CH}$ versus $\ln|\Delta p|$ for $L = 400$.

## 4. Finite-size scaling

$\tau_{CH}$ is finite above, below, and at $p_c$. Consequently one expects a deviation from the power-law behaviour $\tau_{CH} \propto \Delta p^{-q}$ near $p_c$. The deviation from linearity observed in the ln–ln plots of figure 1 is due to some combination of finite size effects and this crossover. To separate out these effects, a finite-size scaling analysis was performed for the $\tau_{CH}$ measurement in two dimensions. This requires measuring $\tau_{CH}$ at $p_c$ for various values of $L$. Assume the scaling form

$$\tau_{CH} = \Delta p^{-q} f(\xi/L) = \Delta p^{-q} f\left(\Delta p^{-\nu}/L\right)$$

where the asymptotic behaviour of $\tau_{CH}$ is given by $\tau_{CH} \propto \Delta p^{-q}$ and $\xi$ is the percolation correlation length. It is clear that $\tau_{CH} \propto L^{q/\nu}$ at $p_c$ where $\Delta p = 0$.

The method used for measuring $\tau_{CH}$ was identical to that used in section 3 except that percolating samples had to be identified and removed. At $p_c$ samples are generated that are both percolating and non-percolating. In order to examine the behaviour of $\tau_{CH}$ as one approaches $p_c$ from below one must weed out the percolating realizations from the set over which data is collected.

The value used for $p_c$ was 0.59275. $\tau_{CH}$ was measured for 22 $L$ values from $L = 6$ to $L = 100$. For $L = 6$ to $L = 22$, 10000 realizations were generated. For $L = 25$ to $L = 100$, 1000 realizations were generated. Error bars on the $\tau_{CH}$ averages were around $\pm0.05$ for $L = 6$ to $L = 22$ and somewhat larger for $L > 22$.

For $L > 20$ there is a noticeable deviation from linearity in the $\ln \tau_{CH}$ versus $\ln L$ plot (see figure 2). Using values between $L = 6$ and $L = 17$ one obtains a slope of $0.948\pm0.004$. This gives $\tau_{CH} \propto \Delta p^{-1.264\pm0.005}$.

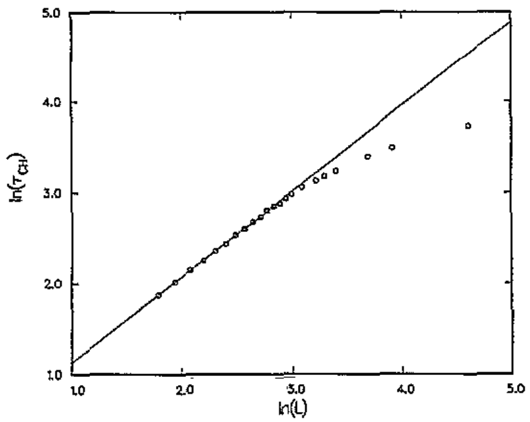


**Figure 2.** A plot of $\ln \tau_{CH}$ versus $\ln L$ at $p = p_c$.

## 5. Calculation of $D$

In this section, the results of sections 3 and 4 are used to calculate the transport coefficient for $\tau_\alpha > \tau_p$ and $p < p_c$. When $\tau_\alpha > \tau_p$, the distance traveled in the time $\tau_\alpha$ is limited to $\xi'$ the average size of finite clusters. This gives

$$D = \frac{\langle r^2(\tau_\alpha)\rangle}{\tau_\alpha} = \frac{\xi'^2}{\tau_\alpha}.$$

The initial intention was to obtain values of $\xi'$ appropriate to the lattice sizes used in section 3 for determining $\tau_{CH}$. It was found that $\tau_{CH}$ suffered much less from finite-size effects than did $\xi'$. Figure 3($a$) shows a plot of $\ln \tau_{CH}$ versus $\ln|\Delta p|$ for the three lattice sizes. One can see that the $L = 200$ and $L = 400$ data points agree fairly well for $|\Delta p| \geqslant 0.03$. Figure 3($b$) shows a similar plot for the $\xi'$ data. In light of this, $\xi' = \Delta p^{-\nu+\frac{1}{2}\beta}$, with $\nu - \frac{1}{2}\beta$ equal to the exact value $\frac{91}{72}$ that was used in the calculation of $D$. With $\tau_\alpha = (1/\alpha)|\Delta p|^{-1.266\pm0.033}$, one obtains $D = \alpha|\Delta p|^{-1.262\pm0.033}$. Using the $\tau_{CH}$ value from the finite-size scaling analysis in two dimensions one obtains $D = \alpha|\Delta p|^{-1.264\pm0.005}$.

This value for the exponent $s$ is in good agreement with series expansion results (Adler *et al* 1990) and random walk methods (Adler *et al* 1984, Bunde *et al* 1984). It falls outside of the very precise values obtained via finite-size scaling/transfer matrix methods by Normand and Herrmann (1988).

In three dimensions, using $\xi' = |\Delta p|^{-0.68}$ and $\tau_\alpha = (1/\alpha)|\Delta p|^{-0.63\pm0.05}$ from section 3 one has $D = \alpha|\Delta p|^{-0.73\pm0.05}$. This value for the exponent $s$ is likely to be on the high side due to the small lattice size used in determining $\tau_\alpha$. It is, however, in agreement with other determinations (Normand and Herrmann 1990).

