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AC conductivity for the two-dimensional bond-percolation problem

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Abstract. The frequency-dependent conductivity for the bond-percolation model in two dimensions is determined on a 300×200 square lattice in the frequency range $10^{-3} \leqslant \omega \leqslant 5$. Close to $p_c = 0.5$ the real and imaginary parts of the conductivity can be fitted by power laws for a certain frequency range: $\sigma_R \sim \omega^{x_R}$, $\sigma_I \sim \omega^{x_I}$, where $x_R = 0.345 \pm 0.005$, $x_I = 0.318 \pm 0.005$. The difference in x_R and x_I is in contrast to recent theories on anomalous diffusion on percolation clusters which predict $x_R = x_I$. The result for x_R supports arguments which, contrary to the Alexander-Orbach rule, suggest $\mu/\nu = 1$ in $d = 2$.

Considerable interest has been devoted recently to the problem of anomalous diffusion on percolation clusters (Gefen *et al* 1983, Alexander and Orbach 1982, Ben-Avraham and Havlin 1982, Aharony and Stauffer 1984, Laibowitz and Gefen 1984, Pandey *et al* 1984, Harris *et al* 1984). At intermediate frequencies and close to p_c the diffusing particles are expected to reveal the fractal structure of the clusters in the system. Using scaling arguments, Gefen *et al* (1983) show that for $\omega\xi^{2+\theta} \gg 1$

$$\sigma_{AC} \sim (i\omega)^x \tag{1}$$

where

$$x = (2+\theta)\mu/\nu \qquad \text{and} \qquad \theta = (\mu - \beta)/\nu.$$

ξ is the correlation length, which diverges as $\xi \sim |p - p_c|^{-\nu}$ close to p_c. The exponents μ and β describe the behaviour of the DC conductivity $\sigma_{DC} \sim (p - p_c)^\mu$ and the probability to belong to the infinite cluster $P_\infty \sim (p - p_c)^\beta$ respectively (for a review on percolation theory see e.g. Stauffer (1979)).

Alexander and Orbach (1982) have observed that for percolation clusters there is a unique 'fraction' dimensionality $\bar{d} = \frac{4}{3}$ for $d > 2$. Taking the 'Alexander-Orbach rule' seriously, one obtains

$$\mu/\nu = \tfrac{3}{2}(d - \tfrac{4}{3} - \beta/3\gamma), \tag{2}$$

which at $d = 2$ is

$$\mu/\nu = \tfrac{91}{96} = 0.948. \tag{3}$$

For the AC conductivity exponent x one obtains

$$x_{AO} = \tfrac{1}{3}. \tag{4}$$

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Aharony and Stauffer (1984), however, recently conjectured that relation (2) should be replaced by

$$\mu/\nu = d - 1 \tag{5}$$

for $d \leqslant 2.1$. Using this value for μ/ν one obtains at $d = 2$

$$x_{AS} = 0.3453. \tag{6}$$

Accurate Monte Carlo simulations at $d = 2$ give e.g.

$$\mu/\nu = 0.973 \pm 0.005 \tag{7}$$

(Zabolitzky 1984, see also Hong *et al* 1984, Lobb and Frank 1984, Herrmann *et al* 1984) which excludes both equations (2) and (5).

In a recent paper (Biller 1984) I have presented a simple and accurate procedure to determine the frequency-dependent conductivity for a variety of one-dimensional diffusive systems. It turns out that this procedure can be easily extended to the two-dimensional case (for lattices of up to 300×200 sites), and that it is particularly useful to determine the AC conductivity in the so-called anomalous region, where the fractal structure of the large clusters is important.

Similarly to the one-dimensional case, the simulation starts by generating a square lattice of 300×200 sites, where the bonds are occupied according to a probability p. Then the discretised version of the two-dimensional diffusion equation is solved for 100 000 time steps with an equilibrium density of particles $P_n = 1$ at time $t = 0$, an electrical field of the form $E_x = \delta_{t,0}$ and periodic boundary conditions. At each time step the spatially averaged current in the x direction is determined, which is finally Fourier transformed to give the complex AC conductivity for $\omega \geqslant 10^{-3}$.

This algorithm is well suited for parallel processing, and thus a single run only takes about 12 minutes on a Cyber 205 vector processor. Error sources due to the finite network, the finite number of time steps, and the finite discretisation parameter were tested and found to be small for the frequencies considered here.

Figures 1 and 2 give an impression of the results obtained using this simulation method. Obviously for p close to $p_c = 0.5$ and $5 \times 10^{-3} \leqslant \omega \leqslant 10^{-1}$ both the real and

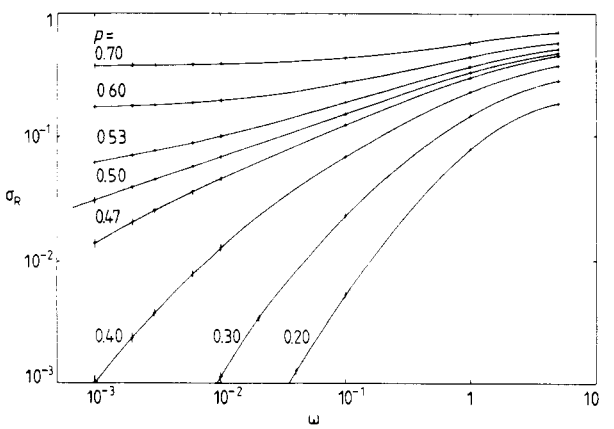

Figure 1. Real part of the frequency-dependent conductivity (σ_R) for various p and $10^{-3} \leqslant \omega \leqslant 5$. Some data points are drawn explicitly to indicate the error bars.

