Biased random walks on lattices with diluted disorder

1989 J. Phys. A: Math. Gen. 22 5231

(http://iopscience.iop.org/0305-4470/22/24/012)

J. Phys. A: Math. Gen. **22** (1989) 5231–5248. Printed in the UK

Biased random walks on lattices with diluted disorder

M H Ernst † and Th M Nieuwenhuizen ‡

† Institute for Theoretical Physics,Princetonplein 5, PO Box 80006, 3508 TA Utrecht, The Netherlands

‡ Institut für Theoretische Physik, RWTH, Templergraben 55, 5100 Aachen, Federal Republic of Germany

Received 2 May 1989, in final form 3 August 1989

Abstract. In bond or site percolation models for 'myopic ants' the jumps of a random walker are biased to attempt only open passages, whereas an unbiased walker ('blind ant') tries open and blocked ones equally. The present paper generalises these concepts to impurity problems. One parameter describes the conductivity of the impurity, which may be higher or lower than that of the host sites or bonds. Another parameter describes a weak or strong bias to move away or stay close to impurities. This provides a more general description for, e.g., flow in porous media, oil in sands or gas in rocks. The models are analysed to first order in the concentration of impurities. Results are presented for the static diffusion coefficient and the velocity autocorrelation function. It is found that the bias parameter mainly enters the short- and intermediate-time regime.

1. Introduction

In standard percolation problems [1, 2] an unbiased random walker ('blind ant') attempts to jump at times $t = 1, 2, 3, \ldots$ to any of its nearest-neighbour (NN) sites with equal probability, say $\frac{1}{4}$ for a square lattice. If the attempted bond or site is excluded or blocked ('contains an impurity'), the random walker (RW) remains on its original site and makes a new attempt on the next time step. With this stochastic dynamics the blind ant will spend a substantial amount of time in regions with a high concentration of impurities, without exploring neighbouring regions.

To stimulate it to move away from these high concentration regions, one may bias the RW ('myopic ant') to attempt only a NN jump to any of the l open or not-excluded sites or bonds ($l = 1, 2, 3, 4$) with probability $1/l$. If the site is completely surrounded by impurities the RW cannot move. This biased RW will always jump and the total probability for leaving a site, not totally surrounded, is uniform over the whole lattice, independent of the local surroundings. Such systems have been investigated in great detail near the percolation threshold [3] and also at low impurity concentration [4–12].

These models have also been generalised to random resistor networks and all types of RW on disordered lattices in bond and site versions [2, 8–11]. This can be done by replacing a fraction c of sites or bonds in the host lattice by impurities with non-vanishing hopping rates, $\psi = 1 - b$, which may be larger ($b < 0$) or smaller ($0 < b \leq 1$) than those in the host lattice.

At low concentrations such models of unbiased RW have been investigated in great detail. Both for bond randomness [4–7] and for site randomness [8–11] an

0305-4470/89/245231+18$02.50

expansion up to $\mathcal{O}(c^2)$ was performed. Computer simulations by Frenkel for the site and bond percolation model [13] and by Breij *et al* [14] for bond percolation at low concentrations of disorder gave good agreement both for the diffusion coefficient and for the time dependence of the velocity autocorrelation function (VACF). Simulations of the diffusion coefficient in site and bond problems [15] were found to be well described by the low concentration expansion up to $\mathcal{O}(c^2)$ for concentrations not too close to the percolation threshold [4, 8].

In the present paper we generalise the above classes of models such that the RW is strongly or weakly biased to look for the easier passages, or—on the contrary—to have a bias to remain close to impurity sites. The purpose of the present paper is to calculate analytically the frequency dependent diffusion coefficient and the VACF of such biased RW at low concentration of impurities, and to investigate to what extent this bias affects the transport coefficients and the long-time behaviour of the VACF. This will be done for both bond and site problems.

In a series of papers [4–11] a systematic theory was developed for calculating the above properties for the unbiased RW up to $\mathcal{O}(c^2)$ in the impurity concentration. Here that method is extended to biased RW on lattices with a low concentration c of randomly placed impurities. For the bond problem the response function is calculated in section 2, the density expansion to $\mathcal{O}(c)$ is treated in section 3, and diffusion and VACF are treated in section 4, where also the results are discussed. The same is done for the site problem in sections 5 and 6. The last section contains a discussion of the results.

2. Master equation–bond problem

We shall consider independent particles or random walkers (RW) making nearest-neighbour (NN) jumps on a hypercubic lattice in d dimensions. A small fraction c of the bonds, taken at random, is replaced by impurities. The hopping rates across impurity bonds differ from those across host lattice bonds.

For a fixed configuration of impurities the probability distribution of the RW to be at site n at time t of the lattice can be described by the master equation

$$\dot{p}_n = \frac{1}{2d}\sum_{\alpha}\left[\psi_n^{\alpha}\left(\frac{p_{n+e_\alpha}}{x_{n+e_\alpha}} - \frac{p_n}{x_n}\right) + \psi_{n-e_\alpha}^{\alpha}\left(\frac{p_{n-e_\alpha}}{x_{n-e_\alpha}} - \frac{p_n}{x_n}\right)\right]. \tag{2.1}$$

Greek indices $\alpha, \beta, \ldots$ $(= 1, 2, \ldots d)$ label cartesian components of d-vectors and tensors, and e_α is a set of d unit vectors pointing along the positive α axis.

To specify the configuration of impurities we assign to each bond $(n, n+e_\alpha)$ a random variable c_n^{α}, with values

$$c_n^{\alpha} = \begin{cases} 1 & \text{with probability } c \\ 0 & \text{with probability } 1-c \end{cases} \tag{2.2}$$

to indicate that the bond is an impurity bond or a host lattice bond respectively. The random variables ψ_n^{α} and $\psi_{n-e_\alpha}^{\alpha}$ indicate the hopping rates across the bonds $(n, n+e_\alpha)$ and $(n-e_\alpha, n)$ respectively. We choose units of time such that $\psi_n^{\alpha} = 1$ for a host lattice bond and $\psi_n^{\alpha} = 1-b$ for an impurity bond:

$$\psi_n^{\alpha} = 1 - bc_n^{\alpha} \tag{2.3}$$

with $b < 0$ or $0 < b \leq 1$ for impurities that respectively have a 'higher conductivity' or 'lower conductivity' than the host lattice bonds. The value $b = 1$ refers to blocked bonds ('insulating impurities') or to the bond percolation problem. The random variable x_n in (2.1) is defined as

$$x_n = 1 - \frac{a}{2d}\sum_{\alpha}(c_n^{\alpha} + c_{n-e_\alpha}^{\alpha}) \equiv 1 - az_n \tag{2.4}$$

where z_n is the fraction of nearest-neighbour bonds of site n, that contain impurities ($z_n = l/2d; l = 0, 1, 2, ..., 2d$). The basic idea of the 'myopic ant models' is that the random walker can optimise its jump trials by inspecting its nearest-neighbour bonds and give a *positive bias* to easy passages (bonds with higher jump rates). By setting $a = 0$ in (2.4), one has the standard model of the unbiased random walker ('blind ant'). Consider the total rate for leaving site n:

$$w_n = \frac{1}{2d}\sum_{\alpha}\frac{\psi_n^{\alpha} + \psi_{n-e_\alpha}^{\alpha}}{x_n} = \frac{1 - bz_n}{1 - az_n}. \tag{2.5}$$

Consider first the case of low conductivity impurities ($0 < b \leq 1$) (with jump rates smaller than those in the host). To have a physically meaningful model, one should observe that the total rate out of a site cannot be increased by replacing high-conductivity bonds by low-conductivity bonds; consequently $0 \leq a \leq b \leq 1$. In the case of high-conductivity impurities ($b < 0$) one can repeat the above argument with both types of bonds interchanged; consequently $|a| \leq |b|$. In case $a = b$ the total rate in (2.5) is unity, irrespective of the presence of impurities. The bond percolation model $a = b = 1$ is known in the literature as the 'myopic ant' model. It is mainly studied near the percolation threshold.

