Numerical simulation of continuous percolation conductivity*

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The electrical conductivity at a continuum percolation transition is derived by evaluating the limit of a sequence of results obtained for conductance networks with increasing range of correlation. The conductivity obeys the power law $\sigma(c) \propto (C - C^*)^{\gamma}$, with $C^* = 0.145 \pm 0.05$ and $\gamma = 1.4$.

In our previous work[1] (I), the simulation of electrical conductivity in a random inhomogeneous medium was carried out by incorporating correlation between values of conductances initially randomly assigned to adjacent bonds of a simple-cubic network. This was done by employing a procedure which can be iterated progressively, and which results in the formation of regions of constant conductivity extending over several lattice distances. In the case of a noncorrelated network, each bond is assigned a random number $0 < r^{(1)} < 1$, so that the distribution function $P^{(1)}(r)$ of the set $\{r^{(1)}\}$ is given by

$$P^{(1)}(r) = \begin{cases} 1, & 0 < r^{(1)} < 1 \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

In order to obtain a noncorrelated conductance distribution in which a fraction C and $1 - C$ of the bonds are assigned the values $g = 1$ and $g = x$, respectively, all bonds with $r^{(1)} > r_0^{(1)} = 1 - C$ are assigned the value $g = 1$ while the others are characterized by $g = x$. Let us specify each vertex by the triplet of zeroes, positive, or negative integers $\vec{l}$ and each bond between vertices by the vector pairs $\vec{l} + \vec{i}, \vec{l}$, where $\vec{i}$ is drawn from the set of nearest-neighbor separations $(\pm 1, 0, 0)$, $(0, \pm 1, 0)$, $(0, 0, \pm 1)$. The first step of the six-band correlation process [Fig. 1(a)] consists of assigning an r value to each vertex, $r_{\vec{l}}^{(2)}$, obtained by averaging the $r^{(1)}$ values of all six bonds sharing it:

$$r_{\vec{l}}^{(2)} = \frac{1}{6} \sum_{\vec{i}} r_{\vec{l}+\vec{i},\vec{l}}^{(1)} . \tag{2}$$

The second step consists of assigning r values to the bonds according to the prescription

$$\begin{aligned} r_{\vec{l}+\vec{i},\vec{l}}^{(2)} &= r_{\vec{l}}^{(2)}, \quad \operatorname{sgn} i = 1 \\ r_{\vec{l}+\vec{i},\vec{l}}^{(2)} &= r_{\vec{l}+\vec{i}}^{(2)}, \quad \operatorname{sgn} i = -1 \end{aligned} \tag{2a}$$

where i is the nonvanishing component of $\vec{i}$. Thus in Fig. 1(a), we have

$$r_1^{(2)} = r_2^{(2)} = r_3^{(2)} \neq r_4^{(2)} \neq r_5^{(2)} \neq r_6^{(2)} .$$

The distribution function $P^{(2)}(r^{(2)})$ of the new set $\{r^{(2)}\}$, peaks around $C = 0.5$. The above procedure may be iterated to obtain the set $\{r^{(n)}\}$. The distribution function becomes more narrowly peaked around $C = 0.5$ as n increases.

In order to obtain a sample in which a fraction C of the bonds have the value $g = 1$, we have to assign this value to bonds for which $r^{(n)} > r_0^{(n)}(C)$. The parameter $r_0^{(n)}(C)$ is determined by means of a closed loop procedure so that the following relation is obeyed:

$$\frac{1}{N_b} \sum_{i=1}^{N_b} \Theta^{(n)}(r_i) = C , \tag{3a}$$

where

$$\Theta^{(n)}(r_i) = \begin{cases} 1, & r_i > r_0^{(n)}(C) \\ 0, & r_i < r_0^{(n)}(C) \end{cases} \tag{3b}$$

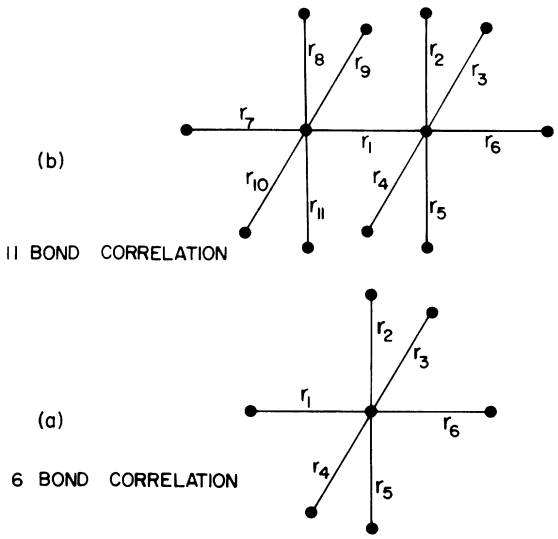


FIG. 1. Schematic depiction of the correlation procedure: (a) six-bond correlation, (b) eleven-bond correlation.

and N_b is the total number of bonds in the lattice.

