

# Random Walks on Cubic Lattices with Bond Disorder

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*Received July 7, 1986; revision received September 12, 1986*

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We consider diffusive systems with static disorder, such as Lorentz gases, lattice percolation, ants in a labyrinth, termite problems, random resistor networks, etc. In the case of diluted randomness we can apply the methods of kinetic theory to obtain systematic expansions of dc and ac transport properties in powers of the impurity concentration  $c$ . The method is applied to a hopping model on a  $d$ -dimensional cubic lattice having two types of bonds with conductivity  $\sigma$  and  $\sigma_0 = 1$ , with concentrations  $c$  and  $1-c$ , respectively. For the square lattice we explicitly calculate the diffusion coefficient  $D(c, \sigma)$  as a function of  $c$ , to  $O(c^2)$  terms included for different ratios of the bond conductivity  $\sigma$ . The probability of return at long times is given by  $P_0(t) \approx [4\pi D(c, \sigma) t]^{-d/2}$ , which is determined by the diffusion coefficient of the disordered system.

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**KEY WORDS:** Lorentz gas; random walk on a disordered lattice; ant in a labyrinth; termite problem; bond percolation; random resistor network.

## 1. INTRODUCTION

Kinetic theory methods for obtaining density expansions<sup>(1)</sup> of static and frequency-dependent transport properties can be applied successfully to lattice models with quenched disorder, at least for densities not too close to a percolation threshold. This is shown by the results for the diffusion coefficient and the velocity autocorrelation function (VACF) in 2D lattice models with site<sup>(2,3)</sup> or bond<sup>(4)</sup> disorder.

Diffusive systems with static disorder, such as Lorentz gases, dynamic percolation, ants in a labyrinth, termite problems, random barrier models, random resistor networks, or the closely related lattice dynamics problems with normal and superelastic springs, etc., have received much recent atten-

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tion. Such problems can be modeled by random walks on disordered lattices which are equivalent to lattice dynamics of disordered harmonic crystals.

For the case of diluted randomness, where only a random fraction  $c$  of bonds or sites of the host lattice have been replaced by impurities, we develop a kinetic theory for diffusion phenomena on random lattices. In particular, we study a random walk on a square lattice with two types of bonds: impurity bonds with a transition rate ("conductance")  $\sigma$  and bonds of the host lattices with conductance  $\sigma_0 = 1$ . The model describes bond percolation for  $\sigma = 0$  and the termite problem for  $\sigma \gg 1$ .

Different methods to study these problems have already been discussed in Ref. 4. Here we only mention the effective medium approximation<sup>(5-8)</sup> and the single-impurity approximation,<sup>(9,10)</sup> which yield results identical to those of kinetic theory in linear order in the impurity concentration.

The basic quantity to be studied in this paper is the probability distribution  $P_n(t)$  for a displacement  $n$  in a time  $t$ , averaged over the quenched disorder, for a hopping model on a cubic lattice with unit lattice distance. From this quantity one can obtain the moments of displacement and related quantities. The most important one is the mean square displacement  $\langle n_x^2 \rangle(t)$  and the related time-dependent diffusion coefficient

$$\tilde{D}(t) = \frac{1}{2} (\partial/\partial t) \langle n_x^2 \rangle(t) = \int_0^t d\tau \phi(\tau) \quad (1.1)$$

where  $\tilde{D}(\infty) = D$  is the static diffusion and  $\phi(t)$  is the lattice analog of the VACF

$$\phi(t) = \langle v_x(0) v_x(t) \rangle = \frac{1}{2} (\partial/\partial t)^2 \langle n_x^2 \rangle(t) \quad (1.2)$$

The macroscopic conductivity in these bond models is directly proportional to the static diffusion coefficient  $D$ .

In this section we first present a detailed description of the model, and recall some symmetry properties. We consider a hopping model on a lattice, where an unbiased random walker (blind ant) makes nearest neighbor hops and is hindered by the presence of randomly distributed bond impurities (scatterers). The lattice is a  $d$ -dimensional simple cubic lattice with unit lattice distance, with  $N = L^d$  sites and periodic boundary conditions. A site is labeled by  $n = (n_x, n_y, \dots, n_d)$  and its second nearest neighbors are labeled by  $n + \rho$ .

A fraction  $c$  of bonds in the host lattice (having "conductivity"  $\sigma_0 = 1$ ) is replaced by impurity bonds with "conductivity"  $\sigma$ . The impurity bonds

may be nonconducting ( $\sigma = 0$ , “hard scatterers”) or have a nonvanishing conductivity  $\sigma$  which may be larger or smaller than that of the host lattice. If  $\sigma \gg 1$  we have the case of “superconducting” bonds or the “termite problem.”<sup>(11)</sup> When moving on a connected cluster of superconducting bonds, the RW makes on the average a jump every  $1/\sigma$  time units (fast time scale). However, the RW will leave the superconducting cluster after an average number of  $\sigma$  jumps, and moves onto the connected cluster of normal-conducting bonds, where it makes on the average a jump in one unit of time (slow time scale). The above arguments apply only to small (impurity) clusters of size  $l = 1, 2, \dots$ , which is the case of interest in a low-density theory to  $O(c')$ .

Here we choose the formulation of continuous-time random walks (CTRW), where the RW pauses after every hop during a time interval  $\tau$ , which is a random variable with an exponential distribution. Such CTRW can be described by the master equation with a continuous time,<sup>(12)</sup> where the transition rate across a bond is proportional to its conductivity, which has either the value  $\sigma_0 = 1$  or  $\sigma \equiv 1 - b$ . The probability distribution  $p_n(t)$  to find the RW on site  $n$  at time  $t$  is then described by

$$\dot{p}_n = (1/2d) \sum_{\rho} \psi_{n,n+\rho} (p_{n+\rho} - p_n) \tag{1.3}$$

Here we have assigned to every bond  $(n, n + \rho)$  a random variable

$$\psi_{n,n+\rho} = 1 - bc_{n,n+\rho} \tag{1.4}$$

where  $b = 1 - \sigma \leq 1$  and where

$$c_{n,n+\rho} = \begin{cases} 1 & \text{with probability } c \\ 0 & \text{with probability } 1 - c \end{cases} \tag{1.5}$$

The solution of the master equation depends on the set of random variables  $\{c_n\}$ , and the quantity of physical interest is obtained by averaging this solution over the probability distribution of  $\{c_n\}$ . The most basic quantity is the average probability of displacements  $P_n(t)$ , whose Fourier–Laplace transform is the response function  $F(q, z)$ .

These functions obey symmetry relations based on the interchange of the two types of conductors.<sup>(13)</sup> We first note that the master equation is invariant under the mapping  $\sigma \rightarrow \sigma' = 1/\sigma$ , and  $c_{n,n+\rho} \rightarrow c'_{n,n+\rho} = 1 - c_{n,n+\rho}$  and  $t \rightarrow t' = \sigma t$ . If we map in addition the probability distribution (1.5) as  $c \rightarrow c' = 1 - c$ , then the average quantities possess the following symmetry:

$$P_n(t, c, \sigma) = P_n(\sigma t, 1 - c, 1/\sigma) \tag{1.6}$$

This implies the following symmetry relations for the diffusion coefficient and VACF due to (1.1) and (1.2):

$$\begin{aligned} D(c, \sigma) &= \sigma D(1 - c, 1/\sigma) \\ \varphi(t, c, \sigma) &= \sigma^2 \varphi(\sigma t, 1 - c, 1/\sigma) \end{aligned} \quad (1.7)$$

Analogous symmetry relations hold for  $\tilde{D}(t)$  in (1.1). We note that  $D(0, \sigma)$  is the diffusion coefficient of the host lattice without impurities. Measured in the length and time units used in this paper,  $D(0, \sigma) = 1/2d \equiv D_0$ .

The above symmetry relations apply for general dimensionality. In the two-dimensional case we have an additional symmetry, since the square lattice with a random mixture of two different types of bonds (conductances) is self-dual, as shown by Straley.<sup>(13)</sup> This yields

$$D(c, \sigma) D(c, 1/\sigma) = D_0^2 \quad (1.8)$$

Combination of both symmetries yields

$$D(c, \sigma) D(1 - c, \sigma) = \sigma D_0^2 \quad (1.9)$$

From there the exact value for the half-filled lattice follows as  $D(\frac{1}{2}, \sigma) = \sigma^{1/2} D_0$ .

The plan of the paper is as follows. In Section 2 we develop a resolvent formalism for the master equation  $\dot{p}_n = -(Lp)_n$  and make a  $T$ -matrix expansion of the average resolvent  $\langle (z + L)^{-1} \rangle$ . In Section 3 the response function is evaluated to linear and quadratic order in the impurity concentration  $c$ . As an application, we obtain the coefficients in the  $c$  expansion of the diffusion coefficient (Section 4) and of the long-time behavior of the return probability (Section 5) and present the numerical results for these coefficients obtained by performing 2D lattice sums. In our analytic and numerical calculations in the present and in a subsequent article we also need short-time expansions of the response function and transport quantities derived from it. The coefficients in these expansions will be calculated for general impurity concentration and general dimensionality in Section 6. We further need many properties of the basic Green's functions for the square lattice, which can be derived along the lines of Ref. 14 and are given in Appendix A. In Appendix B a certain lattice sum is calculated analytically, whereas Appendix C calculates the ring collision integral and the return probability on an impurity-free lattice.

## 2. T-MATRIX EXPANSION

In this section the hopping model is cast in the language of kinetic theory by developing a  $T$ -matrix expansion of the response function.