Instead of a *positive bias* for hopping *away* from regions of high concentration of low-conductivity impurities (myopic ants) one may also consider models with a *negative bias*, i.e. the RW is biased to be at sites adjacent to low conductivity impurities, corresponding to $a < 0$ for $b > 0$ or $a > 0$ for $b < 0$. In summary: the model parameters are limited to

$$a \leq b \leq 1 \qquad \text{if } 0 < b \leq 1$$
$$b \leq a < 1 \qquad \text{if } b < 0.$$

In the following we need the stationary solution p_n^0 of the master equation, given by

$$p_n^0 = \text{constant} \times x_n = x_n\Big(\sum_m x_m\Big)^{-1}. \tag{2.6}$$

For large systems with N sites this becomes

$$p_n^0 = \frac{x_n}{N\langle x_n\rangle} = \frac{x_n}{N(1 - ac)}. \tag{2.7}$$

We consider an ensemble of RW and take (2.6) as the probability that any of them starts at $t = 0$ at site n. To calculate the moments of displacement we study the joint probability $p(nt; m) = P_{nm}(t)p_m^0$ that the RW be at m at $t = 0$ and at n at t. The

conditional probability $P_{nm}(t)$ with $P_{nm}(0) = \delta_{nm}$ also satisfies the master equation (2.1), which in matrix form is

$$\dot{P}(t) = -LX^{-1}P(t) \tag{2.8}$$

with

$$L = \frac{1}{2d}\sum_{\alpha}(S_\alpha^{-1} - 1)\Psi^\alpha(S_\alpha - 1) \tag{2.9}$$

or explicitly

$$L_{nm} = \frac{1}{2d}\sum_{\alpha}[\psi_n^\alpha(\delta_{n,m} - \delta_{m,n+e_\alpha}) + \psi_{n-e_\alpha}^\alpha(\delta_{n,m} - \delta_{m,n-e_\alpha})]. \tag{2.10}$$

The matrix $(S_\alpha)_{nm} = \delta_{m,n+e_\alpha}$ represents a translation over the lattice vector e_α. Furthermore, we will be using the diagonal matrices $A = \{X, \Psi^\alpha, C^\alpha\}$ with $A_{nm} = a_n\delta_{nm}$.

Next we introduce the response function as the generating function of the average moments of displacement

$$\begin{aligned} F(q,z) &= \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-zt}\sum_{n,m}\mathrm{e}^{-\mathrm{i}q(n-m)}\langle p(nt;m)\rangle \\ &= \frac{1}{N\langle x\rangle}\sum_{n,m}\mathrm{e}^{-\mathrm{i}q(n-m)}\left\langle \frac{1}{z + LX^{-1}}X\right\rangle_{nm} \end{aligned} \tag{2.11}$$

where we used the formal solution (2.1) and the stationary distribution (2.7) in matrix notation. The angle brackets $\langle\cdots\rangle$ denote an average over the quenched disorder (2.2). It depends only on $(n-m)$ because of translational invariance. It is therefore convenient to write (2.11) in Fourier representation

$$F(q,z) = \frac{1}{\langle x\rangle}\left\langle X\frac{1}{zX + L}X\right\rangle_{qq} \tag{2.12}$$

where $A_{qq'}$ denotes the Fourier representation of the matrix A,

$$A_{qq'} = \frac{1}{N}\sum_{n,m}\mathrm{e}^{-\mathrm{i}nq + \mathrm{i}mq'}A_{nm}. \tag{2.13}$$

For later calculations it is convenient to write the response function as

$$F(q,z) = \frac{1}{z} - \left(\frac{1-bc}{1-ac}\right)\frac{\omega(q)}{z^2} + \frac{1}{z^2(1-ac)}\left\langle L\frac{1}{zX + L}L\right\rangle_{qq}. \tag{2.14}$$

The first term is the only one which survives at $q = 0$ and expresses particle number conservation ($\sum_n p_n(t) = 1$). The second term

$$\omega(q) = 1 - \frac{1}{d}\sum_{\alpha=1}^{d}\cos q_\alpha \tag{2.15}$$

is the structure factor of the pure lattice and $\langle\psi\rangle\omega(q) = (1-bc)\omega(q) = \langle L\rangle_{qq}$ is the Fourier transform of the average of (2.8). The calculation of (2.10) up to O(c) will be reported in the next section.

3. Density expansion bond problem

The purpose of this section is to expand (2.12) up to linear order in the concentration c of impurities. We first outline the general procedure. To that purpose the matrices in (2.12) are split into a part referring to the impurity free lattice (all $c_n^\alpha = 0$) and a part linear in the fluctuating density c_n^α of impurities

$$L = L^0 - V \qquad zX + L = z + L^0 - W. \tag{3.1}$$

Then the average in (2.12) is expanded into a formal power series in $\langle V W^l \cdots \rangle$. In the multiple sums over products $c_n^\alpha c_m^\beta c_r^\gamma \cdots$ we retain only those terms that contain one single impurity bond, using the relation $\langle (c_n^\alpha)^l \rangle = \langle c_n^\alpha \rangle = c$. All terms involving different impurities are at least of $\mathcal{O}(c^2)$. In this procedure we take into account all the walks that repeatedly visit a single impurity.

To carry out this programme we use the Fourier representation, where $L^0_{qq'} = \omega(q)\delta_{qq'}$ on account of (3.1), (2.10) and (2.13) and

$$\begin{aligned} V_{qq'} &= \sum_\alpha C^\alpha_{qq'} v_{qq'} \equiv \sum_\alpha C^\alpha_{qq'} \varepsilon^+_\alpha(q) \cdot \mathbf{v} \cdot \varepsilon_\alpha(q') \\ W_{qq'} &= \sum_\alpha C^\alpha_{qq'} w_{qq'} \equiv \sum_\alpha C^\alpha_{qq'} \varepsilon^+_\alpha(q) \cdot \mathbf{w} \cdot \varepsilon_\alpha(q') \end{aligned} \tag{3.2}$$

where $C^\alpha_{qq'}$ is the Fourier transform (2.13) of the matrix $C^\alpha_{nm} = c^\alpha_n \delta_{nm}$. Here $\varepsilon^+_\alpha(q)$ is the Hermitian adjoint of the 2-vector with components $\varepsilon_{\alpha,i}(q)$ $(i = 1, 2)$:

$$\varepsilon_\alpha(q) = \begin{pmatrix} \exp(iq_\alpha) \\ 1 \end{pmatrix} \tag{3.3}$$

and $\mathbf{v}$ and $\mathbf{w}$ are 2×2 matrices.

$$\mathbf{v} = \frac{b}{2d} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \qquad \mathbf{w} = \frac{1}{2d} \begin{pmatrix} b + za & -b \\ -b & b + za \end{pmatrix}. \tag{3.4}$$

We denote the propagator of the host lattice by

$$g_{qq'} \equiv \left(\frac{1}{z + L^0} \right)_{qq'} = \delta_{qq'} g(q) = \delta_{qq'} (z + \omega(q))^{-1} \tag{3.5}$$

and write the average in (2.11) as

$$\begin{aligned} \left\langle L \frac{1}{zX + L} \right\rangle_{qq} &= \left\langle (L^0 - V) g \frac{1}{1 - Wg} (L^0 - V) \right\rangle \\ &= \omega^2(q) g(q) \left\langle \frac{1}{1 - Wg} \right\rangle_{qq} \\ &\quad - \omega(q) \left(\left\langle Vg \frac{1}{1 - Wg} \right\rangle_{qq} + \left\langle g \frac{1}{1 - Wg} V \right\rangle_{qq} \right) \\ &\quad + \left\langle Vg \frac{1}{1 - Wg} V \right\rangle_{qq}. \end{aligned} \tag{3.6}$$

