ac Hopping Conductivity of a One-Dimensional Bond-Percolation Model

T. Odagaki
Department of Physics, City College of the City University of New York, New York, New York 10031

and

M. Lax
Department of Physics, City College of the City University of New York, New York, New York 10031, and Bell Laboratories, Murray Hill, New Jersey 07974

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The exact frequency dependence of the ac hopping conductivity of a one-dimensional chain with random interruptions is obtained. The real and imaginary parts of the ac conductivity are shown to vanish quadratically and linearly, respectively, with frequency at the static limit. Critical behavior of the ac conductivity in the limit of no interruptions is discussed.

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Carrier or exciton transport and spectral diffusion on one-dimensional random chains have been extensively studied from both theoretical and experimental view points.[1-5] Randomness in the chain gives rise to localization of carrier eigenstates.[6] Therefore, transport or diffusion on the chain with sufficient randomness takes place by hopping from one localized center to another rather than by propagation of Bloch waves. If there exist impurities or defects in the chain, they may interrupt the hopping path and the dc conductivity will vanish. ac conductivity at nonzero frequencies, however, can be nonvanishing even if many interruptions of the hopping channel exist, since the carrier can always respond to an ac field. The frequency dependence of the ac conductivity and diffusion constant is determined by the distribution of random interruptions.

The bond-percolation model is one of the most simplified models which describe the effect mentioned above. In the present paper, we solve exactly the bond-percolation model for hopping conduction on a one-dimensional chain, where the nearest-neighbor hopping rate of a bond is broken at random with probability $1-p$. If we regard a set of sites that are connected to each other by unbroken bonds as a cluster, then the chain is divided into a set of finite clusters except for the limiting case $p=1$. As we shall see below, the ac conductivity of the whole system is given by a weighted average of the conductivity associated with finite clusters and each finite-cluster problem is solved rigorously. It will be shown that at the static limit the real and imaginary parts of the ac conductivity vanish quadratically and linearly, respectively, with frequency, and at the high frequencies both approach their own plateau values.

Recently, Heinrichs[7] investigated the same problem. However, except for the pair case, he treats finite clusters using periodic boundary conditions (PBC) as an approximation. His PBC result for a finite cluster shows quite a large deviation over some frequency range from our exact solution for properly terminated clusters.

As shown by Scher and Lax,[8] the hopping conductivity for one-dimensional system can be reduced to

$$\sigma(\omega)=(ne^2/kT)D(\omega), \tag{1}$$

where the generalized diffusion constant $D(\omega)$ is given by

$$D(\omega)=-\frac{\omega^2}{2}\sum_{x,x_0}(x-x_0)^2\tilde{P}(x,i\omega|x_0)f(x_0). \tag{2}$$

Here, n is the density of effective carriers, T is the absolute temperature, ω is the frequency, x denotes a site position in the chain, and $f(x_0)$ the equilibrium distribution function for the initial carrier position will, in this paper, be assumed to be $1/L$, where L is the total number of sites. $\tilde{P}(x,u|x_0)$ is the Laplace transform of the transition probability $P(x,t|x_0,0)$ which denotes the probability of finding a carrier at site x at time t if it started at site x_0 at time $t=0$. The Laplace transform $\tilde{P}$ is assumed to obey the usual random-walk equation

$$(u+W_{x,x+1}+W_{x,x-1})\tilde{P}(x,u|x_0)-W_{x,x+1}\tilde{P}(x+1,u|x_0)-W_{x,x-1}\tilde{P}(x-1,u|x_0)=\delta_{x,x_0} \tag{3}$$