We start with the master equation (1.3), which reads in a notation more convenient for our purposes

$$\begin{aligned} \dot{p}_n &= (1/2d) \sum_x [\psi_n^\alpha(p_{n+\rho_x} - p_n) + \psi_{n-\rho_x}^\alpha(p_{n-\rho_x} - p_n)] \\ &= -(1/2d) \sum_x (1 - E_x^{-1}) \psi_n^\alpha (1 - E_x) p_n \\ &= -\sum_m \hat{L}_{nm} p_m = -(\hat{L}p)_n \end{aligned} \tag{2.1}$$

where  $\hat{L}_{nm}$  is the coordinate representation of the linear master operator  $L$ . From now on we label the bond  $(n, n + \rho_x)$  by  $(n, \alpha)$ , and the random variable (1.6) and (1.7) will be denoted by

$$\psi_n^\alpha = 1 - bc_n^\alpha \tag{2.2}$$

The vector  $\rho_x$  is a lattice vector in the  $\alpha$  direction ( $\alpha = x, y, \dots, d$ ) and  $E_x$  is a shift operator, defined as  $E_x A(n) = A(n + \rho_x)$ . We further note for later convenience that the stationary solution of (2.1), properly normalized, reads  $p_n^0 = 1/N$ .

The average concentration of impurities is

$$c = (dN)^{-1} \sum_{n\alpha} c_n^\alpha = \langle c_n^\alpha \rangle$$

Here and in the sequel brackets  $\langle \dots \rangle$  imply an average over the probability distribution of the random variables  $\{c_n^\alpha\}$ . The case  $b = 1$  in (2.2) corresponds to nonconducting bonds (percolation problem, “pure ant” model); the case  $b = 0$  represents the ordinary RW on a uniform lattice. The limit  $b \rightarrow -\infty$  corresponds to superconducting bonds (“pure ter-mite” model).

The quantity of main interest, which describes all transport properties, is the probability distribution  $\langle p(nt; m0) \rangle = P_{n-m}(t)$  for a displacement  $n - m$  averaged over the random impurities. An equivalent description can be given in terms of its moments of displacement:

$$\langle (n_x - m_x)^l \rangle = \sum_{n,m} (n_x - m_x)^l \langle p(nt; m0) \rangle \tag{2.3}$$

The two-time probability distribution  $p(nt; m0)$  can be expressed in terms of the conditional probability  $p(nt|m0)$  multiplied by the initial distribution  $p_m(0)$ , which is always taken to be the stationary solution of (2.1), viz.  $p_m(0) = p_m^0 = 1/N$ . Thus, we write the formal solution of (2.1) as

$$p(nt; m0) = p(nt|m0) p_m^0 = N^{-1} (\exp - t\hat{L})_{nm}$$

The generating function for the (Laplace-transformed) moments of displacement—mostly referred to as response function—is then

$$\begin{aligned} F(q, z) &= N^{-1} \left\langle \sum_{n,m} e^{iq(n-m)} \hat{p}_z(n|m) \right\rangle \\ &= \langle (z + L)^{-1} \rangle_{qq} \end{aligned} \quad (2.4)$$

The propagator  $\hat{p}_z(n|m) = ((z + \hat{L})^{-1})_{nm}$  is the Laplace transform of  $p(nt|m0)$ , and we have introduced the Fourier representation  $A_{qq'}$  of a matrix  $\hat{A}_{nm}$  in coordinate representation as

$$A_{qq'} = N^{-1} \sum_{n,m} e^{inq} \hat{A}_{nm} e^{-imq'} \quad (2.5)$$

where  $q$  is a reciprocal lattice vector in the first Brillouin zone (1BZ). All  $q$  sums in this paper extend over 1BZ. For later reference we quote the orthogonality relations:

$$N^{-1} \sum_n e^{in(q-q')} = \delta_{qq'}; \quad N^{-1} \sum_{q \in 1BZ} e^{iq(n-m)} = \delta_{nm} \quad (2.6)$$

The function  $P_n(t)$  is the lattice analog of Van Hove's  $G(r, t)$  function in the theory of liquids; its Fourier-Laplace transform  $F(q, z)$  is the scattering function. In Eq. (2.4) we have cast the response function in a form very similar to and very suitable for kinetic theory analysis,<sup>(1)</sup> which we will develop in the remaining part of this section.

To proceed, we decompose  $L$  in (2.1) according to (2.2) into a part  $L^0$  referring to the uniform lattice and a perturbation  $-\delta L$  describing the impurities, i.e.,  $L = L^0 - \delta L$ , with

$$\begin{aligned} (L^0 a)_n &= (1/2d) \sum_x (1 - E_x^{-1})(1 - E_x) a_n \\ (\delta L a)_n &= (b/2d) \sum_x (1 - E_x^{-1}) c_n^x (1 - E_x) a_n \end{aligned} \quad (2.7)$$

We further define  $g = (z + L^0)^{-1}$  as the propagator of the uniform lattice. In the Fourier representation (2.5) these quantities have the form

$$\begin{aligned} L_{qq}^0 &= \omega(q) \delta_{qq'} \\ g_{qq'} &= g(q) \delta_{qq'} = [z + \omega(q)]^{-1} \delta_{qq'} \end{aligned} \quad (2.8)$$

where

$$\omega(q) = (1/2d) \sum_x \varepsilon_x^*(q) \varepsilon_x(q) = (1/d) \sum_x (1 - \cos q_x) \quad (2.9)$$

The asterisk denotes complex conjugation and  $\varepsilon_x(q) = 1 - \exp(-iq_x)$ . For the perturbation we find similarly

$$\delta L_{qq'} = (b/2dN) \sum_{n,\alpha} c_n^\alpha e^{i(q-q')n} \varepsilon_x^*(q) \varepsilon_x(q') \tag{2.10}$$

where only the impurity bonds contribute to the  $(n, \alpha)$  sum. The formal perturbation expansion of  $F(q, z)$  follows with the help of

$$(z + L^0 - \delta L)^{-1} = g \sum_{l=0}^{\infty} (\delta L g)^l$$

and (2.4) and (2.8) yield

$$\begin{aligned} F(q, z) &= g(q) + g^2(q) M(q, z) \\ M(q, z) &= \sum_{l=0}^{\infty} \langle (\delta L g)^l \delta L \rangle_{qq} \end{aligned} \tag{2.11}$$

Each  $\delta L$  contains a sum over impurities. The terms in the perturbation expansion can be regrouped by adding successive terms referring to the same impurity by the so-called  $T$ -matrix resummation. To that purpose we consider

$$[(\delta L g)^l \delta L]_{qq'} = \sum_{q_1 \dots q_l} \delta L_{qq_1} g_1 \delta L_{q_1 q_2} g_2 \dots \delta L_{q_{l-1} q_l} g_l \delta L_{q_l q'}$$

where  $g_i = g(q_i)$  as defined in (2.8) and all  $q$  sums run over 1BZ. Next we insert (2.10), with the result

$$\begin{aligned} & [(\delta L g)^l \delta L]_{qq'} \\ &= N^{-1} (b/2d)^{l+1} \sum_{n_1 \alpha_1} \dots \sum_{n_l \alpha_l} \sum_{m \beta} c_{n_1}^{\alpha_1} \dots c_{n_l}^{\alpha_l} c_m^\beta \\ & \times \exp(iqn_1 - iq'm) \varepsilon_{\alpha_1}^*(q) G_{\alpha_1 \alpha_2}(n_1 - n_2) \\ & \times G_{\alpha_2 \alpha_3}(n_2 - n_3) \dots G_{\alpha_l \beta}(n_l - m) \varepsilon_\beta(q') \end{aligned} \tag{2.12}$$

Here we have introduced the quantity

$$G_{\alpha\beta}(n, z) = \int_q e^{-iqn} \varepsilon_\alpha(q) g(q, z) \varepsilon_\beta^*(q) \tag{2.13}$$

with the short-hand notation

$$\int_q \dots = N^{-1} \sum_{q \in 1\text{BZ}} \dots \underset{N \rightarrow \infty}{\approx} (2\pi)^{-d} \int \dots \int_{-\pi}^{\pi} d^{(d)}q \dots \tag{2.14}$$

In the thermodynamic limit ( $N \rightarrow \infty$ ) the  $q$  summation may be replaced by an integral over the 1BZ. The quantity  $G_{\alpha\beta}(n, z)$  is essentially (apart from the goniometric factors  $\varepsilon_\alpha \varepsilon_\beta^*$ ) the probability for a displacement  $n$  on a uniform lattice.

Suppose that two successive bond labels  $(n, \alpha)$  and  $(m, \beta)$  refer to the same bond; then  $c_n^\alpha c_m^\beta = (c_n^\alpha)^2 = c_n^\alpha$  and  $G_{xx}(0, z)$  is essentially the probability of return to the same site or bond on a uniform lattice. If we sum all possible returns to the impurity bond  $(n\alpha)$ , we have the single-impurity  $T$ -matrix

$$T(z) = (b/2d) \sum_{l=0}^{\infty} [bG_{xx}(0, z)/2d]^l = (b/2d)[1 - bJ(z)]^{-1} \quad (2.15)$$

The  $T$ -matrix is a scalar in the present bond model and is independent of  $\alpha$  ( $\alpha = x, y, \dots, d$ ) because of cubic symmetry, where we have introduced

$$\begin{aligned} J(z) &= (1/2d) G_{xx}(0, z) = (1/d) \int_q g(q)(1 - \cos q_x) \\ &= (1/d) \int_q \omega(q)/[z + \omega(q)] \end{aligned} \quad (2.16)$$

and we used the cubic symmetry together with (2.13) and (2.9).

In order to carry out the  $T$ -matrix resummation in (2.11), we average (2.12) over the probability distribution of the impurities, and obtain with the help of (2.15) the final result of this section:

$$\begin{aligned} M(q, z) &= N^{-1} \sum_{n\alpha} \langle c_n^\alpha \rangle T(z) \varepsilon_\alpha^*(q) \varepsilon_\alpha(q) \\ &+ N^{-1} \sum_{l=1} \sum_{n_1\alpha_1} \sum_{n_2\alpha_2} \cdots \sum_{n_l\alpha_l} \sum_{m\beta} \langle c_{n_1}^{\alpha_1} c_{n_2}^{\alpha_2} \cdots c_{n_l}^{\alpha_l} c_m^\beta \rangle e^{iq(n_1 - m)} \\ &\times \varepsilon_{\alpha_1}^*(q) T(z) G_{\alpha_1\alpha_2}(n_1 - n_2) \\ &\times T(z) G_{\alpha_2\alpha_3}(n_2 - n_3) T(z) \cdots G_{\alpha_l\beta}(n_l - m) T(z) \varepsilon_\beta(q) \end{aligned} \quad (2.17)$$

The primes on the summation signs indicate that any pair of consecutive bond labels is different.

