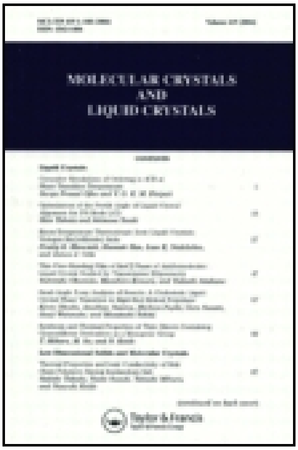

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QUASI-LOCALIZATION EFFECTS IN RANDOM ONE-DIMENSIONAL HOPPING SYSTEMS

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Based on a master equation description, we investigate the classical dc hopping conductivity, g_L, in random one-dimensional systems of finite length L. In particular, we determine the $L\to\infty$ asymptotic properties of its probability distribution, $\rho_L(g)$, and we compare these exact results with the predictions from scaling arguments and with numerical simulations. The limiting behavior of $\rho_L(g)$ is non-universal, and interesting quasi-localization effects are observed if the probability density $\rho(w)$ of the random near neighbor hopping rates behaves singularly as $w\to 0$. We speculate on the experimental observability of these effects, and we point out the similarities and differences with respect to the effects of quantum localization.

I. INTRODUCTION

One-dimensional transport is strongly affected, and sometimes dominated, by the effects of randomness. This is true for quantum mechanical as well as for classical transport, but the respective consequences of disorder exhibit quite different characteristics.

In quantum systems, the zero temperature resistance, for example, has been shown[1,2] to increase exponentially with L, the length of the one-dimensional system. Careful investigations[2-4], however, indicate that quantities such as resistance or conductance do not have well behaved probability distributions in the limit as $L\to\infty$. In particular, the associated ratios (standard deviation)/(mean) diverge with increasing L.

The present paper is concerned with an investigation of the analogous effects for classical transport in random one-dimensional systems. Our model[5,6] is based on a master equation description of classical hopping-type transport on a one-dimensional lattice,

$$\frac{dP_n}{dt} = W_{n,n-1}\,(P_{n-1}-P_n) + W_{n,n+1}\,(P_{n+1}-P_n) \quad . \tag{1}$$

$P_n(t)$ is the probability of finding a hopping particle at site n at time t, and the near neighbor hopping rates, $W_{n,n+1} = W_{n+1,n} \geq 0$, are assumed to be mutually independent random variables, distributed according to a probability density $\rho(w)$.

The behavior of $\rho(w)$ near $w=0$ enters crucially into the asymptotic (e.g. large L, low frequency, long time) properties of transport quantities[5,6], and we shall concentrate on the three representative classes of probability densities that have been considered in previous investigations[5,6]:

Class (a): $\rho(w)$ such that

$$W_{av}^{-1} \equiv \int_0^\infty dw\, \rho(w) w^{-1} < \infty \quad . \tag{2a}$$

Class (b):

$$\rho(w) \to \rho_0 = \text{const.} > 0 \quad , \quad \text{as } w \to 0 \quad . \tag{2b}$$

Class (c):

$$\rho(w) = \begin{cases} (1-\alpha)w^{-\alpha} & 0 \leq w \leq 1 \\ 0 & \text{else} \end{cases} \quad ; \quad 0 < \alpha < 1 \quad . \tag{2c}$$

Class (a) probability densities either have a lower cutoff, or at least go to zero as $w\to 0$. As a special case, class (a) contains the ordered system, $\rho(w) = \delta(w-W_0)$. As long as we are only interested in the asymptotic dependences on the relevant variable, and not in prefactors, class (c) can be extended to contain all $\rho(w)$ that exhibit a power law singularity as $w\to 0$. Most distributions $\rho(w)$ of interest for physical problems either belong to one of the above classes, or are of percolation type, $\rho(w) = p\delta(w)+(1-p)\delta(w-W_o)$. For comparison, we shall therefore also include percolation systems (and the ordered system) into our discussion.

