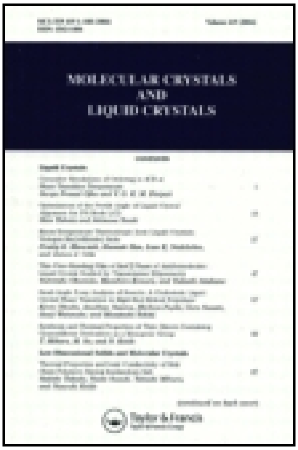

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HOPPING CONDUCTION IN ONE-DIMENSIONAL RANDOM CHAINS*

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Hopping conduction in one-dimensional chains is studied for two types of random distribution of the nearest neighbor jump rate w. The exact frequency dependence of the ac conductivity is obtained for a bond-percolation model where the jump rate vanishes randomly. The real and imaginary part of the ac conductivity are shown to vanish quadratically and linearly with the frequency, respectively. Critical behaviors at the percolation threshold are discussed. A distribution $\rho w^{\rho-1}/w_0^{\rho}$ $(0 \leqslant w \leqslant w_0,\ \rho > 0)$ for the jump rate is used to describe hopping conduction among randomly-located sites, where ρ is the dimensionless number density of the sites. Using the coherent medium approximation, it is shown that an insulator-to-metal transition takes place at $\rho = 1$. Five regimes, depending on the value of ρ, are possible for the low frequency behavior of the conductivity, the ac part of the conductivity at low frequencies is quasi-symmetric around $\rho = 1$ and for $0 < \rho \leqslant 1$ a carrier can disappear from its initial site even though the dc conductivity vanishes.

I. INTRODUCTION

In this paper, we study stochastic transport due to hopping of carriers on one-dimensional chains, in which the motion of carriers is governed by the usual random walk equation with random elementary jump rates. Let $P(x,t\,|\,x_0,0)$ be the conditional probability that one finds a carrier at site x at time t if it was at

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site x_0 at t=0. We assume that the Laplace transform $\tilde{P}(x, u \mid x_0)$ of $P(x, t \mid x_0, 0)$,

$$\tilde{P}(x, u \mid x_0) = \int_0^\infty P(x, t \mid x_0, 0)\, e^{-ut}\, dt \,, \tag{1.1}$$

obeys a master equation

$$(u + w_{x+1,x} + w_{x-1,x})\tilde{P}(x, u \mid x_0) - w_{x,x-1}\tilde{P}(x-1, u \mid x_0)$$

$$- w_{x,x+1}\tilde{P}(x+1, u \mid x_0) = \delta(x, x_0) \,. \tag{1.2}$$

Here, we have neglected carrier-hops beyond nearest neighbors. We assume, for simplicity, $w_{x,x+1} = w_{x+1,x}$. It has been shown in the linear response regime that when $kT << \hbar\omega$ the ac conductivity $\sigma(\omega)$ due to the hopping motion can be expressed in the form of a generalized Einstein relation[1,2]

$$\sigma(\omega) = \frac{ne^2}{kT} D(\omega) \,, \tag{1.3}$$

where the generalized diffusion constant $D(\omega)$ is given by the second spatial moment of $\tilde{P}(x, u \mid x_0)$

$$D(\omega) = -\frac{\omega^2}{2} \sum_x (x-x_0)^2 < \tilde{P}(x, i\omega \mid x_0) > \,, \tag{1.4}$$

where n is the number density of the carrier with a charge e, k is the Boltzmann constant, T is the absolute temperature and $<\cdots>$ denotes an ensemble average over possible jump rates.