### 3. DENSITY EXPANSION

The first term in (2.17) involves encounters of the RW with a single impurity only. It is therefore linear in the impurity concentration  $\langle c_n^\alpha \rangle = c$  and simplifies to  $2dc T(z) \omega(q)$  due to (2.9). All remaining terms in (2.17)



involve at least two different impurities, so that  $\langle c_n^\alpha c_n^{\alpha'} \cdots c_m^\beta \rangle$  is at least quadratic in  $c$ . Thus, the response function (2.11) to linear order in  $c$  is given by

$$M(q, z) = 2dc T(z) \omega(q) = cb\omega(q)/[1 - bJ(z)] \quad (3.1)$$

The term in (2.17) with  $l=1$  contains an encounter of the RW with impurity  $(n, \alpha) \equiv 1$  and a subsequent one with a different impurity  $(m, \beta) \equiv 2$ , formally denoted by the collision sequence [12]. The term with  $l=2$  involves the sequence of encounters [12*k*], which contains a two-impurity contribution [121] and a three-impurity contribution [123]. All terms with  $l \geq 2$  contain at least two impurity contributions. They are of  $O(c^2)$  since  $\langle c_n^\alpha c_m^\beta c_n^\alpha \cdots \rangle = \langle c_n^\alpha c_m^\beta \rangle = c^2$ . The two-impurity contributions in higher order terms involve the following encounter sequences with impurities (1) and (2): [12], [121], [1212], [12121],..., and contain respectively one, two, three, four, ..., crossings between the impurity pair (12). To evaluate the contributions of such sequences to  $M(q, z)$  in (2.17), we have to consider separately the terms with an odd number of crossings, denoted by  $M^{(\text{odd})}(q, z)$ , where the RW starts at impurity (1) and ends at impurity (2); and  $M^{(\text{even})}(q, z)$  with an even number of crossings, where the RW returns to the first impurity. We begin with the odd number of crossings, where starting position  $n$  and final position  $m$  are different:

$$M^{(\text{odd})}(q, z) = (c^2/N) \sum_{(n\alpha) \neq (m\beta)} \sum e^{iq(n-m)} \\ \times T \varepsilon_\alpha^*(q) R_{\alpha\beta}(n-m) R_{\beta\alpha}(m-n) \cdots R_{\alpha\beta}(n-m) \varepsilon_\beta(q) \quad (3.2)$$

and we have introduced

$$R_{\alpha\beta}(n, z) = G_{\alpha\beta}(n, z) T(z) = R_{\beta\alpha}(-n, z) \quad (3.3)$$

Since the summand in (3.2) depends only on  $(n-m)$ , we can trivially carry out one of the lattice sums. Using the symmetry (3.3), we find for the total contribution of two impurities with an odd number of crossings in between

$$M^{(\text{odd})}(q, z) = c^2 T \sum'_{n\alpha\beta} e^{iqn} \varepsilon_\beta(q) \varepsilon_\alpha^*(q) [1 - R_{\alpha\beta}^2(n)]^{-1} R_{\alpha\beta}(n) \quad (3.4)$$

For the total two-impurity contribution of an even number of crossings one finds similarly

$$M^{(\text{even})}(q, z) = c^2 T \sum'_{n\alpha\beta} |\varepsilon_\alpha(q)|^2 [1 - R_{\alpha\beta}^2(n)]^{-1} R_{\alpha\beta}^2(n) \\ = 2dT c^2 \omega(q) \sum'_{n\beta} R_{\alpha\beta}^2(n)/[1 - R_{\alpha\beta}^2(n)] \quad (3.5)$$

In the last equality we have used the fact that the coefficient of  $|\varepsilon_\alpha(q)|^2$  is a lattice sum  $\sum_{n\beta} \{\dots\}_{\alpha\beta}$ , independent of  $\alpha$ , because of cubic symmetry. Next, the  $\alpha$  sum is performed with the help of (2.9) and yields the factor  $2d\omega(q)$ .

Combination of (3.1), (3.4), and (3.5) yields the total contribution to (2.11), exact up to  $O(c^2)$  terms included,

$$M(q, z) = 2cdT\omega(q) \left\{ 1 + c \sum'_{n\beta} R_{x\beta}^2(n)/[1 - R_{x\beta}^2(n)] \right\} \\ + c^2T \sum'_{n\alpha\beta} e^{iqn} \varepsilon_\beta(q) \varepsilon_\alpha^*(q) R_{\alpha\beta}(n)/[1 - R_{\alpha\beta}^2(n)] \quad (3.6)$$

where the prime on the summation signs indicates the constraint  $(n\beta) \neq (0x)$  and  $(n\beta) \neq (0\alpha)$ , respectively.

The result (3.6) together with  $F(q, z) = g(q) + g^2(q) M(q, z)$  determines the response function exact to  $O(c^2)$  and can be used to calculate the distribution of displacements  $P_n(t)$  or its moments  $\langle n_x^l \rangle$ , the diffusion coefficients, the VACF, and related time correlation functions. It is the basic result of this paper, and serves as a starting point for deriving explicit expressions for the above quantities in terms of lattice sums. Then the lattice sums have to be evaluated, partly analytically, partly numerically. In the present article this program is carried out for the static diffusion coefficient in Section 4 and for the long-time behavior of the return probabilities in Section 5.

#### 4. STATIC DIFFUSION COEFFICIENT

In the previous section we have obtained the response function or moment-generating function (2.11), where  $M(q, z)$  has been calculated in (3.6) to  $O(c^2)$  in the concentration of impurities. In this section we concentrate on the mean square displacement  $\langle n_x^2 \rangle$ , the diffusion coefficient  $D$ , and the VACF  $\varphi(t)$ . Denoting the Laplace transform of the VACF as  $\Phi(z)$ , we have for the static diffusion coefficient  $D = \Phi(z=0)$ . The quantity  $\Phi(z)$  can be considered as the frequency-dependent diffusion coefficient, and we have, according to (1.1), (1.2), (2.3), and (3.4),

$$\Phi(z) = \frac{1}{2}z^2 \langle n_x^2 \rangle(z) = -\frac{1}{2}z^2 F''(0, z) \quad (4.1)$$

where  $\langle n_x^l \rangle(z)$  represents the Laplace transform of the  $l$ th moment of the displacement and where we have used the abbreviation

$$A''(0, z) = (\partial/\partial q_x)^2 A(q, z)|_{q=0}$$

Expressed in  $M(q, z)$ , this becomes  $\Phi(z) = (2d)^{-1} - \frac{1}{2}M''(0, z)$ , and we obtain after some calculation, using Eq. (3.6),

$$\Phi(z) = (2d)^{-1} - cT(z) \left\{ 1 + c \sum'_{n\beta} R_{x\beta}^2(n, z) / [1 - R_{x\beta}^2(n, z)] + c \sum_{n \neq 0} R_{xx}(n, z) / [1 - R_{xx}^2(n, z)] \right\} \quad (4.2)$$

This expression represents the Laplace transform of the VACF, exact to  $O(c^2)$  terms included. The static diffusion coefficient follows by taking the limit as  $z \rightarrow 0$ . Thus, we have to evaluate the  $d$ -dimensional lattice sums in (4.2) at  $z = 0$ , where the functions  $R_{\alpha\beta}(n, 0) = T(0) G_{\alpha\beta}(n, 0)$  decay as  $O(|n|^{-d})$  for  $|n| \gg 1$ , where  $|n|^2 = n_x^2 + n_y^2 + \dots + n_d^2$ . A detailed analysis of this behavior for the two-dimensional case is given in Appendix A. Therefore the lattice sum  $\sum_n |R_{xx}(n, 0)|$  diverges logarithmically, and one is not allowed to interchange the lattice summation with the limit as  $z \rightarrow 0$ . However, the slowly convergent terms in (4.2), which originate from a single crossing of the RW between two impurities, can be summed analytically using the relation  $\sum_n R_{xx}(n, z) = 0$ . It can be obtained from (3.3), (2.13), and (2.6), and the relevant lattice sum becomes

$$\sum_{n \neq 0} \frac{R_{xx}(n, z)}{1 - R_{xx}^2(n, z)} = -2dT(z) J(z) + \sum_{n \neq 0} \frac{R_{xx}^3(n, z)}{1 - R_{xx}^2(n, z)}$$

where we have used the relation  $R_{xx}(0, z) = T(z) G_{xx}(0, z)$  together with (2.16). The summand of the  $d$ -dimensional lattice sum at  $z = 0$  decreases as  $O(|n|^{-3d})$  and we can calculate the sum by first setting  $z = 0$  and next performing the lattice sum.