Let us denote the numerical results for the conductivity on the noncorrelated lattice by $f_1(x, C) = \sigma_1(x, C)/\sigma(C=1)$. $f_1(x, C)$ is thus the first term in a sequence of functions $f_n(x, C)$ which represent the conductivity of the progressively correlated networks. In our previous work[1] we have concentrated on deriving the values of $f_2(x, C)$, the nearest-neighbor correlation case, and $f_3(x, C)$, the conductivity of the second-order correlated network.

In this note we proceed beyond second-order correlation, and study higher correlated networks up to $n=5$. From our results we can extrapolate the sequence $f_n(x, C)$ to $n \to \infty$ and thus achieve a close approach to the simulation of the conductivity of a continuous random system. In particular, in the case $x \ll 1$, we obtain information on the behavior of electrical conductivity near a continuous percolation transition.

Information on higher terms of the sequence $f_n(x, C)$ in the limit $x \to 0$ in the concentration range $0 < C < 0.3$ is important for the determination of C^*, the continuous percolation threshold. To achieve a better convergence of the sequence of successive correlations in this limit we have employed in this case an enhanced correlation procedure. The set of random numbers $\{r^{(n)}\}$ is now obtained from the set $\{r^{(n-1)}\}$ by means of the following transformation:

$$r_1^{(n)} = \frac{1}{11} \sum_{j=1}^{11} r_j^{(n-1)} \quad . \tag{4}$$

The ten bonds $r_2, \ldots, r_{11}$ are all the bonds which share a common vertex with r_1 as demonstrated in Fig. 1(b). In the covering lattice[2] of our cubic lattice, which is the lattice formed by all the midpoints of the bonds in the original lattice, the ten corresponding points are the nearest neighbors of the point which corresponds to r_1. In contrast to the six-bond correlation process, each bond gets a different value of $r^{(2)}_{\vec{l}+\vec{l},\vec{l}}$ (and $r^{(2)}_{\vec{l}+\vec{l},\vec{l}}$, generally) following the 11-bond correlation procedure. This difference between the two schemes is immaterial because similar configurations of metallic and nonmetallic regions are generated by both after sufficient iteration.

For the study of $f_n(x, C)$ down to $C=0$ we had to increase the lattice size to $30\times30\times30$ in order to avoid the large fluctuations which characterize the results calculated on different samples of smaller size in this region. We managed to achieve this increase by densely packing several numbers into one word of the CDC 6600 memory, which is conventionally reserved for one number. A careful optimization of the overrelaxation parameter Ω