We expand these terms in powers of $C^{\alpha}_{qq'}$ and keep only terms involving powers of c^{α}_n referring to a single impurity bond. For example

$$\left\langle Vg\frac{1}{1-Wg}V\right\rangle_{qq} = \sum_{l=0}^{\infty}\langle Vg(Wg)^lV\rangle_{qq}$$

$$= \sum_{l=0}^{\infty}\frac{1}{N}\sum_{n\alpha}\langle(c^{\alpha}_n)^{l+2}\rangle\frac{1}{N^{l+1}}\sum_{q_0}\cdots\sum_{q_l}\exp[\mathrm{i}(q-q_0)n+\mathrm{i}(q_0-q_1)n+\cdots+\mathrm{i}(q_l-q)n]$$

$$\times\ v_{qq_0}g(q_0)w_{q_0q_1}\cdots w_{q_{l-1}q_l}g(q_l)v_{q_lq}. \tag{3.7}$$

Here $\langle(c^{\alpha}_n)^l\rangle = \langle c^{\alpha}_n\rangle = c$ and the product of exponents $\exp(\mathrm{i}q'n)$ cancel. For large lattices ($N\to\infty$) the q-sums over the first Brillouin zone (1BZ) can be replaced by integrals, and we use the convention

$$\int_q\cdots = \lim_{N\to\infty}\frac{1}{N}\sum_{q\in 1\mathrm{BZ}}\cdots = \int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi}\frac{\mathrm{d}^{(d)}q}{(2\pi)^d}\cdots.$$

We define the 2×2 matrix $\mathbf{G}$ with elements

$$G_{ij} = \int_q \varepsilon_{\alpha,i}(q)g(q)\varepsilon^{*}_{\alpha,j}(q). \tag{3.8}$$

It has the form

$$\mathbf{G} = \begin{pmatrix}\gamma_1 & \gamma_2\\ \gamma_2 & \gamma_1\end{pmatrix} \tag{3.9}$$

with components

$$\gamma_1 = \int_q\frac{1}{z+\omega(q)} \equiv L(z) \qquad \gamma_2 = \int_q\frac{\cos q_{\alpha}}{z+\omega(q)} = (1+z)L(z)-1 \tag{3.10}$$

independent of α because of the cubic symmetry. With the help of this notation (3.7) reduces to:

$$\sum_{l=0}^{\infty}\langle Vg(Wg)^lV\rangle_{qq} = c\sum_{\alpha}\sum_{l=0}^{\infty}\varepsilon^{\dagger}_{\alpha}(q)\cdot\mathbf{vG}(\mathbf{wG})^l\mathbf{v}\cdot\varepsilon_{\alpha}(q)$$

$$= c\sum_{\alpha}\varepsilon^{\dagger}_{\alpha}(q)\cdot\mathbf{vG}\frac{1}{\mathbf{1}-\mathbf{wG}}\mathbf{v}\cdot\varepsilon_{\alpha}(q)+\mathcal{O}(c^2).$$

In the same way the remaining terms of (3.6) can be evaluated as

$$\sum_{l=0}^{\infty}\langle(Wg)^lW\rangle_{qq} = c\sum_{\alpha}\varepsilon^{\dagger}_{\alpha}(q)\cdot\frac{1}{\mathbf{1}-\mathbf{wG}}\mathbf{w}\cdot\varepsilon_{\alpha}(q)+\mathcal{O}(c^2)$$

$$\sum_{l=0}^{\infty}\langle V(gW)^l\rangle_{qq} = c\sum_{\alpha}\varepsilon^{\dagger}_{\alpha}(q)\cdot\mathbf{v}\frac{1}{\mathbf{1}-\mathbf{wG}}\cdot\varepsilon_{\alpha}(q)+\mathcal{O}(c^2)$$

$$\sum_{l=0}^{\infty}\langle(Wg)^lV\rangle_{qq} = c\sum_{\alpha}\varepsilon^{\dagger}_{\alpha}(q)\cdot\frac{1}{\mathbf{1}-\mathbf{wG}}\mathbf{v}\cdot\varepsilon_{\alpha}(q)+\mathcal{O}(c^2).$$

The matrices $\mathbf{v}, \mathbf{w}$ and $\mathbf{G}$ have the general form (3.9) and therefore commute. Collecting terms yields

$$\left\langle L\frac{1}{zX+L}L\right\rangle_{qq} = \omega^2(q)g(q)$$

$$+ c\sum_{\alpha}\varepsilon_{\alpha}^{\dagger}(q)\cdot\frac{1}{\mathbf{1}-\mathbf{wG}}(\mathbf{G}\mathbf{v}^2 - 2\omega(q)g(q)\mathbf{v} + \omega^2(q)g^2(q)\mathbf{w})\cdot\varepsilon_{\alpha}(q). \tag{3.11}$$

Next the propagator is evaluated:

$$(\mathbf{1}-\mathbf{wG})^{-1} = (r_1^2 - r_2^2)^{-1}\begin{pmatrix} r_1 & r_2 \\ r_2 & r_1 \end{pmatrix} \tag{3.12}$$

where r_1 and r_2 satisfy

$$r_1 + r_2 = 1 - (b + \tfrac{1}{2}za)J(z) \qquad r_1 - r_2 = 1 - \tfrac{1}{2}za\,K(z). \tag{3.13}$$

The functions $J(z)$ and $K(z)$ follow from (3.10) as

$$J(z) = \frac{1}{d}(\gamma_1 - \gamma_2) = \frac{1}{d}\int_q \frac{\omega(q)}{z+\omega(q)} \qquad K(z) = \frac{1}{d}(\gamma_1 + \gamma_2) \tag{3.14}$$

and are independent of a and b. We may write the matrix $(\mathbf{1}-\mathbf{wG})^{-1}\cdots$ in (3.11) as

$$\frac{1}{2d}\begin{pmatrix} A+B & -A \\ -A & A+B \end{pmatrix}.$$

Collecting terms results in

$$A(q,z) = \frac{1}{r_1(z)+r_2(z)}[b^2J(z) - 2b\omega(q)g(q,z) + b\omega^2(q)g^2(q,z) - r_2(z)B(q,z)]$$

$$B(q,z) = \frac{za\omega^2(q)g^2(q,z)}{r_1(z)-r_2(z)} \tag{3.15}$$

where $g(q,z) = 1/(z+\omega(q))$. By performing the sum over α in (3.11), we finally obtain for the response function

$$F(q,z) = \frac{1}{z} - \frac{\omega(q)(1-bc)}{z^2(1-ac)} + \frac{\omega^2(q)g(q,z)}{z^2(1-ac)} + \frac{c}{z^2}(A(q,z)\omega(q) + B(q,z)) + \mathcal{O}(c^2). \tag{3.16}$$

We note that the q dependence only enters through $\omega(q)$. Taylor expansion of (3.16) in powers of q yields the moments of displacement and transport properties on account of (2.11). They will be calculated in the next section.

