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Anomalous transport properties for random-hopping and random-trapping models

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Previous work on anomalous transport is extended to two and three dimensions. Using critical-path analysis it is shown that random-hopping models always lead to a finite dc conductivity and diffusion constant and thus to normal asymptotic behavior above 1D. For RT models anomalous behavior is shown to be possible with indices in agreement with the Scher-Lax theory, above 2D. It is also pointed out that such behavior is to be expected for an exponential tail of traps and the temperature dependence is predicted.

The purpose of this paper is to discuss the asymptotic behavior of transport coefficients in amorphous systems. Anomalies in these coefficients are fairly frequently observed and are usually described phenomenologically in the framework of Scher-Lax-Montroll theory.[1,2] This approach maps the random medium on a periodic effective medium with suitably chosen local properties. The physical models of interest are mainly of two types:

(a) Random-hopping (RH) models with symmetric two-site transfer rates

$$W_{i\to j}=W_{j\to i} \tag{1}$$

and a distribution of these rates.

(b) Random trapping (RT) models for which

$$(W_{i\to j}/W_{j\to i})=e^{-(\Delta_i-\Delta_j)/k_BT}\ , \tag{2}$$

where the trap depths (Δ_i) are the dominant random variables.

Within the above effective-medium approaches the two types of problems seem, in essence, equivalent. Both lead to anomalous transport coefficients for sufficiently singular distributions of the random variables. This is obvious in the original waiting function formalism of Scher and Lax,[1] but applies also to similar more complex effective-medium approaches,[3] which use averages of the short-distance properties of the random system to define the properties of the effective medium. Thus Scher and Lax calculate the local average

$$\psi(t)=\left\langle \exp\left[-\left(\sum_j W_{i\to j}\right)t\right]\right\rangle \tag{3}$$

to determine the average probability that a particle has not left its original site in a time t.

For 1D systems these prescriptions are not correct in detail but not wrong in a rough qualitative way. We have shown elsewhere[4-7] how one can construct a correct (nonlocal effective-medium approximation in this case. In 1D one can also show that there is symmetry (though not exact equivalence) between RH and RT models.[6,8] For two- or three-dimensional systems the apparent symmetry between RH and RT models is intuitively surprising. If one waits long enough in an RT model a diffusing particle should eventually fall into deep traps even if they are very rare. The trapping rate is even enhanced as one goes from 1D to 2D to 3D.[9,10] Thus, the long-time behavior of an RT model will always be dominated by the deepest traps. The situation for RH models is quite different. In 1D there is no way around a high (low W) barrier but for higher dimensionalities a low concentration of such barriers can always be avoided. This is indeed the conclusion implied by the critical-path analyis of Ambegaokar, Halperin, and Langer.[11] Following a similar line of analysis we shall show that the RH and RT models are indeed qualitatively different whenever the percolation density is smaller than one (i.e., above 1D). Only the RT models can show anomalous asyptotic behavior.

To estimate the actual transport coefficients we use a self-consistent scheme developed elsewhere[5-7] for one-dimensional problems. This enables us to set a lower limit on the dc conductivity for RH models and to relate the anomalous power laws in RT models to the temperature and trap distribution. Since we have discussed anisotropic (quasi-1D) systems elsewhere[7,12] the discussion is restricted to isotropic systems.

THE RH MODEL

We consider a master equation on a lattice

$$\frac{d\vec{P}}{dt}=\hat{W}\vec{P}\ , \tag{4}$$

where $\vec{P}$ is a vector whose components

$$P_{\vec{i}}=P_{(i_1,i_2,\ldots,i_d)} \tag{5}$$

are the occupation probabilities of the relevant sites (on a d-dimensional lattice). The random matrix $\hat{W}$ describes the transport process. To conserve particle number, one must have

$$\sum_{\vec{j}} W_{\vec{i}\vec{j}} = 0, \; \frac{d}{dt}\left(\sum_{i} P_{\vec{i}}\right) = 0 \; . \tag{6}$$

For random hopping (RH) one further assumes symmetry [Eq. (1)]

$$W_{\vec{i}-\vec{j}} = W_{\vec{j}-\vec{i}} \; . \tag{1'}$$

For simplicity we finally assume that W only couples nearest neighbors on the lattice

$$\begin{aligned} W_{\vec{i},\vec{j}} &= w \text{ for } \vec{i}, \vec{j} \text{ as nearest neighbors} \\ W_{\vec{i}\vec{i}} &= \sum_{j} W_{\vec{i}\vec{j}} \\ &= 0 \text{ otherwise.} \end{aligned} \tag{7}$$

Finally, we assume the values of the transfer rates (w) to be independent random variables on each bond with a random distribution $\rho(w)$.

