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Conductivity for one-dimensional disordered classical systems: A computer simulation

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Abstract. A simple computer simulation for one-dimensional, classical, disordered systems with symmetric hopping rates is presented, which is well suited for vectorised programming.

The data for the frequency-dependent conductivity are compared to analytical results for various classes of distributions of the transfer rates. In particular, for singular distributions of the form $\rho(W) \sim W^{-\alpha}$, $0 \leqslant W \leqslant 1$, it is demonstrated that the well known effective medium theory is an excellent approximation for $-1 \leqslant \alpha \leqslant 0.9$.

1. Introduction

Recently considerable interest has been devoted to the study of one-dimensional (1D), disordered, classical systems (Alexander *et al* 1981a). These studies provide a rather good explanation for conductivity measurements in the 1D superionic conductor Hollandite and the quasi-1D conductor $Qn(TCNQ)_2$ (Alexander and Bernasconi 1979, Alexander *et al* 1981c).

Depending on the class of disorder under consideration, a variety of methods has been presented to determine the frequency-dependent conductivity for these systems: rigorous results have been obtained for non-singular distributions, where all moments and inverse moments of the distribution of the transfer rates exist (Zwanzig 1982, Denteneer and Ernst 1983, Biller 1984a). These systems show a universal long-time behaviour and the DC conductivity is given by the first inverse moment of the distribution of the transfer rates. For systems, where all (or at least some) of the inverse moments do not exist, the situation is less clear: apart from the effective medium theory and a simple scaling argument (Alexander *et al* 1981a, Alexander and Bernasconi 1979) there exists a rigorous solution for the low-frequency autocorrelation function for these systems, which can be connected with the conductivity by a scaling relation (Bernasconi *et al* 1980). Stephen and Kariotis (1982), using the replica trick, obtain the same result. Although all of these methods predict the same non-universal low-frequency conductivity for distributions of the form $\rho(W) \sim W^{-\alpha}$, $0 \leqslant W \leqslant 1$, all of them are based on assumptions to determine this quantity.

An exact solution however, can be given for another class of systems: the 1D bond-percolation model (Odagaki and Lax 1980). I will use this system later on to demonstrate the quality of my simulations.

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The intention of this work is not only to provide a test for analytical results so far obtained for singular distributions, but also to present a simple procedure for simulating these systems. This procedure is well suited for parallel processing on a Cyber 205 vector processor. It should also be applicable to two- and three-dimensional systems.

2. Model equations and analytical results

We consider the following set of coupled rate equations, connecting the change in particle density $\partial_t P_n$ at site n, with the current to sites n and $n-1$ (Biller 1984a)

$$\partial_t P_n + j_n - j_{n+1} = 0 \tag{1}$$

where, assuming symmetric hopping rates,

$$j_n = -W_n(P_{n+1} - P_n - E(t)). \tag{2}$$

Using linear response theory, I have included an external field $E(t)$ explicitly in the current (Biller 1984b). Note that P_n may not only be interpreted as the change in particle density due to the external field E, but also as the particle density itself, because only the difference in the P_n matters. The W_n are assumed to be random transfer rates which are uncorrelated in space, having one of the following distributions.

Class (A): $\rho(W)$ such that all $\langle W^m \rangle$ and all $\langle 1/W^m \rangle$ exist (non-singular distributions). As an example, we will consider the following distribution

$$\rho(W) = \tfrac{1}{2}[\delta(W - \tfrac{1}{2}) + \delta(W - \tfrac{3}{2})]. \tag{3}$$

Class (B): $\rho(W)$ such that only the first r inverse moments exist: $\langle 1/W^m \rangle$ finite for $m \leqslant r$, and $\langle 1/W^m \rangle^{-1} = 0$ for $m > r$. A particular example ($r = 1$) for this class of distributions is the following form

$$\rho(W) = (1-\alpha)W^{-\alpha}, \qquad 0 \leqslant W \leqslant 1, \qquad -1 \leqslant \alpha < 0. \tag{4}$$

Class (C): $\rho(W)$ such that no inverse moment exists: $\langle 1/W^m \rangle^{-1} = 0$ for $m \geqslant 1$. Here we will consider a similar form as for class (B) (Alexander *et al* 1981a)

$$\rho(W) = (1-\alpha)W^{-\alpha}, \qquad 0 \leqslant W \leqslant 1, \qquad 0 \leqslant \alpha < 1. \tag{5}$$

Class (D):

$$\rho(W) = (1-p)\delta(W) + p\delta(W-1), \qquad 0 \leqslant p \leqslant 1. \tag{6}$$

This is the bond-percolation model (Odagaki and Lax 1980), where we have a finite probability for the W to be zero.

