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A numerical study of diffusion and conduction in a 2D random medium

J M Luck

Service de Physique Théorique, CEN-Saclay, 91191 Gif-sur-Yvette, Cedex, France

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Abstract. We investigate numerically the diffusion and conduction properties of a two-dimensional random lattice hopping model. Our results are compared with a recent field theoretical renormalisation group approach, showing that two is the upper critical dimension for such models. The predicted scaling law with a universal logarithmic behaviour of the velocity is clearly observed. The finiteness of the diffusion constant as well as its regular dependence versus the strength of randomness are evenly in good agreement with analytical results. We also determine the frequency dependence of the AC conductivity tensor.

1. Introduction

Diffusion and conduction properties of random media have been the subject of much recent interest. Disordered conductors are usually represented by a lattice hopping model (see Alexander *et al* 1981 and references therein). The general model with non-symmetric hopping rates exhibits a very rich structure in one dimension (Kesten *et al* 1975, Solomon 1975, Sinaï 1982, Derrida and Pomeau 1982, Bernasconi and Schneider 1983, Derrida 1983). Randomness induces two remarkable effects in one-dimensional diffusion: there exists generally a whole 'critical phase' where the velocity vanishes, and where some critical exponents vary continuously with the strength of disorder; moreover different physical quantities are, in general, singular at different points.

The hopping model in dimension d higher than one has been studied through a weak disorder expansion (Derrida and Luck 1983), and through a perturbative renormalisation group (RG) analysis (Luck 1983). These papers are referred to as (I) and (II) in the following. The upper critical dimensionality is $d_c = 2$. For $d > 2$, any weak disorder is irrelevant; a classical diffusive behaviour is observed. For $d < 2$, a small randomness in the hopping rates changes the long-time behaviour of certain physical quantities, which obey universal scaling laws with non-trivial critical exponents. Very similar results have been obtained in the 'true self-avoiding walk problem' (Amit *et al* 1983, Obukhov and Peliti 1983, Peliti 1983).

In the two-dimensional case, the perturbative RG approach (II) predicts universal logarithmic corrections to the classical diffusion and conduction laws. These logarithms are characteristic of whatever model at its upper critical dimension.

The aim of the present paper is to study a particular example of a 2D random lattice hopping model, by solving exactly the steady-state equations on finite lattices, as explained in (I). We shall consider successively the velocity induced by a constant

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exterior field, the diffusion tensor, and the AC (frequency dependent) conductivity tensor. We discuss for each quantity how the present numerical results compare with the analytical predictions of the weak disorder expansion, and the renormalisation group analysis.

2. The model

We shall follow throughout this paper the notation of (I). The hopping model is defined by a collection of hopping rates $\{W_{y,x}\}$: $W_{y,x}\,dt$ is the probability of jumping from site x to site y during the infinitesimal time dt. The $W_{y,x}$ are distributed according to a given translationally invariant measure.

Our particular choice of hopping rates is as follows: every site of the infinite square lattice is of type A with probability $p_A = p$, and of type B with probability $p_B = 1 - p$. The attribution of a type label (A or B) to a given site is done independently for each site.

Let $\hat{1}$ and $\hat{2}$ denote the unit vectors in both directions on the lattice. The $W_{y,x}$ read

$$\text{for } x \text{ of type A:} \begin{cases} W_{x+\hat{1},x} = W_{x+\hat{2},x} = \frac{1}{4}(1+b) \\ W_{x-\hat{1},x} = W_{x-\hat{2},x} = \frac{1}{4}(1-b) \end{cases} \tag{1.A}$$

$$\text{for } x \text{ of type B:} \begin{cases} W_{x+\hat{1},x} = W_{x+\hat{2},x} = \frac{1}{4}(1-b) \\ W_{x-\hat{1},x} = W_{x-\hat{2},x} = \frac{1}{4}(1+b) \end{cases} \tag{1.B}$$

where the bias b lies between 0 and 1. Figure 1 shows one site of each type, where the magnitude of the associated rates is symbolised by arrows.