4. VACF and the diffusion bond problem

The diffusion coefficient and velocity autocorrelation function (VACF) can be defined most conveniently in terms of the moments of displacement. They are generated by the q expansion of the response function (2.11) as

$$F(q,z) = 1 - \tfrac{1}{2}q_\alpha q_\beta \langle \Delta n_\alpha \Delta n_\beta \rangle(z) + \frac{1}{4!} q_\alpha q_\beta q_\gamma q_\delta \langle \Delta n_\alpha \Delta n_\beta \Delta n_\gamma \Delta n_\delta \rangle(z) + \cdots \tag{4.1}$$

where $\alpha, \beta, \gamma, \delta$ label cartesian components and where $\langle \cdots \rangle(z)$ denotes the Laplace transform of the moments of displacement:

$$\langle \Delta n_\alpha \Delta n_\beta \cdots \rangle_t = \sum_{n,m} \langle (n_\alpha - m_\alpha)(n_\beta - m_\beta) \cdots p(nt;m) \rangle. \tag{4.2}$$

The average $\langle \cdots \rangle$ is over the quenched disorder (2.2). The second moment is proportional to $\delta_{\alpha\beta}$ because of the cubic symmetry. Its long time behaviour defines the diffusion coefficient $\langle (\delta n_x)^2 \rangle_t \sim 2Dt$ $(t \to \infty)$ and its second derivative the VACF

$$\varphi(t) = \langle v_x(0) v_x(t) \rangle \equiv \frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \langle (\Delta n_x)^2 \rangle_t.$$

Its Laplace transform is

$$\Phi(z) = \tfrac{1}{2} z^2 \langle (\Delta n_x)^2 \rangle(z). \tag{4.3}$$

Since (4.1) can be written as

$$F(q,z) = z^{-1} - (q/z)^2 \Phi(z) + \cdots \tag{4.4}$$

we deduce from (3.14) that the Laplace transform of the VACF is

$$\Phi(z) = \frac{1}{2d} \left(1 + c(a-b) - \frac{cb^2 J(z)}{1 - (b + \frac{1}{2}za) J(z)} \right) + \mathcal{O}(c^2). \tag{4.5}$$

The diffusion coefficient follows by setting $z = 0$:

$$D = \Phi(0) = \frac{1}{2d} \left[1 + c \left(a - \frac{db}{d-b} \right) + \mathcal{O}(c^2) \right]. \tag{4.6}$$

The VACF can be obtained by Laplace inversion of (4.5). As follows from the large-z behaviour of (4.3) and (2.12), the VACF contains a term proportional to a Dirac delta function $\delta_+(t)$ with normalisation $\int_0^\infty \mathrm{d}t \delta_+(t) = 1$. Hence

$$\varphi(t) = D_{\mathrm{E}} \delta_+(t) + \varphi_+(t) + \mathcal{O}(c^2) \tag{4.7}$$

where $D_{\mathrm{E}} = (1/2d)(1 - bc)/(1 - ac)$ is the Enskog or short-time diffusion coefficient, and $\varphi_+(t)$ is negative for all $t > 0$ and linear in c.

In two dimensions $J(z)$ is known analytically through (3.14) and (3.10) [5], yielding

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

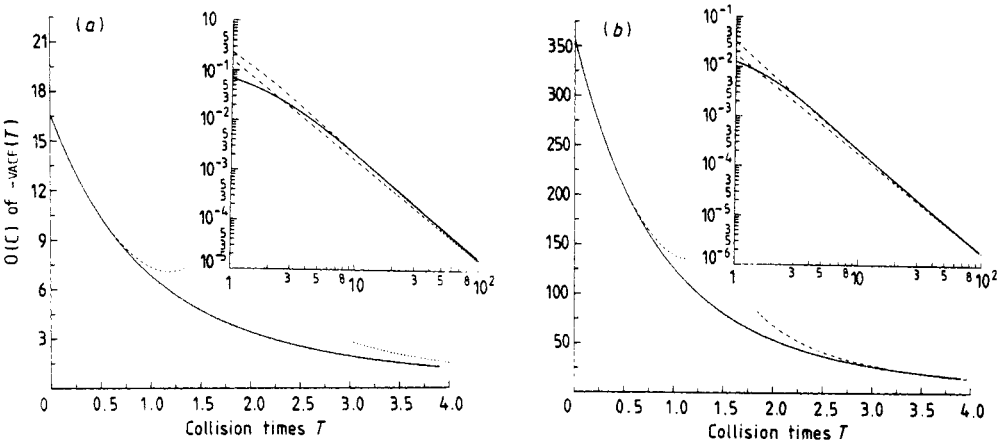

Figure 1. VACF for myopic ants. (*a*) The model with excluded bonds and $a = b = 1$. (*b*) The model with impurity bonds of low conductivity and $a = b = 0.5$. In both cases the broken curve represents the short-time expansion to order t^3 and the insets display the situation for large time, the broken curve being given by equation (4.9).

where $K(m)$ is the complete elliptic integral of the first kind [16]. Numerical inversion of the Laplace transform (4.5) yields the VACF. However, from the leading small-z singularity of $K(z)$ and $J(z)$ one can determine the long time behaviour of the VACF analytically. This yields [5]

$$J(z) = \tfrac{1}{2}[\tfrac{1}{2} + (z/2\pi)(1 - \tfrac{1}{2}z)\ln(z/8) + \cdots]. \tag{4.8}$$

With the help of Tauberian theorems, derived in [6], one finds for the long-time tail

$$\varphi(t) \simeq -\frac{cb^2t^{-2}}{2\pi(2-b)^2}\left[1 + \frac{4bt^{-1}}{(2-b)\pi}\ln(t/\tau_1) - \frac{a}{2}\left(\frac{6-b}{2-b}\right)t^{-1} + \cdots\right] \tag{4.9}$$

with

$$\tau_1 = \frac{1}{8}\exp\left(\frac{3}{2} - \gamma + \frac{\pi}{4} - \frac{\pi}{2b}\right) \tag{4.10}$$

where γ is Euler's constant.

To obtain the long-time tail for general dimensionality ($d > 2$), we determine the small-z singularities of $J(z)$ by studying the integrand in (3.14) at small values of q. The result is [5]

$$J(z) \simeq \frac{1}{d}(1 - zL(0) + \cdots) + \tfrac{1}{2}\Gamma\left(-\frac{d}{2}\right)\left(\frac{dz}{2\pi}\right)^{d/2}(1 - \tfrac{1}{4}dz + \cdots) \tag{4.11}$$

valid for $d > 2$ with $d = 2n + \epsilon$ ($\epsilon \downarrow 0$) for d even. Here $L(0) = \hat{p}_d(\mathbf{0};0)$ is a lattice Green function. Its value for $d = 3$ is $L(0) = \hat{p}_3(\mathbf{0};0) \simeq 1.516\,386\,06$ [17]. The corresponding long-time tail is

$$\varphi(t) \simeq -\frac{cb^2d}{4(d-b)^2}t^{-1-d/2}\left(\frac{d}{\pi}\right)^{d/2}\left(1 + \frac{\tau_1^{(d)} - a\tau_2^{(d)}}{t} + \cdots\right) \tag{4.12}$$

with

$$\tau_1^{(d)} = \frac{d(d+2)}{8} + \frac{(d+2)(2bL(0) - a)}{2(d-b)} \qquad \tau_2^{(d)} = \frac{(d+2)(3d-b)}{4d(d-b)}. \tag{4.13}$$

Next we briefly discuss the results for the bond problem. The VACF (4.5) and the diffusion coefficient D in (4.6) show some interesting features. By setting $a = 0$ one recovers the results for the unbiased RW of [5]. They are in good agreement with existing computer simulations for bond percolation models [13, 14]. For positive values of a the diffusion coefficient decreases, because the RW is biased to move out of regions of high impurity concentration. For $a = 0, b = 1$ one has the standard model of blind ants and Kirkpatrick's effective medium value [15] of diffusion coefficient is recovered, $D = [1 - dc/(d-1)]/(2d)$. For $a = 0, b < 0$ the impurities are high quality conductors and the diffusion coefficient is enhanced. For $a = b = 1$ the model describes myopic ants in a percolation model. The diffusion coefficient is larger than that for blind ants in the same model. In the limit $b \longrightarrow -\infty$ the bonds become superconducting and $D = [1 + c(d+a)]/(2d)$. Finally for large negative a the diffusion coefficient quickly vanishes, because the particles get stuck at impurities. This can be seen from the stationary distribution (2.7).