For later reference let me quote the analytical results obtained for the various classes of distributions. For class (A) there exists an expansion for the conductivity in the low- and high-frequency limit (Zwanzig 1982, Denteneer and Ernst 1983, Biller 1984a)

$$\sigma(\omega) = \langle W^{-1} \rangle^{-1}[1 + m_{-2} z^{1/2} + (\tfrac{11}{24} m_{-2}^2 - \tfrac{1}{4} m_{-3}) z + O(z^{3/2})] \tag{7}$$

$$z = \langle i\omega W^{-1} \rangle, \qquad m_{-n} = \langle (W^{-1} - \langle W^{-1} \rangle)^n \rangle / \langle W^{-1} \rangle^n$$

$$\sigma(\omega) = \langle W \rangle [1 - 2m_2 s^{-1} + 2m_3 s^{-2} + O(s^{-3})]$$

$$s = i\omega \langle W \rangle^{-1}, \qquad m_n = \langle (W - \langle W \rangle)^n \rangle / \langle W \rangle^n. \tag{8}$$

For class (B) and (C) systems the conductivity may be determined from the well known effective medium (EM) relation (Alexander *et al* 1981a) which reads

$$\langle (W-\sigma_{\text{eff}})/[W+\tfrac{1}{2}(g_{\text{eff}}+\mathrm{i}\omega)]\rangle = 0, \tag{9}$$

where g_{eff} is related to σ_{eff} by

$$\sigma_{\text{eff}} = g_{\text{eff}}(g_{\text{eff}}+\mathrm{i}\omega)/\mathrm{i}\omega.$$

I will compare iterative solutions of this relation with my simulations later on.

Using for (9) the expansion procedure of Bernasconi and Schneider (1984) one has asymptotically for class (B) systems (see also Richards and Renken 1980)

$$\sigma_{\text{eff}}(\omega) = \sigma_{\text{DC}}(1+F_\alpha\cdot(\mathrm{i}\omega)^{|\alpha|/2}), \qquad -1<\alpha<0, \qquad \mathrm{i}\omega\to 0 \tag{10}$$

where

$$F_\alpha = \frac{\pi(1+|\alpha|)}{2^{|\alpha|}\sin(\pi|\alpha|)}\sigma_{\text{DC}}^{1+|\alpha|/2}$$

and

$$\sigma_{\text{DC}} = |\alpha|/(1+|\alpha|).$$

The result for class (C) systems obtained by Bernasconi *et al* (1980) via a scaling assumption reads

$$\sigma(\omega) = D_0(C_\alpha^{-2})(\mathrm{i}\omega)^{\alpha/(2-\alpha)} \tag{11}$$

where $D_0 \simeq \frac{1}{4}$ and C_α can be determined exactly, but is rather well described by the effective medium result

$$C_{\alpha,\text{eff}} = \tfrac{1}{2}[\pi(1-\alpha)2^\alpha/\sin\pi\alpha]^{1/(2-\alpha)}. \tag{12}$$

Stephen and Kariotis have obtained equivalent results, using the replica trick.

For $\alpha = 0$, where the crossover from class (C) to class (B) occurs, Alexander *et al* (1981a) obtain

$$\sigma(\omega) \simeq -(2/\rho(0))(1/\ln(\mathrm{i}\omega)). \tag{13}$$

For class (D) systems the exact result for the conductivity is given by Odagaki and Lax. The limiting form for small frequencies reads

$$\sigma(\omega) = \frac{p}{2(1-p)^2}\mathrm{i}\omega + \frac{p(1+p)^2}{4(1-p)^4}\omega^2. \tag{14}$$

3. Simulation procedure

The simulation procedure now works as follows: (1) is discretised in time

$$P_n(t+\tau) = P_n(t) - \tau(j_n(t) - j_{n-1}(t)) \tag{15}$$

where $\tau < \frac{1}{2}$, to keep the simulation stable, and t from now on is understood as a discrete variable. $j_n(t)$ is still given by (2). We take a system of 60 000 sites with periodic boundary conditions. The W_n are determined at the beginning of the simulation with a pseudo-random number generator, according to one of the distributions (A)-(D) equations (3)-(6).