We first want to show that an RH model always has a finite dc conductivity. We do this by setting a lower limit on this quantity. We are interested in the effect of small W on the transport properties. Consider for definiteness the mean square and width of the distribution

$$\langle X^2(t)\rangle = \sum_{j} \vec{j}^2 P_{\vec{j}}(t), \;\; P_{\vec{j}}(0) = \delta(\vec{j}) \tag{8}$$

For a normal system

$$\lim_{t\to\infty} \langle X^2(t)\rangle = Dt \; , \tag{9}$$

where D is a constant. Anomalous behavior would show up if one had instead

$$\lim_{t\to\infty} \langle X^2(t)\rangle \propto t^{2\nu} \tag{10}$$

where $\nu < \frac{1}{2}$. On a 1D chain this occurs when $\rho(W)$ is sufficiently singular,[4] i.e., when

$$\lim_{w\to 0} \rho(w) \propto w^{-\alpha}, \;\; 0 \leq \alpha < 1 \; . \tag{11}$$

Such distributions lead, in 1D, to an anomalous $\nu[=(1-\alpha)/(2-\alpha)]$ and to a frequency-dependent diffusion constant and conductivity[4-7,13]

$$\sigma(\omega) \propto (-i\omega)^{\alpha/(2-\alpha)}, \;\; \omega \to 0 \; . \tag{12}$$

On the other hand, when $\rho(W)$ is such that

$$\langle 1/W\rangle = \int dw[\rho(w)/w] \tag{13}$$

is defined, one has $\nu = \frac{1}{2}$ and

$$\lim_{\omega\to 0} \sigma(\omega) \propto \langle 1/W\rangle^{-1} \; . \tag{14}$$

Now for an RH model the conductance of a (2D or 3D) lattice cannot be smaller than that of a bundle of disconnected 1D strings placed in parallel. For example, the conductance on a cubic lattice along the x axis cannot be smaller than that of the 1D strings one obtains if one only keeps connections along x and disconnects parallel rods. Equality holds for an ordered system but, in general, not in the presence of disorder. Analogous constructions are always possible and it follows that the existence of a finite dc conductivity for a given $\rho(w)$ in 1D is sufficient to assure that it is also finite for higher dimensionalities. Thus, anomalous behavior cannot occur for distributions which lead to (13). The actual value of the conductivity is, of course, always higher than would be implied by Eq. (14), because the small W will tend to be shunted out by parallel connections. We emphasize that this argument does not apply to RT models. It is thus sufficient to consider singular distributions [Eq. (11)] which would lead to anomalous behavior in 1D.[5-7] In analogy to the procedure we have used for the 1D situation, we introduce a lower curoff into $\rho(w)$, for example W_m, and remove all W smaller than W_m from the lattice. This defines a percolation problem. The total density of removed bonds is:

$$\int_0^{W_m} \rho(w)dw = 1 - P. \tag{15}$$

On the resulting percolation network of (bond density ρ), the W are distributed according to

$$\tilde{\rho}(w;W_m) = \begin{cases} P^{-1}\rho(w), & w > W_m \\ 0, & w < W_m \; . \end{cases} \tag{16}$$

Obviously the conductivity of this network $[\sigma(W_m)]$ is a lower bound on σ. The removal of the small W ($< W_m$) cannot increase the conductivity. Thus

$$\sigma > \sigma(W_m). \tag{17}$$

To have a finite $\sigma(W_m)$ one wants

$$1 > p(W_m) > p_c \; ,$$

where p_c is the critical percolation density. We now want to estimate $\sigma(W_m)$. For p close to p_c the conducting skeleton of the percolation network consists of long 1D strands between junctions whose length is

$$l \propto (p - p_c)^{(d-2)\nu_d - t_d} \; , \tag{18}$$

where t^d and ν^d are the conductivity and correlation length exponents for percolation. These strands have an average conductance W_{eff}/l where

$$W_{eff} = (\langle 1/W \rangle_{W_m})^{-1} , \tag{19}$$

$$\langle 1/W_m \rangle_{W_m} = \int dw [\tilde{p}(w, W_m)/w] . \tag{20}$$

The conductivity of a network with the same p for which all W are replaced by W_{eff} is a lower bound on $\sigma(W_m)$

$$\sigma(W_m) > W_{eff}(p - p_c)^{t_d} . \tag{21}$$

For small $(p - p_c)$ (i.e., when l is large) the right-hand side of Eq. (21) should be a good approximation. Specifically, when

$$l \gg W_m^{\alpha - 1} , \tag{22}$$

the variance of the strand conductances becomes small. When this is not the case, one still has a lower bound. High-conductance strands are weighted more heavily than those with low conductance in the network conductivity.