## 6. Discussion

Based on the results for the transport coefficients, it appears that the proposed mechanism correctly describes the asymptotic transport observed below $p_c$. In addition, the role of the hotspots in forming the paths of least resistance is correctly identified. Also verified is

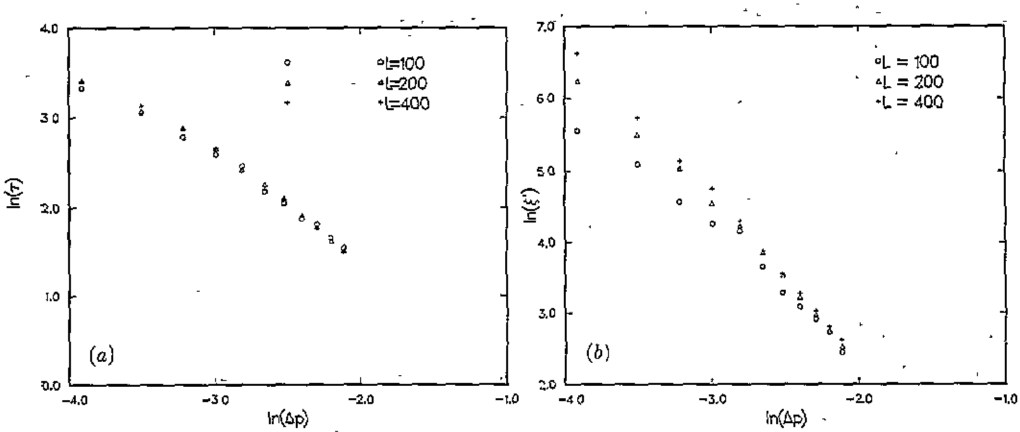


**Figure 3.** (*a*) A plot of $\ln \tau_{CH}$ versus $\ln|\Delta p|$ for various values of $L$; (*b*) a similar plot of $\ln \xi'$ versus $\ln|\Delta p|$.

the identification of the $\alpha$-dependent time scale relevant to this problem as $\tau_\alpha = (1/\alpha)\tau_{CH}$ where $\tau_{CH}$ is the time between visits to hotspots on the same cluster. According to the theory presented by Efros and Shklovskii (1976) and Straley (1976), the region in the parameter space $(|\Delta p|, \alpha)$ for which $D = \alpha|\Delta p|^{-s}$ is given by $|\Delta p| \gg \alpha^{1/(s+t)}$. This may be rewritten as $|\Delta p|^{-(t+2\nu-\beta)} \ll (1/\alpha)|\Delta p|^{s-2\nu+\beta}$. In terms of time scales, this is $\tau_p \ll \tau_\alpha$ where $(1/\alpha)|\Delta p|^{s-2\nu+\beta}$ is identified as $\tau_\alpha$, in agreement with the results presented here.

If $\tau_\alpha$ scales as $(1/\alpha)|\Delta p|^{-\nu+\frac{1}{2}\beta}$, then $D = \alpha|\Delta p|^{-\nu+\beta/2}$, which is the Alexander–Orbach conjecture (1982). The results obtained here do not rule this out.

A very modest amount of computer time was used to obtain these results. An unoptimized code was run on the Cray XMP. The running times per realization were approximately 3.2 min, 13.4 s, and 1.20 s for $L^2/2$ walks on the $L = 400$, $L = 200$ and $L = 100$ lattices, respectively. The time required for two-dimensional analysis is

$$N_R\left[aL^{3.95} + bL^2\right]$$

where $a = 1.145 \times 10^{-8}$, $b = 1.105 \times 10^{-5}$ and $N_R$ is the number of realizations of the $L \times L$ lattice. The number of walks per $L$ value for each realization is taken to be $L^2/2$.

This method, combined with finite-size scaling, provides a very computationally efficient way of determining the conductivity exponent $s$. Data for a finite-size scaling analysis, obtained by Lobb and Frank (1984), was reported to require under two hours on an IBM 3081. A finite-size scaling determination of $s$ by the method presented here, using the same values of $L$ with comparable error, would take about 600s on a Cray XMP. A finite-size scaling study comparable in extent to that presented by Herrmann *et al* (1984) would require $\approx 70$ s.

The theory of Efros, Shklovskii and Straley predicts that $D = \alpha|\Delta p|^{-s}$ will be valid for $|\Delta p|^{s+t} \gg \alpha$. It should be possible to satisfy this criterion for any small $\Delta p$ by suitable choice of $\alpha$. Two possibilities may explain the deviation from linearity observed in the $\ln \tau_{CH}$ plots. One possibility is that $r(\tau_\alpha)$ also changes its dependence on $\Delta p$ and L in this region in such a way as to preserve the form of $D$. Another is that one is already in the crossover region where the transport phenomena change. Future plans include an investigation of the distance traveled before exit from a cluster as a function of $\Delta p$ and $L$

investigation of the distance traveled before exit from a cluster as a function of $\Delta p$ and $L$ for some fixed, small $\alpha$. Also of interest might be a thorough investigation of the hotspot dimensionality as a function of $\Delta p$ for $p < p_c$. In addition, I believe that a method similar to that employed here for the determination of s may be used to determine the conductivity exponent at $p = p_c$ where $D = \alpha^u$.

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