Diffusion in a one-dimensional disordered system

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The low-frequency properties of a disordered one-dimensional diffusion model are determined. Of particular interest is the case where the distribution of hopping elements diverges for small values of the hopping elements. The density of states and the leading correction terms are calculated at low frequencies and the diffusion constant and correlation length are determined. The scaling assumptions of Alexander et al. are verified. The model considered is also one for phonons with random force constants and the localization length for low-frequency phonons is determined. The case where there is both off-diagonal and diagonal disorder is considered.

I. INTRODUCTION

The properties of a random one-dimensional chain have been widely studied since Dyson's[1] pioneering work. A review of work on this problem has been given by Alexander et al.[2] This type of problem arises in a variety of situations of physical interest: particle diffusion in a random one-dimensional material, low-temperature properties of a random Heisenberg magnetic chain, excitation transfer along a one-dimensional array of traps, phonons on a random chain, etc. The general type of problem considered here is described by a diffusion equation of the form

$$C_r \frac{\partial p_r}{\partial t} = W_{r,r-1}(p_{r-1} - p_r)$$
$$+ W_{r,r+1}(p_{r+1} - p_r) , \qquad (1.1)$$

where r denotes the lattice sites and $p_r(t)$ the probability of finding a particle at site r at time t. The hopping rates (or bonds) $W_{r,r+1} = W_{r+1,r}$ may be independent random variables distributed according to a probability density $\rho(W)$. In addition, the C_r (the sites) may be random variables.

This is exactly the problem considered by Alexander et al.[2] They were concerned with the low-frequency or long-time behavior. In the case of the random-bond problem they considered three different types of distributions.

Case (a): $\rho(W)$ is such that

$$W_a^{-1} = \int_0^\infty dW \rho(W) W^{-1} < \infty . \qquad (1.2)$$

Case (b): $\rho(W)$ is such that $\rho(W) \to 1$ as

$$W \to 0 . \qquad (1.3)$$

Case (c):

$$\rho(W) = \begin{cases} (1-\alpha)W^{-\alpha}, & 0 \le W \le 1 \\ 0, & 1 < W \end{cases} \qquad (1.4)$$

with $0 < \alpha < 1$.

An exact asymptotic solution for the single-site Green's function in these three cases was achieved by Bernasconi et al.[3] From this the low-energy density of states can be obtained. With the assumption of a single characteristic length, Alexander et al.[2] were able to obtain expressions for the transport properties.

The reason for reconsidering this problem here is that using the replica procedure we are able to solve the resulting integral equations in a straightforward manner at low frequencies. In this way we obtain not only the leading terms in the density of states, but also the leading correction terms.[4] In addition, the diffusion constant and correlation length are determined explicitly without any scaling assumptions. Where they overlap, our results are in agreement with those of Alexander et al. Furthermore, our results verify that the scaling assumption made by them is valid. We do not believe there are any difficulties associated with the replica method and the $n \to 0$ limit in this problem. It is a way of generalizing the problem which leads to useful simplifications.

In Sec. II we summarize some necessary results and introduce the replica procedure and generating function. This is based on previous work.[5] In Sec. III the integral equation for random bonds is derived and solved in the asymptotic limit in the above three cases. In Secs. IV and V the diffusion constant and correlation length are calculated. In Sec. VI we discuss phonons and the phonon locali-

zation length. In Sec. VII the random-site problem and case where both sites and bonds are random variables are considered. Finally in Sec. VIII the results are discussed.

II. GENERATING FUNCTION

We begin by summarizing some useful formulas. The Laplace transform of the rate Eq. (1.1) with the initial condition $p_r(t) = \delta_{r,0}$ is

$$\omega P_r - W_{r,r-1}(P_{r-1} - P_r) - W_{r,r+1}(P_{r+1} - P_r)$$
$$= \delta_{r,0} + U_r , \quad (2.1)$$

where

$$P_r(\omega) = \int_0^\infty e^{-\omega t} p_r(t) dt . \quad (2.2)$$

We have included an external potential U_r on the right-hand side of (2.1) for convenience. The solution of (2.1) up to terms of order U can be written $P_r = P_r^{(0)} + \delta P_r$ where

$$P_r^{(0)} = G_{r0}(\omega) , \quad (2.3)$$

$$\delta P_0 = \sum_r G_{0r}(\omega) U_r , \quad (2.4)$$

where G_{rs} is the Green's function. The average density of states is given by

$$N(\omega) = -\frac{1}{\pi} \text{Im} \langle G_{00}(-\omega + i\delta) \rangle , \quad (2.5)$$

where $\langle \ \rangle$ indicates an average over the random elements W.