II. INFINITE SYSTEMS

Previous investigations[5,6] have mainly been concerned with time- and frequency-dependent properties of an infinite system described by Eqs.(1). If at time t=0 a particle is placed at the origin, i.e.

$$P_n(0) = \delta_{n,o} \quad , \tag{3}$$

the decay of the initial probability amplitude is given by $\langle P_o(t)\rangle$, and the mean-square displacement by(the lattice constant is unity)

$$\langle x^2(t)\rangle = \sum_{n=-\infty}^{\infty} n^2 \langle P_n(t)\rangle \quad , \tag{4}$$

where $\langle\ldots\rangle$ denotes an average over the (independent) random variables $W_{n,n+1}$ (i.e. an ensemble average). The frequency-dependent hopping conductivity $\sigma(\omega)$ is related to $\langle x^2(t)\rangle$ as follows[5,6](fluctuation-dissipation theorem):

$$\sigma(\omega) = \frac{n_o e^2}{kT} \langle g(\omega)\rangle = \frac{n_o e^2}{kT} \langle D(-i\omega)\rangle \quad , \tag{5}$$

$$\langle D(z)\rangle = \frac{1}{2} z^2 \int_o^\infty dt\, e^{-zt} \langle x^2(t)\rangle \quad , \tag{6}$$

where n_o and e denote density and charge of the hopping particles, and T is temperature. $\langle D(-i\omega)\rangle$ is thus a (frequency-dependent) diffusion constant, and in the following we shall refer to $g(\omega)$ as the normalized conductivity corresponding to a single chain.

The asymptotic properties of $\langle P_o(t)\rangle$, $\langle x^2(t)\rangle$, and $\langle g(\omega)\rangle$ have been shown to be non-universal, i.e. they depend on the probability distribution $\rho(w)$ of the hopping rates. Class (a) systems exhibit the same asymptotic behavior as an ordered system, with an average transfer rate equal to W_{av} (defined in Eq.(2a))[5,6]:

$$<P_o(t)> \approx (4\pi\, W_{av})^{-1/2}\, t^{-1/2} \quad , \quad t \to \infty \quad , \tag{7a}$$

$$<x^2(t)> \approx 2\, W_{av}\, t \quad , \quad t \to \infty \quad , \tag{7b}$$

$$<g(\omega)> \approx W_{av} \quad , \quad \omega \to 0 \quad . \tag{7c}$$

Class (c) systems, on the other hand, exhibit a completely different asymptotic behavior[5,6],

$$<P_o(t)> \propto t^{-(1-\alpha)/(2-\alpha)} \quad , \quad t \to \infty \quad , \tag{8a}$$

$$<x^2(t)> \propto t^{2(1-\alpha)/(2-\alpha)} \quad , \quad t \to \infty \quad , \tag{8b}$$

$$<g(\omega)> \propto (-i\omega)^{\alpha/(2-\alpha)} \quad , \quad \omega \to 0 \quad , \tag{8c}$$

The class (b) behavior is intermediate[5,6] with logarithmic corrections to the class (a) behavior. We note that the results for $<P_o(t)>$ are exact, whereas those for $<x^2(t)>$ and $<g(\omega)>$ rely on the validity of a scaling hypothesis[5,6].

If $\rho(w)$ does not belong to class (a), the decay of $<P_o(t)>$ and the increase of $<x^2(t)>$ are thus slower than in an ordered system, and $<g(\omega)>$ exhibits an anomalous low-frequency behavior, leading to a vanishing dc conductivity, $<g(0)> = 0$. These effects result from a slowing down, or quasi-localization, of the hopping particles, induced by the randomness of the hopping rates.

III. SYSTEMS OF FINITE LENGTH

If the dc conductivity, $<g(0)>$, vanishes for the infinite system, it is of interest to study its decay with increasing sample length. In the following, we therefore concentrate on finite systems, and on the dc conductivity,

$$g_L \equiv \lim_{\omega \to 0} g_L(\omega) \quad , \tag{9}$$

where L denotes the length of the system. To be definite, we define $g_L(\omega)$ as the normalized conductivity of an infinite system that consists of periodical repetitions of an array of L hopping rates, $(W_1, W_2, \ldots, W_L)$. From its definition, see Eqs.(4)-(6), and by performing the limit $\omega \to 0$, it follows[7] that g_L is simply given by

$$g_L = L \cdot G_L = L \cdot \left[\sum_{n=1}^{L} W_n^{-1} \right]^{-1} \quad . \tag{10}$$

We note that this result, despite its simplicity, is nontrivial, and that its derivation[7] is rather involved. It allows, however, for a very obvious interpretation. If the W_n are considered to represent "conductances", G_L is the "equivalent conductance" corresponding to a network which consists of L conductances in series.