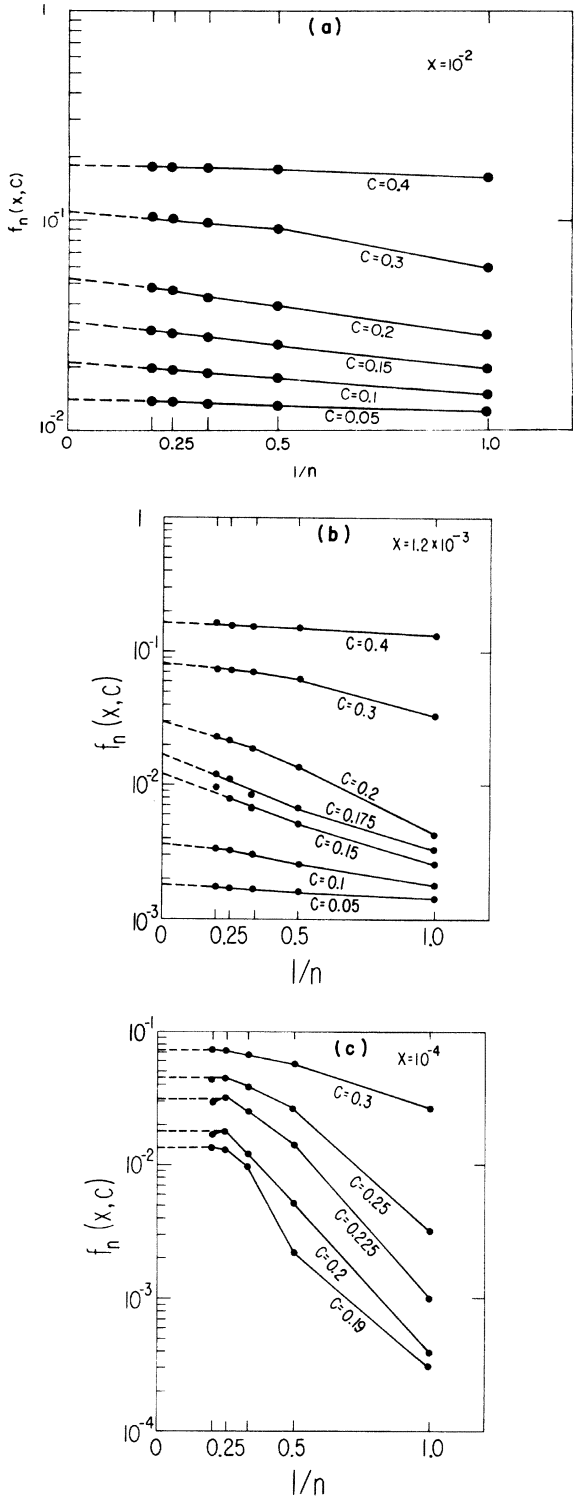


FIG. 2. Conductivity of nth-order correlated networks plotted against $1/n$: (a) $x = 10^{-2}$, lattice sizes $15\times15\times15$ and $18\times18\times18$, (b) $x = 1.2\times10^{-3}$, lattice sizes $15\times15\times15$ and $18\times18\times18$, (c) $x = 10^{-4}$, lattice size $30\times30\times30$.

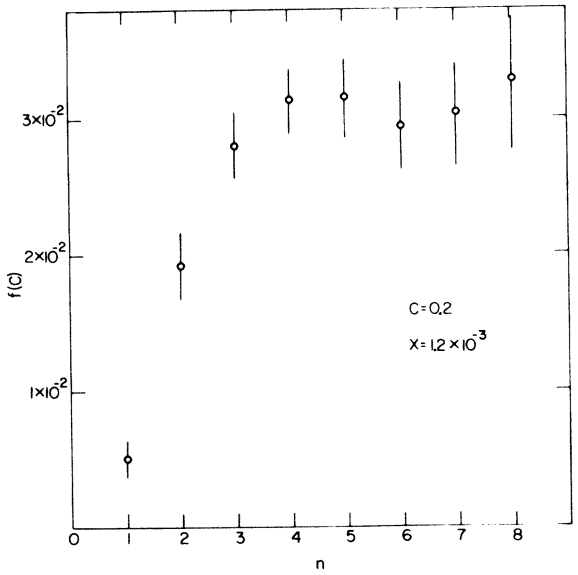


FIG. 3. Effect of high-order correlations up to $n = 8$ on the conductivity. Lattice size $30\times30\times30$.

(defined in I) was needed to reach a reasonable convergence rate.

In Fig. 2 the sequence of $f_n(x, C)$ for $n = 1-5$ is plotted vs $1/n$ for several values of x. Each point in Figs. 2(a) and 2(b) for $x = 10^{-2}$ and $x = 1.2\times10^{-3}$ represents the average of numerical results for 12–24 correlated networks derived from different initial random sets $\{r^{(1)}\}$, while each point in Fig. 2(c) for $x = 10^{-4}$ corresponds to an average of six