With the introduction of the Fourier transforms

$$\langle G_{rs}(\omega) \rangle = \frac{1}{N} \sum_k e^{ik(r-s)} G(k,\omega) ,$$
$$U_r = \frac{1}{\sqrt{N}} e^{ikr} U , \quad (2.6)$$

where N is the number of sites, the Fourier transform of the average response is

$$\langle \delta P(k,\omega) \rangle = G(k,\omega) U . \quad (2.7)$$

The diffusion constant $D(\omega)$ can be obtained by expansion of $G(k,\omega)$ in powers of k:

$$G(k,\omega) \simeq \frac{1}{\omega} - \frac{D(\omega)}{\omega^2} k^2 + \cdots . \quad (2.8)$$

We now introduce a "partition function"

$$Z = \left\langle \int (dV) e^{-H(V)} \right\rangle , \quad (2.9)$$

where the $\vec{V}$ are n component variables and

$$H(V) = \frac{1}{2} \sum_{rs} \vec{V}_r G_{rs}^{-1} \vec{V}_s + \sum_r \vec{U}_r \cdot \vec{V}_r$$
$$= \sum_r \left[\frac{\omega}{2} \vec{V}_r^2 + \frac{1}{2} W_{r,r+1} (\vec{V}_r - \vec{V}_{r+1})^2 \right.$$
$$\left. + \vec{U}_r \cdot \vec{V}_r \right] . \quad (2.10)$$

In what follows it is understood that the $n \to 0$ limit is to be taken. To determine the average Green's functions we introduce a generating function[5]

$$s_0(\vec{p},\omega) = \left\langle \int (dV) e^{-i\vec{p} \cdot \vec{V}_0} e^{-H} \right\rangle , \quad (2.11)$$

where $\vec{p}$ is an n component vector. The integral in (2.11) is easily evaluated and in the $n=0$ limit (omitting terms of order U^2)

$$s_0(p) = \left\langle \exp \left[-\frac{p^2}{2} G_{00} + i\vec{p} \sum_r G_{0r} \vec{U}_r \right] \right\rangle . \quad (2.12)$$

The average Green's function and response function are then given by

$$\langle G_{00}(\omega) \rangle = - \left[\frac{\partial^2}{\partial p_\alpha^2} s_0(p) \right]_{p=U=0} , \quad (2.13)$$

$$\langle \delta P_0 \rangle = -i \left[\frac{\partial}{\partial p_\alpha} \delta s_0(p) \right]_{p=0} , \quad (2.14)$$

where δs_0 is the part of s_0 linear in U.

It is convenient to introduce the Fourier transform on $\vec{p}$ of (2.11)

$$s_0(\vec{V},\omega) = \frac{1}{(2\pi)^n} \int e^{i\vec{p} \cdot \vec{V}} s(\vec{p},\omega) . \quad (2.15)$$

In terms of this function the density of states is

$$N(\omega) = -\frac{1}{\pi} \text{Im} \int V_\alpha^2 d\vec{V} s_0(V, -\omega + i\delta) \quad (2.16)$$

and the response function (2.7)

$$G(k,\omega) = -\frac{1}{U} \int V_\alpha d\vec{V} \delta s_k(V,\omega) , \quad (2.17)$$

where δs_k is the spatial Fourier transform of δs_r.

III. INTEGRAL EQUATION AND DENSITY OF STATES

An integral equation which determines $s_0(V)$ is easily written down. We focus attention on site 0

and in the generating function (2.11) (for $U=0$) represent everything on the left and right of this site by $Q(V)$. Thus,

$$s_0(V) = e^{-(\omega/2)V^2} Q^2(V) . \qquad (3.1)$$

From translational invariance $Q(V)$ satisfies the integral equation

$$Q(V) = \int d\vec{V}' \langle e^{-(W/2)(\vec{V}-\vec{V}')^2} \rangle e^{-(\omega/2)\vec{V}'^2} Q(V') . \qquad (3.2)$$

When the external field $U=0$, $Q(V)$ only depends on V^2 and then it is possible to carry out the angular integral in (3.2) and take the $n=0$ limit with the result

$$Q(V) = \langle e^{-(W/2)V^2} \rangle$$
$$+ \int_0^\infty dV' \langle WVI_1(WVV') e^{-(W/2)(V^2+V'^2)} \rangle$$
$$\times e^{-(\omega/2)V'^2} Q(V') , \qquad (3.3)$$

where I_1 is the Bessel function. However, the solution of the integral equation is much simplified if we keep it in the form (3.2). We now consider the solution of (3.2) in the various cases of interest.

(A) Pure system. When there is no disorder

$$Q(V) = e^{-(a_0/2)V^2} \qquad (3.4)$$

and substitution in (3.2) requires that a_0 satisfy

$$a_0 = \frac{W(\omega+a_0)}{W+\omega+a_0} . \qquad (3.5)$$

The appropriate solution of this equation is

$$a_0 = \tfrac{1}{2}[-\omega+(\omega^2+4W\omega)^{1/2}] . \qquad (3.6)$$

From (3.1) and (2.16) the density of states is

$$N(\omega) = \frac{1}{\pi\omega^{1/2}(4W-\omega)^{1/2}} \qquad (3.7)$$

This result is of course well known.[2] One important feature is that $a_0 \sim \omega^{1/2}$ for small ω so that Q is slowly varying for small ω.

