Computer simulations of conductance noise in a dynamical percolation resistor network

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(Received 11 March 1994; revised manuscript received 25 July 1994)

Computer simulations of a dynamical bond percolation model in the form of a random resistor network are described. The conductance of a two-dimensional random resistor network is calculated using the transfer matrix approach when the network is at the percolation threshold. Keeping the total number of broken bonds fixed, a fraction of broken bonds are allowed to exchange places with adjacent unbroken bonds, and the conductance of the network is recalculated. This procedure is repeated a great many ($\sim 10^3$) times, and the Fourier transform of the resulting time trace of the conductance yields the spectral density of the dynamical percolation network. The dynamical percolation noise has a Lorentzian power spectra with a characteristic lifetime that represents the regeneration rate of the lattice.

PACS number(s): 64.60.Ak, 61.43.Bn, 73.50.Td

Percolation networks have been successfully employed to model the dynamics and electronic properties of disordered systems [1–5]. A prototypical percolation network is a series of bonds (resistors) on a lattice which are either randomly broken (infinite resistance) or filled (finite resistance). The percolation threshold corresponds to the minimum fraction of filled bonds which form a continuous path across an infinite network. Noise processes and in particular $1/f$ noise in percolation networks have been recently studied, both theoretically [6–9] and experimentally [10,11], in order to improve our understanding of the mechanisms responsible for conductance fluctuations in disordered solids. The time dependence of the conductance in nearly all of these studies arises either from random walks along the backbone of the percolation filament (which has a fractal geometry) [12,13] or from the intrinsic noise mechanisms of the material which comprises the percolation network. In the latter systems the magnitude and the finite size scaling of the noise power is studied as the percolation threshold is approached [6,7,10,11].

An alternative source of conductance fluctuations, termed dynamical percolation [14,15], allows broken bonds and unbroken bonds in a random resistor network to exchange places as a function of time, keeping the total number of broken bonds constant. Such models describe the influence of atomic or electronic hopping on the conductance of a disordered lattice, and are applicable to a variety of systems including ionic conduction in polymeric solid electrolytes, hydrogen motion in amorphous silicon, and vortex motion in high temperature superconductors. In addition, growth patterns of solidification fronts and domain walls have been successfully modeled by finding the optimal path through a percolation network [16,17], however, the effect of subsequent bonding rearrangements on the interface profile would be described by a dynamical percolation process. Despite the importance of hopping models for studying diffusion and electronic conduction in such systems, dynamical percolation networks have received less attention than static percolation problems.

In this paper, we describe computer simulations of the conductance fluctuations of a time dependent random resistor network. The conductance of a two-dimensional rectangular lattice is calculated for which half of the bonds are broken, corresponding to the percolation threshold. Dynamics are introduced into this system by allowing a small fraction of the conducting bonds to diffuse through the lattice, altering the conduction paths while keeping the total number of broken bonds conserved. The conductivity of the network is then recalculated, and the procedure is repeated a large number ($\sim 10^3$) of times, yielding a time trace of the conductance of the percolation network. The noise power spectra of the dynamical percolation network is then obtained from Fourier transforms of these conductance fluctuations.

Previous studies of dynamical percolation have involved analytical calculations of diffusion on a lattice at the percolation threshold where either the transition rates for hopping between nearest neighbor sites are allowed to randomly change with time [14], or the entire lattice is renewed at various intervals with random reassignment of hopping probabilities after each renewal [15]. In contrast, the simulations described in this paper model the effect of a structural rearrangement due to the diffusion of broken bonds, which subsequently modifies the connectivity and electronic properties of the conducting filaments in the host medium. These simulations were motivated by our interest in understanding conductance fluctuations in hydrogenated amorphous silicon (*a*-Si:H) [18] though the results are relevant to other experimental systems ranging from high T_c superconductors [19] to sound propagation in granular media [20]. In the case of hydrogen diffusion in *a*-Si:H, where the motion of bonded hydrogen enables defect creation and removal which in turn changes the electronic conductivity of the film [21], the flipping of broken and unbroken bonds represents the hopping of hydrogen atoms from one bonding configuration to another.