A study of the L-dependence of the dc conductivity g_L thus amounts to an investigation of the properties of the inverse of a sum of L independent random variables. For a given probability density $\rho(w)$ of the hopping rates, we denote the probability density of the conductivity g_L by $\rho_L(g)$, and our aim is the determination of the $L \to \infty$ asymptotic behavior of $\rho_L(g)$. In particular, we shall be interested in the asymptotic behavior of corresponding averages, such as the average conductivity,

$$\langle g_L \rangle = \int_0^\infty dg \; \rho_L(g) \; g \quad , \tag{11}$$

and the standard deviation,

$$\Delta g_L = \left[\langle g_L^2 \rangle - \langle g_L \rangle^2 \right]^{1/2} \quad . \tag{12}$$

For an <u>ordered system</u> the problem is trivial, and one has $g_L = W_0$, independent of L. <u>Percolation systems</u> are also easily investigated, and it follows that

$$\rho_L(g) = (1-e^{-\lambda L})\delta(g) + e^{-\lambda L}\,\delta(g-W_0) \tag{13}$$

for any finite L, where $\lambda \equiv -\ln(1-p)$. The average conductivity thus decreases exponentially, $\langle g_L \rangle = W_0 \exp(-\lambda L)$, but the standard deviation exhibits a slower decrease, so that $\Delta g_L / \langle g_L \rangle \approx \exp(\lambda L/2)$ diverges as $L \to \infty$.

For more interesting hopping rate distributions, i.e. for the classes (a),(b), and (c) above, we have recently been able[7] to derive the exact asymptotic behavior of

$\rho_L(g)$. The corresponding results will be summarized in section V, but in the next section we shall first analyze the predictions of a qualitative scaling approach.

IV. SCALING ARGUMENTS

The scaling arguments presented in this section are very similar to those used in previous investigations[6,8] to describe the low frequency and long time asymptotic properties of infinite systems. We first observe that for class (a) distributions, one expects from Eq.(10) that $\langle g_L \rangle \approx W_{av}$ as $L\to\infty$, where W_{av} is defined in Eq.(2a).

For probability densities $\rho(w)$, for which W_{av} does not exist, we choose some small cutoff hopping rate W_c. The average length $L(W_c)$ of a segment for which all W_n are larger than W_c is then given by

$$L \approx \left[\int_0^{W_c} dw\ \rho(w)\right]^{-1} \quad , \tag{14}$$

if W_c is small enough. For systems of length L, we can therefore approximate the true $\rho(w)$ by a corresponding distribution which has a lower cutoff at $W_c = W_c(L)$, given by Eq.(14). For this truncated distribution, however, $W_{av} = W_{av}(W_c)$ exists, and we can approximate $\langle g_L \rangle$ by

$$\langle g_L \rangle \approx W_{av}(W_c) \approx \left[\int_{W_c}^{\infty} dw\ \rho(w) w^{-1}\right]^{-1} \quad . \tag{15}$$

The cutoff W_c, which defines our length scale, can now be eliminated from Eqs.(14) and (15), leading to a qualitative prediction for the decay of $\langle g_L \rangle$ with increasing L. Applied to class (b) and class (c) distributions, this procedure leads to the following explicit expressions for the $L\to\infty$ asymptotic decay of $\langle g_L \rangle$:

$$\langle g_L \rangle \approx (\rho_0 \ \ell n\ L)^{-1} \qquad [\text{class (b)}] \quad , \tag{16a}$$

$$\langle g_L \rangle \approx \frac{\alpha}{1-\alpha}\ L^{-\alpha/(1-\alpha)} \qquad [\text{class (c)}] \quad . \tag{16b}$$

The predictions can be compared with numerical simulations, and in Fig.1 we present results for two different

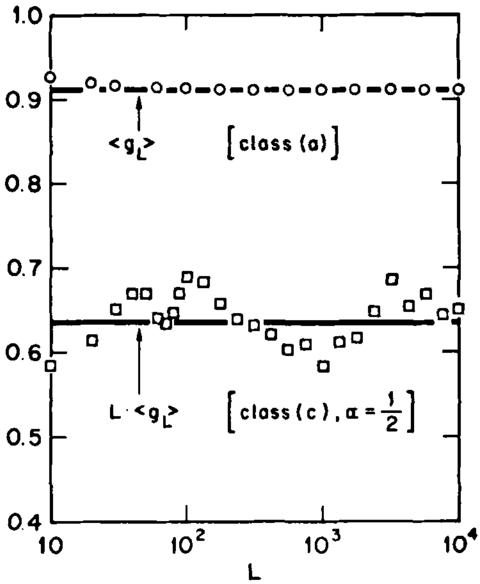

FIGURE 1 Average dc conductivity $<g_L>$ vs. sample length L for a class (a) and a class (c) distribution of hopping rates (see text). Numerical simulations (○ and □) represent averages over 10^3 samples, and the horizontal lines indicate the exact asymptotic limits.