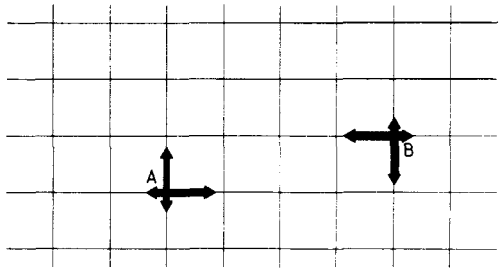

Figure 1. One site of each type (A and B) present in our model. The length of the arrows represents the magnitude of the hopping rates to nearest neighbours in the corresponding direction.

This problem is non-symmetric, because $W_{x,y}$ and $W_{y,x}$ depend respectively on the types of sites y and x, which are independent. The $W_{y,x}$ have been chosen such that $\Sigma_y W_{y,x} = 1$ for all x. This convenient normalisation sets the microscopic time scale of the model equal to unity.

We have chosen the following numerical procedure.

(a) Firstly manufacture a finite (square $N \times N$) sample according to the preceding rules, with periodic boundary conditions.

(b) Secondly, determine the physical quantities through a numerical resolution of the steady-state equations derived in (I). The most efficient way to deal with these N^2

or $2N^2$ coupled linear equations seems to be the standard relaxation method, using as a starting point the translationally invariant solution of the steady state in a pure medium. We shall describe explicitly this relaxation method in the case of the velocity. We always get a reasonable accuracy ($\sim 1\%$) on the physical quantities after 300 to 600 steps.

(c) Thirdly, average the physical quantities over M distinct samples.

Although we do not know of any *a priori* optimal choice of M and N (at fixed total computer time), we have found an empirical compromise between statistical errors and relaxation times for lattice sizes around $N = 50$ to 100. Reasonable error bars are then obtained for $M = 5$ to 50.

The statistical errors cannot be reduced by an appreciable amount without using roughly 100 times more computer time; that seems to be an unreasonable enterprise, since the present work has used roughly one hour CP time on a CRAY.

3. The velocity

According to (I), the components V_μ of the velocity are given by

$$V_\mu = \sum_{x,y} (y_\mu - x_\mu) W_{y,x} Q_x \tag{2}$$

where Q_x is the solution of

$$\sum_y (W_{x,y} Q_y - W_{y,x} Q_x) = 0 \tag{3}$$

satisfying the normalisation condition

$$\sum_x Q_x = 1. \tag{4}$$

We have solved equation (3) by a standard relaxation method, starting from the solution corresponding to the pure medium:

$$Q_x^{(0)} = N^{-2}$$

updating the Q_x according to the formula

$$Q_x^{(n+1)} = \sum_y W_{x,y} Q_y^{(n)}$$

(since $\Sigma_y W_{y,x} = 1$ for all x) and normalising the solution according to (4) after each sweep of the whole lattice. The method gives a reasonable convergence of the velocity after several hundreds of sweeps ($\leqslant 600$ sweeps).

In our model, both components V_μ of the velocity are equal, on whatever finite sample:

$$V_1 = V_2 = V. \tag{5}$$

The weak disorder expansion up to first order predicts

$$V = V_0[1 - (4/\pi) g \ln \Lambda / V_0 + \ldots] \tag{6}$$

where Λ is some cut-off of order unity, and where the 'bare velocity' V_0 and the

'coupling constant' g are simply related to the parameters b and p defining our model:

$$V_0 = b(p - \tfrac{1}{2}) \tag{7}$$

$$g = \tfrac{1}{4}b^2. \tag{8}$$

The domains of variation of these parameters read:

$$0 \leqslant p \leqslant 1 \qquad 0 \leqslant b \leqslant 1 \qquad -\tfrac{1}{2} \leqslant V_0 \leqslant \tfrac{1}{2} \qquad 0 \leqslant g \leqslant \tfrac{1}{4}. \tag{9}$$

This notation is consistent with that of (I) and (II).