The network studied here consists of four million bonds (resistors) in a two-dimensional rectangular lattice 10^5 bonds long and 20 bonds wide. Finite size effects were checked by using lattices of different size. Infinitely

conducting strips are placed across the top and bottom edges of the lattice. If a hypothetical voltage drop is applied across these electrodes then the conductance may be calculated using the transfer matrix method [16]. The resistance values of the bonds in the network have a Gaussian distribution with a mean resistance value of unity and a standard deviation corresponding to 0.1 in arbitrary units.

A small section (~ 70 bonds long) of the resistor network is shown in Fig. 1, those resistors which reside on filaments which extend from the top of the grid to the bottom, and hence contribute to the conductance of the network are indicated by darkened bonds. While for an infinitely large network at the percolation threshold there will be only one conducting filament which spans the entire lattice [2], in a finite network there are many filaments which extend across the lattice at the percolation threshold. By imaging random sections of the lattice, we estimate that a two-dimensional $L \times H$ grid 10^5 bonds long and 20 bonds high contains approximately 2×10^3 filaments which are continuous across the top and bottom electrodes. An alternative method for calculating the filament number N uses an expression for the correlation length calculated by Derrida and De Seze [22]. In this case, the filament width may be estimated from the correlation length, $\xi \sim 4H/\pi$. Since the filaments are separated by nonconducting regions of approximately the same width there exists approximately 1 conduction path in a region 2ξ wide on the lattice. This results in approximately, $N \sim L/(2\xi)$, or 1963 filaments, in good agreement with our estimates based upon imaging random sections of the network.

An inherent feature of the transfer matrix method is the long and narrow lattices which allow a large number of filaments to conduct in parallel. The width and length of the random resistor lattice was chosen to eliminate boundary effects and yields convergence of the conductivity toward its limit value to within 0.3%. We believe that this model provides a reasonable approximation to a network of inhomogeneous current paths proposed to be responsible for the conductance fluctuations in a-Si:H [18]. The cross-sectional area of these current microchannels is estimated to be comparable to the a-Si:H film thickness, justifying a two dimensional simulation. The natural geometrical similarities between the lattice used in a two-dimensional transfer matrix method and the proposed current filament model in a-Si:H motivated our use of this approach over other traditional techniques that employ relaxation methods or systematic node elimination. In addition, the transfer matrix method is a computationally faster technique for investigating the quantities of interest in this dynamical percolation study. Using these lattice sizes a typical time trace of over 1000 time steps requires 10 h of CPU time on a Cray X-MP.

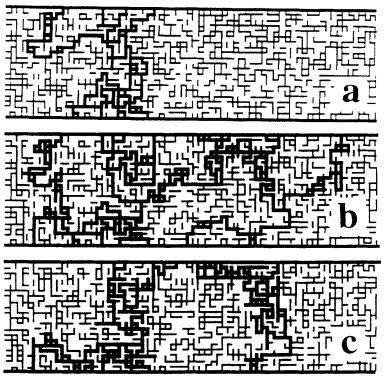

FIG. 1. Sketch of a small section of the two-dimensional random resistor network used in the computer simulations. The entire lattice is 10^5 bonds (resistors) long and 20 bonds wide; the conductance of the network is calculated across the lattice's width using the transfer matrix technique. Half of the resistors are removed, corresponding to the percolation threshold; those bonds which span the grid's width and contribute to the conductance are darkened. The initial configuration is shown in (a). After allowing at random 4% of the broken bonds to exchange places with adjacent unbroken bonds, a lattice is generated. (b) and (c) show the resulting changes in the network after repeating the bond exchange process 6 and 11 times, respectively.