A formal solution of the master equation (1.2) is readily written as the (x,x_0) matrix element of a *random walk propagator* $(u\mathbf{1} - \mathbf{H})^{-1}$,

$$\tilde{P}(x, u \mid x_0) = \{(u\mathbf{1} - \mathbf{H})^{-1}\}_{xx_0} \,, \tag{1.5}$$

where $\mathbf{H}$ is the tridiagonal hopping matrix of infinite dimension

$$\mathbf{H} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & w_{-2-1} & \Gamma_{-1} & w_{-10} & 0 & 0 & \cdot \\ \cdot & 0 & w_{0-1} & \Gamma_0 & w_{01} & 0 & \cdot \\ \cdot & 0 & 0 & w_{10} & \Gamma_1 & w_{12} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \tag{1.6}$$

with $\Gamma_x = -w_{x-1,x} - w_{x+1,x}$ and $\mathbf{1}$ is the unit matrix. The jump rates $\{w_{x,x+1}\}$ are random variables which have a distribution suitable for individual systems.

II. EXACT RESULTS FOR A BOND-PERCOLATION MODEL

In actual one-dimensional chains, hopping of carriers may be prohibited by infinitely high barriers or disruptions. The simplest model to describe the effects of the disruptions is the bond-percolation model where each jump rate obeys a distribution

$$P(w_{x,x+1}) = p\,\delta(w_{x,x+1} - w_0) + (1-p)\,\delta(w_{x,x+1}) \ . \tag{2.1}$$

Here, $\delta(w)$ is a Dirac δ-function and $w_0 \neq 0$. An important consequence of the distribution (2.1) is that the hopping matrix is reduced to a block-diagonal form and an N-site block has a structure

$$\mathbf{H}_N = \begin{bmatrix} -w_0 & w_0 & 0 & \cdot & \cdot & 0 \\ w_0 & -2w_0 & w_0 & \cdot & \cdot & \cdot \\ 0 & w_0 & -2w_0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & -2w_0 & w_0 \\ 0 & \cdot & \cdot & \cdot & w_0 & -w_0 \end{bmatrix} \tag{2.2}$$

for $N = 2, 3, \cdots$ and $\mathbf{H}_1 = [0]$. Each block corresponds to a finite cluster which is separated from the rest of the system by two broken bonds at both ends of the cluster. Therefore, the transition probability $\tilde{P}(x,u\,|\,x_0)$ vanishes unless x and x_0 belong to the same cluster and the diffusion constant (1.4) reduces to a weighted average of those of finite clusters:[3,4]

$$D(\omega) = \sum_{N=1} N(1-p)^2 p^{N-1}\, D_N(\omega) \ , \tag{2.3}$$

where the diffusion constant for an N-site cluster $D_N(\omega)$ is defined by

$$D_N(\omega) = -\frac{\omega^2}{2N} \sum_{x,x_0}^{N} (x - x_0)^2 \{(i\omega \mathbf{1}_N - \mathbf{H}_N)^{-1}\}_{x,x_0} \tag{2.4}$$

and the factor $N(1-p)^2\,p^{N-1}$ is the probability that a given site is a member of an N-site cluster. Here, $\mathbf{1}_N$ is an $N\times N$ unit matrix. It is elementary to evaluate the matrix elements of $(i\omega \mathbf{1}_N - \mathbf{H}_N)^{-1}$ and $D_N(\omega)$ is given[3] by

$$D_N(\omega)/a^2 w_0 = 1 + N^{-1}\{1 - (4/\tilde{\omega})i\}^{1/2}\{(z_+^{2N} + 1)^{-1} - (z_-^{2N} + 1)^{-1}\} \ , \tag{2.5}$$

where $z_\pm = (\sqrt{i\tilde{\omega}} \pm \sqrt{i\tilde{\omega}+4})/2$, $\tilde{\omega} = \omega/w_0$ and a is the lattice constant. The average of $D_N(\omega)$, Eq. (2.3), was carried out numerically to yield the frequency dependence of $D(\omega)$ shown in Fig. 2.1. We notice three typical behaviors; (i) a level-off at the high frequency limit; (ii) the real and imaginary parts of $\tilde{D}(\omega)$ vanish quadratically and linearly in frequency at the static limit, respectively, and (iii) a gradual transition from the low frequency to the high frequency regimes. Actually, the limiting behaviors read as