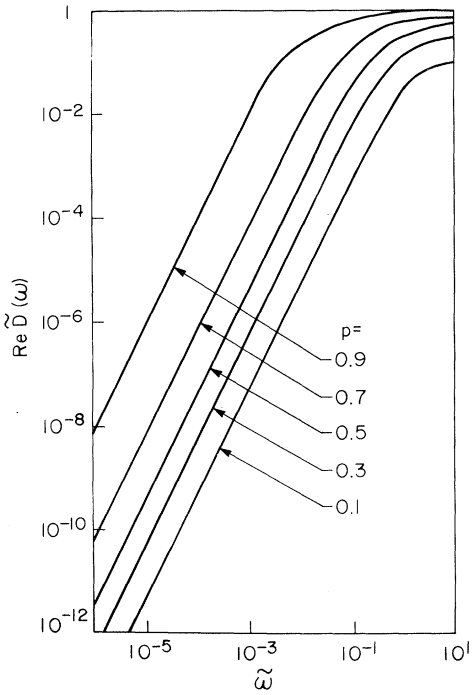

FIG. 1. The dependence of real part of $\tilde{D}(\omega)$ on frequency for various values of p.

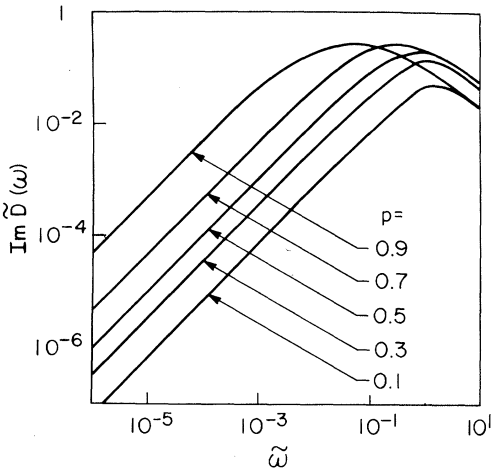

FIG. 2. The dependence of imaginary part of $\tilde{D}(\omega)$ on frequency for various values of p.

The jump rate $W_{x,x'}$ from x' to x is zero unless x and x' are nearest neighbors and is assumed to satisfy $W_{x,x+1}=W_{x+1,x}$.

The bond-percolation model is characterized by a probability function of the jump rate $W_{x,x+1}$ such that

$$P(W_{x,x+1}) = p\delta(W_{x,x+1}-W_0)+(1-p)\delta(W_{x,x+1}) \tag{4}$$

with a nonzero constant jump rate W_0, namely, each bond is broken at random with probability $1-p$. If $p\neq 1$, the chain is composed of a set of segments; each segment is a cluster of sites which are connected to each other by unbroken bonds.

Now it is clear that $P(x,t|x_0,0)$ and hence $\tilde{P}(x,u|x_0)$ are zero unless x and x_0 belong to the same cluster. Therefore, Eq. (2) can be reduced to a sum over clusters of different sizes:

$$D(\omega)=\sum_{N=1}^{\infty} NC_N D_N(\omega) \tag{5}$$

and the diffusion constant $D_N(\omega)$ of the cluster of size N is given by

$$D_N(\omega)=-\frac{\omega^2}{2N}\sum_{x,x_0}^{N}(x-x_0)^2\tilde{P}(x,i\omega|x_0). \tag{6}$$

The probability of finding a cluster of size N ($N-1$ bonds terminated by a broken bond at each end) is given by

$$C_N=(1-p)^2p^{N-1}. \tag{7}$$

Thus, the complete diffusion constant is expressed as a weighted average of the finite-cluster diffusion constants.

For a finite system, Eq. (3) is expressed in a compact with use of vector and matrix notations as

$$\underline{A}\vec{\tilde{P}}(u,x_0)=\vec{\delta}(x_0), \tag{8}$$

where $A_{x,x'}=(u+2W_0)\delta_{x,x'}-W_0(\delta_{x-1,x'}+\delta_{x+1,x'})$, $A_{1,x'}=(u+W_0)\delta_{1,x'}-W_0\delta_{2,x'}$, $A_{N,x'}=-W_0\delta_{N-1,x'}+(u+W_0)\delta_{N,x'}$, for $2\leq x\leq N-1$ and $1\leq x'\leq N$, and $[\vec{\tilde{P}}(u,x_0)]_x=\tilde{P}(x,u|x_0)$, $[\vec{\delta}(x_0)]_x=\delta_{x,x_0}$. Since the eigenvector and the eigenvalue of the $N\times N$ tridiagonal matrix A are given by $(C_m,C_{3m},\ldots,C_{(2N-1)m})$ and $u+2W_0(1-C_{2m})$, respectively, with $C_m=\cos m\pi/2N$ and $m=0,1,\ldots,N-1$, it is easy to see that