We have thus determined a lower bound for σ:

$$\sigma > \sigma(W_m) > W_{eff}(p - p_c)^{t_d} . \tag{23}$$

We can improve this somewhat by maximizing the right-hand side of (23) with respect to W_m. From Eqs. (11), (16), and (19) one has

$$W_{eff}(W_m) \propto W_m^{\alpha} , \tag{24}$$

and from (15)

$$p - p_c \propto \int_{W_m}^{W_c} w^{-d} dw \propto W_c^{1-d}(1 - \lambda_m^{1-\alpha}) , \tag{25}$$

where we have defined

$$p(W_c) = p_c , \quad \lambda_m = W_m/W_c . \tag{26}$$

Thus

$$W_{eff}(p - p_c)^t = W_c^{\alpha + (1-\alpha)t} \lambda_m^{\alpha} (1 - \lambda_m^{1-\alpha})^t . \tag{27}$$

The maximum of this limit is found for

$$\lambda_m = \{\alpha / [\alpha + (1 - \alpha)t]\}^{1/(1-\alpha)} , \tag{28}$$

giving

$$(p - p_c)/p_c = \frac{(1 - \alpha)t}{\alpha + (1 - \alpha)t} \tag{29}$$

and

$$\sigma > W_c^{\alpha + (1-\alpha)t} \alpha^{\alpha} [(1 - \alpha)t]^t / [\alpha + (1 - \alpha)t]^{\alpha + t} . \tag{30}$$

This is in the same spirit as the Ambegaokar, Halperin, and Langer limit.[11] As pointed out earlier, this is probably not very good as a numerical estimate except for $\alpha \lessapprox 1$ when $p - p_c$ becomes small [Eq. (29)]. This is also true for another reason. In 3D p_c is quite low (~0.15). Thus the low-W behavior [Eq. (11)] is not really meaningful near p_c except in the most singular limit $\alpha \approx 1$.

We emphasize that we have assumed a singular distribution with no lower cutoff [i.e., Eq. (11)] which would lead to anomalous behavior if used, e.g., in the Scher-Lax analysis [Eq. (3)].

The fact that we have shown that the dc conductivity must be finite obviously does not imply that no anomalies will be observed in random systems at higher frequencies. Such anomalies are, in fact, very common. For anisotropic systems they can be described very well as crossover effects from anomalous one-dimensional to normal three- (or two-) dimensional behaviors and comparison with experiment seems very satifactory.[7,12] For an isotropic 3D system the situation is more complex.[15] The very-short-time behavior can, of course, be determined from a cluster expansion. For longer times one is tempted to generalize the critical-path analysis to finite frequencies. There are, however, two difficulties. Even for diffusion on a percolation network, the short-time behavior is not well understood. There is obviously a crossover when the mean-square distance traveled becomes comparable to the connectivity correlation length and the high-frequency behavior cannot be deduced from the dc conductivity. In the present problem, one has an additional scale introduced by the random distribution. Thus, a naive approach does not seem very meaningful.

RANDOM-TRAPPING MODELS

As emphasized above, there is a fundamental difference between RT and RH models above 1D. This reflects the qualitatively different dimensional dependence of the two problems. As d increases it becomes easier to *avoid* a low-W bond. This is reflected in the fact that the critical percolation density decreases

$$\frac{dp_c(d)}{d(d)} < 0 . \tag{31}$$

On the other hand, the trapping probability $\pi(t)$ *increases* with d (for a given concentration of traps). The upper critical dimensionality for this problem is two.[9,10] For $d > 2$

$$\frac{d\pi}{dt} = Ac_t\,, \quad \pi(t) \propto t\,, \quad t \to \infty \tag{32}$$

where A is a (lattice-dependent) constant of order 1 and c_t is the trap concentration. This is to be contrasted with the much slower 1D behavior

$$\pi(t) \propto t^{1/2}\ . \tag{33}$$

[In 2D there are logarithmic corrections to $\pi(t)$ and the situation is somewhat more complex.]