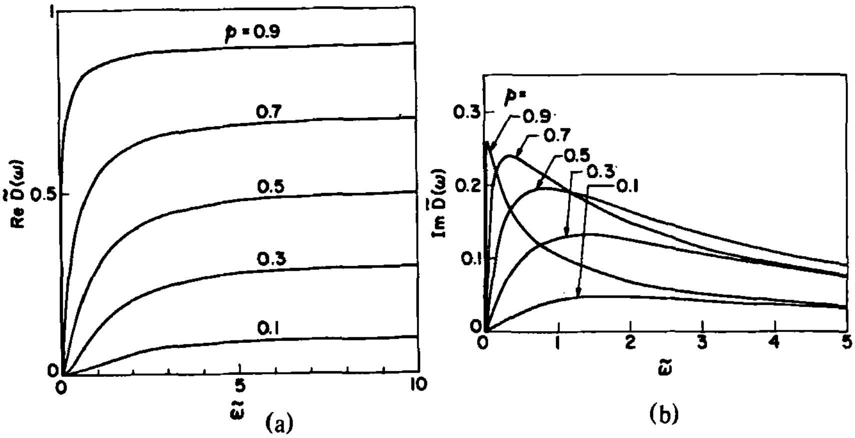
$$\tilde{D}(\omega) \sim p + \frac{2p(1-p)}{\tilde{\omega}}\, i - \frac{2p(1-p)}{\tilde{\omega}^2} \qquad \text{as } \omega \to \infty \ , \tag{2.6}$$

and

$$\tilde{D}(\omega) \sim \frac{p}{2(1-p)^2}\,\tilde{\omega} i + \frac{p(1+p)^2}{4(1-p)^4}\,\tilde{\omega}^2 \qquad \text{as } \omega \to 0 \ . \tag{2.7}$$

Therefore, $\tilde{D}(\omega)$ shows the following critical behaviors at the percolation threshold $p = p_c$ ($p_c = 1$):

$$\lim_{\tilde{\omega}\to 0} \frac{\mathrm{Re}\,\tilde{D}(\omega)}{\tilde{\omega}^2} \propto (p_c - p)^{-4} \quad \text{and} \quad \lim_{\tilde{\omega}\to 0} \frac{\mathrm{Im}\,\tilde{D}(\omega)}{\tilde{\omega}} \propto (p_c - p)^{-2} \ . \tag{2.8}$$



(a) (b)

FIGURE 2.1 The frequency dependence of the dimensionless diffusion constant $\tilde{D}(\omega) \equiv D(\omega)/a^2 w_0$ for the bond-percolation model in a chain; (a) the real part of $\tilde{D}(\omega)$ and (b) the imaginary part of $\tilde{D}(\omega)$.

The divergence of $\mathrm{Im}\,\tilde{D}(\omega)/\tilde{\omega}$ at $p=p_c$ implies that the dielectric constant also diverges at $p=p_c$.

We can also easily calculate the probability that a carrier will remain at its initial site:[5]

$$\langle P(x_0,\infty \mid x_0,0)\rangle_{x_0} = 1 - p \ . \tag{2.9}$$

III. COHERENT MEDIUM APPROXIMATION

Recently, we have applied the idea of the coherent potential approximation[6] to obtain an approximate ensemble average of the random walk propagator.[2] The essential idea of the coherent medium approximation is the following: Suppose we try to find a coherent hopping matrix $\mathbf{H}_c$ defined by

$$\langle (u\mathbf{1} - \mathbf{H})^{-1}\rangle = (u\mathbf{1} - \mathbf{H}_c)^{-1} \ . \tag{3.1}$$