The convergence can be improved further by subtracting the double crossings of the RW between two impurities and summing them analytically. The required lattice sum  $\sum R_{\alpha\beta}^2(n, z)$  is calculated in Appendix B. In the remaining lattice sums the summands are at large  $|n|$  proportional to  $R_{x\beta}^3(n, 0) \sim O(|n|^{-3d})$  and converge very rapidly. We simply quote the final expression for the VACF for the  $d$ -dimensional cubic lattice, exact up to  $O(c^2)$ :

$$\Phi(z) = (2d)^{-1} - cT - c^2T \left\{ -2dTJ + 4d^2T^2[J - J^2 + zJ'] + \sum_{n \neq 0} \frac{R_{xx}^3(n, z)}{1 - R_{xx}^2(n, z)} + (d-1) \sum_{n \neq 0} \frac{R_{xy}^4(n, z)}{1 - R_{xy}^2(n, z)} \right\} + O(c^3) \quad (4.3)$$

where  $J'(z) = dJ(z)/dz$  and  $T(z)$  and  $R_{\alpha\beta}(n, z)$  are respectively defined in (2.15), (2.16), and (3.3). The resulting expression for the diffusion coef-

ficient in a  $d$ -dimensional cubic lattice follows from (4.3) by setting  $z = 0$ , and using the relations  $T(0) = \frac{1}{2}b/(d-b)$  and  $J(0) = 1/d$  derived from (2.15) and (2.16). It has the form of an expansion in powers of the impurity concentration:

$$D(c) = D_0(1 + \alpha_1 c + \alpha_2 c^2 + \dots) \quad (4.4)$$

where  $D_0 = 1/2d$  and

$$\begin{aligned} \alpha_1 &= -db/(d-b) \\ \alpha_2 &= -\frac{db}{d-b} \left[ -\frac{db(1-b)}{(d-b)^2} + \sum_{n \neq 0} \frac{R_{xx}^3(n, 0)}{1 - R_{xx}(n, 0)} \right. \\ &\quad \left. + (d-1) \sum_{n \neq 0} \frac{R_{xy}^4(n, 0)}{1 - R_{xy}^2(n, 0)} \right] \end{aligned} \quad (4.5)$$

The zeroth-order term  $D_0 \equiv 1/2d$  is the diffusion coefficient of the uniform lattice without impurities; the coefficient  $\alpha_1$  of the linear term in  $c$  represents the contribution from scattering by a single impurity; and the coefficient  $\alpha_2$  of the  $O(c)$  term describes the contribution from scattering by two different impurities. For the 1D case one verifies that  $R_{xx}(n, 0) = 0$  for  $n \neq 0$  and the density expansion (4.5) is in agreement with the exact result<sup>(4,16)</sup> for the 1D random barrier model, where  $D_0/D = \langle 1/\psi \rangle = 1 + cb/(1-b)$ . For the explicit evaluation of the  $O(c^2)$  terms we restrict ourselves to the 2D square lattice. Due to the square symmetry one has the symmetry relation at the site  $(n_x, n_y)$ :

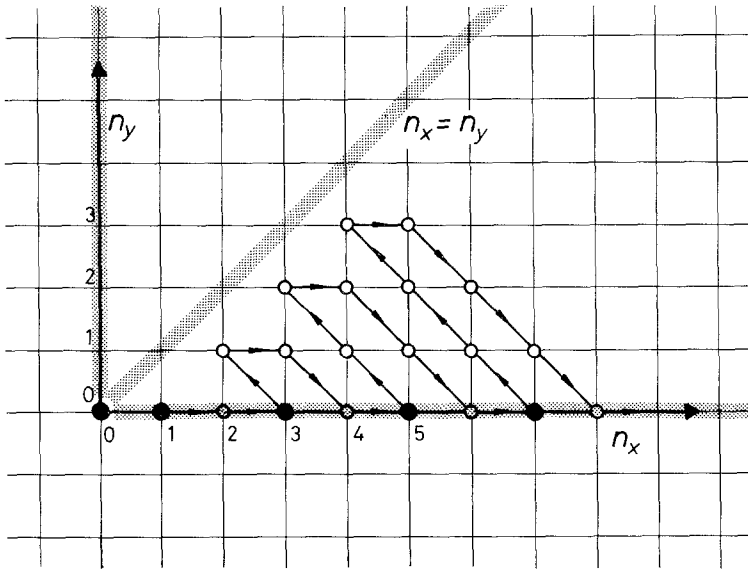
$$R_{xx}(n_x, n_y; 0) = -R_{xx}(n_y, n_x; 0) \quad (4.6)$$

as follows from (A3) and (A9). After symmetrizing the lattice sum in (4.5), we find for the coefficient  $\alpha_2$  in the square lattice

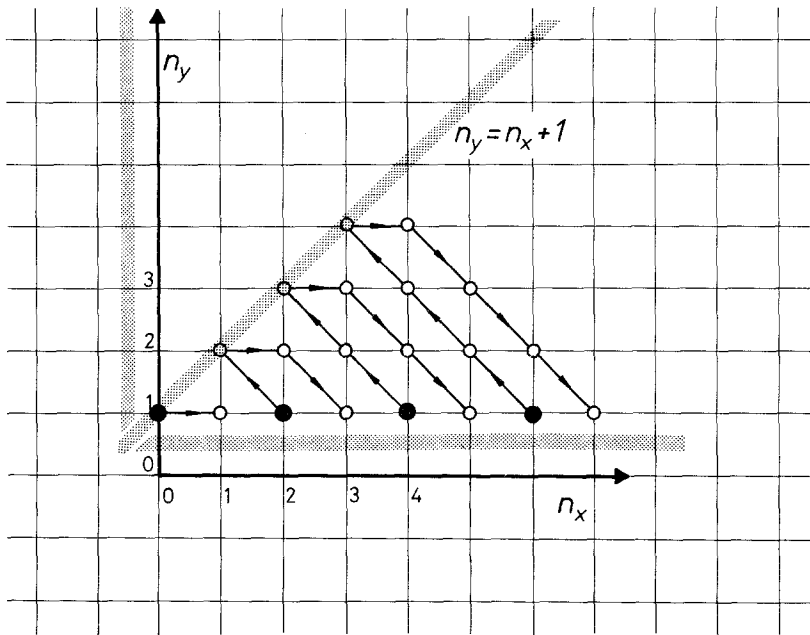
$$\begin{aligned} \alpha_2 &= -[2b/(2-b)][-2b(1-b)/(2-b)^2 \\ &\quad + \sum_{n \neq 0} H(n_x, n_y) + \sum_n K(n_x, n_y)] \end{aligned} \quad (4.7)$$

where the summands are

$$\begin{aligned} H(n_x, n_y) &= R_{xx}^4(n, 0)/[1 - R_{xx}^2(n, 0)] \\ K(n_x, n_y) &= R_{xy}^4(n, 0)/[1 - R_{xy}^2(n, 0)] \end{aligned} \quad (4.8)$$



(a)



(b)

Fig. 1. Two-dimensional square lattice with summation region (a)  $\{n_x \geq n_y \geq 0\}$  and (b)  $\{n_x \geq n_y - 1 \geq 0\}$  in (4.7) involving lattice Green's functions (a)  $G_{xx}(n, z=0)$  and (b)  $G_{xy}(n, z=0)$ , respectively. The shaded lines denote the lines of reflection symmetry. The arrows denote the scheme for solving the recursion relations (A10) for  $G_{xx}(n, z)$  and  $G_{xy}(n, z)$  in Appendix A. The Greens' functions at the sites marked with black dots are used as initial values in solving the recursion relations.

The summations in (4.7) can be reduced to triangular region indicated in Fig. 1a and 1b, respectively:

$$\begin{aligned} \sum_{n \neq 0} H(n, m) &= 4 \sum_{n \geq 1} H(n, 0) + 8 \sum_{n > m \geq 1} H(n, m) \\ \sum_n K(n, m) &= 4 \sum_{n \geq 0} K(n, n + 1) + 8 \sum_{n \geq m \geq 1} K(n, m) \end{aligned}$$

based on the symmetry properties

$$\begin{aligned} H(n, n) &= 0; & H(n, m) &= H(m, n) \\ H(n, m) &= H(-n, m) = H(n, -m) \end{aligned}$$

as follows from (3.3), (A4), and (B10), and

$$\begin{aligned} K(n, m) &= K(-n - 1, m) = K(n, -m + 1) \\ K(n, m) &= K(m - 1, n + 1) \end{aligned}$$

The lines of reflection symmetry for the functions  $H$  and  $K$  are indicated respectively in Fig. 1a and 1b. The quantities  $H$  and  $K$  are expressed in terms of  $R_{\alpha\beta}(n, 0) = [\frac{1}{2}b/(2 - b)] G_{\alpha\beta}(n, 0)$  with the help of (3.3) and (2.15), and the integrals  $G_{\alpha\beta}(n, 0)$  have been calculated in Appendix A. Their numerical values are listed in Table I, and we can calculate the coefficients  $\alpha_1$  and  $\alpha_2$  in the density expansion of the diffusion coefficient.

The two-dimensional lattice sums in (4.7) converge very rapidly, as  $\sum_n |n|^{-8}$ , where  $|n|^2 = n_x^2 + n_y^2$ . The first term in each of the sums, viz.  $4H(1, 0)$  and  $4K(0, 1)$ , determines essentially the value of the complete sum, as one can easily verify by using the values

$$\begin{aligned} R_{xx}(1, 0; 0) &= [b/(2 - b)](1 - 4/\pi) \\ R_{xy}(1, 0; 0) &= [b/(2 - b)](1 - 2/\pi) \end{aligned}$$

from Table I and comparing the results with Table II. The remaining terms in (4.9) contribute less than 1.3% over the whole range of  $b$  values ( $b \leq 1$ ). Thus we have the approximate analytical expression for  $\alpha_2$  (correct within 1.3%)

$$\begin{aligned} \alpha_2(b) \approx \frac{-4b^2}{(2 - b)^3} \left[ b - 1 + \frac{b^3(4 - \pi)^4}{2\pi^2(\pi - 2b)(\pi - \pi b + 2b)} \right. \\ \left. + \frac{b^3(\pi - 2)^4}{2\pi^2(\pi - b)(\pi - \pi b + b)} \right] \end{aligned} \tag{4.9}$$

Because of the symmetry (1.7) between high and low concentrations upon interchanging the conductances ( $\sigma \leftrightarrow 1/\sigma$ ), we also have an expansion of  $D$

Table I. Values of  $G_{xx}(n_x, n_y; 0) = A + B/\pi$  and  $G_{xy}(n_x, n_y; 0) = C + D/\pi$

$(n_x, n_y)$	$A$	$B$
(1, 0)	2	-8
(2, 0)	10	-32
(3, 0)	50	-472/3
(4, 0)	258	-2432/3
(5, 0)	1362	-64184/15
(2, 1)	-6	56/3
(3, 1)	-34	320/3
(4, 1)	-190	8852/15
(3, 2)	10	-472/15
	$C$	$D$
(0, 1)	-2	4
(1, 1)	-4	12
(2, 1)	-20	188/3
(3, 1)	-104	980/3
(4, 1)	-552	26012/15
(1, 2)	2	-20/3
(2, 2)	8	-76/3
(3, 2)	52	-2452/15
(2, 3)	-2	92/15
(3, 3)	-12	564/15

in powers of  $1 - c$ . The combined expansion possibly allows us to estimate the complete  $c$  dependence of  $D$  by interpolation between the high- and low-density results. The numerical value of the coefficient  $\alpha_2$  is listed in Table II for the related pairs of parameters  $(\sigma, \sigma' = 1/\sigma)$  or

Table II. Coefficient  $\alpha_2$  in (4.4) for Several Values of  $b = 1 - \sigma$

$b$	$\alpha_2(b)$	$b' = b/(b - 1)$	$\alpha_2(b')$
1	-0.21075	$-\infty$	4.2108
9/10	0.16944	-9	2.5082
7/8	0.21189	-7	2.2079
4/5	0.27047	-4	1.5073
3/4	0.27291	-3	1.1671
1/2	0.14737	-1	0.29707
1/3	0.06394	-1/2	0.09606
1/4	0.03497	-1/3	0.04666
1/5	0.02194	-1/4	0.02744

( $b, b' = b/(b - 1)$ ), where  $\sigma = 1 - b$ . The final results for the diffusion coefficient  $D(c, \sigma)$  are plotted in Fig. 2 for the whole range of  $c$  values.