We start with the initial condition for $P_n(0)=0$ (or $P_n(0)=1$) and use for $E(t)$ either $E(t)=1/\tau\cdot\delta_{t,0}$ or $E(t)=\theta(t)$. Then $j_n(t)$ and $P_n(t+\tau)$ are determined for up to 200 000 time steps. At each time step the average current in the system is evaluated:

$$j_{\mathrm{av}}(t)=\frac{1}{N}\sum_{n=1}^{N} j_n(t). \tag{16}$$

Because of the large system size of $N=60\,000$ the fluctuations in j_{av} due to different realisations of the same ensemble are small, typically of the order of 2%. Now $\sigma(t)$ is determined from $j_{\mathrm{av}}(t)$. The result of course does not depend on the form chosen for $E(t)$. A final Fourier transform of $\sigma(t)$ then gives $\sigma(\omega)$ for ω down to 10^{-4}.

The above procedure is particularly well suited for parallel processing on a Cyber 205 vector processor. Thus it takes only about 13 minutes to determine $j_{\mathrm{av}}(t)$ for 100 000 time steps and a system size of 60 000 sites.

Error sources in this simulation are

(i) the finite discretisation parameter τ, which becomes particularly important at high frequencies;

(ii) the finite number of time steps N_t, which is of influence at small frequencies;

(iii) the finite systems size N, which, I believe, is only important in the class (D) case at p close to p_c; and

(iv) numerical errors: a test for these errors is the particle number conservation. The largest deviation I observed for $1/N\,\Sigma_n P_n(t=\tau N_t)$ was 10^{-7}, which is small and unimportant for our results.

Altogether, for all figures displayed in this paper, the error should be of about the size of the symbols used for the graphs.

4. Results and discussion

4.1. Class (D) *systems*

Let us start the discussion with the bond-percolation model (Odagaki and Lax 1980). Figure 1 shows the simulation results for the real and imaginary parts of the conductivity $(\sigma_{\mathrm{R}}(\omega), \sigma_{\mathrm{I}}(\omega))$ for various values of p compared with the exact solution (equation (10) in the work of Odagaki and Lax). The system size was $N=60\,000$ sites and the number of time steps was $N_t=50\,000$. There are virtually no deviations from the exact result, apart from some small errors in σ_{I} for $\omega\simeq 1$, which could be removed by taking a smaller time constant τ! I should mention, however, that deviations do occur for p close to $p_c=1$. Thus for $p=0.98$ and $N_t=100\,000$ I observed an error of about 15% for $\omega=2\times10^{-4}$, which was down at about 2% by taking a different realisation. These errors originate in fluctuations, which become large for p close to p_c, and also in the fact that close to p_c the current decays very slowly.

Thus, if one were interested in the conductivity close to p_c the system size N and the number of time steps N_t should be increased. Here numerical errors may finally become important. Still the critical behaviour for σ_{R} and σ_{I} as predicted by equation (14) can be observed.

4.2. Class (A) *systems*

A simple class (A) system is given by (3), where the bonds can assume only two finite values. This system was simulated for $N_t=100\,000$, using different parameters τ for

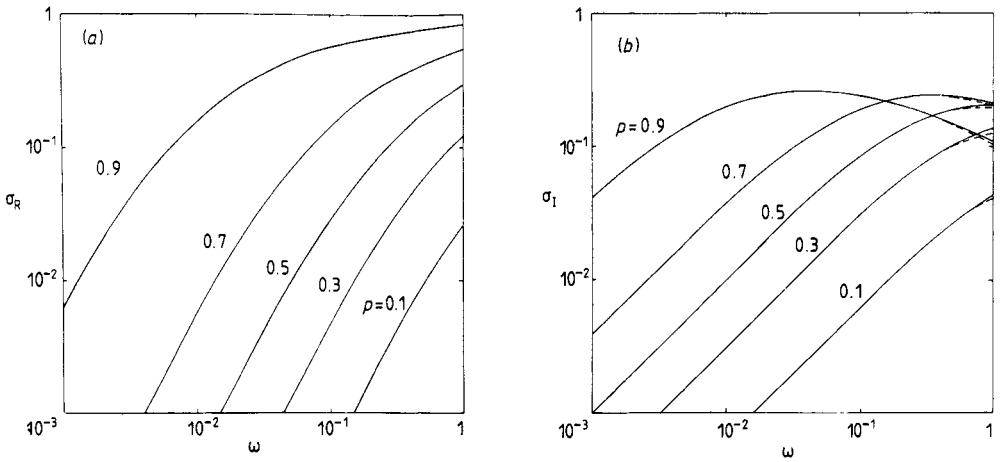

Figure 1. Real and imaginary part of the conductivity (*a*) $\sigma_R(\omega)$, (*b*) $\sigma_I(\omega)$ for the bond-percolation model (class (D), equation (6)) for various values of p. The simulation results (——) are compared to the exact solution (- - - -) (Odagaki and Lax 1980).

