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Brief Reports

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Diffusion in one-dimensional disordered systems: An effective-medium approximation

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The effective-medium approximation is shown to give the correct frequency-dependent diffusion coefficient for small frequencies in a one-dimensional disordered system with a nonsingular distribution of transfer rates. This confirms the scaling hypothesis which has been proposed to study diffusion in such a system.

A wide class of dynamical processes in random systems can be described by a master equation for a lattice characterized by random values of transfer rates $W_{nn'} = W_{n'n}$ between pairs of nearest-neighbor sites,[1]

$$\dot{P}_n(t) = \sum_{\substack{n' \\ \text{NN of } n}} [W_{nn'}P_{n'}(t) - W_{n'n}P_n(t)] \quad . \tag{1}$$

Here $P_n(t)$ is the probability for the excitation to be on site n at time t given that it starts on $n=0$ at time $t=0$. The values of W assigned to the lattice bonds are random variables distributed according to a probability density $\rho(W)$.

Among the processes to which Eq. (1) (or a modified version of it) is related are dispersive hopping transport in amorphous semiconductors,[2–4] the migration of localized electronic excitation among impurities embedded in a host,[5,6] and frequency-dependent conductivity in superionic conductors.[1,7]

Recently, much attention has been given to the solutions of Eq. (1) for one-dimensional systems.[1,8,9] In this case, exact results for asymptotically long times were obtained for $\langle P_0(t)\rangle$, the probability of the excitation to be at the origin at time t. Here $\langle \cdots \rangle$ denotes an average over the ensemble of random configurations. The results for $\langle P_n(t)\rangle$ which are required for the study of the excitation transport were derived by invoking the following scaling hypothesis[8]:

$$\langle \tilde{P}_n(\omega)\rangle \approx \langle \tilde{P}_0(\omega)\rangle F(n/\xi(\omega)); \quad \omega \to 0 \quad , \tag{2}$$

where $\langle \tilde{P}_n(\omega)\rangle$ is the Laplace transform of $\langle P_n(t)\rangle$, and $F(Z)$ is an arbitrary scaling function which is normalized to satisfy $F(0)=1$. The physical idea leading to this scaling hypothesis is that for each ω there is a length $\xi(\omega)$ such that the diffusion at times $t >> 1/\omega$ and over distances $n > \xi$ is insensitive to the details of the randomness in the system. In Ref. 9 a renormalization-group calculation is derived for the long-time diffusion coefficient.

Recently, one of us[10] proposed a self-consistent effective-medium approximation (EMA) for solving Eq. (1) in all dimensions. We apply this EMA for one-dimensional systems and show that, for randomness characterized by a nonsingular $\rho(W)$,[1] the EMA gives exact results for $\langle \tilde{P}_n(\omega)\rangle$ in the limit of small ω and consequently for the long-time diffusive behavior. This result confirms that the scaling hypothesis, Eq. (2), is exact for the $\rho(W)$ we use here.

The Laplace transform of Eq. (1) is

$$\omega\tilde{P}_n(\omega) = \sum_{n'} [W_{nn'}\tilde{P}_{n'}(\omega) - W_{n'n}\tilde{P}_n(\omega)] + \delta_{n0} \quad , \tag{3}$$

or, in matrix representation,

$$\hat{A}(\omega)\hat{P}(\omega) = \hat{1} \quad , \tag{4}$$

where, using "bracket" notation,

$$\hat{P}(\omega) = \sum_n \tilde{P}_n(\omega)|n\rangle \quad , \tag{4a}$$

$$\tilde{P}_n(\omega) = \int e^{-\omega t}P_n(t)\,dt \quad , \tag{4b}$$

and

$$\hat{A}(\omega) = \sum_{\substack{k,l \\ (\text{NN})}} |k\rangle \left[\left(\omega + \sum W_{ik}\right)\delta_{kl} - W_{kl}\right]\langle l| \quad . \tag{5}$$

The information concerning the diffusion process can be obtained from $\langle \tilde{P}_n(\omega) \rangle$:

$$\langle \tilde{P}_n(\omega) \rangle = \langle \hat{A}^{-1}(\omega) \rangle_{0n} \ . \quad (6)$$