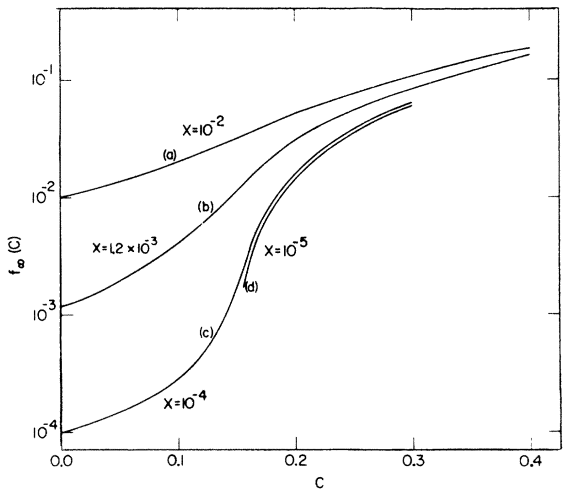
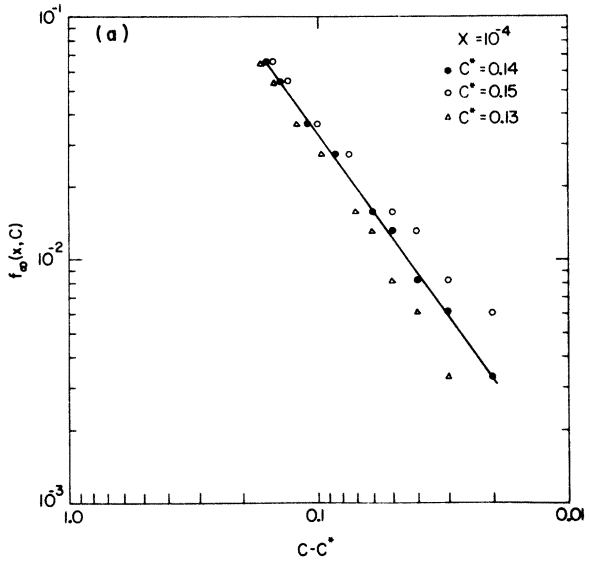


FIG. 4. Extrapolated value $f_\infty(x, C)$ of the sequence $f_n(x, C)$ for (a) $x = 10^{-2}$, lattice sizes $15\times15\times15$ and $18\times18\times18$, (b) $x = 1.2\times10^{-3}$, lattice sizes $15\times15\times15$ and $18\times18\times18$, (c) $x = 10^{-4}$, lattice size $30\times30\times30$, (d) $x = 10^{-5}$, lattice size $30\times30\times30$.



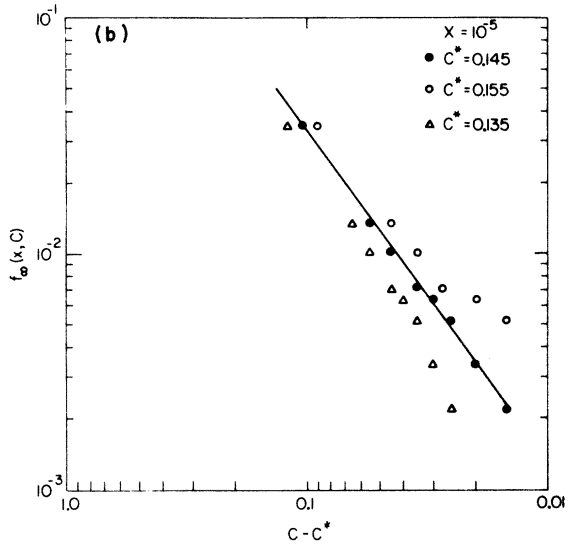


FIG. 5. Log-log plot of $f_\infty(x, C)$ vs $C-C^*$: (a) $x = 10^{-4}$, (b) $x = 10^{-5}$.

numerical results for different random samples. The cubic network studied were of sizes $15\times15\times15$, $18\times18\times18$, and $30\times30\times30$. We deduce $f_\infty(x, C)$ by extrapolating each sequence of $f_n(x, C)$ vs $1/n$ at fixed C to $1/n \to 0$. For $0.4 < C < 1$ $f_n(x, C)$ is practically independent of n in agreement with our previous results in I. It is interesting to note that the extrapolated values of $f_n(x, C)$ as $1/n \to 0$ are not significantly different from the values of f_4 and f_5. We get the impression that the sequence flattens out for $n = 4$, and that $f_n(x, C)$ does not increase any further as $1/n \to 0$, but fluctuates around an average value. This property of $f_n(x, C)$ is manifested by the sequence of values in Fig. 3

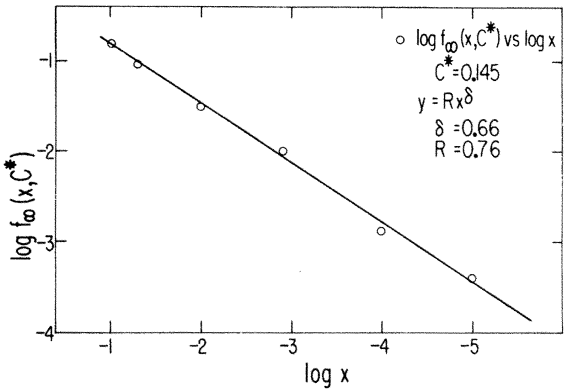


FIG. 6. Log $f_\infty(x, C^*)$ vs log x.