For the square lattice the diffusion coefficient obeys an additional symmetry relation (1.8) based on self-duality, which relates the diffusion coefficient  $D(c, \sigma)$  at the parameter value  $\sigma = 1 - b$  to the diffusion coefficient  $D(c, 1/\sigma)$  at the parameter value  $\sigma' = 1/\sigma$  or  $b' = b/(b - 1)$ . Hence, the expansion coefficients  $\alpha_i(\sigma)$  and  $\alpha_i(1/\sigma)$  in (4.4) are related through

$$\alpha_1(1/\sigma) = -\alpha_1(\sigma), \quad \alpha_2(1/\sigma) = \alpha_1^2(\sigma) - \alpha_2(\sigma) \quad (4.10)$$

which is a consequence of self-duality (1.8). One can verify that the explicit results derived in (4.7) and (4.8) for the square lattice indeed satisfy the requirements of self-duality, since  $R_{\alpha\beta}(n, 0)$  only changes sign under the mapping  $\sigma \leftrightarrow 1/\sigma$ .

Since the symmetry relation (1.9) provides us with the exact value of the diffusion coefficient for the half-filled square lattice, viz.

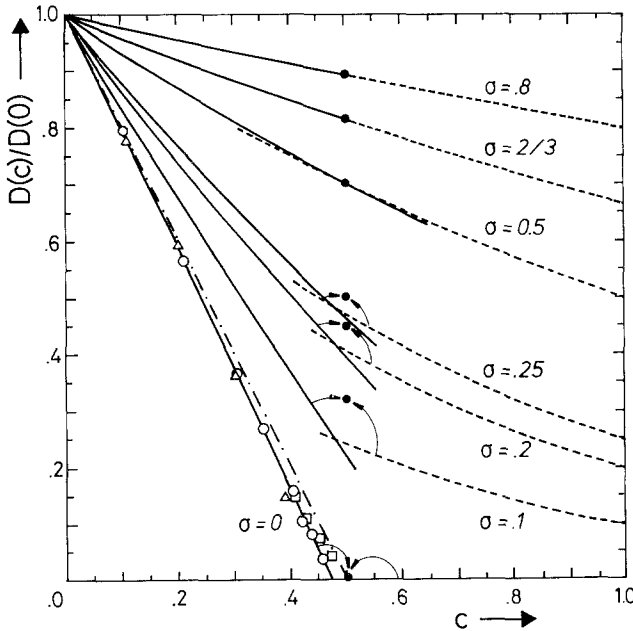


Fig. 2. Diffusion coefficient  $D(c)/D(0)$  versus concentration  $c$  of impurity bonds for several values of the impurity conductance  $\sigma$ . (—) The  $c$  expansion (4.4) with coefficients given in Table II; (- -) the  $(1 - c)$  expansion obtained from the symmetry relation (1.7). (●) Exact value  $D(\frac{1}{2}, \sigma) = \sigma^{1/2}D(0) = \sigma^{1/2}/4$ . For bond percolation ( $\sigma = 0$ ) the threshold  $D(\frac{1}{2}, 0) = 0$  is also exact. (—) The new results for bond percolation are compared with the simulation results of Kirkpatrick<sup>(5)</sup> and (- - -) with effective medium theory, where  $D(c, 0) = (1 - 2c)/4$ .



$D(\frac{1}{2}, \sigma) = \sigma^{1/2} D_0$ , we have a test on the accuracy of the extrapolations between high and low densities, as indicated in Fig. 2.

A further test on the accuracy of the extrapolations follows from the rigorous bounds on the following quantity:

$$\Delta(c, \sigma) = D(c, \sigma)/D_0 = 2d D(c, \sigma) \tag{4.11}$$

derived by Golden and Papanicolaou,<sup>(19)</sup> in particular their Eq. (6.12), reading

$$\sigma m(1 - c, 1/\sigma) \leq \Delta(c, \sigma) = \sigma \Delta(1 - c, 1/\sigma) \leq m(c, \sigma) \tag{4.12}$$

valid for  $\sigma < 1$ ; for  $\sigma > 1$  the inequality signs are reversed. We also introduced

$$\begin{aligned} m(c, \sigma) &= 1 + c[(\sigma - 1)^{-1} + (1 - c)/d]^{-1} \\ &= 1 - dbc/[d - b(1 - c)] \end{aligned} \tag{4.13}$$

with  $\sigma = 1 - b$ . For the one-dimensional case upper and lower bound coincide with the exact value, derived below (4.5). Comparison of (4.12) and (4.13) with (4.4) and (4.5) also shows  $\alpha_2(\sigma) \leq db^2/(d - b)^2$  for  $\sigma < 1$ , with the equality sign reversed for  $\sigma > 1$ .

For the 2D percolation case ( $\sigma = 0, b = 1$ ) the rigorous bounds reduce to  $0 \leq \Delta(c, 0) \leq (1 - c)/(1 + c)$ , which are clearly satisfied, as shown by Fig. 2. The test appears to be most critical for *small* nonvanishing  $\sigma$  values. In Table III we have compared the upper bound (ub) and lower bound (lb) with the extrapolated expansion  $D^{(2)}(c, \sigma)$  at low density ( $c$  expansion) and at high density [ $(1 - c)$  expansion] for the value  $\sigma = 0.1$ , where the exact value for  $\Delta(1/2, \sigma) = \sqrt{\sigma} \approx 0.316$ .

If we consider the interpolation formula

$$\hat{D}(c, \sigma) = \max\{D^{(2)}(c, \sigma), \sigma D^{(2)}(1 - c, 1/\sigma)\} \tag{4.14}$$

**Table III. Comparison of Upper and Lower Bounds (ub and lb) on  $\Delta(c, \sigma)$  with Results from  $c$  Expansion and  $(1 - c)$  Expansion at  $\sigma = 0.1$ . Where  $\Delta(1/2, \sigma) = \sqrt{\sigma} \approx 0.316$**

$c$	lb	$c$ Expansion	$(1 - c)$ Expansion	ub
0.40	0.294	0.373	0.206	0.507
0.475	0.251	0.261	0.255	0.440
0.50	0.239	0.224	0.245	0.419
0.55	0.217	0.151	0.224	0.379
0.60	0.197	0.079	0.206	0.341

as an estimate for the  $c$  dependence of the diffusion coefficient over the whole range of  $c$  values, then we may conclude that  $\hat{D}(c, \sigma)$  satisfies the rigorous bounds for all values of  $c$  and  $\sigma$ .

**5. RETURN OR STAYING PROBABILITY**

As a second application of our result, exact up to  $O(c^2)$ , for the response function  $F(q, z)$  in (3.8), we consider the probability distribution  $P_0(t)$  for zero displacement, the so-called return or staying probability. In fact, we are able to calculate the whole average probability distribution  $P_n(t)$  through Fourier inversion. For the Laplace-transformed quantity  $\hat{P}_n(z)$  we find from (2.4)

$$\hat{P}_n(z) = \int_q e^{-iqn} F(q, z) \tag{5.1}$$

This yields, in particular, for the return probability

$$\begin{aligned} \hat{P}_0(z) = & \int g + \int g^2 \omega B(z) \\ & + c^2 \sum'_{n\alpha\beta} R_{\alpha\beta}(n, z) R_{\alpha\beta}^{(2)}(n, z) / [1 - R_{\alpha\beta}^2(n, z)] \end{aligned} \tag{5.2}$$

where we have used (2.11) with  $M(q, z)$  from (3.6) and we introduced

$$B(z) = 2cdT \left\{ 1 + c \sum'_{n\beta} R_{x\beta}^2(n, z) / [1 - R_{x\beta}^2(n, z)] \right\} \tag{5.3}$$

and

$$\begin{aligned} R_{\alpha\beta}^{(2)}(n, z) &= R_{\beta\alpha}^{(2)}(-n, z) \\ &= T \int e^{-iqn} \varepsilon_\alpha(q) \varepsilon_\beta^*(q) g^2(q) \\ &= -T \frac{d}{dz} [G_{x\beta}(n, z)] \end{aligned} \tag{5.4}$$

On the impurity-free host lattice the return probability is given by the first term on the rhs of (5.2),  $P_0(z) = \int g$ , with a long-time behavior of the form  $P_0(t) \approx (4\pi D_0 t)^{-d/2}$  as  $t \rightarrow \infty$ , with  $D_0 = (2d)^{-1}$ .

In order to determine the long-time behavior of  $P_0(t)$  on the disordered lattice, we need to know the dominant small- $z$  behavior of the remaining terms in  $\hat{P}_0(z)$  in (5.2). In the second term the dominant small- $z$

singularity is contained in the integral  $\int g^2\omega = -(d/dz) \int g\omega$ . This corresponds in time language to

$$(-t d/dt) \int e^{-\omega t} \approx (d/2)(2\pi D_0 t)^{-d/2} \quad \text{as } t \rightarrow \infty$$

The factor  $B(z)$ , defined in (5.3), approaches a constant  $B(0)$  as  $z \rightarrow 0$  [compare with (4.2)].