$\hat{A}(\omega)$ in Eq. (5) can be represented as a sum of a homogeneous term and a term which contains the random fluctuations

$$\hat{A}(\omega) = \hat{A}_M(\omega) - \delta\hat{A}(\omega) \ , \quad (7)$$

where

$$\hat{A}_M(\omega) = \sum_{\substack{k,l \\ (\mathrm{NN})}} |k\rangle \{[\omega + 2W_M(\omega)]\delta_{kl} - W_M(\omega)\Delta_{kl}\} \langle l| \ . \quad (8)$$

Here[10]

$$\delta\hat{A}(\omega) = \sum_{\substack{k,l \\ (\mathrm{NN})}} 2[W_{kl} - W_M(\omega)]\hat{Q}_{kl} \ , \quad (9a)$$

$$\hat{Q}_{kl} = \tfrac{1}{2}(|k\rangle - |l\rangle)(\langle k| - \langle l|) \ , \quad (9b)$$

and

$$\Delta_{kl} = \begin{cases} 1, & \text{if } k,l \text{ are nearest neighbors} \\ 0, & \text{otherwise.} \end{cases} \quad (9c)$$

$\hat{A}^{-1}$ can now be expressed as[11,12]

$$\hat{A}^{-1} = G_M + G_M T G_M \ , \quad (10)$$

where $G_M \equiv \hat{A}_M^{-1}$ is the lattice Green's function for a homogeneous medium with $W_{kl} = W_M(\omega)$.

$$T = \sum_{k \neq l} t_{kl} + \sum_{k,l \neq m,n} t_{kl} G_M t_{mn} + \sum_{\substack{k,l \neq m,n \\ m,n \neq p,q}} t_{kl} G_M t_{mn} G_n t_{pq} + \cdots \ , \quad (11)$$

and the t matrix for the kl bond is

$$t_{kl} = \frac{(|k\rangle - |l\rangle)(W_M - W_{kl})(\langle k| - \langle l|)}{1 - (\langle k| - \langle l|)G_M(|k\rangle - |l\rangle)(W_M - W_{kl})} \ . \quad (12)$$

From Eq. (12) we obtain

$$\langle \hat{A}^{-1} \rangle^{-1} = \hat{A}_M - \frac{\langle T \rangle}{1 + G_M \langle T \rangle} \ . \quad (13)$$

The effective-medium condition for $W_M(\omega)$ is[10,12]

$$\langle t \rangle = \int t(W, W_M)\rho(W)\, dW = 0 \ . \quad (14)$$

Due to the summation restrictions in Eq. (11) and the random assignment of values of W to different bonds, this condition leads to the vanishing of the first three terms in $\langle T \rangle$ so that the first nonzero term is of fourth order in t.

Using Eq. (12), Eq. (14) can be written explicitly for any dimensionality:

$$\int \rho(W) \frac{(W - W_M)\, dW}{W[1 - \omega G_M^0(\omega)] + W_M[z/2 - 1 + \omega G_M^0(\omega)]} = 0 \ , \quad (15)$$

where

$$G_M^0(\omega) = \langle 0 | G_M(\omega) | 0 \rangle \ ,$$

and z is the lattice coordination number. For a one-dimensional lattice $z = 2$ and Eq. (15) reduces to[1,13]

$$\int \rho(W) \frac{(W - W_M)\, dW}{W + (W_M - W)\omega G_M^0(\omega)} = 0 \quad (16)$$

and

$$G_M^0(\omega) = \frac{1}{\{\omega[\omega + 4W_M(\omega)]\}^{1/2}} \ . \quad (17)$$

From Eqs. (16) and (17) one obtains the following result for $W_M(\omega)$ up to order ω:

$$W_M(\omega) = W_M(0) + W_{M1}\sqrt{\omega} + W_{M2}\omega + \cdots \ , \quad (18)$$

where

$$W_M(0) = \left\langle \frac{1}{W} \right\rangle^{-1} \ ,$$

$$W_{M1} = \tfrac{1}{2} \left\langle \left[\frac{1}{W} - \frac{1}{W_M(0)} \right]^2 \right\rangle W_M^{5/2}(0) \ , \quad (19)$$

$$W_{M2} = \tfrac{3}{8} \left\langle \left[\frac{1}{W} - \frac{1}{W_M(0)} \right]^2 \right\rangle^2 W_M^4(0) - \tfrac{1}{4} \left\langle \left[\frac{1}{W} - \frac{1}{W_M(0)} \right]^3 \right\rangle W_M^3(0) \ .$$