distributions of hopping rates. The first corresponds to a $\rho(w)$ which is one for $1/2 \leq w \leq 3/2$, and zero otherwise. It belongs to class (a), with $\overline{W_{av}} = 1/\ell n3 \simeq 0.910$, and we see that the numerical results converge very rapidly to this limiting value. The second is a class (c) distribution, and we have chosen $\alpha=1/2$, so that Eq.(16b) would predict $L<g_L> \to 1$ as $L \to \infty$. The numerical results indicate that the above scaling arguments seem to give the correct L-dependence, $<g_L> \propto L^{-1}$, but also that they fail to predict the correct limit for $L<g_L>$, which turns out to be $2/\pi$ (see section V). In addition, the scattering of the data, which represent an average over 1000 samples, is much larger than for the class (a) distribution. This shows that it is not sufficient to study the average of g_L, but that we also have to determine the asymptotic properties of its probability distribution, $\rho_L(g)$, which is beyond the scope of such scaling arguments.

V. EXACT RESULTS

The asymptotic form of $\rho_L(g)$ can, in fact, be determined exactly, at least for the three classes of hopping rate distributions defined above [Eqs.(2a)-(2c)]. The mathematical details will be presented in separate publications[7], and in the following we only give a brief summary of the main results.

As $L\to\infty$, $\rho_L(g)$ approaches a homogeneous function representation,

$$\rho_L(g) = \lambda_L \; h(\lambda_L g) \quad , \tag{17}$$

where the scaling factor λ_L, as well as the limiting scaling function $h(x)$, are functionals of the hopping rate distribution $\rho(w)$.

For <u>class (a)</u> distributions one obtains $h(x) = \delta(x-1)$, and $\lambda_L = W_{av}^{-1}$. It follows that

$$\lim_{L\to\infty} \langle g_L\rangle = W_{av} \quad , \quad \lim_{L\to\infty} \Delta g_L = 0 \quad , \tag{18}$$

and we note that W_{av}, Eq.(2a), is independent of L.

In <u>class (b)</u> systems one still has $h(x) = \delta(x-1)$, but now $\lambda_L = \rho_0 \,\ell n L$. This implies that the asymptotic decay of $\langle g_L\rangle$ is exactly given by Eq.(16a), and that $\Delta g_L/\langle g_L\rangle$ still vanishes as $L\to\infty$.

For <u>class (c)</u> distributions, finally, $h(x)$ is no longer universal. It depends on α, $h(x) = h_\alpha(x)$, and can be expressed in terms of a generalized hypergeometric function[7]. The scaling factor λ_L is given by $\lambda_L = L^{\alpha/(1-\alpha)}$, and the asymptotic decay of $\langle g_L\rangle$ follows a power law,

$$\langle g_L\rangle \approx \gamma\Gamma(\gamma)\Gamma(\alpha)^{-\gamma} \cdot L^{-\alpha/(1-\alpha)} \quad , \tag{19}$$

where $\gamma = 1/(1-\alpha)$. The standard deviation Δg_L, finally, becomes proportional to $\langle g_L\rangle$,

$$\lim_{L\to\infty} \Delta g_L/\langle g_L\rangle = \left[\gamma^{-1}\,\Gamma(2\gamma)\Gamma(\gamma)^{-2} - 1\right]^{1/2} \quad , \tag{20}$$

so that $\Delta g_L/\langle g_L\rangle$ never becomes small. This reflects the fact that for class (c) distributions the limiting scaling function $h_\alpha(x)$ is not a delta function.