(B) Case (a). When the distribution $\rho(W)$ is such that at least the low moments $\langle W^{-n} \rangle$ exist $(n=1,2,3,...)$ then (3.2) can be solved by the steepest-descent method. The slowly varying factors $e^{-(\omega/2)V'^2} Q(V)$ are expanded around $V'=V$. To leading order in ω/W, $Q=Q_0$ where Q_0 satisfies the equation

$$\tfrac{1}{4}Q_0 = \frac{1}{\omega W_a} \frac{\partial^2 Q_0}{\partial(V^2)^2} \qquad (3.8)$$

and $1/W_a = \langle 1/W \rangle$. The solution is of exactly

the same form as for the pure system (3.4)

$$Q_0 = e^{-(a/2)V^2}, \quad a = \sqrt{\omega W_a} . \qquad (3.9)$$

The higher terms in this solution are easily obtained:

$$Q = Q_0 \left[1 + A\omega V^2 + \tfrac{1}{2}B\omega a V^4 + \frac{1}{3!}C\omega^2 a V^6 \right.$$
$$\left. + \frac{1}{4!}D\omega^2 a^2 V^8 + \cdots \right] . \qquad (3.10)$$

After some algebra we find

$$A = A_0 + \frac{\omega}{a}A_1 ,$$
$$B = B_0 + \frac{\omega}{a}B_1 . \qquad (3.11)$$

Introducing the moments

$$m_2 = 1 - W_a^2 \langle \frac{1}{W^2} \rangle ,$$
$$m_3 = 1 - W_a^3 \langle \frac{1}{W^3} \rangle , \qquad (3.12)$$

We have

$$A_0 = \tfrac{1}{4}(1 + \tfrac{3}{4}m_2) ,$$
$$A_1 = -\tfrac{1}{16}(1 - 7m_2 + \tfrac{59}{16}m_2^2 + \tfrac{7}{3}m_3) ,$$
$$B_0 = -\tfrac{1}{16}m_2 ,$$
$$B_1 = \tfrac{1}{16}(1 - \tfrac{7}{2}m_2 + \tfrac{61}{16}m_2^2 + \tfrac{5}{3}m_3) , \qquad (3.13)$$
$$C = \tfrac{1}{64}(m_2 - \tfrac{23}{4}m_2^2 - \tfrac{4}{3}m_3) ,$$
$$D = \tfrac{3}{256}m_2^2 .$$

As $V^2 \sim 1/\omega^{1/2}$ we have kept terms in (3.10) up to order ω. This is sufficient to give us the leading correction in the density of states which from (2.16) and (3.10) is

$$N(\omega) = \frac{1}{2\pi(\omega W_a)^{1/2}}$$
$$\times \left[1 + \frac{\omega}{W_a}(\tfrac{1}{8} - \tfrac{3}{8}m_2 + \tfrac{15}{128}m_2^2 + \tfrac{1}{8}m_3) \right] . \qquad (3.14)$$

(C) Case (c). In this case the distribution $\rho(W)$ is singular and the steepest-descent method fails. However, for small ω we can reduce (3.2) to a differential equation. Introduce

$$\vec{U} = \omega^\beta \vec{V}, \quad x = W/\omega^{2\beta} , \qquad (3.15)$$

where β is to be determined. After subtracting $e^{-(\omega/2)V^2}Q(V)$ from both sides of (3.2) we get

$$Q(U)[1-f(U)]=(1-\alpha)\omega^{2\beta(1-\alpha)}\int d\vec{U}'\int_0^{\omega^{-2\beta}}x^{-\alpha}dx\,e^{-(x/2)(\vec{U}-\vec{U}')^2}[f(U')Q(U')-f(U)Q(U)]\,,$$

$$(3.16)$$

where $f(U)=e^{-(\omega^{1-2\beta}/2)U^2}$. To leading order in ω we set $Q=Q_0$, and keeping only leading terms in (3.16) we find

$$\tfrac{1}{2}U^2Q_0(U)=(1-\alpha)$$
$$\times\int d\vec{U}'\int_0^\infty x^{-\alpha}dx\,e^{-(x/2)(\vec{U}-\vec{U}')^2}$$
$$\times[Q_0(U')-Q_0(U)]$$

$$(3.17)$$

and

$$\beta=\frac{1}{2(2-\alpha)}\,.$$

$$(3.18)$$

The kernel in this integral equation is a difference kernel, and (3.17) is reduced to a differential equation by taking its Fourier transform with respect to $\vec{U}$,

$$\hat{Q}_0(q)=\int e^{-i\vec{q}\cdot\vec{U}}Q_0(U)d\vec{U}\,.$$

$$(3.19)$$

Then $\hat{Q}_0(q)$ satisfies

$$\nabla_q^2\hat{Q}_0(q)=2^\alpha\Gamma(\alpha)q^{2-2\alpha}\hat{Q}_0(q)\,.$$

$$(3.20)$$

As $\hat{Q}_0(q)$ depends only on q^2 we may take the $n=0$ limit of this equation:

$$\left[\frac{\partial^2}{\partial q^2}-\frac{1}{q}\frac{\partial}{\partial q}\right]\hat{Q}_0(q)=2^\alpha\Gamma(\alpha)q^{2-2\alpha}\hat{Q}_0(q)\,.$$

$$(3.21)$$

The change of variables

$$q=(A_\alpha z)^{2\beta},\quad A_\alpha=\frac{2-\alpha}{2^{\alpha/2}\Gamma^{1/2}(\alpha)}$$

$$(3.22)$$

reduces (3.21) to Bessel's equation. The solution that vanishes as $q\to\infty$ and is normalized such that $\hat{Q}(q=0)=1$ is

$$\hat{Q}_0(q)=\frac{2}{2^{2\beta}\Gamma(2\beta)}z^{2\beta}K_{2\beta}(z)\,,$$

$$(3.23)$$

where K is a Bessel function of the second kind. The normalization condition $\hat{Q}_0(q=0)=1$ corresponds to $Q(V=0)=1$, the required condition. This relation is an artifact of the $n=0$ limit.