small and high frequencies. The result is shown in figure 2. The crossover from low- to high-frequency behaviour, where the analytical expansion breaks down, can be clearly seen. Note that Monte Carlo simulations previously done for this class of systems only determined $\langle x^2(t)\rangle$ (and higher moments), whereas here $\sigma(\omega)$ is given directly for more than six decades in ω (Richards and Renken 1980, Haus *et al* 1982).

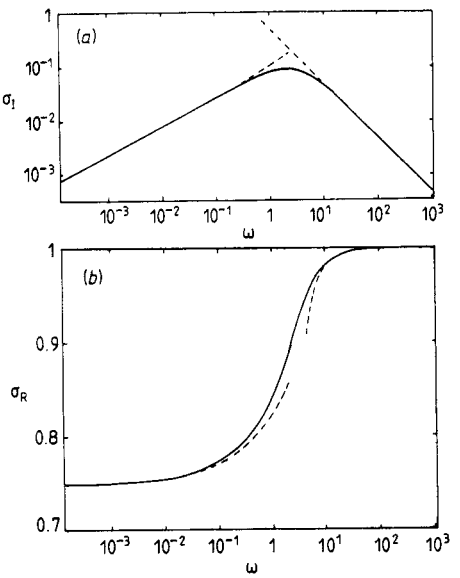

Figure 2. (*a*) $\sigma_R(\omega)$, (*b*) $\sigma_I(\omega)$ for a particular class (A) distribution (equation (3)). Simulation results (——), analytical results (- - - -) equations (7) and (8) for low and high frequencies, respectively.

4.3. Class (C) *and class* (B) *systems*

The most interesting class of distributions is given by class (C) systems (5), because there, the first inverse moment does not exist, and σ is expected to show a non-universal α-dependent low-frequency behaviour (Alexander *et al* 1981a, Bernasconi *et al* 1979, Alexander and Bernasconi 1979, Bernasconi *et al* 1980, Stephen and Kariotis 1982). Our choice for a class (B) system (4) should, however, be interesting too: although there is a finite DC conductivity given by $\sigma_{DC} = \langle W^{-1} \rangle^{-1}$ one expects non-universal behaviour in $(\sigma - \sigma_{DC})$ due to the fact that m_{-2} and all higher inverse moments diverge for this distribution (Richards and Renken 1980, Bernasconi and Beyelen 1980).

Let us first concentrate on class (C) systems: figure 3 shows the long-time behaviour of $\sigma(t)$ for various values of α compared with the theoretically expected dependence of $\sigma_{th} \sim t^{-2/(2-\alpha)}$. The curves were fitted such that $\sigma_{th}(N_t) = \sigma(N_t)$. Obviously the slopes agree well for intermediate values of α, whereas deviations occur at α close to zero and one. In figure 4 the real and imaginary parts of $\sigma(\omega)$ are compared with expression (11). As with the long-time behaviour of $\sigma(t)$, one observes that the theoretical result (11) agrees well with our data for intermediate values of α. However, it has already been pointed out by Richard and Renken and Bernasconi and Beyeler, that for small α relation (11) is not sufficient, but higher-order terms in the expansion of σ become important for the frequencies we are able to consider here. The same thing happens for $(1-\alpha) \ll 1$, I was told by Bernasconi and Schneider (1984). Thus for $0 < \alpha \leqslant 0.3$ and $0.9 \leqslant \alpha < 1$ the limiting form (11) can only be seen for extremely small frequencies, out of reach for our simulations. However, one may solve the EM-relation (9) iteratively (see figure 4). The excellent agreement with the numerical