We assume $\mathbf{H}_c$ has a form

$$\mathbf{H}_c = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & w_c & -2w_c & w_c & 0 & 0 & \cdot \\ \cdot & 0 & w_c & -2w_c & w_c & 0 & \cdot \\ \cdot & 0 & 0 & w_c & -2w_c & w_c & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}, \tag{3.2}$$

where w_c is a coherent jump rate and can be a function of u. Now, we replace one of the coherent jump rates w_c in the coherent medium by an actual jump rate, say, w_{12}. The hopping matrix $\mathbf{H}_A$ of this system can be written as

$$\mathbf{H}_A = \mathbf{H}_c + \mathbf{V} \ , \tag{3.3}$$

where the perturbation $\mathbf{V}$ is given by a matrix of infinite dimension whose nonvanishing elements are only an 2×2 submatrix,

$$\mathbf{V} = \begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & 0 & 0 & 0 & 0 & \cdot \\ \cdot & 0 & w_c - w_{21} & w_{12} - w_c & 0 & \cdot \\ \cdot & 0 & w_{21} - w_c & w_c - w_{12} & 0 & \cdot \\ \cdot & 0 & 0 & 0 & 0 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} . \tag{3.4}$$

The coherent jump rate w_c is approximately determined by a self-consistency condition

$$\left\langle (u\mathbf{1} - \mathbf{H}_A)^{-1} \right\rangle = (u\mathbf{1} - \mathbf{H}_c)^{-1} \ , \tag{3.5}$$

where the average is taken over possible w_{12}. It is easy to see that condition (3.5) yields a single scalar equation for w_c

$$\frac{1 - u\bar{P}(x_0,u \,|\, x_0)}{2w_c} \equiv \frac{1}{\Xi + 2w_c} = \int \frac{P(w_{12})}{\Xi + 2w_{12}} \, d\, w_{12} \ , \tag{3.6}$$

where Ξ is defined by the lefthand side and the diagonal matrix element $\bar{P}(x_0,u \,|\, x_0)$ of the coherent random walk propagator is given by

$$\bar{P}(x_0, u \,|\, x_0) = (u^2 + 4uw_c)^{-1/2} \ . \tag{3.7}$$

The diffusion constant of our coherent medium is simply given by

$$D(\omega) = a^2 w_c \ . \tag{3.8}$$

The ensemble average of the probability that a carrier will remainat its initial position can be evaluated from $\bar{P}(x_0,u \,|\, x_0)$ by

$$\lim_{t\to\infty} \left\langle P(x_0,t \,|\, x_0) \right\rangle_{x_0} = \lim_{u\to 0} u \, \bar{P}(x_0,u \,|\, x_0) \ . \tag{3.9}$$

IV. A POWER LAW DISTRIBUTION

Suppose a chain on which hopping sites are randomly located. The distance r between adjacent hopping sites obeys a Poisson distribution

$$p(r) = n_s \exp(-n_s r) \ , \tag{4.1}$$

if hopping sites are uniformly distributed with a fixed number density n_s. We assume that hopping of carriers is important only between adjacent sites and negligible between further neighbors, and also assume that a jump rate $w(r)$ between adjacent sites depends exponentially on the distance r between these sites;

$$w(r) = w_0 \exp(-r/R_d) \ . \tag{4.2}$$

Here, w_0 and R_d are relevant scaling parameters of frequency and distance. Equations (4.1) and (4.2) imply that the jump rate between adjacent sites x and

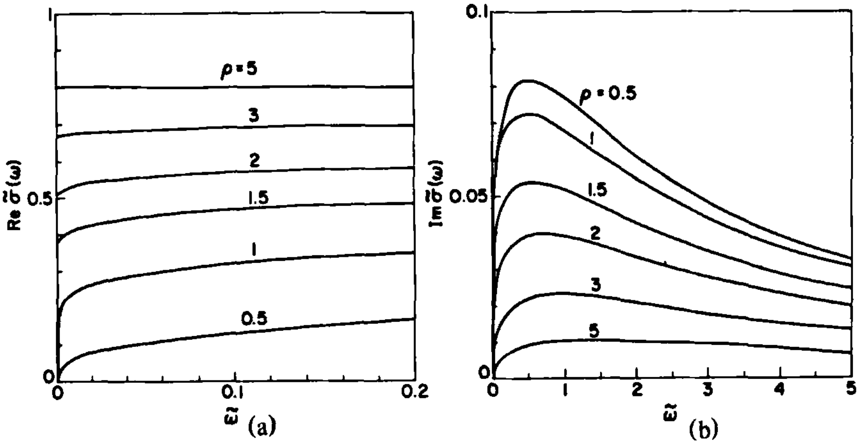


FIGURE 4.1 The frequency dependence of the dimensionless conductivity $\tilde{\sigma}(\omega) = \sigma(\omega)kT/ne^2$ for the power law distribution; (a) the real part of $\tilde{\sigma}(\omega)$ and (b) the imaginary part of $\tilde{\sigma}(\omega)$. $\tilde{\omega} \equiv \omega/w_0$.