The leading term in the density of states is now from (2.16), (3.1), and (3.19),

$$N_0(\omega)=\frac{\sin 2\pi\beta}{\pi\omega^{2\beta}}\int_0^\infty q^{-1}dq\left|\frac{\partial\hat{Q}_0}{\partial\alpha}\right|^2,\quad(3.24)$$

and substituting (3.23),

$$N_0(\omega)=\frac{C_\beta^{(0)}}{\omega^{2\beta}}\,,$$

$$(3.25)$$

where

$$C_\beta^{(0)}=\frac{1-2\beta}{2^{4\beta}\beta\Gamma^2(2\beta)A^{4\beta}}\,.$$

$$(3.26)$$

The ω dependence in (3.25) agrees with the result of Bernasconi et al.[3] $C_\beta^{(0)}$ has recently been obtained by Bernasconi[10] in agreement with (3.26).

It is possible to calculate the leading corrections to (3.25). We go back to (3.16) and let $Q=Q_0+Q_1$ and retain the leading corrections in ω in the equation. It turns out that there are two types of correction terms which vary as $\omega^{\alpha/2-\alpha}$ and $\omega^{(1-\alpha)/(2-\alpha)}$. The first dominates when $\alpha<\tfrac{1}{2}$ and Q_1 satisfies

$$L(q)\hat{Q}_1(q)=-\frac{1-\alpha}{\alpha}\omega^{\alpha/(2-\alpha)}q^2\hat{Q}_0(q)\,,$$

$$(3.27)$$
$$\alpha<\tfrac{1}{2}$$

and when $\alpha>\tfrac{1}{2}$

$$L(q)\hat{Q}_1(q)=-\omega^{(1-\alpha)/(2-\alpha)}L_1(q)\nabla_q^2\hat{Q}_0(q)\,,$$

$$(3.28)$$
$$\alpha>\tfrac{1}{2}$$

where

$$L(q)=\nabla_q^2-2^\alpha\Gamma(\alpha)q^{2-2\alpha}\,,$$

$$(3.29)$$

$$L_1(q)=\tfrac{1}{4}\nabla_q^2-2^{\alpha-1}\Gamma(\alpha)q^{2-2\alpha}\,.$$

Equations (3.27) and (3.28) can be solved by introducing the change of variables (3.22) and then by making use of the Green's function for Bessel's equation. We will omit the details and quote the results for the leading corrections to the density of states $N(\omega)=N_0(\omega)+N_1(\omega)$ where

$$N_1(\omega)=\begin{cases}-\dfrac{C_\beta^{(1)}}{\omega^{1-2\beta}},&\alpha<\tfrac{1}{2}\\[2ex]-\dfrac{C_\beta^{(2)}}{\omega^{4\beta-1}},&\alpha>\tfrac{1}{2}\,.\end{cases}$$

$$(3.30)$$

The constants C are given by

$$C_\beta^{(1)} = \frac{2^{4(1-\beta)}\beta(2\beta+1)A_\alpha^{4\beta}}{\pi(4\beta-1)\Gamma^2(2\beta)}\sin2\pi\beta$$

$$\times I(8\beta+1,\beta) ,$$

(3.31)

$$C_\beta^{(2)} = \frac{\sin4\pi\beta}{\pi(4\beta-3)2^{4\beta}\Gamma^2(2\beta)A_\alpha^{8\beta}}$$

$$\times I(5-4\beta,\beta) ,$$

where

$$I(\gamma,\beta) = \tfrac{1}{2}\int^\infty dz\, z^\gamma[2K_{2\beta}^2K_{2\beta-2}I_{2\beta}$$

$$-K_{2\beta}K_{2\beta-1}(I_{2\beta}K_{2\beta-1}$$

$$-K_{2\beta}I_{2\beta-1})]$$

(3.32)

In the case $\alpha=\tfrac{1}{2}$ ($\beta=\tfrac{1}{3}$) both the terms (3.30) contribute in leading order to the density of states.