As V_0 goes to zero, the perturbative series (6) becomes singular. The renormalisation group approach (II) predicts a universal scaling behaviour:

$$V/V_0 = f(x) \qquad x = (g \ln(1/V_0))^{-1} \tag{10}$$

with

$$f(x) \sim Cx \qquad \text{as } x \to 0 \tag{11}$$

for $V_0 \ll \Lambda$ and small g.

In other words, a static field V_0 induces a current V which vanishes more rapidly than V_0 by one power of $\ln V_0$.

We have computed V for different values of g, and for V_0 up to $0.05 \ll 1$. Figure 2 shows a plot of V/V_0 as a function of $(g \ln(1/V_0))^{-1}$. Different symbols indicate different values of b. Their meaning will be kept throughout all the figures. A good agreement with (10)–(11) is observed, namely

(a) the existence of a scaling function f is clear

(b) the asymptotic behaviours of f:

$$f(x) \sim 1 - (4/\pi x) \qquad (x \to \infty) \tag{12}$$

$$f(x) \sim Cx \qquad (x \to 0) \text{ with } C \sim 0.21 \tag{13}$$

coincide with (6) and (10)–(11) respectively. This value of C is empirically determined by drawing a straight line on figure 2.

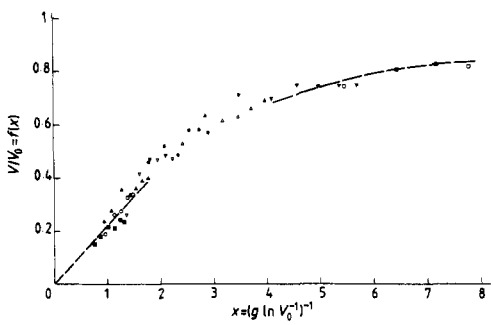

Figure 2. The scaling function of the velocity. The broken curve at large values of x is the first-order weak coupling expansion. The broken line at small values of x gives an estimate of the slope C (see equations (11)–(13)). The values of b are denoted by: □, 0.40; ▼, 0.50; △, 0.60; ●, 0.70; ▽, 0.80; ▲, 0.90; ○, 0.95; ■, 1.

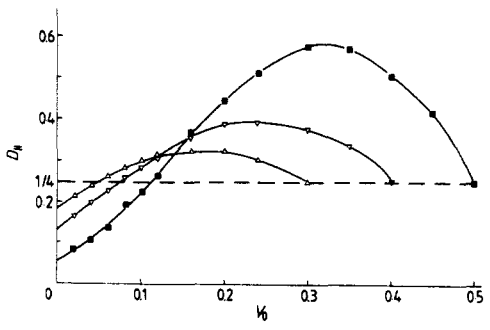

Figure 3. The parallel diffusion constant $D_\parallel$ as a function of V_0 for different values of b (△, 0.60; ▽, 0.80; ■, 1). Note the existence of a finite limit D_0 as $V_0 \to 0$.

This scaling analysis is only valid for $g \to 0$, while some data correspond to $g = \frac{1}{4}$. On the other hand, the best choice for the cut-off Λ is certainly not the value $\Lambda = 1$ we have adopted.

We think that these two small systematic deviations from scaling are quite negligible compared with the statistical errors on our data.

Likewise, the systematic finite-size effects are negligible as far as the velocity is concerned: we have not noticed any systematic deviation by comparing sizes $N = 20$ to 200. A compromise between statistical errors and relaxation times led us to use mostly 50×50 and 100×100 lattices.

We shall examine systematically the finite-size effects for other quantities in the following.