We now examine the corrections to $\hat{A}_M(\omega)$ in Eq. (13) by considering the nonvanishing terms in $\langle T \rangle$. The magnitude of the first such term is of fourth order in t can be written as

$$\sum_{p \neq q} \langle t_{p,p+1}^2 \rangle \langle t_{q,q+1}^2 \rangle (\Gamma_{p,p+1;q,q+1})^3 \ , \quad (20)$$

where

$$\Gamma_{p,p+1,q,q+1} = \langle p | G_M | q \rangle + \langle p+1 | G_M | q+1 \rangle - \langle p | G_M | q+1 \rangle - \langle p+1 | G_M | q \rangle \ . \quad (21)$$

For small ω,[1]

$$\langle p | G_M | q \rangle = \frac{1}{2\sqrt{\omega W_M(0)}} \left[\frac{1}{1 + [\omega / W_M(0)]^{1/2}} \right]^{|p-q|} \ . \quad (22)$$

Hence

$$\Gamma_{p,p+1;q,q+1} \sim -\frac{\sqrt{\omega}}{2W_M(0)^{3/2}} + O(\omega) \ . \quad (23)$$

In the limit $\omega \to 0$, t_{kl}^2 becomes ω independent and therefore the correction term in Eq. (20) is of order $\omega^{3/2}$. The rest of the series consists of terms of higher order in ω. Therefore the lowest order of ω in the correction to the EMA result is $\omega^{3/2}$. Successive terms in the series contain higher-order moments of

$1/W$ which we assumed to exist.

The diffusion coefficient $D(\omega)$ is given by[10] $W_M(\omega)$, and $\langle R^2(t)\rangle$, the mean-squared displacement is

$$\langle R^2(t)\rangle = \mathcal{L}^{-1}\left(\frac{2D(\omega)}{\omega^2}\right) . \tag{24}$$

$\mathcal{L}^{-1}$ is the inverse Laplace transform. From the above arguments, it follows that the results derived by Machta,[9] Alexander and Orbach,[14] and Van Beijeren,[15] are exact to order $\sqrt{\omega}$. The relation[1]

$$D(\omega) = \frac{1}{4\omega\langle\tilde{P}_0(\omega)\rangle^2} , \tag{25}$$

which follows from the effective-medium picture, is also exact at least for the $\rho(W)$ discussed here. From Eq. (22) one can easily obtain the following expression for $\langle\tilde{P}_n(\omega)\rangle$ in the limit $\omega\to 0$:

$$\langle\tilde{P}_n(\omega)\rangle = \langle 0|G_M(\omega)|n\rangle . \tag{26}$$

So

$$\langle\tilde{P}_n(\omega)\rangle \sim \langle\tilde{P}_0(\omega)\rangle \exp(-\sqrt{\omega/W_M}|n|) . \tag{27}$$

Since we have shown that the diffusion can be exactly described by $W_M(\omega)$ given by Eq. (19), it follows that the scaling hypothesis of Bernasconi *et al.*,[8] Eq. (2), is asymptotically exact with

$$F(n/\xi(\omega)) = \exp[-n/\xi(\omega)] , \quad \xi(\omega) = \sqrt{W_M/\omega} . \tag{28}$$

It is important to note that once the diffusion in a random lattice can be represented by an effective medium, a similar scaling relation for $\langle\tilde{P}_n(\omega)\rangle$ follows at all dimensionalities.[10] Thus, in three dimensions,[16]

$$\langle\tilde{P}_n(\omega)\rangle \sim \langle\tilde{P}_0(\omega)\rangle F_3\left(\frac{|\vec{n}|}{\xi(\omega)}\right) , \tag{29}$$

where

$$F_3(y) \sim \frac{e^{-y}}{y} \quad \text{for large } y . \tag{30}$$

In conclusion, we have shown that the effective-medium approximation for diffusion is a well controlled approximation which can be systematically extended and the corrections to which can be obtained. These corrections can be examined in a similar manner for the interesting case where the distribution of transfer rates $\rho(W)$ is such that $\langle 1/W\rangle$ is infinite.[1] The results of this study are planned to be published elsewhere.

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