To determine the dominant singularity of the third term in (5.2), one cannot interchange the small- $z$  limit with the lattice summation. The arguments are the same as those referring to the third term in (4.2), and we proceed similarly by separating it into

$$c^2 \sum'_{n\alpha\beta} R_{\alpha\beta}(n, z) R_{\alpha\beta}^{(2)}(n, z) + c^2 \sum'_{n\alpha\beta} R_{\alpha\beta}^3(n, z) R_{\alpha\beta}^{(2)}(n, z) / [1 - R_{\alpha\beta}^2(n, z)] \quad (5.5)$$

The first term can be evaluated analytically in a manner similar to Appendix B. The result is

$$4c^2 T^2 d^2 \int g^3\omega^2 - 4c^2 T^2 d \int g^2\omega \int g\omega \approx \alpha_1^2 c^2 \left[ \int g^3\omega^2 - (1/d) \int g^2\omega \right] \quad (z \rightarrow 0) \quad (5.6)$$

In the last equality we have only kept the dominant small- $z$  singularity, and used  $\alpha_1 = 2dT(0)$ , as given in (4.5). The long-time behavior corresponding to  $\int g^3\omega^2$  is  $[d(d+2)/8](4\pi D_0 t)^{-d/2}$  as  $t \rightarrow \infty$ .

The second term in (5.5) converges rapidly, so that lattice summation and small- $z$  limit can be interchanged. Here  $R_{\alpha\beta}^{(2)}(n, z)$ , defined in (5.4), contains the dominant small- $z$  singularity, which is independent of the site index  $n$ . The arguments are essentially the same as given in Appendix A4 for the square lattice. For our purpose we may therefore make the following replacement in the second term of (5.5):

$$R_{\alpha\beta}^{(2)}(n, z) \rightarrow \delta_{\alpha\beta} 2T(0) \int g^2\omega$$

and set  $z = 0$  elsewhere.

Combination of the previous results and comparison with (4.4) and (4.5) shows that the long-time behavior of the return probability for the disordered lattice has the anticipated form:

$$P_0(t) \approx [4\pi D(c) t]^{-d/2} \quad (t \rightarrow \infty)$$

where the diffusion coefficient  $D(c)$  is given by the density expansion (4.4) and (4.5). The result also agrees with the exact result<sup>(16)</sup> for the 1D random jump rate model, where  $D(c) = D_0[1 + cb/(1 - b)]^{-1}$ .

### 6. SHORT-TIME EXPANSIONS

The behavior of the response function  $F(q, z)$ , of the probability distribution of displacements  $P_n(t)$ , of the time-dependent diffusion coefficient, the VACF, etc., can be calculated exactly for short times to all orders in the impurity concentration and for arbitrary dimensionality  $d$ , as will be shown in this section.

Starting from (2.4), we write the inverse Laplace transform of the response function as

$$\tilde{F}(q, t) = \langle e^{-tL} \rangle_{qq} = 1 - t \langle L_{qq} \rangle + \frac{1}{2} t^2 \langle L_{qq}^2 \rangle + \dots \tag{6.1}$$

where, due to (2.7)–(2.10),

$$\begin{aligned} L_{qq'} &= \omega(q) \delta_{qq'} - \delta L_{qq'} \\ \delta L_{qq'} &= (1/N) \sum_n c_n^\alpha \exp[i(q - q') n] \varepsilon_\alpha^*(q) \varepsilon_\alpha(q) \\ C_{qq'}^\alpha &= (1/N) \sum_n c_n^\alpha \exp[i(q - q') n] \end{aligned} \tag{6.2}$$

With the help of these relations we can calculate  $\langle L_{qq}^m \rangle$  for  $m = 1, 2, 3, \dots$ . We shall only work out the results for  $m = 1$  and 2, and simply quote those for  $m = 3$ :

$$\begin{aligned} \langle L_{qq} \rangle &= \omega(q)(1 - bc) \\ \langle L_{qq}^2 \rangle &= \omega^2(q)(1 - 2bc) \\ &\quad + (b/2d)^2 \sum_{\alpha\beta} \sum_{q'} \varepsilon_\alpha^*(q) \varepsilon_\alpha(q') \varepsilon_\beta^*(q') \varepsilon_\beta(q) \langle C_{qq'}^\alpha C_{q'q}^\beta \rangle \end{aligned} \tag{6.3}$$

To proceed we use the following fluctuation formulas<sup>(16)</sup>:

$$\begin{aligned} \langle C_{qq'}^\alpha C_{q'q}^\beta \rangle &= (\kappa_2/N) \delta_{\alpha\beta} + \kappa_1^2 \delta_{qq'} \\ \langle C_{qq'}^\alpha C_{q'q'}^\beta C_{q''q}^\gamma \rangle &= (\kappa_3/N) \delta_{\alpha\beta} \delta_{\beta\gamma} \\ &\quad + (\kappa_2 \kappa_1/N) (\delta_{qq'} \delta_{\beta\gamma} + \delta_{qq''} \delta_{\alpha\beta} + \delta_{q'q''} \delta_{\alpha\gamma}) + \kappa_1^3 \delta_{qq'} \delta_{q'q''} \end{aligned} \tag{6.4}$$

where  $\kappa_l$  is the  $l$ th cumulant corresponding to the  $l$ th moment  $\langle (c_n^x)^l \rangle = \langle c_n^x \rangle = c$  and is given by

$$\begin{aligned} \kappa_1 &= \langle c \rangle = c; & \kappa_2 &= \langle (c - \langle c \rangle)^2 \rangle = c(1 - c) \\ \kappa_3 &= \langle (c - \langle c \rangle)^3 \rangle = c(1 - c)(1 - 2c) \end{aligned} \tag{6.5}$$

One thus obtains

$$\langle L_{qq}^2 \rangle = (b^2/d) c(1 - c) \omega(q) + (1 - bc)^2 \omega^2(q) \tag{6.6}$$

and the response function becomes

$$\begin{aligned} \tilde{F}(q, t) &= 1 - t(1 - bc) \omega(q) + \frac{1}{2}t^2 [c(1 - c)(b^2/d) \omega(q) + (1 - bc)^2 \omega^2(q)] \\ &\quad - \frac{1}{6}t^3 \{c(1 - c)(b^2/d^2) [(d + \frac{1}{2})(1 - bc) - b(1 - 2c)] \omega(q) \\ &\quad + c(1 - c)(2b^2/d)(1 - bc) \omega^2(q) + (1 - bc)^3 \omega^3(q)\} + O(t^4) \end{aligned} \tag{6.7}$$

where we have also used the result for  $\langle L_{qq}^3 \rangle$ . The coefficient of  $t^n$  is exact to all orders in the concentration  $c$ . This expansion allows us to obtain the short-time behavior of the moments of displacement, etc. If one replaces  $t^n/n!$  by  $z^{n-1}$  in (6.7) one obtains the high-frequency expansion of the response function  $F(q, z)$ , from which the high-frequency expansion of the VACF  $\Phi(z)$ , ac conductivity, Burnett functions, etc., can be obtained.

As an illustration we consider the time-dependent diffusion coefficient, defined in (1.1), and we deduce from (4.1) and (6.7)

$$\begin{aligned} \tilde{D}(t) &= -\frac{1}{2}(\partial/\partial t)(\partial/\partial q_x)^2 \tilde{F}(q, t)|_{q=0} \\ &= D_E - tc(1 - c)(b^2/2d^2) \\ &\quad + t^2c(1 - c)(b^2/4d^3) [(d + \frac{1}{2})(1 - bc) - b(1 - 2c)] + O(t^3) \end{aligned} \tag{6.8}$$

where the *short-time limit* of  $\tilde{D}(t)$  is referred to as the Enskog value or the high-frequency limit of the diffusion coefficient:

$$D_E = (1 - bc)/2d \tag{6.9}$$

It corresponds to the diffusion coefficient of an *effective uniform lattice* with  $L^0$  replaced by  $\langle L \rangle = (1 - bc) L^0$ , where  $1 - bc$  is the *effective free volume fraction* or the *porosity* of the medium. (Recall that  $b = 1$  corresponds to completely blocked bonds.)

The short-time behavior of the VACF follows from (6.8) and (1.1). As  $\tilde{D}(t)$  for  $t \downarrow 0$  approaches a nonvanishing limit  $\tilde{D}(0) = D_E$ , Eq. (1.1) implies that the VACF contains a term  $D_E \delta_+(t)$ , where  $\delta_+(t)$  is a Dirac delta

function normalized to unity on the positive time interval. Thus, we find for the VACF as  $t \downarrow 0$ :

$$\begin{aligned} \varphi(t) \approx D_E \delta_+(t) - c(1-c)(b^2/2d^2) \\ + tc(1-c)(b^2/2d^3)[(d + \frac{1}{2})(1-bc) - b(1-2c)] + O(t^2) \end{aligned} \quad (6.10)$$

The coefficients in the short-time expansions (6.7)–(6.10) are exact to all orders in the impurity concentration. Furthermore, one easily verifies that the symmetry relations (1.6)–(1.7) between high and low densities are indeed satisfied.

## 7. CONCLUSION

Using the methods of kinetic theory,<sup>(1)</sup> we have studied the random resistor network or a lattice version of a Lorentz model, or the problem of an unbiased random walk (RW) on a random  $d$ -dimensional cubic lattice with two types of bonds: host lattice bonds having conductivity  $\sigma_0 = 1$  and concentration  $1 - c$  and impurity bonds (scatterers having conductivity  $\sigma = 1 - b$  and concentration  $c$ ). We have set up a systematic expansion of transport properties in powers of the impurity concentration. The results to  $O(c)$  are determined by summing all possible visits of the RW to a single scatterer (called “repeated ring collisions” in kinetic theory). The  $O(c^2)$  terms are determined by summing all possible sequences of visits of the RW to a pair of scatterers. For the 1D case the results to  $O(c^l)$  coincide with the  $c$  expansion of the exact result  $D_0/D(c, \sigma) = 1 - cb/(1 - b)$  for the random barrier model, as discussed in Section 4.