(D) Case (b). This is the marginal case. We can proceed as in (C) above, setting $\beta=\tfrac{1}{4}$, except that in the second integral in (3.16) it is not possible to set the upper limit to infinity. The differential equation replacing (3.21) is now

$$\left[\frac{\partial^2}{\partial q^2}-\frac{1}{q}\frac{\partial}{\partial q}\right]\hat{Q}_0(q)$$

$$=q^2[1-\gamma-\ln(\tfrac{1}{2}q^2\omega^{1/2})]\hat{Q}_0(q) , \quad (3.33)$$

where γ is Euler's constant. The ln terms may be removed by the substitution

$$q=\frac{1}{L^{1/4}}\left[1-\frac{\ln L}{8L}-\cdots\right]q' , \quad (3.34)$$

where $L=|\ln\omega^{1/2}|$. Then

$$\left[\frac{\partial^2}{\partial q'^2}-\frac{1}{q'}\frac{\partial}{\partial q'}\right]\hat{Q}_0(q')=q'^2\hat{Q}_0(q') , \quad (3.35)$$

which can be reduced to Bessel's equation by substituting $q'=\sqrt{2z}$. The solution in normalized form is

$$\hat{Q}_0(q')=\frac{(2z)^{1/2}}{\Gamma(\tfrac{1}{2})}K_{1/2}(z) . \quad (3.36)$$

The density of states is then found to be

$$N(\omega)=\frac{1}{2\pi}\left[\frac{L}{\omega}\right]^{1/2}\left[1+\frac{\ln L}{4L}+\cdots\right] , \quad (3.37)$$

up to terms of order $(\ln L)/L$.

IV. THE DIFFUSION CONSTANT

In this section we consider the response of the generating function (2.11) to a slowly varying potential. Again focusing attention on site 0 we can write

$$S_0(V)=e^{-(\omega/2)V^2-\vec{U}_0\cdot\vec{V}}Q_{L0}Q_{R0} , \quad (4.1)$$

where Q_L and Q_R represent the effect of all sites to the left and right of 0, respectively. Q_R satisfies the integral equation

$$Q_{R0}(V)=\int d\vec{V}'\langle e^{-(W/2)(\vec{V}-\vec{V}')^2}\rangle$$

$$\times e^{-(\omega/2)V'^2-\vec{U}_1\cdot\vec{V}'}Q_{R1}(V') . $$

(4.2)

Q_L satisfies a similar equation with U_{-1} replacing U_1. We only require the linear response to the potential U so that we can set

$$Q_{Rr}=Q+\delta Q_{Rr} , \quad (4.3)$$

where Q satisfies (3.2) and δQ is proportional to U. Substituting (4.3) in (4.2) and keeping terms of order U only gives

$$\delta Q_{R0}=\int dV'\langle e^{-(W/2)(V-V')^2}\rangle e^{-(\omega/2)V'^2}$$

$$\times[\delta Q_{R1}(V')-\vec{U}_1\cdot\vec{V}'Q_0(V')] .$$

(4.4a)

Introducing the Fourier transform (2.6) and

$$Q_{Rr}=\frac{1}{\sqrt{N}}e^{ikr}\delta Q_k \quad (4.4b)$$

in (4.4a) gives

$$e^{-ik}\delta Q_k=\int d\vec{V}'\langle e^{-(W/2)(\vec{V}-\vec{V}')^2}\rangle e^{-(\omega/2)V'^2}$$

$$\times[\delta Q_k(V')-\vec{U}\cdot\vec{V}'Q_0(V')] .$$

(4.5)

There is a corresponding equation for δQ_L and this is obtained by replacing k by $-k$. When (4.3) and (4.4b) are substituted in (4.1) we find δs_k, the Fourier transform of the part of s_0 linear in U is given by

$$\delta s_k=e^{-(\omega/2)V^2}[-\vec{U}\cdot\vec{V}Q^2+Q(\delta Q_k+\delta Q_{-k})] . $$

(4.6)

We now require the solution of the integral equation (4.5) and again we consider the different cases.

(A) Case (a). For a uniform field ($k=0$) the transformation $V\to V-U/\omega$ in (2.10) served to re-

move terms linear in U. When this transformation is applied to (2.15) it shows that the solution of (4.5) for $k=0$ must be

$$\delta Q_{k=0} = \frac{1}{\omega} \vec{U} \cdot \frac{\partial Q}{\partial \vec{V}} \ . \tag{4.7}$$

This suggests that we try a solution of (4.5):

$$\delta Q_k = \frac{A_k}{\omega} \vec{U} \cdot \frac{\partial Q}{\partial \vec{V}} \ . \tag{4.8}$$

This can be shown to be correct for small ω when Q can be replaced by Q_0 [Eq. (3.9)] and

$$A_k = \frac{\omega}{a(e^{-ik}-1)+\omega} \ . \tag{4.9}$$

Then substituting (4.8) in (4.6) and using (2.17) we find for small ω and k that

$$G(k,\omega) = \frac{1}{\omega + W_a k^2} \ . \tag{4.10}$$

This result is of the same form as in the pure system and the diffusion constant is W_a.