4. The diffusion tensor

The component $D_{\mu\nu}$ of the diffusion tensor is given by (I):

$$D^{\mu\nu} = \tfrac{1}{2} \sum_{x,y} [(y^\mu - x^\mu) T_x^\nu + (y^\nu - x^\nu) T_x^\mu] W_{y,x} + \tfrac{1}{2} \sum_{x,y} [(y^\mu - x^\mu)(y^\nu - x^\nu) W_{y,x} Q_x] - \tfrac{1}{2} \left(V^\mu \sum_x T_x^\nu + V^\nu \sum_x T_x^\mu \right) \tag{14}$$

where Q_x has already been defined and used to compute V_μ, and where T_x^μ is the solution of

$$\sum_y [W_{x,y} T_y^\mu - W_{y,x} T_x^\mu + (x^\mu - y^\mu) W_{x,y} Q_y] = V^\mu Q_x. \tag{15}$$

In the present case, only one component of $D_{\mu\nu}$ is non-trivial.

Let ε_μ be the unit vector parallel to V_μ:

$$\varepsilon_\mu = V_\mu / |V| = (1/\sqrt{2}, 1/\sqrt{2}). \tag{16}$$

We have then, on an arbitrary finite sample,

$$D_{\mu\nu} = (\delta_{\mu\nu} - \varepsilon_\mu \varepsilon_\nu) D_\perp + \varepsilon_\mu \varepsilon_\nu D_\parallel \tag{17}$$

and moreover

$$D_\perp = \tfrac{1}{4}. \tag{18}$$

Only $D_\parallel$ deserves some interest. Figure 3 shows a plot of $D_\parallel$ as a function of V_0 for three different values of b: $b = 0.6$, 0.8 and 1.

For a given value of b, V_0 reaches its maximal value for $p \to 1$:

$$V_{0\,\max} = \tfrac{1}{2} b. \tag{19}$$

Since this value corresponds to a pure A phase, it is very easy to check that we have

$$D_\parallel = D_\perp = \tfrac{1}{4} \qquad \text{at } V_0 = V_{0\,\max}. \tag{20}$$

The RG analysis predicts a very weak singularity in $D_\parallel(V_0)$ as $V_0 \to 0$:

$$D_\parallel \sim D_0(1 - \text{constant}/\ln(\Lambda / V_0)) \tag{21}$$

in an exponentially small critical region.

Although we cannot see this singularity in our numerical data, we have, nevertheless, this interesting result: $D_0 = D_{\|}(V_0 = 0)$ is finite.

Let us now consider the variations of D_0 with g in some more detail. This quantity is expected to be a regular function of g. The weak coupling expansion predicts

$$D_0 = \tfrac{1}{4} - (2/\pi)g + O(g^2). \tag{22}$$

We take into account the eventual systematic finite-size effects in the following way. D_0 is computed for different lattice sizes, and the data are extrapolated to $N = \infty$. Figure 4 illustrates the convergence of this method. Even at large disorder ($b = 0.9$) and for small lattices ($N = 10$ to 40), these finite-size effects are small and regular in $1/N$.

The straight line corresponds to a least-squares fit. The size of the error bars is $\mathcal{N}^{-1/2}$, where $\mathcal{N} = MN^2$ is the total number of sites used in the computation of a point. The statistical errors are clearly less than that crude estimate.

Figure 5 shows the variations of D_0 (extrapolated as we have just explained) as a function of g. The broken line represents the weak-disorder expansion (22).

The agreement between analytical and numerical results is again very good. Let us recall that even the existence and finiteness of D_0 at $g \neq 0$ is a recent non-trivial result (II).

In the limiting case $b = 1$ ($g = \frac{1}{4}$), where every W is either 0 or 1 (that is therefore a very wildly disordered medium), D_0 reaches a finite limit:

$$D_{0\,\mathrm{lim}} \sim 0.053 \tag{23}$$

which is roughly five times smaller than in the absence of randomness.