Equations (4.9) and (4.12) show the *negative* long-time tail typical for the Lorentz gas [18, 19]. Hence, there is an increased probability that the RW returns to regions that were visited before—i.e. where a possible path has been realised—as compared with entering new regions. The VACF $\varphi_+(t)$ in (4.7) in hopping models is negative for *all* $t > 0$, whereas in the continuous Lorentz gas $\varphi(t)$ goes negative after a finite time.

The dominant tail of the VACF is independent of the bias a. This can be seen from (4.5) because a enters only in the combination $(b + \frac{1}{2}az)$, and hence will only show up in the subleading tail. It adds a positive (negative) contribution to the coefficient of $t^{-2-d/2}$ for a positive (negative) bias a, because for $a > 0$ particles get away faster from the scatterer and $\varphi(t)$ is less negative.

The function $\varphi_+(t) \equiv -c\varphi_1(t)$ has been calculated by numerically inverting the Laplace transform in (4.5). This has been done for the two-dimensional case, along the lines in [5, 6]. In figure 1(*a*) we present the short- and long-time behaviour, for myopic ants in a model with excluded bonds ($a = b = 1$). In figure 1(*b*) we show the same for myopic ants in a model with impurity parameters ($a = b = \frac{1}{2}$). In figure 2(*a*) the same quantity is plotted for blind ants in a model with excluded bonds ($a = 0, b = -1$). These results are to be compared with figure 1(*a*), where ants are myopic rather than blind. In figure 2(*b*) we consider blind ants in a medium where the conductivity of impurity bonds is half that of host lattice bonds ($a = 0, b = \frac{1}{2}$) to be compared with figure 1(*b*). Figure 2(*c*) shows $\varphi_1(t)$ for blind ants in a medium with superconducting impurities ($a = 0, b = -\infty$).

5. Master equation site problem

In this section we consider systems where disorder is present at the sites of a d-dimensional hypercubic lattice. We study a master equation which generalises myopic and blind ants in a system with excluded sites to a system with impurity sites. The master equation has the form

$$\dot{p}_n = \frac{1}{2d}\sum_{\rho}\left(\psi_n \frac{p_{n+\rho}}{x_{n+\rho}} - \psi_{n+\rho}\frac{p_n}{x_n}\right) \equiv -(LX^{-1}p)_n. \tag{5.1}$$

Here ρ denotes any nearest-neighbour lattice vector and

$$\psi_n = 1 - bc_n \tag{5.2}$$

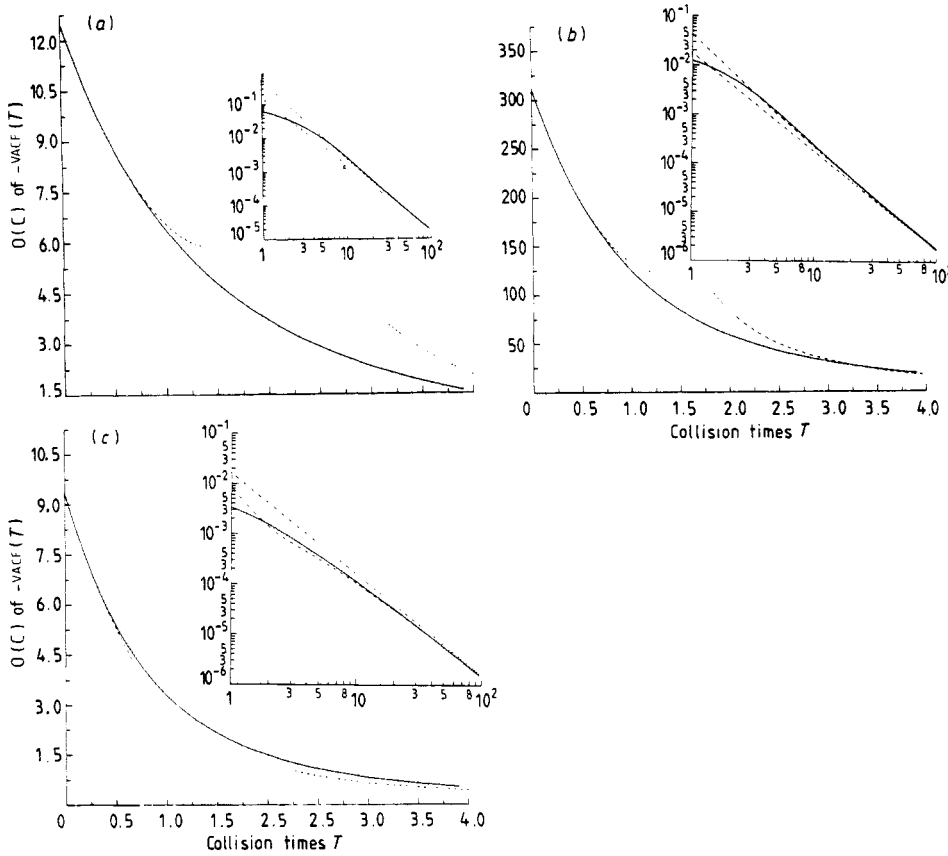

Figure 2. VACF for blind ants. (*a*) The model with excluded bonds and $a = 0$, $b = 1$. (*b*) The model with impurity bonds of low conductivity and $a = 0$, $b = 0.5$. (*c*) The model with superconducting impurity bonds and $a = 0$, $b = -\infty$. In each case the broken curve represents the short-time expansion to order t^3 and the insets display the situation for large time, the broken curve being given by equation (4.9).

where $c_n = 0$ for host sites and $c_n = 1$ for impurity sites. The parameter b models the strength of impurities: for $b = 1$, impurity sites are excluded (site percolation model), for $0 < b < 1$ they are lower quality conductors than the host sites; whereas for $-\infty < b < 0$ they are higher quality conductors. Note that the rate ψ_n depends only on the *end point of the jump* and not on the starting point. In (5.1) the rates ψ_n are modified by local factors x_n, which depend on the number of impurities on nearest-neighbour sites:

$$x_n = 1 - \frac{a}{2d} \sum_{\rho} c_{n+\rho} \tag{5.3}$$

with $-\infty < a \leq b \leq 1$ for $b > 0$ and $b \leq a \leq 1$ for $b < 0$. For $a > 0$ rates are enhanced, whereas they are suppressed for $a < 0$. The unbiased case $a = 0$ is termed 'blind ants' and the biased case $a = b$ 'myopic ants', for which the total rate for leaving a given site is uniform throughout the whole system, despite the presence of disorder, (see the discussion below (2.5)). The matrix L for the site problem in (5.1) is defined as

$$L = \frac{1}{2d} \sum_{\rho} (S_{\rho}^{-1} - 1) \Psi S_{\rho} \tag{5.4a}$$

or explicitly

$$L_{nm} = \frac{1}{2d}\sum_{\rho}(\psi_{n+\rho}\delta_{nm} - \psi_n\delta_{m,n+\rho}) \tag{5.4b}$$

where the translation matrix $(S_\rho)_{nm} = \delta_{m,n+\rho}$. The matrices X, Ψ and C are diagonal with elements x_n, ψ_n and c_n respectively. The stationary distribution can again be found explicitly

$$p_n^0 = \frac{x_n\psi_n}{N\langle x\rangle\langle\psi\rangle} = \frac{x_n\psi_n}{N(1-ac)(1-bc)}. \tag{5.5}$$