(B) Case (c). We can again reduce (4.5) to a differential equation when ω is small. We briefly outline the steps. The inhomogeneous term in (4.5) is $-\vec{U} \cdot \vec{V} Q_0(V)$ as $\omega \to 0$, and then (4.5) becomes

$$\delta Q_k e^{-ik} = -\vec{U} \cdot \vec{V} Q_0(V)$$
$$+ \int d\vec{V}' \langle e^{-(W/2)(\vec{V}-\vec{V}')^2} \rangle$$
$$\times e^{-(\omega/2)V'^2} \delta Q_k(V') \ . $$
$$\tag{4.11}$$

Then proceeding as in case (C) of Sec. III we find the differential equation satisfied by the Fourier transform $\delta \hat{Q}_k(q)$,

$$L(q)\delta Q_k(q) = 2i\omega^{\beta-1}\vec{U} \cdot \vec{\nabla}_q \hat{Q}_0(q)$$
$$+ 2\omega^{2\beta-1}(e^{-ik}-1)\delta \hat{Q}_k(q) \ . $$
$$\tag{4.12}$$

where $L(q)$ is given in (3.29). We were not able to find a closed-form solution to this equation. In order to calculate the diffusion constant from (2.8) we expanded the solution of (4.12) in powers of k up to terms of order k^2. Substitute

$$\delta \hat{Q}_k = i\omega^{\beta-1}\vec{U} \cdot \vec{q}(\hat{Q}_0 + \hat{M}) \tag{4.13}$$

in (4.12), and it is found that $\hat{M}$ satisfies

$$L_2(\alpha,q)\hat{M} = -2ik\omega^{2\beta-1}(\hat{Q}_0+\hat{M}) \ , \tag{4.14}$$

where

$$L_2(\alpha,q) = \frac{\partial^2}{\partial q^2} + \frac{1}{q}\frac{\partial}{\partial q} - \Gamma(\alpha)2^\alpha q^{2-2\alpha} \ . \tag{4.15}$$

Terms of order k^2 have been omitted on the right-hand side of (4.14) as they do not contribute in leading order to the diffusion constant $D(\omega)$. With the introduction of the change of variables (3.22), Eq. (4.14) takes the form

$$\left[z\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} - z \right]\hat{M}$$
$$= -8ik\omega^{2\beta-1}\beta^2 A_\alpha^{4\beta} z^{4\beta-1}(\hat{Q}_0+\hat{M}) \ . \tag{4.16}$$

The Green's function for this equation satisfies

$$\left[z\frac{\partial^2}{\partial z^2} + \frac{\partial}{\partial z} - z \right]\mathscr{G}(z,z') = \delta(z-z')$$

and is

$$\mathscr{G}(z,z') = \begin{cases} -K_0(z)I_0(z'), & z>z' \\ -K_0(z')I_0(z), & z<z' \ . \end{cases} \tag{4.17}$$

This enables us to rewrite (4.16) as an integral equation

$$\hat{M}(z) = -8ik\omega^{2\beta-1}\beta^2 A_\alpha^{4\beta}$$
$$\times \int dz' \mathscr{G}(z,z')z'^{4\beta-1}$$
$$\times [\hat{Q}_0(z')+\hat{M}(z')] \ . \tag{4.18}$$

This equation can now be solved as a power series in k by iteration. From the terms of order k^2 we determine the diffusion constant using (4.6), (2.17), and (2.8) with the result

$$D(\omega) = \omega^{4\beta-1}C_\beta^{(3)} \ , \tag{4.19}$$

where

$$C_\beta^{(3)} = \frac{2^{7-4\beta}\beta^3 A_\alpha^{8\beta}}{\Gamma^2(2\beta)}$$
$$\times \int_0^\infty dz\, dz'(zz')^{6\beta-1}K_{2\beta}(z)K_{2\beta}(z')$$
$$\times \mathscr{G}(z,z') \ . \tag{4.20}$$

In case (b) a very similar calculation gives

$$D = \frac{C_{1/4}^{(3)}}{L(\omega)} \ , \tag{4.21}$$

where $L(\omega) = |\ln\omega^{1/2}|$ and $C_{1/4}^{(3)}$ is obtained from $C_\beta^{(3)}$ by replacing $\beta = \frac{1}{4}$ ($\alpha=0$) and $A_0 \to 2$ (this is necessary because A_α is not defined for $\alpha=0$).

V. CORRELATION FUNCTIONS

In this section we consider the long-distance behavior of the Green's function or correlation

function $\langle G_{r0}(\omega)\rangle$ and define a correlation length through

$$\langle G_{r0}(\omega)\rangle \sim e^{-r/\xi(\omega)}, \quad r\to\infty \ . \tag{5.1}$$

In terms of the partition function (2.9) we can write the correlation function as

$$\langle G_{r0}(\omega)\rangle = \left\langle \int (dV)V_{r\alpha}V_{0\alpha}e^{-H(V)}\right\rangle , \tag{5.2}$$

where, as usual, the limit $n\to 0$ is understood. This correlation function can be expressed in terms of the eigenvalues and eigenvectors of the integral equation with the same kernel as (3.2):

$$\lambda\Psi(\vec{V})= \int d\vec{V}'\langle e^{-(W/2)(\vec{V}-\vec{V}')^2}\rangle e^{-(\omega/2)V'^2}\Psi(\vec{V}') \ . \tag{5.3}$$