$$\tilde{P}(x,u|x_0)=\{1/u+2\sum_{m=1}^{N-1}C_{(2x-1)m}C_{(2x_0-1)m}/[u+2W_0(1-C_{2m})]\}/N. \tag{9}$$

TABLE I. The low-frequency behavior of $\tilde{D}(\omega)$: $\tilde{D}(\omega) = A\tilde{\omega}^2 + B\tilde{\omega}i + O(\tilde{\omega}^3)$.

Method	$\tilde{D}(\omega)$ A	B
CTRW	$p(4-3p)/4(1-p)^4$	$p(2-p)/2(1-p)^2$
CPA	$p(2-p)/8(1-p)^4$	$p(2-p)/4(1-p)^2$
Exact	$p(1+p)^2/4(1-p)^4$	$p/2(1-p)^2$

TABLE II. The high-frequency behavior of $\tilde{D}(\omega)$: $\tilde{D}(\omega) = p - A'/\tilde{\omega}^2 + (B'/\tilde{\omega})i + O(\tilde{\omega}^{-3})$.

Method	$\tilde{D}(\omega)$ A'	B'
CTRW	$p(1-p)$	$p(1-p)$
CPA	$2p(1-p)(2-p)$	$2p(1-p)$
Exact	$2p(1-p)$	$2p(1-p)$

Insertion of this expression into (6) and some elementary algebraic manipulations yield

$$\tilde{D}_N(\omega) \equiv \frac{D_N(\omega)}{a^2 W_0} = \frac{N^2-1}{12} i\tilde{\omega} + \frac{\tilde{\omega}^2}{2N^2} \sum_{m=1}^{N-1} \frac{[1-(-1)^m](1+C_{2m})}{(1-C_{2m})^2[2(1-C_{2m})+i\tilde{\omega}]} \tag{10a}$$

$$= 1 + \frac{(1+4/i\tilde{\omega})^{1/2}}{N}\left(\frac{1}{z_+^{2N}+1} - \frac{1}{z_-^{2N}+1}\right), \tag{10b}$$

where $\tilde{\omega} = \omega/W_0$, $z_\pm = [(i\tilde{\omega})^{1/2} \pm (4+i\tilde{\omega})^{1/2}]/2$, and a denotes the lattice constant of the chain. The diffusion constant of a finite chain $\tilde{D}_N(\omega)$ behaves as

$$\tilde{D}_N(\omega) \to (N^4-1)\tilde{\omega}^2/120 + (N^2-1)i\tilde{\omega}/12 \tag{11a}$$

at the low-frequency limit and

$$\tilde{D}_N(\omega) \to 1 - 1/N - 2/N\tilde{\omega}^2 + 2i/N\tilde{\omega} \tag{11b}$$

at the high-frequency limit.

Now, the normalized ac conductivity or the normalized diffusion constant of the total system $\tilde{D}(\omega) \equiv kT\sigma(\omega)/(ne^2a^2W_0) = D(\omega)/a^2W_0$ can be easily evaluated numerically using Eqs. (5), (7), and (10). Figures 1 and 2 show the frequency dependence of real and imaginary part of $\tilde{D}(\omega)$ for various values of p. The diffusion constant and hence ac conductivity are always zero at the static limit except when $p = 1$ as physically expected; if $p \neq 1$, $\mathrm{Re}\tilde{D}(\omega)$ vanishes quadratically with $\tilde{\omega}$ and $\mathrm{Im}\tilde{D}(\omega)$ vanishes linearly. Explicitly, the frequency dependence of $\tilde{D}(\omega)$ at the static limit is given by

$$\tilde{D}(\omega) \sim \frac{p(1+p)^2}{4(1-p)^4}\tilde{\omega}^2 + \frac{p}{2(1-p)^2}\tilde{\omega}i. \tag{12}$$