$x+1$ obeys a distribution

$$P(w_{x,x+1}) = \begin{cases} \rho(w_{x,x+1})^{\rho-1}/(w_0)^\rho & 0 \leqslant w_{x,x+1} \leqslant w_0 \\ 0 & \text{otherwise} \end{cases} \tag{4.3}$$

with $\rho = n_s R_d$.

Now we study a chain whose lattice constant is $a = 1/n_s$ and the nearest neighbor jump rates obey the distribution (4.3). We solved Eqs. (3.6) and (3.7) with the distribution (4.3) numerically and obtained the frequency dependence of the dimensionless ac conductivity $\tilde{\sigma}(\omega) \equiv \sigma(\omega)kT/ne^2$ shown

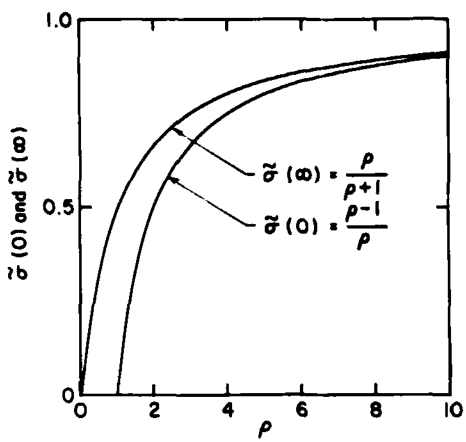


FIGURE 4.2 The ρ-dependence of $\tilde{\sigma}(0)$ and $\tilde{\sigma}(\infty)$. The real part of the ac conductivity $\tilde{\sigma}(\omega)$ shows the frequency dependence bounded by $\tilde{\sigma}(0)$ and $\tilde{\sigma}(\infty)$.

Table 4.1 The low frequency behavior of $\tilde\sigma(\omega)$ for the power law distribution. $\tilde\sigma(\omega) \equiv \tilde\sigma(0) + \tilde\sigma_1(\omega)$ and $\tilde\omega \equiv \omega/w_0$.

ρ	$\tilde\sigma(0)$	$\tilde\sigma_1(\omega) \quad (\omega \sim 0)$
$2 < \rho$	$\frac{\rho-1}{\rho}$	$\left(\frac{\rho-1}{\rho}\right)^{1/2} \frac{1}{2\rho(\rho-2)}(i\tilde\omega)^{1/2}$
$\rho = 2$	$1/2$	$-(1/8\sqrt{2})(i\tilde\omega)^{1/2}\ln(i\tilde\omega)$
$1<\rho<2$	$\frac{\rho-1}{\rho}$	$\left(\frac{\rho-1}{\rho}\right)^{\frac{\rho+1}{2}} \frac{2^{1-\rho}(\rho-1)\pi}{\sin(\rho-1)\pi}(i\tilde\omega)^{\frac{\rho-1}{2}}$
$\rho = 1$	0	$-2/\ln\{-i\tilde\omega/\ln(i\tilde\omega)\}$
$0<\rho<1$	0	$\left(\frac{2^{1-\rho}\rho\pi}{\sin\rho\pi}\right)^{-\frac{2}{1+\rho}}(i\tilde\omega)^{\frac{1-\rho}{1+\rho}}$

in Fig. 4.1.[7] We can see the following characteristics: (i) The real and imaginary part level off at the high frequency limit. (ii) The dc conductivity $\sigma(0)$ is zero if $\rho \leqslant 1$ and nonzero if $\rho > 1$, that is a metal-insulator transition takes place at $\rho=1$. (iii) The so-called ac part $\sigma(\omega)-\sigma(0)$ shows various frequency dependences depending on ρ. In fact, we can easily find at the high frequency limit