The solution with the largest eigenvalue $\lambda=1$ is $\Psi_0=Q$. To determine the correlation function (5.2) we require the next eigenvalue and eigenvector, which we call λ_1 and Ψ_1, respectively. From (5.2) Ψ_1 must have p-type symmetry, i.e., it is of the form $V_\alpha\phi_1(V^2)$. In terms of these eigenvalues and eigenvectors

$$\langle G_{r0}(\omega)\rangle = K^2\lambda_1^r , \tag{5.4}$$

where

$$K= \int d\vec{V}\, e^{-(\omega/2)V^2}\Psi_0 V_\alpha\Psi_1 \ . \tag{5.5}$$

It is assumed that both Ψ_0 and Ψ_1 are normalized:

$$\int d\vec{V}e^{-(\omega/2)V^2}\Psi^2=1 \ . \tag{5.6}$$

(A) Pure system. In this case it is easily shown that

$$\Psi_1\sim V_\alpha e^{-(a_0/2)V^2}, \quad \lambda_1=\frac{W}{W+\omega+a_0} , \tag{5.7}$$

where a_0 is given in (3.6). From (5.4) and (5.1) at low frequencies we find

$$\xi^{-1}(\omega)= \left[\frac{\omega}{W}\right]^{1/2} \ . \tag{5.8}$$

(B) Case (a). For low frequencies we can use the steepest-descent method to reduce (5.3) to a differential equation. It is found that

$$\Psi_1\sim V_\alpha e^{-(a/2)V^2}, \quad \lambda_1=1-(\omega/W_a)^{1/2}-\cdots , \tag{5.9}$$

where a is given in (3.9). The correlation length is given by (5.8) with W_a replacing W.

(C) Case (c). For small ω we assume a solution to (5.3) of the form

$$\Psi_1=V_\alpha\phi_1(V^2), \quad \lambda_1=1-C_\beta\omega^{1-2\beta} , \tag{5.10}$$

where C_β is a constant to be determined. Proceed-

ing as in case (C) Sec. III we can obtain a differential equation for the Fourier transform $\hat{\phi}_1(q)$ of $\phi_1(V^2)$. This equation can be set in the form

$$L_2(q)\hat{f}_1+2C_\beta\hat{f}_1=0 , \tag{5.11}$$

where $\hat{f}_1=(1/q)\hat{\phi}_1'(q)$ and L_2 is given in (4.15). The frequency dependence of the correlation length follows from (5.10):

$$\xi^{-1}(\omega)=C_\beta\omega^{1-2\beta} \ . \tag{5.12}$$

We were not able to determine C_β in closed form. If necessary, a variational method can be used.[6]

In case (b) a similar calculation gives

$$\xi^{-1}=C_{1/4}\omega^{1/2}L^{1/2}(\omega) \ . \tag{5.13}$$

The correlation length is finite for all $\omega>0$. This is characteristic of diffusive processes in general. In cases (b) and (c) the small hopping rates occurring in the distribution have the effect of reducing the correlation length. It should be noted that the eigenvalues C_β of (5.11) are discrete and thus the form of (5.1) is verified.

VI. PHONON LOCALIZATION LENGTH

The model considered in Sec. III is also a model for phonons in one dimension with random force constants. In Eq. (2.1) ω should be replaced by $-\omega^2$ in this case. It is generally accepted that all eigenstates in one-dimensional disordered systems are localized. In this section we calculate the average rate of exponential growth $\gamma(\omega^2)$ of particular phonon states of frequency ω. This is given by (see Ishii[7])

$$\gamma(\omega^2)= \int d\lambda\, N(\lambda)\ln|\omega^2-\lambda| , \tag{6.1}$$

where $N(\lambda)$ is the average density of states. It has been argued by Thouless[8] that $\gamma(\omega^2)$ is the inverse localization length. A more convenient formula than (6.1) is

$$\gamma(\omega^2)=\mathrm{Re}\int^{-\omega^2} d\lambda\langle G_{00}(\lambda)\rangle \ . \tag{6.2}$$

The average Green's function has been determined in Sec. III and we will quote the results

$$\gamma(\omega^2)= \begin{cases} \dfrac{1}{8}\dfrac{m_2}{W_a}\omega^2, & \text{case (a)} \\[3mm] \dfrac{\pi\omega}{4|\ln\omega|^{1/2}}, & \text{case (b)} \\[3mm] C_\beta^{(0)}\dfrac{\pi\cot 2\pi\beta}{1-2\beta}\omega^{2(1-2\beta)}, & \text{case (c)} \end{cases} \tag{6.3}$$

where $C_\beta^{(0)}$ is given in (3.26). As expected the average exponential growth rate is greater in case (c), i.e., the localization length is shorter than in case (a). In each case $\gamma(\omega^2) \to 0$ as $\omega \to 0$, indicating a diverging localization length. Note that case (c) does not go smoothly into case (a), but the coefficient of the leading term vanishes when $\alpha = 0$.