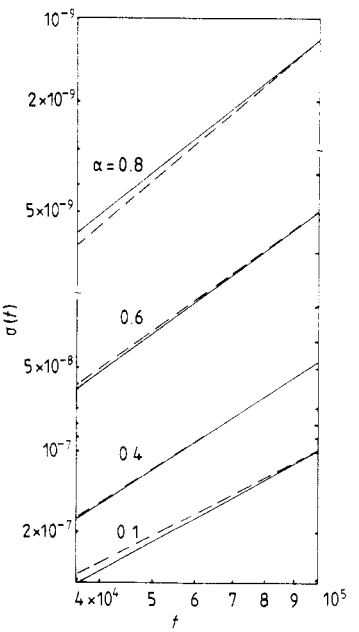

Figure 3. Long-time behaviour of the conductivity $\sigma(t)$ for class (C) systems (equation (5)) for various α. The simulation results (——) are compared with the theoretically expected behaviour $\sigma_{th} \sim t^{-2/(2-\alpha)}$ (- - - -). The curves for σ_{th} were fitted such that $\sigma_{th}(N_t) = \sigma(N_t)$, $N_t = 100\,000$.

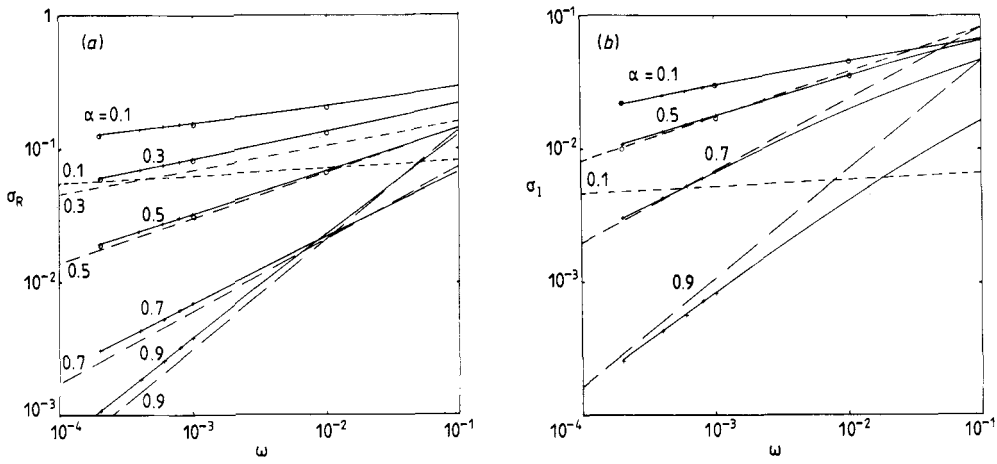

Figure 4. Real and imaginary part of the conductivity (*a*) $\sigma_R(\omega)$, (*b*) $\sigma_I(\omega)$ for class (C) distributions (equation (5)) for various α. Simulation results: +, (——); analytical results (equation (10)): (- - - -); iterative solution of the EM-relation (equation (9)): ○. (The values of σ_R for $\alpha = 0.9$ in (*a*) are enlarged by a factor of 10).

data shows that the effective medium relation (9) is indeed a very good approximation for all values of $\alpha \leqslant 0.9$. This is again demonstrated in figure 5 where the real and imaginary parts of σ are displayed as functions of α for $\omega = 2 \times 10^{-4}$ and $-1.0 \leqslant \alpha \leqslant 0.9$. Note the rather good agreement of the data with (11) (using the EM-result equation (12)) for $0.9 > \alpha > 0.4$ and with the iterative solution of the EM-relation (9).

At $\alpha = 0$ the crossover from class (C) to class (B) occurs. Class (B) systems and the case $\alpha = 0$ are displayed in figure 6. Equation (13) for $\alpha = 0$ and (10) for $0 > \alpha > -1$ are not sufficient for the frequencies considered here, but again the iterative solution of the EM-relation (9) agrees well with our results.