The connectivity of the filaments and hence the conductance of the network varies when bonds are allowed to exchange places, or flip. The flipping rate, defined as the fractional number of bonds switched per time step, in Fig. 1 was 4×10^{-2}, that is, in a single time step one out of every 25 resistors is permitted to flip from its original bonding site into a neighboring unoccupied lattice site. Figure 1(a) shows the initial configuration of this small section of the network, the resulting configurations after 6 and 11 time steps are shown in Figs. 1(b) and 1(c), respectively. After six time steps the single filament in Fig. 1(a) has become ~ 60 bonds wide with a high degree of redundancy along with a large number of critical bonds, the breaking of which causes a large change on the conductance of the filament. After another five time steps the single large filament has evolved into two fairly direct filaments. The variation in filament number and structure with bond exchange gives rise to the conductance fluctuations described below.

The bond switching procedure is repeated and the conductance of the network is recalculated after each time step; the resulting time trace of the conductivity fluctuations is shown in Fig. 2 for a bond flipping rate R_f of 4×10^{-2}. The R_f in Fig. 2 corresponds to an average of $\sim 64\,000$ bonds exchanging places per time step; the average magnitude of the conductance fluctuations is $\Delta G/G \sim 10^{-2}$. The Fourier transform of the conductivity time trace in Fig. 2 yields a power spectrum which is well described by a Lorentzian frequency dependence, as shown in Fig. 3. The solid line is a fit to the spectral density by the expression $S(f) = C\tau/[1+(2\pi f\tau)^2]$, where C, a measure of the magnitude of the fluctuations, is 8.9×10^{-4} and the lifetime, τ, is 3.01. No single power law frequency dependence yields a better fit to the data than the Lorentzian expression. A Lorentzian frequency dependence is found to describe the conductance fluctuations in our simulations for a wide range of flipping rates and for lattices for which the length (and consequently the number of conducting filaments) is varied. For the flipping rate of $R_f = 4 \times 10^{-2}$ in Fig. 3, every filament in

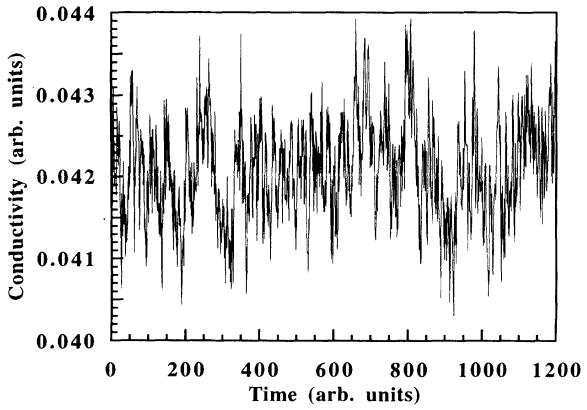

FIG. 2. Time trace of the conductance of the two-dimensional random resistor network described in the text. In each single time step the bond flipping rate was 4%.

the entire resistor network is varied several times in a single time step. The resulting fluctuations were expected to either have a frequency independent spectral density (white noise) indicating uncorrelated fluctuations, or to display $1/f$ noise. The latter would result from the superposition of an ensemble of Lorentzian power spectra, each individual Lorentzian arising from the switching of a single current filament. Since the variation of spatially separated filaments is independent, a broad distribution of lifetimes, leading to $1/f$ noise, would not have been surprising. The fact that the data is described by a single Lorentzian, and not a $1/f$ spectral density, indicates that the distribution of lifetimes for the entire network is fairly narrow.