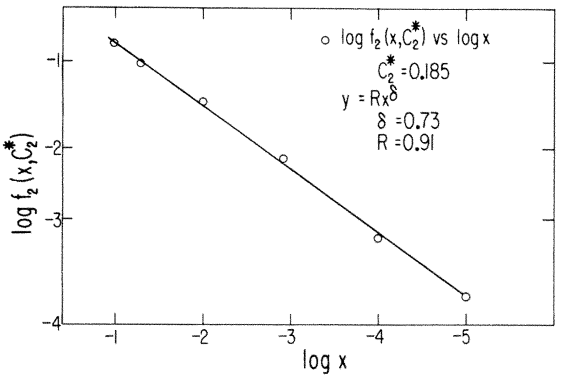


FIG. 7. Log $f_2(x, C_2^*)$ vs log x.

which extends up to $n=8$.

We have calculated $f_4(x, C)$ and $f_5(x, C)$ for $x = 10^{-4}$ and for $x = 10^{-5}$ in the range $0.16 < C < 0.3$. We consider the average of these two functions as a good approximation to the limit $f_\infty(x, C)$.

Figure 4 presents $f_\infty(x, C)$ vs C obtained from the results of the extrapolation procedure of Fig. 2, together with $f_\infty(x, C)$ derived on the $N=30$ lattice for $x=10^{-4}$ and $x=10^{-5}$. Average values of $f_4(x, C)$ and $f_5(x, C)$ determined on several $30\times30\times30$ lattices are plotted on a log-log plot vs $C - C^*$, for $x=10^{-4}$ [Fig. 5(a)] and $x=10^{-5}$ [Fig. 5(b)].

We find that for power law $f_\infty(C) = A_\infty(C - C_\infty^*)^{\gamma_\infty}$ holds for the two x values over the concentration range $0.16 < C < 0.3$ with the following values of A_∞, C_∞^*, and γ_∞:

$$\begin{aligned} &x=10^{-4},\\ &C_\infty^* = 0.140 \pm 0.005,\\ &A_\infty = 1.05 \pm 0.05,\\ &\gamma_\infty = 1.4 \pm 0.05;\\ &x=10^{-5},\\ &C_\infty^* = 0.145 \pm 0.005,\\ &A_\infty = 1.0 \pm 0.05,\\ &\gamma_\infty = 1.4 \pm 0.05. \end{aligned} \tag{5}$$

The final values of C_∞, A_∞, and γ_∞ and their error bounds were estimated as follows. A log-log plot of $f_\infty(x, C)$ vs $C - C^*$ was made for several values of C^*. The value of C^* yielding the best fit to a straight line was taken as C_∞^*. The values of A_∞ and γ_∞ were then derived from this line. Within the range $C^* = 0.145 \pm 0.005$ a straight line can still be fitted for $x=10^{-5}$ (see $C^*=0.135$ and $C^*=0.155$ in Fig. 6). The error bounds on A_∞ and γ_∞ were estimated from the straight lines corresponding to $C^* = 0.145 \pm 0.005$.

We take C_∞^* for $x=10^{-5}$ as the best currently available figure for C^*, the continuous percolation threshold. We note that the value thus obtained for C^*, 0.145 ± 0.005, is lower than any percolation threshold known[2] for a lattice.

Straley[3] has predicted a power-law dependence of $f(x, C^*)$ upon x. From our results we find that the following power law holds in the range $10^{-5} \leq x \leq 10^{-1}$ for continuous percolation, Fig. 6:

$$f_\infty(x, C^*) = Rx^\delta, \tag{6}$$

with $C^* = 0.145$, $\delta = 0.66$, and $R = 0.76$.

We also find for $n=2$ (nearest-neighbor correlation), Fig. 7,

$$f_2(x, C_2^*) = Rx^\delta, \tag{7}$$

with $C_2^* = 0.185$, $\delta = 0.73$, and $R = 0.91$.

We are grateful to S. Kirkpatrick for calling Straley's work to our attention and for suggesting the examination of the critical index behavior of $f(x, C^*)$.

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