Specific RT models have been considered in the literature and shown to lead to anomalous behavior.[14] We have considered the 1D case in Ref. 6. To compare with our random barrier analysis, we consider the analog of Eq. (11):

$$\rho(\theta) \propto \theta^{-\alpha}\,, \quad \theta \to 0 \tag{34}$$

where

$$\theta = \exp[-(\Delta/T)] \tag{35}$$

and θ measures the effectiveness of the trap. It is easy to see that this corresponds to an exponential tail in the trap distribution

$$p(\Delta) \propto \exp[-(\Delta/T_0)]\,, \quad \alpha = (T_0 - T)/T_0\ . \tag{36}$$

This is therefore a very reasonable distribution for amorphous insulators or semiconductors. To simplify the model we assume

$$W_{i\to j} = W\theta_i \tag{37}$$

and for convenience set $W=1$ below.

We try to set limits on the frequency-dependent diffusion θ_m. Now for a walk of N steps on the lattice, the probability of being trapped in a deep trap with $\theta < \theta_m$ is small if

$$N < \left(\int^{\theta_m} \rho(\theta)\,d\theta\right)^{-1} \approx \theta_m^{-(1-\alpha)}\ . \tag{38}$$

On the other hand, for a walk involving only $\theta > \theta_m$ one will observe the average residence time, i.e.,

$$N(t) \propto t\,\theta_{av}\ , \tag{39}$$

where

$$\theta_{av} = (\langle 1/\theta\rangle_{\theta_m})^{-1} \propto \theta_m^{\alpha} \tag{40}$$

if N is sufficiently large so that the variance in transit times becomes small

$$N \gg \langle 1/\theta^2\rangle_{\theta_m} / \langle 1/\theta\rangle^2_{\theta_m} \propto \theta_m^{-(1-\alpha)}\ . \tag{41}$$

This defines a unique relationship between θ_m and N

$$N(\theta_m) \approx \theta_m^{-(1-\alpha)} \tag{42}$$

for which both inequalities (38) and (41) are approximately valid. Using (39) gives

$$\theta_m(t)\,t \approx 1\ , \tag{43}$$

and finally for the actual distance traveled

$$\langle X^2(t)\rangle \propto N(t) \propto t^{1-\alpha}\ , \tag{44}$$

$$\nu = (1-\alpha)/2\ , \tag{45}$$

which is the result one would obtain by applying the Scher-Lax procedure[1] to the same system. This is equivalent to having a frequency-dependent diffusion constant and conductivity

$$D(\omega) \propto \sigma(\omega) \propto \theta_{av} \propto \omega^{\alpha}\ . \tag{46}$$

This should be compared to the 1D result[6]

$$D_{1\text{-}d}(\omega) \propto \sigma_{1\text{-}d}(\omega) \propto \omega^{(\alpha/2-\alpha)}\ . \tag{47}$$

Thus the traps are *more* effective in reducing diffusion than they would be in 1D, reflecting the difference between Eqs. (32) and (33).

Comparing to the physical model for the trap distribution [Eqs. (35) and (36)], one predicts

$$\sigma(\omega, T) \propto \omega^{(T_m - T)/T_m}\ , \tag{48}$$

with anomalous behavior only for $T < T_m$. We note, however, that the assumption (37) implies constant geometrical factors and neglects the expected correlation of the extent of bound trap states with their energy $(-\Delta)$. When this is important, the results would be somewhat modified.

When $\rho(w)$ is such that $\langle 1/W\rangle$ is defined [Eq. (13)], an analogous argument shows that one always has a finite dc conductivity (i.e., a normal situation, in our terminology). Obviously, this does not exclude peculiar temperature dependences (e.g., of the Mott type) or high-frequency anomalies.[15]

CONCLUSIONS

We have extended previous studies of anomalous transport properties in one-dimensional and anistropic systems. Using a critical-path analysis we were able to set a lower limit on the dc conductivity for two- and three-dimensional random-hopping models. We are thus able to show that such models cannot result in anomalous low-frequency transport. The estimates we derive for the conductivity are frequently only qualitative. We were not able to analyze the intermediate frequency regime which would interpolate between the high-frequency cluster expansions and the low-frequency behavior dominated by the dc conductivity. For random-trapping models we find an enhancement of the anomalies found in one dimension. The exponents agree with those obtained from the Scher-Lax analysis. We have thus shown that above one dimension random-hopping and random-trapping models belong to qualitatively different classes. This would also apply to the mathematically equivalent random force constant and random mass lattice models.

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