It follows that, at the percolation point ($p_c = 1$), $\tilde{D}(\omega)$ shows the following critical behaviors:

$$\lim_{\tilde{\omega}\to 0}[\mathrm{Re}\tilde{D}(\omega)/\tilde{\omega}^2] \sim (p_c - p)^{-4}, \tag{13a}$$

$$\lim_{\tilde{\omega}\to 0}[\mathrm{Im}\tilde{D}(\omega)/\tilde{\omega}] \sim (p_c - p)^{-2}. \tag{13b}$$

As the frequency is increased, $\mathrm{Re}\tilde{D}(\omega)$ also increases and eventually reaches its high-frequency limit, while $\mathrm{Im}\tilde{D}(\omega)$ first increases and then decreases to zero after reaching a maximum. Explicit behavior of $\tilde{D}(\omega)$ at the high-frequency limit reads as

$$\tilde{D}(\omega) \sim p - \frac{2p(1-p)}{\tilde{\omega}^2} + \frac{2p(1-p)}{\tilde{\omega}}i. \tag{14}$$

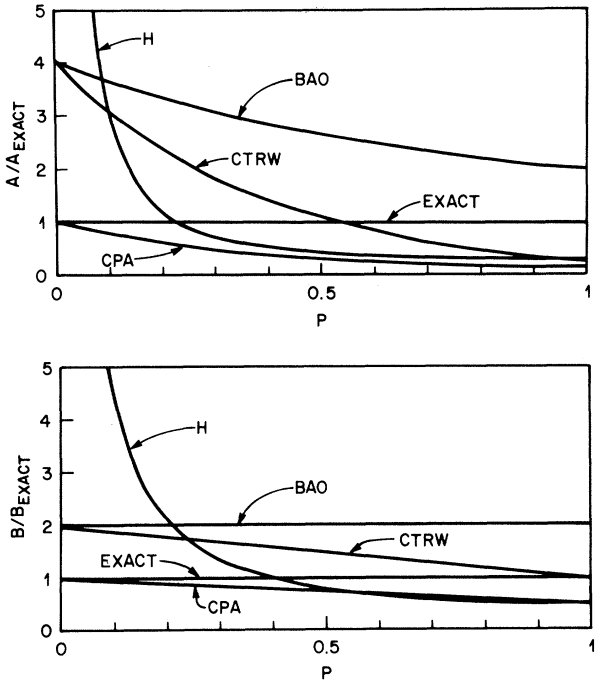

FIG. 3. A comparison of the relative merits of the various approximations in the low-frequency regime: BAO, work of Bernasconi, Alexander, and Orbach (Ref. 2); H, work of Heinrichs (Refs. 7); CTRW, work of Scher and Lax (Ref. 8); CPA, work of Odagaki and Lax (Ref. 9). A and B are defined in Table I.

The principal purpose of the present calculation was to provide an exact solution of a percolation conducting problem as a standard against which approximate methods can be tested.

A comparison between the Scher-Lax continuous-time random walk (CTRW),[8] the coherent-potential approximation (CPA),[9] and the exact results of this paper for the bond-percolation model is presented in Table I for the low-frequency behavior and in Table II for the high-frequency behavior. The CTRW and CPA methods are both found to be qualitatively correct in their dependence on frequency and their singular dependence on p, but quantitative differences with respect to each other and the exact solution are shown to be significant. Figure 3 shows the relative merits of the various approximations[2,7-9] in the low-frequency regime, where the ratio of A/A_{exact} and B/B_{exact} (A and B are defined in Table I) are plotted versus p.

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