In close analogy with section 2 we determine the response function for fluctuations in the stationary state (5.5). The equivalent of (2.11) is

$$F(q,z) = \frac{1}{\langle x\rangle\langle\psi\rangle}\left\langle X\frac{1}{zX+L}X\Psi\right\rangle_{qq}. \tag{5.6}$$

We now perform a density expansion in order to calculate the response function (5.6) to linear order in c, and introduce the fluctuation matrices

$$\begin{aligned} &\Psi = 1-\delta\Psi \qquad X = 1-\delta X \\ &L = L^0 - V \qquad W = V + z\delta X \\ &zX + L = z + L^0 - W. \end{aligned} \tag{5.7}$$

With the help of (2.13) they can be presented in the Fourier representation where $L^0_{qq'} = \omega(q)\delta_{qq'}$ with $\omega(q)$ as in (2.15) and

$$\begin{aligned} &\Psi_{qq'} = C_{qq'}b \qquad \delta X_{qq'} = C_{qq'}\frac{a}{2d}\sum_{\rho}\exp(-\mathrm{i}q\rho + \mathrm{i}q\rho') \\ &V_{qq'} = C_{qq'}\frac{b}{2d}\sum_{\rho}(\exp(-\mathrm{i}q\rho) - 1)\exp(\mathrm{i}q'\rho) \\ &W_{qq'} = C_{qq'}\frac{1}{2d}\sum_{\rho}[(b+za)\exp(-\mathrm{i}q\rho + \mathrm{i}q'\rho) - b\exp(-\mathrm{i}q\rho)] \\ &C_{qq'} = N^{-1}\sum_n c_n\exp[-\mathrm{i}(q-q')n]. \end{aligned} \tag{5.8}$$

Here $q\rho = \sum_\alpha q_\alpha\rho_\alpha$, and similarly for (qn). The response function (5.6) will be transformed by introducing the matrices A and B through

$$X = 1 - gW + gB \qquad X\Psi = 1 - Wg + Ag \tag{5.9}$$

where $g = g(q,z) = 1/(z+\omega(q))$ is the propagator of the pure lattice. In terms of the fluctuations, they are

$$A = V - \delta X L^0 - \delta\Psi g^{-1} + \delta X\delta\Psi g^{-1} \qquad B = V - L^0\delta X \tag{5.10}$$

where the term $\delta X \delta \Psi$ is of order c^2 on account of (5.2) and (5.3) and will be dropped from now on. The response function (5.6), combined with (5.9), then yields

$$F(q,z) = g + g^2[\langle B \rangle_{qq} + \Gamma(q,z)]/(1-ac)(1-bc) \tag{5.11}$$

with

$$\Gamma(q,z) = \langle B \frac{1}{1-gW} gA \rangle_{qq}. \tag{5.12}$$

We represent matrix elements of A, B and W as inner products of $2d$-vectors. From (5.10) and (5.8) it follows that

$$B_{qq'} = C_{qq'} \sum_{\rho} \eta_\rho^*(q)\varepsilon_\rho(q') = C_{qq'} \boldsymbol{\eta}^\dagger(q) \cdot \boldsymbol{\varepsilon}(q') \qquad W_{qq'} = C_{qq'} \boldsymbol{\theta}^\dagger(q) \cdot \boldsymbol{\varepsilon}(q') \tag{5.13}$$

with the $2d$-vectors:

$$\begin{aligned} \epsilon_\rho(q) &= e^{iq\rho} \\ \eta_\rho(q) &= \frac{b}{2d}(e^{iq\rho} - 1) - \frac{a}{2d}\omega(q)e^{iq\rho} \\ \theta_\rho(q) &= \frac{b}{2d}(e^{iq\rho} - 1) + \frac{az}{2d}e^{iq\rho}. \end{aligned} \tag{5.14}$$

The label ρ refers to the $2d$ NN vectors $e_1, e_2, \cdots, e_d, -e_1, e_2, \cdots, -e_d$ respectively. Finally neglecting $\delta X \delta \Psi$ in the expression (5.10) yields

$$A_{qq'} \sim C_{qq'}[\boldsymbol{\varepsilon}^\dagger(q) \cdot \boldsymbol{\eta}(q') - b(z + \omega(q))] \tag{5.15}$$

where we have used the relation

$$V_{qq'} = V_{qq'}^\dagger + b(\omega(q') - \omega(q))C_{qq'}. \tag{5.16}$$

To proceed, we expand (5.10) in powers of W and collect all terms of order c. The analogue of (3.6) and (3.7) is

$$\begin{aligned} \Gamma(q,z) = c \sum_{l=0}^{\infty} \int_{q_0} \cdots \int_{q_l} & \boldsymbol{\eta}^\dagger(q) \cdot \boldsymbol{\varepsilon}(q_0) g(q_0) \boldsymbol{\theta}^\dagger(q_0) \cdot \boldsymbol{\varepsilon}(q_1) g(q_1) \cdots \\ & \times \boldsymbol{\theta}^\dagger(q_{l-1}) \cdot \boldsymbol{\varepsilon}(q_l) g(q_l) \boldsymbol{\varepsilon}^\dagger(q_l) \cdot \boldsymbol{\eta}(q). \end{aligned} \tag{5.17}$$

Here we have also used the fact that the term $b/g(q')$ in (5.15) does not contribute, because $\sum_q \varepsilon_\rho(q) = N\delta_{\rho,0} = 0$. Next it is convenient to introduce $2d \times 2d$ matrices with elements

$$G_{\rho\rho'} = \int_q \varepsilon_\rho(q) g(q) \theta_{\rho'}^*(q) \qquad H_{\rho\rho'} = \int_q \varepsilon_\rho(q) g(q) \varepsilon_{\rho'}^*(q). \tag{5.18}$$

The geometrical sum over l can be performed with the result

$$\Gamma(q,z) = c\boldsymbol{\eta}^\dagger(q) \cdot \frac{1}{\mathbf{1}-\mathbf{G}} \mathbf{H} \cdot \boldsymbol{\eta}(q) + \mathcal{O}(c^2). \tag{5.19}$$

6. VACF and the diffusion site problem

On account of (4.4) the VACF is determined by the coefficient of q^2 in the Taylor expansion of $F(q,z)$ in (5.11) and (5.19). Inserting the small-q expansion, $\eta_\rho(q) = (ib/2d)\sum_\alpha q_\alpha \rho_\alpha + \mathcal{C}(q^2)$, in (5.19) yields the VACF for the site problem

$$\Phi(z) = \frac{1}{2d}\left[1 + c(a-b) - \frac{cb^2}{2d}\sum_{\rho\rho'} \rho_x \left(\frac{1}{\mathbf{1}-\mathbf{G}}\mathbf{H}\right)_{\rho\rho'} \rho'_x\right]. \tag{6.1}$$

In deriving this result we have used the fact that the sum is a second-rank tensor with cubic symmetry, and is therefore proportional to $\delta_{\alpha\beta}$. Also because of cubic symmetry the $2d \times 2d$ matrices $K_{\rho\rho'} = \{H_{\rho\rho'}, G_{\rho\rho'}\}$, where ρ refers to the nearest-neighbour vectors $\rho = \{e_1, e_2, \cdots, e_d, -e_1 - e_2 \cdots, -e_d\}$, have only three independent elements:

$$K_{ii} = K_{xx} \qquad K_{i,d+i} = K_{x\bar{x}} \qquad K_{ij} = K_{xy} \quad (j \neq i, d+i)$$

where $x, \bar{x}$ and y refer respectively to $e_1, -e_1$ and e_2. One easily verifies that the $2d$-vector ρ_x with components $(\rho_x)_i = \delta_{1i} - \delta_{d+1,i}$ is an eigenvector of the cubic symmetric matrix $K_{\rho\rho'}$

$$\sum_{\rho'} K_{\rho\rho'}\rho'_x = (K_{xx} - K_{x\bar{x}})\rho_x \equiv k_1 \rho_x. \tag{6.2}$$