For the square lattice we have given in Table II explicit values for the expansion coefficient  $\alpha_2$  in the density expansion (4.4) of the diffusion coefficient  $D(c, \sigma) = D_0(1 + \alpha_1 c + \alpha_2 c^2)$  for several values of the parameter  $b = 1 - \sigma$ , defined in (1.4). The concentration dependence of  $D(c, \sigma) = \sigma D(1 - c, 1/\sigma)$ , as obtained from a  $c$  expansion and  $(1 - c)$  expansion, are shown in Fig. 2 by a solid and a dashed line respectively. If we denote the quadratic  $c$  approximation by  $D^{(2)}(c, \sigma)$ , we may consider the interpolation formula

$$\hat{D}(c, \sigma) = \max\{D^{(2)}(c, \sigma), \sigma D^{(2)}(1 - c, 1/\sigma)\}$$

as an estimate for the  $c$  dependence of the diffusion coefficient over the whole range of  $c$  values. For the square lattice we have verified in Table III that the estimate  $\hat{D}(c, \sigma)$  satisfies the rigorous upper and lower bounds on  $D(c, \sigma)$  derived by Golden and Papanicolaou.<sup>(19)</sup>

At short times the response function, its moments, time-dependent

transport coefficients, VACF, etc., can be expanded in a Taylor series. The expansion coefficients are exact for all densities and arbitrary dimensionality.

We further investigated (the long-time behavior of) the return probability  $P_0(t)$  on a disordered cubic lattice. Its Laplace transform is directly related to (the low-frequency behavior of) the average spectral density of eigenmodes of the master equation (1.3) or, equivalently, to the spectral density of lattice vibrations of a cubic harmonic lattice with a random mixture of two types of spring constants.<sup>(15,16)</sup>

It was found that the long-time behavior  $P_0(t) \approx [4\pi D(c) t]^{-d/2}$  is completely determined by the diffusion coefficient (4.4) of the disordered lattice. Since  $P_0(t) = \int_0^\infty dE D(E) e^{-Et}$ , an equivalent statement is that the low-frequency part of the average density of vibrational states  $D(\omega^2) d\omega^2 \sim \omega^{d-2} d\omega^2$  is completely determined by the effective elastic constant.

Symmetry properties (homogeneity and self-duality) determine the exact value of the effective diffusion coefficient or effective elastic constant in the 50–50 mixture on a square lattice.

In subsequent publications the present kinetic theory shall be applied to the explicit calculation of the VACF and the time-dependent diffusion coefficient of the square lattice with particular emphasis on their long- and short-time behavior. We shall also modify the hopping rules of the unbiased RW (blind ants) to allow for effects of the impurities present on nearest neighbor sites (myopic ants). The calculations are presently being extended to three-dimensional simple cubic lattices.

## APPENDIX A

### A1. Properties

This appendix deals with the properties of the integral  $G_{\alpha\beta}(n, z)$  with  $(\alpha, \beta, \dots = x, y)$  for the two-dimensional case, where  $n = (n_x, n_y)$ . These quantities are essential to describe the dynamics of the random walker on a square lattice and are defined as

$$\begin{aligned}
 G_{\alpha\beta}(n, z) &= \int_q e^{-inq} g(q) \varepsilon_\alpha(q) \varepsilon_\beta^*(q) \\
 &= \hat{p}(n) - \hat{p}(n + \rho_\alpha) - \hat{p}(n - \rho_\beta) + \hat{p}(n + \rho_\alpha - \rho_\beta) \quad (A1)
 \end{aligned}$$

Here  $g(q) = [z + \omega(q)]^{-1}$  is the response function (2.4) of the uniform lattice with  $\omega(q) = \frac{1}{2}(2 - \cos q_x - \cos q_y)$  and  $\varepsilon_\alpha(q) = 1 - \exp(-iq_\alpha)$  and  $\rho_\alpha$  is a unit vector along the lattice direction  $\alpha = x, y$ . The summation-integration

symbol  $\int_q$  is defined in (2.14) and extends over the first Brillouin zone (1BZ). The integral has been expressed in terms of  $\hat{p}(n, z)$ , which is the Laplace-transformed probability  $P_n(t)$  of a displacement  $n = (n_x, n_y)$  on a uniform lattice, defined as

$$\hat{p}(n, z) = \frac{1}{N} \sum_q e^{-iqn} g(q) = \int_q e^{-iqn} g(q)$$

We first note the obvious properties

$$\begin{aligned} G_{\alpha\beta}(n, z) &= G_{\beta\alpha}(-n, z) \\ G_{xx}(n_x, n_y, z) &= G_{yy}(n_y, n_x, z) \\ G_{xy}(n_x, n_y, z) &= G_{yx}(n_y, n_x, z) \end{aligned} \quad (\text{A2})$$

We further write  $G_{xx}$  in the form

$$\begin{aligned} G_{xx}(n, z) &= G_{xx}(n_x, n_y, z) \\ &= 2 \int g(q) (1 - \cos q_x) \exp(-in_x q_x - in_y q_y) \end{aligned} \quad (\text{A3})$$

This expression is symmetric under reflections in  $n_x = 0$  and  $n_y = 0$ , indicated by the (shaded) lines of reflection symmetry in Fig. 1a:

$$\begin{aligned} G_{xx}(n_x, n_y, z) &= G_{xx}(-n_x, n_y, z) \\ &= G_{xx}(n_x, -n_y, z) = G_{xx}(-n_x, -n_y, z) \end{aligned} \quad (\text{A4})$$

The symmetry of  $G_{xy}(n, z)$  is more clearly exhibited by writing it in the form

$$\begin{aligned} G_{xy}(n_x, n_y, z) &= 4 \int_q g(q) \sin(\tfrac{1}{2}q_x) \sin(\tfrac{1}{2}q_y) \\ &\quad \times \exp[i(n_x + \tfrac{1}{2})q_x + i(n_y - \tfrac{1}{2})q_y] \end{aligned} \quad (\text{A5})$$

This expression is *antisymmetric* under reflection in  $n_x = -\frac{1}{2}$  and  $n_y = \frac{1}{2}$  indicated by the (shaded) lines of reflection symmetry in Fig. 1b:

$$\begin{aligned} G_{xy}(n_x, n_y, z) &= -G_{xy}(-n_x - 1, n_y, z) \\ &= -G_{xy}(n_x, -n_y + 1, z) = G_{xy}(-n_x - 1, -n_y + 1, z) \end{aligned} \quad (\text{A6})$$

and symmetric under reflection in  $n_y = n_x + 1$  (see Fig. 1b):

$$G_{xy}(n_x, n_y, z) = G_{xy}(n_y - 1, n_x + 1, z) \quad (\text{A7})$$



From (2.9) and (A1)

$$G_{xx}(n, z) + G_{yy}(n, z) = 4 \int g(q) \omega(q) e^{-inq}$$

By employing (A2), (2.6), and the relation  $g\omega = 1 - zg$ , we can write it as

$$G_{xx}(n_x, n_y, z) + G_{xx}(n_y, n_x, z) = 4\delta_{n0} - 4z\hat{p}(n, z)$$

Since  $z\hat{p}(n, z) \rightarrow 0$  as  $z \rightarrow 0$  for all  $n$ , we deduce that

$$G_{xx}(n, n, 0) = 2\delta_{n0} \tag{A8}$$

and

$$G_{xx}(n_x, n_y, 0) = -G_{xx}(n_y, n_x, 0) + 2\delta_{n_x 0} \delta_{n_y 0} \tag{A9}$$

Using the relation  $\sum_{\rho} \exp(-iq\rho) = 4[1 - \omega(q)]$ , one derives from (A1) and (2.6)

$$\sum_{\rho} G_{\alpha\beta}(n + \rho, 0) = 4G_{\alpha\beta}(n, 0) - 4[\delta_{n0} - \delta_{n, -\rho_x} - \delta_{n, \rho_y} + \delta_{n, \rho_y - \rho_x}] \tag{A10}$$

where  $n + \rho$  is a nearest neighbor (n.n.) site of  $n$ . The relation (A10) together with the symmetry relations (A4), (A8), and (A9) can be considered as a recursion relation for  $G_{\alpha\beta}(n, 0)$ , and the integrals with  $n = (n_x, n_y = 0)$  are given as initial value (in fact, one needs only input elements with  $n_x = \text{odd}$ ). The solution scheme is indicated in Fig. 1, where black circles represent the input elements. Because of the above symmetries, all sums involving  $G_{xx}(n, 0)$  can be restricted to the triangular region  $\{n_x > n_y \geq 0\}$  indicated in Fig. 1.

For calculating sums involving  $G_{xy}(n, 0)$ , it is sufficient to solve (A10) in the triangular region  $\{n_x \geq 0; 1 \leq n_y \leq n_x + 1\}$ , due to the symmetry properties (A6)–(A7), as indicated in Fig. 2. This can be done once  $G_{xy}(n, 0)$  is given for  $n = (n_x, n_y = 1)$  with  $n_x \geq 0$  (In fact, one only needs input elements with  $n_x = \text{even}$ , as indicated by the black circles in Fig. 2).

### A2. Values of $G_{\alpha\beta}(n, 0)$

For the 3D simple cubic lattice there exists tables<sup>(20)</sup> of the lattice Green's functions  $\hat{p}(n, z=0)$  for sites close to the origin, from which  $G_{\alpha\beta}(n, z=0)$  can be calculated using (A1). Undoubtedly such tables also exist for the square lattice, but we have not found the reference.