The Lorentzian spectral density corner frequency (which is $1/\tau$) separates the white noise at low frequencies from the f^{-2} frequency dependence at higher frequencies. By calculating conductance time traces and their corresponding power spectra at other bond flipping rates, the variation of the Lorentzian spectral density lifetime τ with R_f is obtained. Changing the bond flipping rate can be thought of as increasing an electronic or atomic hopping rate with some external parameter, such as temperature. Since the bond flipping rate is the only time scale introduced into the simulations the expectation is that $\tau=1/R_f$, however, this is in conflict with the data of Fig. 3, where a τ of 3 is observed rather than a τ of 25 for a $R_f=0.04$. The conductance time traces in Figs. 2 and 3 were repeated several times, and the lifetimes observed were always $\tau\sim 3$. A log-log plot of τ against R_f displays a power law relationship $\tau=\kappa/R_f$, where $\kappa\sim 0.10$ for bond flipping rates of $5\times 10^{-3} \leq R_f \leq 10^{-1}$. The lifetime does indeed vary as R_f^{-1}, however, the prefactor κ is much smaller than expected. In order to smooth the data in Fig. 3 the power spectra of three independent conductance time traces for $R_f=0.04$ are octave binned, as shown in Fig. 4. The heavy solid line in Fig. 4 represents the octave integral of a Lorentzian spectral density with a lifetime $\tau=3$, which is an arctangent function. The error bars reflect the variation in noise power magnitudes from one simulation to another and do not reflect the uncertainty in the evaluation of the noise power per octave. The corresponding noise power per octave for $1/f$ noise would be a horizontal line, while white noise would exhibit a noise power per octave which increased at higher frequencies, both of which are excluded by the data in Fig. 4.

One possible explanation for the constant of proportionality κ in terms of a measure of the conducting portion of the lattice is as follows. Only those bonds on the conducting filaments will contribute to the conductance fluctuations and play a role in the power spectrum. The time for which the lattice fluctuations have become uncorrelated (the power spectrum is then frequency independent) is given by τ, it is reasonable that τ also measures the time in which most of the critical conducting bonds have flipped. In this sense, $\tau R_f=\kappa$ estimates the ratio of critical to the total number of bonds. Hence, $\kappa\neq 1$ is an indication that not all the bonds on the lattice must be flipped in order to yield an uncorrelated power

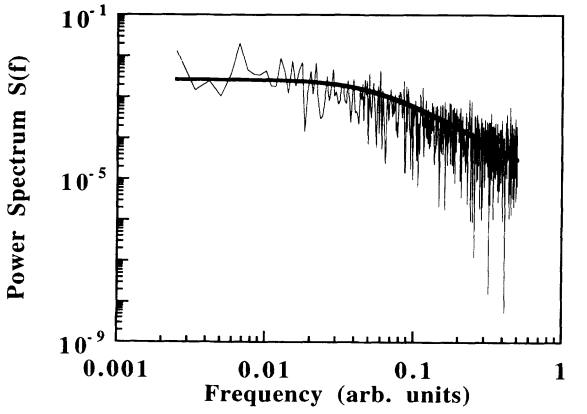

FIG. 3. Log-log plot of the noise power spectrum for the data in Fig. 2 against frequency. The solid line is a fit to the data using a Lorentzian frequency dependence.

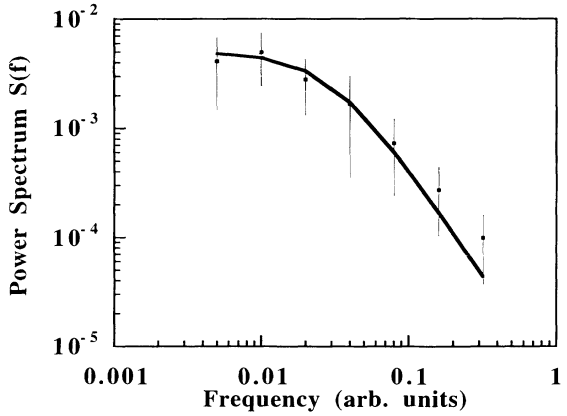

FIG. 4. Log-log plot of the octave binned noise power spectra of three separate simulations of conductance fluctuations for the bond flipping rate in Fig. 3. The solid line is the expected frequency dependence for the noise power per octave of a Lorentzian spectral density. White noise would exhibit a noise power per octave which increased with frequency on this plot, while $1/f$ noise would be represented by a horizontal line.