This eigenvalue k_1 is in fact d-fold degenerate because all ρ_α ($\alpha = 1, 2, \cdots, d$) are eigenvectors with the same eigenvalue. So the matrix $((\mathbf{1}-\mathbf{G})^{-1}\mathbf{H})_{\rho\rho'}$ in (6.1) can be replaced by $h_1/(1-g_1)\delta_{\rho\rho'}$ where h_1 and g_1 are the eigenvalues of $\mathbf{H}$ and $\mathbf{G}$ corresponding to the eigenvector ρ_x. The relation $\sum_\rho \rho_x^2 = 2$ is also needed. The explicit form of the eigenvalues follows from (5.18) and (6.2)

$$h_1(z) = H_{xx} - H_{x\bar{x}} = 2dI(z) \qquad g_1(z) = G_{xx} - G_{x\bar{x}} = (b + az)I(z) \tag{6.3}$$

with

$$I(z) = \int_q \frac{(\sin q_x)^2}{z + \omega(q)}. \tag{6.4}$$

The final result for the VACF in the site model becomes

$$\Phi(z) = \frac{1}{2d}\left(1 + c(a-b) - \frac{2cb^2 I(z)}{1-(b+az)I(z)}\right) + \mathcal{C}(c^2) \tag{6.5}$$

and the diffusion coefficient $D = \Phi(0)$. The function $I(z)$ is known analytically for $d = 2$ [8]

$$I(z) = \tfrac{1}{2}(1+z)\left(1 - \frac{2}{\pi}E((1+z)^{-2})\right) \tag{6.6}$$

where $E(m)$ is the complete elliptic function of the second kind [16], with $I(0) = 1 - 2/\pi$. In the three-dimensional case we only know the value at $z = 0$, namely $I(0) = \frac{1}{6}\{\hat{p}_3(\mathbf{0};0) - \hat{p}_3(2\boldsymbol{e}_1;0)\} \simeq 0.2071712$ [7, 17]. Expression (6.6) has the same

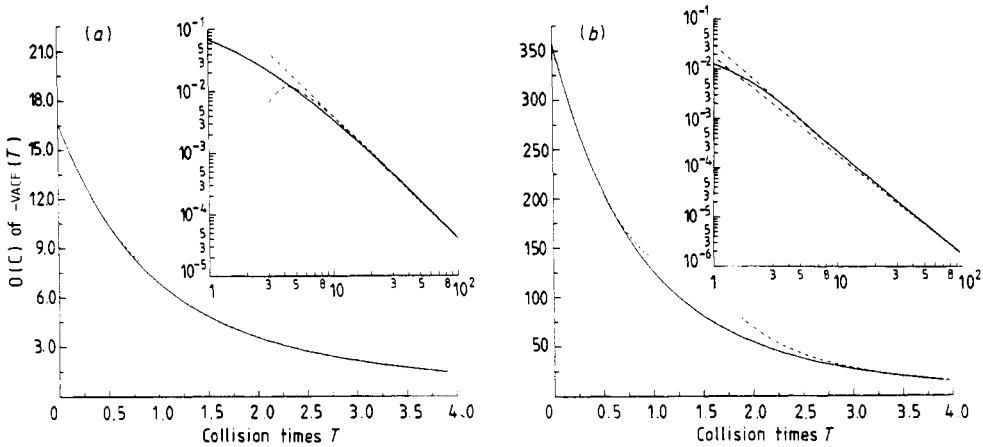

Figure 3. VACF for myopic ants. (*a*) The model with excluded sites and $a = b = 1$. (*b*) The model with impurities of low conductivity and $a = b = 0.5$. In both cases the broken curve represents the short-time expansion to order t^3 and the insets display the situation for large time, the broken curve being given by equation (6.8).

structure as in the random bond model. It reduces to the VACF for the unbiased walker by setting $a = 0$ [8–11], and more particularly for $b = 1$ to the site percolation model [8].

The long-time tail of the VACF follows from the small-z behaviour of (6.6) and is given by [10]

$$I(z) = 1 - \frac{2}{\pi} + z\left(1 - \frac{1}{\pi}\right) + \frac{z}{\pi}(1 + \tfrac{1}{4}z)\ln(z/8) + \cdots. \tag{6.7}$$

Inserting this in (6.5) and determining leading and subleading small-z singularities, one obtains, with the help of Tauberian theorems:

$$\phi(t) \simeq -\frac{cb^2}{2\pi(1 - bI(0))^2}\frac{1}{t^2}[1 + B_1 t^{-1}\ln(t/\tau_1)) - aB_2 t^{-1} + \cdots]$$

$$\tau_1 = \frac{1}{8}\exp\left(\frac{3}{4} - \gamma + \frac{\pi}{8}(b^{-1} + 7)\right)$$

$$B_1 = 4b/[\pi(1 - bI(0))] \qquad B_2 = 2I(0)(3 - bI(0))/[1 - bI(0)]. \tag{6.8}$$

Along the same lines as in (4.9) one can make a small-z expansion of $I(z)$ for general $d > 2$, and derive the analogue of (4.11). Here we only quote the leading terms, i.e.

$$I(z) \simeq I(0) + \left(\frac{d}{2\pi}\right)^{d/2}\Gamma\left(-\frac{d}{2}\right)z^{d/2} + \cdots \tag{6.9}$$

yielding for the dominant tail of the VACF

$$\phi(t) \simeq -\frac{cb^2}{d(1 - bI(0))^2}\left(\frac{d}{2\pi}\right)^{d/2} t^{-1-d/2}. \tag{6.10}$$

As can be seen from (6.8) and (6.9), the coefficient of the leading long-time tail is independent of the bias a, that models the simultaneous interactions of the RW with all NN impurities. The explicit form of the VACF to $\mathcal{O}(c^2)$ included is:

$$\phi(t) = D_E\delta_+(t) + \phi_+(t) + \mathcal{C}(c^2)$$

with $D_E = (1 - bc)/(4 + 4ac)$. The function $\phi_+(t) \equiv -c\phi_1(t)$ can be obtained by numerically inverting the Laplace transform of (6.5). It is presented in figure 3(*a*) for the case of myopic ants in the site percolation model (excluded sites, $a = b = 1$), and in figure 3(*b*) for myopic ants in a system with site impurities. The conductivity of the impurity sites is only half of the host sites ($a = b = \frac{1}{2}$). For comparison figure 3(*c*) shows the VACF for blind ants ($a = 0, b = 1$) in the standard site percolation model, and figure 3(*d*) for blind ants ($a = 0, b = \frac{1}{2}$) and low quality impurity conduction.