To calculate  $G_{xx}(n, 0)$ , we write (A3) in the explicit form

$$G_{xx}(n_x, n_y, 0) = \pi^{-2} \iint_{-\pi}^{\pi} dx dy \\ \times (1 - \cos x) \cos(n_x x) \cos(n_y y) (2 - \cos x - \cos y)^{-1}$$

The  $y$  integration can be performed using Eq. (3.613.1) of Ref. 17 and yields

$$G_{xx}(n_x, n_y, 0) = (4/\pi) \int_0^{\pi} dx \cos(n_x x) [(1 - \cos x)/(3 - \cos x)]^{1/2} \\ \times [2 - \cos x - [(1 - \cos x)(3 - \cos x)]^{1/2}]^{|n_y|} \quad (\text{A11})$$

To solve the recursion relation (A10), we need  $G_{xx}(n, 0)$  for  $n = (n_x, n_y) = (1, 0), (3, 0), \dots$ , as input, as explained in Fig. 1b. The substitution  $u = \cos x$  reduces these integrals to elementary ones, e.g.,

$$G_{xx}(1, 0; 0) = (4/\pi) \int_{-1}^1 du u [(1 + u)(3 - u)]^{-1/2} = 2 - 8/\pi$$

As an example, we apply the recursion relation (A10) for  $G_{nm} \equiv G_{xx}(n, m; 0)$  at  $(n, m) = (1, 0)$  to obtain  $G_{20}$  according to the scheme indicated in Fig. 1a, viz.  $G_{00} + G_{11} + G_{1,-1} + G_{20} = 4G_{10} + 4$ . Since  $G_{00} = 2$  and  $G_{11} = G_{1,-1} = 0$  due to (A8), we find  $G_{20} = 10 - 32/\pi$ . A few integrals are listed in Table I; integrals with larger  $(n_x, n_y)$  values have been calculated numerically.

To solve (A10) for  $G_{xy}(n_x, n_y; 0)$ , we need  $G_{xy}(n_x, 1; 0)$  as input. For that purpose we write (A1) in the form

$$G_{xy}(n, 1; 0) = -\frac{1}{2}\pi^{-2} \iint_{-\pi}^{\pi} dx dy [\cos nx - \cos(nx + x)] \\ \times (1 - \cos y)/(2 - \cos x - \cos y) \\ = -\frac{2}{\pi} \int_0^{\pi} dx [\cos nx - \cos(nx + x)] \\ \times \{1 - [(1 - \cos x)/(3 - \cos x)]^{1/2}\} \\ = -2\delta_{n0} + \frac{1}{2}G_{xx}(n, 0; 0) - \frac{1}{2}G_{xx}(n + 1, 0; 0) \quad (\text{A12})$$

In the second equality we used Eq. (3.613.1) of Ref. 17. The integrals  $G_{xx}$  have been calculated above, and are listed in Table I. The final results for  $G_{xy}(n_x, n_y; 0)$  are also listed in Table I.

**A3. Large- $n$  Behavior of  $G_{\alpha\beta}(n, 0)$**

The large- $n$  behavior of  $G_{\alpha\beta}(n, 0)$  differs from that of the lattice Green's functions  $\hat{p}(n, 0)$ , because the leading large- $n$  terms of  $\hat{p}(n, 0)$  in (A1) cancel. A separate discussion is required and we start the analysis by introducing a new integration variable  $\phi$  in (A11), defined through  $\cos x = 1 - \text{ch } \phi$ . This yields

$$G_{xx}(n_x, n_y, 0) = (4/\pi) \int_0^{\ln(3+2\sqrt{2})} d\phi \exp(|n_y| \phi) \times \cos[n_x \arccos(2 - \text{ch } \phi)] [(\text{ch } \phi - 1)/(3 - \text{ch } \phi)]^{1/2} \tag{A13}$$

The behavior of this integral for large  $|n_y|$  and arbitrary  $n_x$  is determined by small  $\phi$  values, where it reduces to

$$G_{xx}(n_x, n_y; 0) \approx (2/\pi) \int_0^\infty d\phi \phi \cos(n_x \phi) \exp(-|n_y| \phi) \approx (2/\pi)(n_y^2 - n_x^2)/(n_x^2 + n_y^2)^2 \quad (|n_y| \gg 1) \tag{A14a}$$

The finite upper limit in (A13) has been extended toward infinity, which does not affect the leading asymptotic behavior. The integral decays for large distances as  $O(|n_y|^{-2})$ , and the first asymptotic correction is of relative  $O(|n_y|^{-2})$ .

In a similar manner one finds for  $n_y \gg 1$  to relative order in  $1/|n_y|$

$$G_{xy}(n_x, n_y; 0) \approx -(2/\pi) n_x n_y / (n_x^2 + n_y^2)^2 \tag{A14b}$$

**A4. Small- $z$  Behavior of  $G_{\alpha\beta}(n, z)$**

To determine the dominant small- $z$  singularity of  $G_{xx}(n, z)$  it is convenient to take the  $z$  derivative of (A3):

$$\frac{dG_{xx}(n_x, n_y, z)}{dz} = -\frac{2}{(2\pi)^2} \iint_{-\pi}^{\pi} dx dy \frac{(1 - \cos x) \cos(n_x x) \cos(n_y y)}{(z + 1 - \frac{1}{2} \cos x - \frac{1}{2} \cos y)^2}$$

This singularity comes from small  $(x, y)$  values, where the denominator vanishes. By approximating the integrand by its small- $(x, y)$  behavior, one easily determines the dominant singularity as  $dG_{xx}/dz = (2/\pi) \ln z$ , so that

$$G_{xx}(n, z) \approx G_{xx}(n, 0) + (2/\pi) z \ln z + O(z) \tag{A15}$$

We also note that the dominant small- $z$  singularity of  $G_{xx}(n, z)$  at fixed  $n = (n_x, n_y)$  is independent of  $n$ . A similar analysis shows that the dominant small- $z$  singularity of  $G_{xy}(n, z)$  at fixed  $n$  is weaker than  $O(z \ln z)$ , viz.

$$G_{xy}(n, z) \approx G_{xy}(n, 0) + O(z) \tag{A16}$$

**APPENDIX B**

This appendix contains the analytic evaluation of the lattice sum  $\sum R_{x\beta}^2(n, z)$ . We obtain, with the help of (3.3) and (2.13),

$$\sum'_{n\beta} R_{x\beta}^2(n, z) = T^2 \sum_{\beta} \int g^2 |\varepsilon_x|^2 |\varepsilon_{\beta}|^2 - T^2 \left[ \int g |\varepsilon_x|^2 \right]^2 \tag{B1}$$

The prime on the summation sign indicates the restriction that the bond label  $(n, \beta)$  be different from  $(0, x)$ . In deriving this equality we have used (2.6) in the form

$$\sum'_n e^{in(q+q')} = N\delta_{-q,q'} - \delta_{\beta,x}$$

The  $\beta$  summation can be performed using (2.9), and  $|\varepsilon_x|^2$  appearing under integral signs may be replaced by  $2\omega$  because of the cubic symmetry. Finally, we find from (2.16)

$$\int g^2 \omega^2 = \int g\omega - z \int g^2 \omega = d\{J(z) + zJ'(z)\}$$

where  $J'(z) = dJ(z)/dz$ . Combination of the above results yields the required relation:

$$\sum'_{n\beta} R_{x\beta}^2(n, z) = 4d^2 T^2 (J + zJ' - J^2) \tag{B2}$$

**APPENDIX C**

The behavior of the diffusion coefficient and VACF to linear order in the impurity concentration is determined by the integral  $J(z)$ , defined in (2.16). For the square lattice this integral can be calculated exactly<sup>(14)</sup> and we determine its small- $z$  behavior. We introduce

$$J(z) = \frac{1}{2} \int g\omega = \frac{1}{2} [1 - zL(z)] \tag{C1}$$

and obtain from (2.16) and (2.9)

$$L(z) \equiv \int g(q) = (2\pi)^{-2} \int_{-\pi}^{\pi} dq_x \int_{-\pi}^{\pi} dq_y \times (z + 1 - \frac{1}{2} \cos q_x - \frac{1}{2} \cos q_y)^{-1} \tag{C2}$$

where  $L(z)$  is the Laplace transform of the return probability on a uniform lattice, and we show that it is given by

$$L(z) = (2/\pi)(1 + z)^{-1} K((1 + z)^{-2}) \tag{C3}$$

where  $K(x)$  is the complete elliptic integral of the first kind, given by<sup>(18)</sup>

$$K(x) = \int_0^{\pi/2} dt (1 - x \cos^2 t)^{-1/2} = \frac{1}{2}\pi {}_2F_1(\frac{1}{2}, \frac{1}{2}; 1; x) \tag{C4}$$

The expression in terms of Gauss' hypergeometric function  ${}_2F_1$  follows from Ref. 18 and is convenient in view of later expansions around  $x = 1$ . To derive (C3), we change in (C2) to new integration variables  $\alpha = \frac{1}{2}(q_x + q_y)$  and  $\beta = \frac{1}{2}(q_x - q_y)$  and use the invariance of the integrand under the transformations  $(\alpha, \beta) \rightarrow (\beta, \alpha) \rightarrow (\pi - \alpha, \pi - \beta)$ . This transforms (C2) into

$$\begin{aligned} L(z) &= (1/\pi^2) \int_0^{\pi} d\alpha \int_0^{\pi} d\beta (z + 1 - \cos \alpha \cos \beta)^{-1} \\ &= (1/\pi) \int_0^{\pi} d\alpha [(z + 1)^2 - \cos^2 \alpha]^{-1/2} \\ &= (2/\pi)(1 + z)^{-1} K((1 + z)^{-2}) \end{aligned} \tag{C5}$$

Formula (15.3.10) of Ref. 17 in combination with (C4) determines the *small-z behavior* of  $L(z)$  for the square lattice as

$$L(z) \approx -(1/\pi)(1 - \frac{1}{2}z) \ln(z/8) + (1/2\pi)z + \dots \quad (z \rightarrow 0) \tag{C6}$$

and (C1) yields

$$J(z) \approx \frac{1}{2} - (1/4\pi)z^2 + \dots + (1/2\pi)(1 - \frac{1}{2}z)z \ln(z/8) + \dots \quad (z \rightarrow 0) \tag{C7}$$

**ACKNOWLEDGMENT**

One of us (M. E.) thanks Dr. J. Machta for his helpful comments concerning the return probability.

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