$$\tilde\sigma(\infty) = \rho/(\rho+1) \; , \tag{4.4}$$

and at the static limit

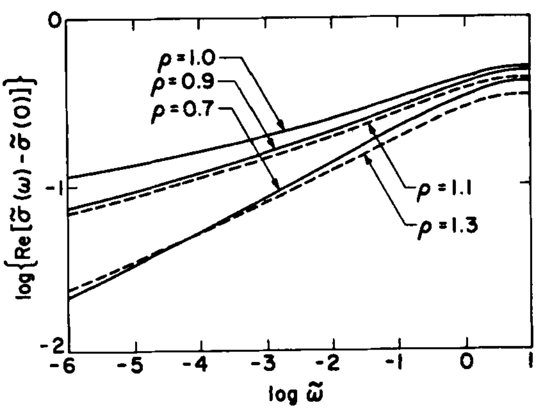


FIGURE 4.3 The low frequency behavior of the real part of $\tilde\sigma_1(\omega) \equiv \tilde\sigma(\omega) - \tilde\sigma(0)$ for $\rho=1$, 1 ± 0.1, 1 ± 0.3. The ac part $\tilde\sigma_1(\omega)$ for $\rho=1\pm\epsilon$ behaves similarly when $\epsilon << 1$.

$$\tilde{\sigma}(0) = (\rho - 1)/\rho \quad \text{if} \quad \rho > 1 \quad \text{and} \quad \tilde{\sigma}(0) = 0 \quad \text{if} \quad 0 < \rho \leqslant 1 \ . \quad (4.5)$$

Figure 4.2 shows the ρ-dependence of $\tilde{\sigma}(0)$ and $\tilde{\sigma}(\infty)$. The real part of the ac condutivity for a given ρ is bounded by $\tilde{\sigma}(0)$ and $\tilde{\sigma}(\infty)$. For the low frequency behavior, we found five regimes classified by the value of ρ, which are summarized in Table 4.1. When $\tilde{\omega} \equiv \omega / w_0 << 1$, the ac part of $\tilde{\sigma}_1(\omega) \equiv \tilde{\sigma}(\omega) - \tilde{\sigma}(0)$ shows a power law dependence on the frequency as $\tilde{\sigma}_1(\omega) = A(i\tilde{\omega})^s$ except for $\rho = 1$ and 2. The factor A and the index s are approximately symmetric near $\rho=1$. [See Figs. 6 and 7 in ref. 7.] Actually, the real parts of $\tilde{\sigma}_1(\omega)$ for $\rho = 1 \pm \epsilon$ ($\epsilon << 1$) behave similarly at low frequencies as depicted in Fig. 4.3.

Using Eq. (3.9) we can easily show that for any $\rho > 0$ $P(x_0, \infty \,|\, x_0, 0) = 0$. Therefore, if $0 < \rho \leqslant 1$ a carrier diffuses infinitely after an infinite time even though the dc conductivity is zero.[8–10]

V. REMARKS

The ac hopping conductivity and the decay of carrier from its initial site of the system described by the master equation (1.1) have been extensively studied by Bernasconi et al[9–12] using scaling arguments and effective medium-type approximations. Their second effective medium approach turns out to be identical to our CMA for one-dimensional chains, although the former is based on the effective medium treatment of a resister network[13] whose Kirchhoff equation is equivalent to the master equation (1.3). In particular, they have studied the power law distribution (4.3) as a prototype of a general distribution for the jump rate, and they obtained three classes according to $\rho \gtreqless 1$.[9,12] However, as we have shown in Section 4, the low frequency behavior of the ac conductivity can be classified into five regimes. A careful analysis shows that there are six regimes of the low frequency behavior for a general distribution if one includes a case where jump rates vanish randomly. These regimes are classified according to the first and second moment of the inverse of the jump rate.[14,15]

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