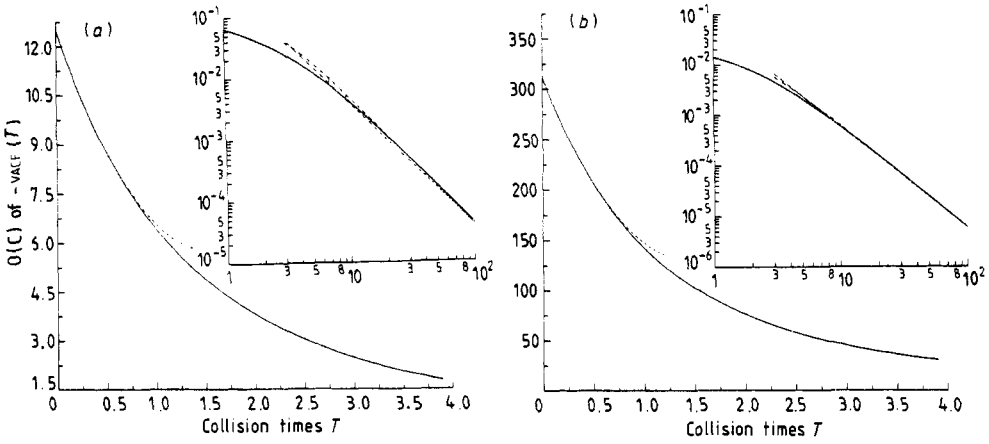

Figure 4. VACF for blind ants. (*a*) The model with excluded sites and $a = 0$, $b = 1$. (*b*) The model with impurities of low conductivity and $a = 0$, $b = 0.5$. In both cases the broken curve represents the short-time expansion to order t^3 and the insets display the situation for large time, the broken curve being given by equation (6.8).

7. Summary

In the present paper we consider diffusion in a medium with a small amount of impurity bonds or sites. The impurity jump rates differ from the host value by an amount proportional to the parameter b. For $0 < b < 1$ the conductivity of impurities is lower than that of the host and for $b = 1$ they are inaccessible (missing bonds or missing sites); for $-\infty < b < 0$, on the other hand, impurities conduct better than the host. Our model also contains a bias parameter a ($0 \leq a \leq b$ for $b > 0$ or $b \leq a \leq 1$ for $b < 0$), which models the effect of multi-impurity interactions of the RW. For $a = 0$ the RW tries to jump with equal likelihood to impurity states and to host sites ('blind ant'). For $a \neq 0$ there is either an enhanced or a diminished rate for hopping to better conducting regions, see section 2. The special case $a = b = 1$, where jumps are fully biased and impurities are non-conducting, is known in the literature as the problem of myopic ants. The model considered here allows for a more general description of the dynamical properties of, e.g., flow in porous media, oil in sands, gas in rocks or conductivity in disordered media.

The bias parameter a mainly affects the short- and intermediate-time behaviour of the VACF. At low densities it has minor influence on the long-time tail because it only enters the subleading terms. The value of the diffusion coefficient is shifted by an amount proportional to the parameter a and the concentration c. It can be verified that the bias parameter a does enter the leading long-time tail of higher correlation

functions. Let us consider, for instance, the long-time tail of the modified Burnett function $\Delta_{xx}(t)$, which is a four-point velocity correlation function defined in [6]. This quantity can be calculated from the q^4-terms of the response function. In the case of bond disorder it behaves as

$$\Delta_{xx}(t) \sim \frac{a^2 c}{4d^3}\left(\frac{d}{2\pi t}\right)^{d/2} \qquad t \to \infty;\ a \neq 0$$

which obviously vanishes if and only if $a = 0$. Then the behaviour is proportional to $t^{-1-d/2}$ [6, 20]. In the system with site disorder the tail of Δ_{xx} is of order $t^{-d/2}$ both for $a \neq 0$ and for $a = 0$. See [11, 20] for the two-dimensional situation with $a = 0$.

In the random bond problem we encountered 2×2 matrices, since each bond connects two sites. In the random site problem there appear $2d \times 2d$ matrices, because to each random site $2d$ bonds are connected.

In the study of systems with quenched bond or site disorder, it turns out that several *ad hoc* approximations are accurate, and others are rather poor. For instance, the effective medium theory gives a very good description of the static conductivity [15], but a poor description of the low-frequency behaviour or, equivalently, of the long-time tails in the velocity autocorrelation function (VACF) *at finite impurity concentration* [21]. In view of these observations it would be of interest to treat our models by a method in the spirit of Watson and Leath [22] or by a generalised effective medium approach, in the spirit of the one proposed by Haus and Kehr [23]. This could give predictions valid in a rather large regime of concentrations. Also a calculation of c^2 terms would be desirable for the same reason. One can also apply a self-consistent method based on Enskog renormalisation methods developed by Cichocki and Felderhof [24].

For many lattice models with simple bond or site disorder computer simulations have been performed. The statistical accuracy of the existing methods [13, 14] seems in general to be sufficient to make a quantitative comparison between theory and simulations for the diffusion coefficient and the long-time tail in the VACF, at least to lowest order, $O(c)$, in the impurity concentration. However, comparison with $O(c^2)$ has only become feasible through a new algorithm of Frenkel that increases the statistical accuracy by a factor 10^3 and enables one to extend the calculation of the VACF to 500–1000 time steps. Frenkel's simulations seem to indicate that the long-time tails in the VACF to $O(c^2)$ in bond problems are in complete agreement with theoretical predictions but there seems disagreement in $O(c^2)$-terms in lattice models with site disorder [25]. A possible explanation is that the true asymptotic regime has not been reached for 500–1000 time steps.

As our biased random walks are, to some extent, hybrids of bond and site disordered systems, it would be very interesting to perform computer simulations to test the present theory and its extensions to higher densities, as well as Watson–Leath and effective medium type theories.

Acknowledgments

The authors thank Peter van Velthoven for performing the numerical work on the VACF and for preparing the figures presented in this paper.

References

[1] Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)

[2] Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695
[3] Pandey R B, Stauffer D, Margolina A and Zabolitsky J G 1986 *J. Stat. Phys.* **34** 427
[4] Ernst M H, van Velthoven P F J and Nieuwenhuizen Th M 1987 *J. Phys. A: Math. Gen.* **20** 949
[5] Ernst M H and van Velthoven P F J 1986 *J. Stat. Phys.* **45** 1001
[6] Ernst M H 1987 *J. Stat. Phys.* **48** 645
[7] van Velzen G A and Ernst M H 1987 *J. Stat. Phys.* **48** 677
[8] Nieuwenhuizen Th M, van Velthoven P F J and Ernst M H 1986 *Phys. Rev. Lett.* **57** 24577
[9] Nieuwenhuizen Th M, van Velthoven P F J and Ernst M H 1987 *J. Phys. A: Math. Gen.* **20** 4001
[10] Ernst M H, Nieuwenhuizen Th M and van Velthoven P F J 1987 *J. Phys. A: Math. Gen.* **20** 5335
[11] Nieuwenhuizen Th M 1989 *Physica* **157A** 1101
[12] Haus J W and Kehr K W 1987 *Phys. Rep.* **150** 262
[13] Frenkel D 1987 *Phys. Lett.* **121A** 385
[14] Breij J J, Gomez Ordonez J and Santos A 1988 *Phys. Lett.* **127A** 5
[15] Kirkpatrick S 1973 *Rev. Mod. Phys.* **45** 574
[16] Abramowitz M and Stegun I A 1970 *Handbook of Mathematical Functions* (New York: Dover)
[17] Montet G L 1970 *Phys. Rev.* **B7** 650
[18] Ernst M H and Weijland A 1971 *Phys. Rev. Lett.* **34A** 39
[19] van Beijeren H 1982 *Rev. Mod. Phys.* **54** 195
[20] Machta J, Ernst M H, van Beijeren H and Dorfman J R 1984 *J. Stat. Phys.* **34** 477
[21] van Velzen G A, Ernst M H and Dufty J W 1988 *Physica* **154A** 34
[22] Watson B P and Leath P J 1974 *Phys. Rev.* **B9** 4893
[23] Haus J W and Kehr K W 1987 *Phys. Rev. Lett.* **36** 5639
[24] Cichocki B and Felderhof B U 1988 *J. Stat. Phys.* **51** 57
[25] Frenkel D 1990 *Fundamental Problems in Statistical Mechanics* vol VII, ed H van Beijeren (Amsterdam: North-Holland)