spectrum. The magnitude of κ can then be estimated by considering the ratio of critical to total bonds on a conducting filament. In a region of height H and of width 2ζ, there exists on average one filament as stated earlier. The number of bonds on the conducting backbone of this filament in two dimensions is $\sim H^D$, where D, the fractal dimension, is 1.6 [5]. If this number of conducting bonds on the filament is divided by the total number of bonds contained in this region (consisting of the backbone current carrying bonds plus the dangling bonds on the filament which do not carry current, yielding a total of $2\zeta H$ bonds) then the fraction of bonds contributing to the conductance is $\kappa = H^D/(2\zeta H)$. For a resistor network of height $H = 20$ and $\zeta = 25.46$ this yields $\kappa \sim 0.12$, in good agreement with the observed value. A simple test of κ would involve changing the height of the lattice, which would change the number of conducting filaments, or alternatively changing the fraction of broken bonds to be either greater than or less than the percolation threshold which again would change the number of filaments in the network. Unfortunately neither approach is computationally feasible. Since the fraction of conducting bonds varies with the height of the lattice as $\kappa \propto H^{-0.4}$, one would have to extend the network by a factor of 10^2 in order to observe an order of magnitude change in κ, which would require correspondingly longer simulation times than for the data in Fig. 2.

Conductance time traces in many disordered systems such as high T_c superconductors and amorphous semiconductors exhibit two-state or multistate switching between discrete resistance levels, termed random telegraph switching noise [18,19,23,24], which is not observed in our simulations of a dynamical percolation resistor network. In the simulations described here, all broken bonds with adjacent unbroken resistors are equally likely to exchange places, corresponding to uncorrelated nearest neighbor atomic or electronic hopping on a disordered lattice. While this simple form of hopping is a natural starting point to investigate time dependent fluctuations in a percolation network, it clearly lacks the crucial element of trapping, present in all real disordered solids. In high T_c superconductors, the resistance switching noise is suggested to arise from the collective motion of magnetic flux vortices [19], while in amorphous silicon, as mentioned above, the motion of bonded hydrogen is believed to enable bonding rearrangements, leading to conductance fluctuations [18]. In both of these systems there will be a distribution of binding energies for vortex pinning sites or silicon-hydrogen traps and, consequently, in contrast to the simulations described here, not all vortices or hydrogen atoms have identical hopping probabilities. We have begun an investigation of the influence of trapping on the conductance fluctuations in a dynamical percolation network; preliminary results on smaller random resistor lattices are encouraging. When a certain fraction of lattice sites in the resistor network are labeled as "traps" forcing any bond that flips onto that site to remain there for a fixed length of time, regardless of the global bond flipping rate, there is no dramatic change in the conductance noise of the network other than a decrease in the effective bond flipping rate. However, when a distribution of trapping times is introduced, and, in particular, when the trapping energies have the same exponential dependence on energy believed to govern the multiple trapping for hydrogen diffusion in a-Si:H, then sharp telegraph switching events are observed in the simulations. Further studies of the influence of a variety of trapping distributions on conductance fluctuations in dynamical percolation networks are presently underway, and will be described in detail in a later publication.

In summary, computer simulations of a dynamical random resistor network at the bond percolation threshold have been performed. The conductance of the network is calculated using the transfer matrix approach, and a fraction of the broken bonds and adjacent unbroken bonds are allowed to exchange places, after which the conductance is recalculated. Repeating this process many times yields a time trace of the conductance fluctuations of the network. Despite the large number of independent filaments within the lattice, there is no evidence of a distribution of time constants, rather, the power spectra of the conductance fluctuations are well described by a Lorentzian frequency dependence where the characteristic lifetime τ reflects the regeneration rate of the conducting portion of the lattice.

This research was supported in part by the NSF DMR-9055722 and the Minnesota Supercomputer Institute. We thank B. Shklovskii for helpful comments.

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