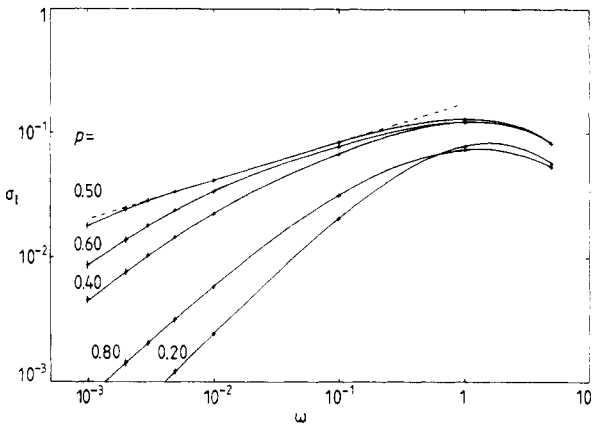

Figure 2. As figure 1, but for the imaginary part of the conductivity, σ_I.

the imaginary part of the conductivity can be fitted by power laws for anomalous diffusion: $\sigma_R \sim \omega^{x_R}$, $\sigma_I \sim \omega^{x_I}$.

At $\omega \simeq 1$ the crossover to the high frequency limit $\sigma_\infty = p$ takes place. Well below p_c and at low frequencies the conductivity follows the asymptotic form $\sigma \sim a i\omega + b\omega^2$ (Odagaki *et al* 1983). The condition for the anomalous regime to develop (Gefen *et al* 1983),

$$\omega \xi^{(2+\theta)} \gg 1,$$

is seen to be very stringent: although e.g. for $p = 0.47$ one obtains a crossover frequency $\omega_c \simeq 10^{-6}$, deviations from power law behaviour can already be seen for $\omega \leqslant 10^{-2}$ (figure 1).

The error bars in figures 1 and 2 are due to the fluctuations one expects from different realisations for a given p. Note that close to p_c and at intermediate frequencies the fluctuations are small, which shows that the fractal structure of the clusters is insensitive to different realisations.

To determine the slopes of the complex conductivity in the anomalous diffusion regime I did 24 independent runs at or close to p_c, i.e. $|p - p_c| \leqslant 10^{-2}$. The results of two of these runs are shown in figure 3. Note that the anomalous region is less developed in σ_I than in σ_R. This might be due to the fact that correction terms to the scaling form (1) are more important in σ_I than in σ_R. It is also obvious that σ_I has a different slope from σ_R in the anomalous region. Using a least squares fit to determine these slopes, I obtained the following average values:

$$x_R = 0.345 \pm 0.005, \qquad 5 \times 10^{-3} \leqslant \omega \leqslant 10^{-1} \tag{8}$$

$$x_I = 0.318 \pm 0.005, \qquad 5 \times 10^{-3} \leqslant \omega \leqslant 5 \times 10^{-2}. \tag{9}$$

The deviation between x_R and x_I cannot be explained by the scaling arguments of Gefen *et al* (1983). However, this deviation might also be due to corrections to the simple scaling form (1).

Note that the relative value of the imaginary to the real part of the conductivity is roughly in accordance with what one expects from equation (1)

$$\sigma_I / \sigma_R = \tan(\tfrac{1}{2}\pi x), \tag{10}$$

for the anomalous region.

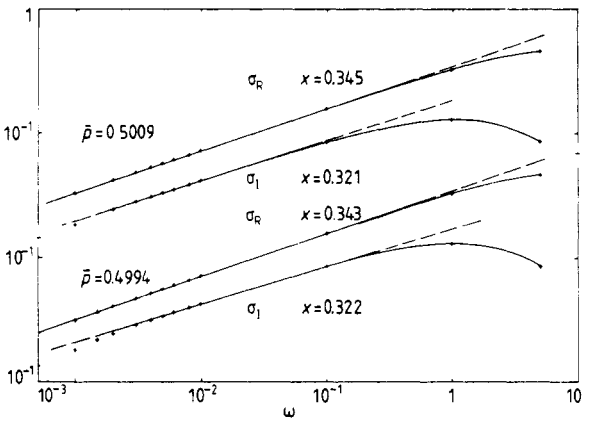

Figure 3. Two examples of the AC conductivity at $p_c = 0.5$. $\bar{p}$ is the average occupancy of the sites generated by the run. The slopes of the broken lines were determined by a least squares fit. Some data points are shown to indicate the error due to the finite lattice and the discretisation of the diffusion equation in time.

For some runs at p_c, I have also determined the slope of the time-dependent conductivity which should behave as

$$\sigma_t \sim t^{-(1+x)}. \tag{11}$$

Typical values for x were of the order of $x \simeq 0.35$, but they were scattering widely (± 0.05) from run to run.

Because the anomalous region is best developed in σ_R it is most appropriate to compare the exponent x_R (8) with the theoretical predictions (4), (6). In contrast to Zabolitzky's (1984) work, this simulation clearly supports the argumentation of Aharony and Stauffer, as can be seen from the close agreement of equations (6) and (8).

In conclusion, I have used a simple simulation procedure to determine the slopes of the real and imaginary parts of the AC conductivity for the two-dimensional bond-percolation problem in the anomalous diffusion region where $\omega\xi^{(2+\theta)} \gg 1$. I have shown that the slopes of σ_R and σ_I differ appreciably, which cannot be accounted for by simple scaling arguments (Gefen *et al* 1983). I have also shown that the anomalous diffusion regime is less developed in σ_I than in σ_R and that the condition for the anomalous region to develop, $\omega\xi^{(2+\theta)} \gg 1$, is very stringent.

My result for the exponent of the real part of the conductivity x_R shows that the Alexander-Orbach rule breaks down at $d = 2$. It is in agreement with arguments which suggest $\mu/\nu = 1$ in $d = 2$ (Aharony and Stauffer 1984).

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