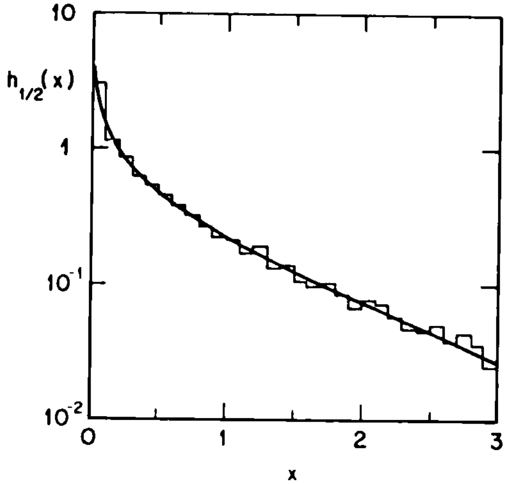

FIGURE 2 Limiting scaling function of the probability density $\rho_L(g)$ for a class (c) hopping rate distribution with α=1/2. The exact asymptotic result for $h_{1/2}(x)$, Eq.(21), is compared with a histogram (10^4 samples) for $h_L(x)$ = $L^{-1}\ \rho_L(L^{-1}x)$ with L=100.

For α=1/2, for example, we have

$$h_{1/2}(x) = \frac{1}{2}\, x^{-1/2} \exp\,(-\,\frac{\pi}{4}\, x) \quad , \tag{21}$$

and

$$\lim_{L\to\infty} L\langle g_L\rangle = \frac{2}{\pi} \quad . \tag{22}$$

The exact asymptotic limit of Eq.(22) is indicated in Fig. 1, and $h_{1/2}(x)$ is plotted in Fig.2, together with a histogram obtained from a numerical evaluation of g_L for 10^4 samples of length L=100. The comparison shows that the corresponding $\rho_L(g)$ is already very close to its limiting behavior.

VI. DISCUSSION

The exact limit theorems for $\rho_L(g)$ imply that the average dc hopping conductivity, $\langle g_L\rangle$, always decays to zero with increasing L, if the minus first moment, W_{av}^{-1}, of the hopping rate distribution $\rho(w)$ does not exist. We thus observe interesting quasi-localization effects in a classical one-dimensional system. The asymptotic properties of the conductivity distribution $\rho_L(g)$ are, however, non-universal. Class (a) systems behave as an ordered system asymptotically, and quasi-localization is not observed at all. For class (b) distributions the decay of $\langle g_L \rangle$ is only logarithmic, and $\Delta g_L/\langle g_L \rangle$ goes to zero, whereas in class (c) systems $\langle g_L \rangle$ exhibits a power law decay, and $\Delta g_L/\langle g_L \rangle$ approaches a finite constant. In percolation systems, finally, $\langle g_L \rangle$ decreases exponentially, and $\Delta g_L/\langle g_L \rangle$ diverges with increasing L.

These non-universal results can be contrasted with the effects of quantum localization[1-4], which occur for any type of disorder, and which are always exponential. In one-dimensional quantum systems one has to analyze a product of random matrices, whereas our classical case requires an investigation of the inverse of a sum of random variables. The peculiar asymptotic properties exhibited by the respective probability distributions are, however, of a rather similar nature, at least in a qualitative, mathematical sense.

Finally, it is interesting to speculate whether classical quasi-localization effects could actually be observed in real physical systems. The best candidates seem to be one-dimensional superionic conductors such as hollandite, whose anomalous transport properties have successfully been analyzed in terms of our classical hopping model. An idealized random barrier model has been shown[9] to lead to a remarkably accurate and detailed description of the experimental results for $\sigma(\omega,T)$ over a wide frequency and temperature range. This model corresponds to a class (c) probability density $\rho(w)$, with a temperature dependent exponent α, $\alpha = 1-T/T_m$. Eq.(19) would thus imply that with increasing sample length L, the dc ionic conductivity should decrease as

$$\sigma_{dc}(T,L) = \sigma_0(T)\cdot L^{-(T_m-T)/T} \quad , \quad T < T_m \quad . \tag{23}$$

For hollandite, where $T_m \approx 450K$ [9], we would thus predict a $L^{-1/2}$ decay of σ_{dc} at T=300K. The magnitude of σ_{dc} at room temperature, however, turns out to be about $10^{-11}(\Omega cm)^{-1}$ for L=10mm, if we use the same model parameters as in Ref.9. A very small lower cutoff in the idealized hopping rate distribution, which cannot be excluded from the ac investigations, would thus prevent an observation of the L-dependence in samples of reasonable length.

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