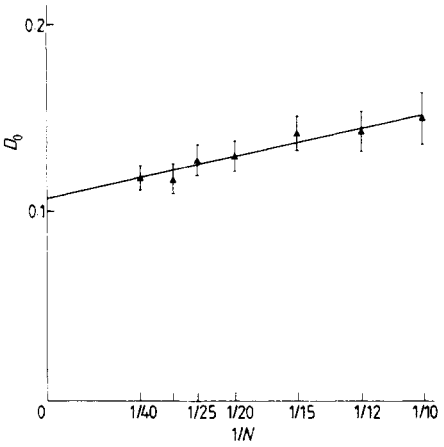

Figure 4. An example of the extrapolation of the finite lattice data to the thermodynamical limit for the quantity D_0 at $b = 0.9$. Systematic finite-size effects are small.

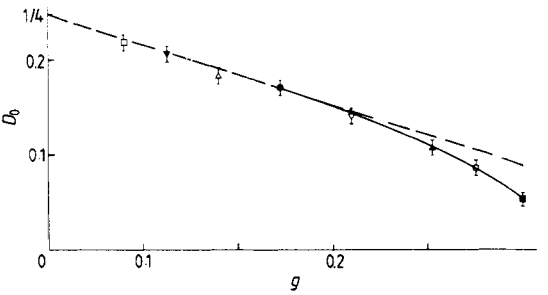

Figure 5. The extrapolated $D_0 = D_{\|}$ ($V_0 = 0$) as a function of g. The broken curve is the result of the weak coupling expansion up to first order.

5. The AC conductivity tensor

The components $\sigma_{\mu\nu}(\omega)$ of the AC conductivity tensor at frequency $f = \omega/2\pi$ are given by (I):

$$\sigma^{\mu\nu}(\omega) = \sum_{x,y} (y^\mu - x^\mu) W_{y,x} [(y^\nu - x^\nu) Q_x + R_x^\nu(\omega)] \tag{24}$$

where $R_x^\nu(\omega)$ is the solution of

$$i\omega R_x^\nu = \sum_y (W_{x,y} R_y^\nu - W_{y,x} R_x^\nu) + \sum_y [W_{x,y}(x^\nu - y^\nu) Q_y - W_{y,x}(y^\nu - x^\nu) Q_x]. \tag{25}$$

Let us restrict ourselves in this section to the case $V_0 = 0$ ($p = \frac{1}{2}$). The continuous theory (II) predicts indeed that V_0 and $\sqrt{\omega}$ are two very analogous relevant variables, at least in $d = 2$ (and $2 - \varepsilon$). We have not been interested in the eventual *crossover* effects occurring when both $V_0 \neq 0$ and $\omega \neq 0$ remove the system from criticality.

In our case, the conductivity tensor takes the following form:

$$\sigma_{\mu\nu}(\omega) = \begin{bmatrix} \frac{1}{2} + \Sigma_1(\omega) & \Sigma_2(\omega) \\ \Sigma_1(\omega) & \frac{1}{2} + \Sigma_2(\omega) \end{bmatrix} \tag{26}$$

on a finite sample. But the two functions $\Sigma_1(\omega)$ and $\Sigma_2(\omega)$, which generally take different values on a given sample, become identical in the thermodynamical limit ($N \to \infty$), or equivalently if they are averaged over a large number M of finite samples. We have therefore

$$\overline{\sigma_{\mu\nu}(\omega)} = \begin{bmatrix} \frac{1}{2} + \Sigma(\omega) & \Sigma(\omega) \\ \Sigma(\omega) & \frac{1}{2} + \Sigma(\omega) \end{bmatrix}. \tag{27}$$

Notice that $\Sigma(\omega)$ is generally complex. Σ is identically zero in the non-random case ($g = 0$), where $\sigma_{\mu\nu}$ is independent of ω. The symmetry of $\sigma_{\mu\nu}(\omega)$ is particular to our model, and by no means a general property of hopping models (see I).