VII. RANDOM SITE AND BOND PROBLEMS

In this section we consider the random-site problem [random C_r in Eq. (1.1)]. We first consider the case where the bonds are not random, i.e., $W_{r,r+1} = W$ for all r. Dyson[1] showed that the random-site and bond problems reduce to the same type of integral equation. The generating function (3.1) is now of the form

$$s_0(V) = \langle e^{-\omega C_0 V^2/2} \rangle Q^2(V) , \tag{7.1}$$

where $Q(V)$ satisfies the integral equation analogous to (3.2):

$$Q(V) = \int d\vec{V}' e^{(W/2)(V-V')^2} \langle e^{-(C/2)V'^2} \rangle Q(V') . \tag{7.2}$$

We introduce a new function

$$R(V) = \langle e^{-(C/2)V^2} \rangle Q(V) . \tag{7.3}$$

Then it is easily shown that the Fourier transform $\hat{R}(q)$ of $R(V)$ satisfies

$$\hat{R}(q) = \int d\vec{q}' \langle e^{-(1/2\omega C)(\vec{q}-\vec{q}\,')^2} \rangle e^{-q'^2/2W} \hat{R}(q') \tag{7.4}$$

The transformation $q = \sqrt{\omega}\vec{q}$ then shows that $\hat{R}$ satisfies an integral equation identical to that of the bond case (3.2) with $W \to 1/C$. The cases (a), (b), and (c) in Eqs. (1.2)–(1.4) then correspond to distributions of C for which

(a) $\langle C \rangle$ finite;

(b) $\rho(C) \sim C^{-2}$, $C \to \infty$;

(c) $\rho(C) \sim C^{2-\alpha}$, $1 < C < \infty$.

The density of states, diffusion constant, and correlation length then have the same behavior as in the random-bond case discussed in Secs. III–V.

Finally we consider the case where both W and C have singular distributions

$$\rho(W) = \frac{1-\alpha}{W^\alpha}, \quad 0 < W < 1$$

$$\rho(C) = \frac{1-\gamma}{C^{2-\gamma}}, \quad 1 < C < \infty \tag{7.5}$$

when $0 < \alpha < 1$ and $0 < \gamma < 1$. The integral equation satisfied by Q is given by (3.16) with $f(U)$ replaced by

$$\langle f(U) \rangle = \langle e^{-(\omega^{1-2\beta}/2)CU^2} \rangle . \tag{7.6}$$

In the low-frequency limit

$$1 - \langle f(U) \rangle = (\tfrac{1}{2}U^2\omega^{1-2\beta})^{1-\gamma} \Gamma(\gamma) , \tag{7.7}$$

and substituting this in (3.16) we find

$$\beta = \frac{1-\gamma}{2(2-\alpha-\gamma)} . \tag{7.8}$$

Introducing the Fourier transform (3.19) the equation satisfied by $\hat{Q}_0(q)$ is now

$$\left[-\frac{\partial^2}{\partial q^2} + \frac{1}{q}\frac{\partial}{\partial q} \right]^{1-\gamma} \hat{Q}_0(q)$$

$$= -2^{\alpha-\gamma}\frac{\Gamma(\alpha)}{\Gamma(\gamma)}q^{2-2\alpha}\hat{Q}_0(q). \tag{7.9}$$

This equation is not easy to solve. The frequency dependence of the quantities of interest follow from (7.8). In order to preserve the symmetry between the bond and site problems we define the density of states by

$$N(\omega) = -\frac{1}{\pi}\text{Im}\langle C_0 G_{00}(-\omega+i\delta) \rangle$$

$$\sim \omega^{-(1-\alpha\gamma)/(2-\alpha-\gamma)} . \tag{7.10}$$

It is also easily shown that the diffusion constant and correlation length have the following frequency dependence:

$$D(\omega) \sim \omega^{(\alpha+\gamma-2\alpha\gamma)/(2-\alpha-\gamma)} ,$$

$$\xi^{-1}(\omega) \sim \omega^{[(1-\alpha)(1-\gamma)]/(2-\alpha-\gamma)} . \tag{7.11}$$

VIII. DISCUSSION

The low-frequency behavior of a one-dimensional diffusion model with random hopping elements has been determined. The use of the replica procedure leads to a considerable simplification in the solution of the resulting integral equations. Exact asymptotic results have been obtained for the density of states, diffusion constant, and correlation length. These results extend those obtained by Alexander et al.[2] In particular, we are able to verify their assumption of a single correlation length and determine the length.

The assumption of a correlation length allows us to relate the exponents determining the frequency

dependence of the correlation length, the diffusion constant, and the density of states. In the present context the scaling assumption can be expressed as follows: The inverse Green's function (2.6) has the scaling form

$$G^{-1}(k,\omega) = \omega f(k\xi(\omega)) , \qquad (8.1)$$

where for small k

$$f(k\xi) = 1 + ck^2\xi^2 + \cdots , \qquad (8.2)$$

where c is a constant. The diffusion constant is thus

$$D(\omega) \sim \omega \xi^2(\omega) . \qquad (8.3)$$

The density of states is

$$N(\omega) = \int \frac{dk}{2\pi} G(k,\omega) \sim \frac{1}{\omega\xi(\omega)} . \qquad (8.4)$$

The relations (8.3) and (8.4) are satisfied by (3.25),

(4.19), and (5.11), and also by (7.10) and (7.11). There is thus one exponent in the model, that of the correlation length. Arguments for this exponent leading to (5.12) have been put forward by Alexander and Bernasconi[9] and Alexander et al.[2]

The correlation length is finite for all $\omega > 0$. This is characteristic of diffusion processes. The effect of distributions of type (c) is to reduce the correlation length for a given value of ω. In this paper we have calculated average quantities. For finite ω as the correlation length is finite, these average quantities should be well defined.

ACKNOWLEDGMENT

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