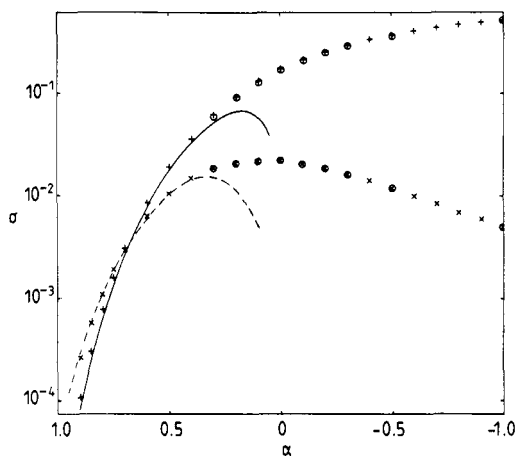

Figure 5. Real and imaginary part of $\sigma(\omega)$ for $\omega = 2 \times 10^{-4}$ as a function of α for $0.9 \geqslant \alpha \geqslant -1$. Simulation results: σ_R: +, σ_I: x; analytical results (equation (10)): σ_R: ——, σ_I: - - - - -; iterative solution of the EM-relation (9): ○.

In figure 6, I have subtracted the theoretically expected value for σ_{DC} from σ_R (σ_{DC} is of course poorly determined by the simulation) to show the non-universal behaviour in $(\sigma_R - \sigma_{DC})$, which can also be seen in σ_I (figure 6(*b*)). It should be noted that, for $\alpha < -1$, one expects non-universal behaviour in higher terms of the expansion of σ (see (9)).

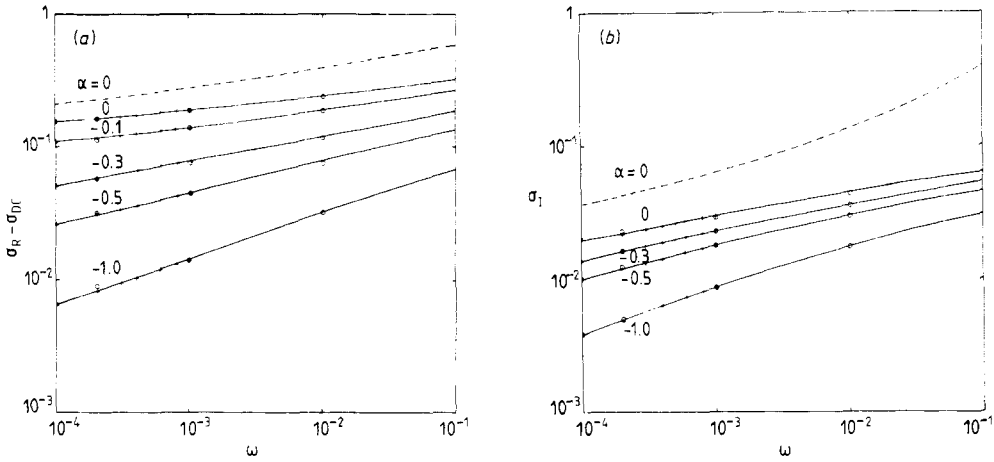

Figure 6. Real and imaginary part of the conductivity (*a*) $\sigma_R(\omega) - \sigma_{DC}$, (*b*) $\sigma_I(\omega)$ for class (B) distributions (4) for various α and the case $\alpha = 0$. Simulation results: +, ——; analytical results (12): - - - - -; iterative solution of the EM-relation: ○.

5. Summary

I have presented a simple simulation procedure to determine directly the frequency-dependent conductivity for 1D disordered, classical systems. This procedure is suited for vectorisation on a Cyber 205 vector processor. Therefore, large systems of 60 000 sites can be simulated in a reasonable amount of time. The quality of the simulations was demonstrated in a comparison with exact results for the bond-percolation model (class (D)) (Odagaki and Lax 1980) and for a model with a non-singular distribution of the transfer rates (class (A)) (Biller 1984a). For systems with distributions of the transfer rates of the form $p(W) = (1-\alpha)W^{-\alpha}$, $0 \leq W \leq 1$, $-1 \leq \alpha < 1$, (class (B) and (C)), I have shown that the well known effective medium relation (Alexander *et al* 1981a) is in good agreement with the data for $\alpha \leq 0.9$. For class (B) systems $(-1 \leq \alpha < 0)$, I have demonstrated that $(\sigma - \sigma_{DC})$ shows non-universal behaviour.

My procedure should also allow the simulation of certain asymmetric hopping models (Derrida and Orbach 1983, Biller 1984b). Of course there the stationary state should be established first, before one applies an external field to determine σ.

One might also try to find out about crossover effects due to nonlinearities in the external field E for class (C) and (D) systems (Alexander *et al* 1981b, Movaghar *et al* 1984, Prigodin and Samukhin 1983).

Finally, I think the procedure can be generalised to study transport problems in disordered systems in higher dimensions (e.g. the bond-percolation model).

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