We have determined numerically $\Sigma(\omega)$ for different values of b and over the whole range $0 < \omega < \infty$. On each finite sample, we get two results $\Sigma_1(\omega)$ and $\Sigma_2(\omega)$ which are always very close, in agreement with a naive formula like

$$\overline{(|\Sigma_1(\omega) - \Sigma_2(\omega)|^2)}^{1/2} \sim K(\omega)/N \tag{28}$$

following directly from the central limit theorem.

For small ω, the effective range of equations (24)–(25) diverges as (II):

$$\xi \sim 1/\sqrt{\omega}. \tag{29}$$

We have, therefore, to analyse more carefully the data corresponding to zero frequency, making use of the extrapolation method described in § 4 in the case of D_0. Figure 6 illustrates an example of convergence of the quantity $\Sigma(0)$ as the lattice size N is varied.

The statistics on each point is roughly the same as in the case of D_0. The straight line is again a least-squares fit.

Figure 7 shows the variations of $\Sigma(\omega)$ in the complex plane for four different values of b. As ω grows from zero to infinity, $\Sigma(\omega)$ varies from a real negative value $\Sigma(0) < 0$ to zero. Its imaginary part is maximal for $\omega \sim 1$ (in our reduced units). The point $\omega = 1$ is indicated by an arrow for each value of b.

The renormalisation group (II) predicts that $\sigma_{\mu\nu}(\omega)$ develops as $\omega \to 0$ the same type of singularity as $D_\parallel(V_0)$ as $V_0 \to 0$. This very weak logarithmic correction is unobservable in our data. These show nevertheless that randomness induces a non-trivial ω-dependence of the conductivity tensor, which is frequency independent in a pure diffusive medium.

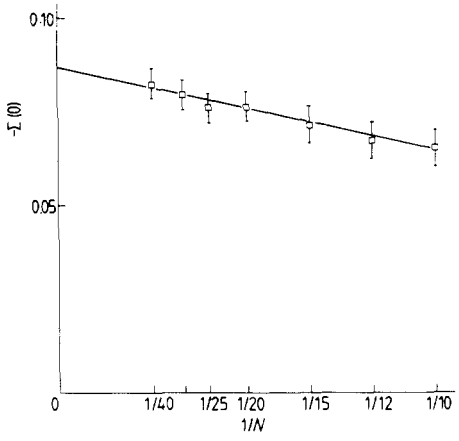

Figure 6. The same as figure 4, for the zero frequency conductivity at $b = 0.40$. Finite-size effects are again very small.

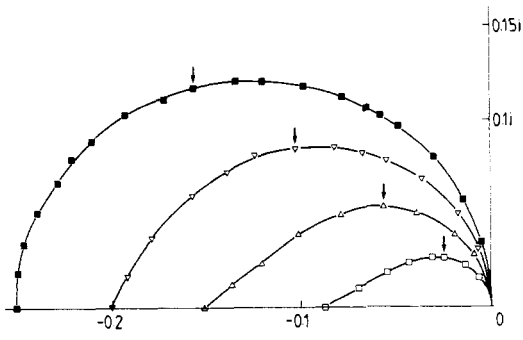

Figure 7. Variations of the quantity $\Sigma(\omega)$ in the complex plane for $0 < \omega < \infty$ and for different values of b. (□, 0.40; △, 0.60; ▽, 0.80; ■, 1). $\Sigma(\omega)$ starts from a real negative value at $\omega = 0$ and goes to 0 at large ω. The points corresponding to $\omega = 1$ are indicated by arrows.

6. Conclusion

We have seen how the random hopping model on a finite lattice is easily numerically tractable through the steady-state equations derived in (I). The systematic finite-size effects are regular enough to be easily taken into account. The statistical errors are small enough to allow us to extract the quantities of interest from the data. These errors cannot be considerably reduced.

The present results are in very good agreement with the predictions of the weak disorder expansion, and of the renormalisation group analysis. In particular, the scaling function of the velocity and its universal logarithmic behaviour, and the finiteness of the diffusion constant at vanishing velocity, are encouraging confirmations of the quoted recent analytical results.

Acknowledgments

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