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LETTER TO THE EDITOR

A phase transition in the dynamics of an exact model for hopping transport

Shlomo Havlin†, Benes L Trus and George H Weiss
National Institutes of Health, Bethesda, MD 20892, USA

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Abstract. We analyse an exact model for hopping transport of a random walker in the presence of randomly distributed deep trapping sites. For an exponential distribution of the depth of traps we find a phase transition in the diffusive behaviour as a function of temperature. We show that above a critical temperature transport is purely diffusive while below it, one finds anomalous diffusion characterised by a diffusion exponent that increases with decreasing temperature. The analysis combines theory with accurate simulation in one and two dimensions. Our analytical and numerical results indicate that the upper critical dimension is $d_c = 2$, i.e. for $d \geq d_c = 2$ the mean-field theory can be applied.

A number of investigators have proposed and analysed models for dispersive transport in amorphous solids [1–5]. The principal qualitative features of such transport are believed to be governed by the residence of otherwise mobile particles at trapping sites until their subsequent release. In particular, it has been shown by cited authors that the choice of appropriate residence time densities can lead to anomalous diffusion in amorphous solids, i.e. diffusion in which the mean square displacement $\langle r^2 \rangle$ is proportional to t^{2/d_w} with $d_w > 2$. Similar ideas have appeared in the literature of chromatography [6]. All of the theoretical work on these problems can be regarded as mean-field approximations in which the complicated structure of a random medium is modelled in terms of translationally invariant residence time densities at the trapping sites.

In the present letter we present and analyse a model for diffusion in random media in the presence of a random concentration, c, of traps that allow release of the particles held in them. The release process is assumed to be first order with a rate constant of the form

$$W = W_0 \exp(-\beta V) \tag{1}$$

where $\beta = 1/(kT)$, V is an energy and W_0 is the (uniform) release rate at infinite temperature. The energies, $V(\boldsymbol{r})$, in (1) are assumed to be random variables depending on the position of the trap, and for the probability density of each $V(\boldsymbol{r})$ we choose the form

$$p(V) = (1/\bar{V}) \exp(-V/\bar{V}) \tag{2}$$

where $\bar{V}$ is the mean value of V. The model represented by (1) and (2) at $T = 0$ corresponds to pure trapping for which exact results are available [7]. We show that there exists a critical temperature, T_c, such that for $T > T_c$ the motion of a random walker is purely diffusive, i.e. $\langle r^2 \rangle \sim t$. When $T < T_c$ the diffusion becomes anomalous,

† Permanent address: Department of Physics, Bar-Ilan University, Ramat-Gan, Israel.

characterised by a temperature-dependent diffusion exponent, d_w, that increases with decreasing temperature. The model represented by (1) and (2) cannot be solved exactly for any dimension d but a phenomenological theory has been developed and checked against accurate simulations in $d = 1$ and 2, based on the method of exact enumeration [8, 9].

Several one-dimensional systems were found recently to have a dynamical phase transition. (a) The temperature dependence of the dynamical conductivity exponent observed in the one-dimensional superionic conductor hollandite was explained [10] as a result of a dynamical phase transition. In this system the conduction by classical charge carriers is assumed to be interrupted by *barriers* with a random distribution of activation energies. (b) Anomalous relaxation in spin glasses can be interpreted in terms of stochastic motion in phase space with a power law distribution of free energy barriers [11]. This corresponds to diffusion in the presence of a one-dimensional hierarchical set of barriers [12] for which a dynamical phase transition was found [13]. (c) The problem of biased diffusion in random structures such as the random comb or the percolation cluster can be mapped [14, 15] on biased diffusion in a linear chain with a power law distribution of transition rates. In this case a phase transition in the dynamics occurs as a function of the bias field.

The analysis of the present model represents a generalisation and more exact version of many models of trap-controlled hopping in amorphous solids [1-5]. The earlier models contain no analogue of temperature as in (1) and can be regarded as mean-field approximations to the present model at a fixed temperature. It is interesting, nevertheless, to see whether a transition between ordinary and anomalous diffusion can be expected from the mean-field approximation (MFA) to the present theory. That MFA shows anomalous diffusion when the mean residence time in a trap is infinite. The mean residence time for our model is

$$\left\langle \frac{1}{W} \right\rangle = (1/W_0 \bar{V}) \int_0^\infty \exp[(\beta - 1/\bar{V})V]\, \mathrm{d}V \tag{3}$$

which is infinite for $T < (\bar{V}/k)$. Thus the mean-field theory predicts a transition as does the present theory. It does not permit the calculation of $\langle r^2 \rangle$ below T_c so that we cannot expect it to predict the correct diffusion exponents without further assumptions being made. Let us first consider the diffusive behaviour and estimate the diffusion constant, D, together with its dependence on β and $\bar{V}$. Machta [16] and Zwanzig [17] have considered the problem of diffusion in one-dimensional random media, finding that in the long-time limit the diffusion constant can be expressed as

$$\frac{1}{D} = \frac{1}{N} \sum_{j=1}^{N} \frac{1}{W_j} \tag{4}$$

where W_i is the release rate at site i. In the present case we can rewrite this for large N as

$$\frac{1}{D} = \frac{1}{N} \left(\sum_{j=1}^{N}{}' \frac{1}{W_j} + (1-c)N \right) \tag{5}$$

where the prime on the sum indicates that it is to be taken over trapping sites only. The sum over W_j^{-1} will be replaced by

$$\frac{1}{N} \sum{}' \frac{1}{W_j} \sim c \int_{W_{\min}}^{W_0} \frac{\rho(W)}{W}\, \mathrm{d}W \tag{6}$$

where $\rho(W)$ is the probability density for the rates and $W_{\min}$ is the minimum value of W. This quantity will be found later.

The calculation of $\rho(W)$ makes use of the relation

$$\rho(W) = p(V)\left|\frac{\mathrm{d}V}{\mathrm{d}W}\right| = \frac{1}{\beta\bar{V}W_0^{1/(\beta\bar{V})}}\frac{1}{W^\alpha} \tag{7}$$

where $\alpha = 1 - 1/(\beta\bar{V}) \equiv 1 - T/T_c \leq 1$ and T_c is the critical temperature. Normal diffusion occurs either when the integral in (6) is independent of N, i.e. for $\alpha < 0$, or when $c = 0$. In order to determine the behaviour of the integral it is necessary to determine the value to be assigned to the lower limit, $W_{\min}$. For this purpose let us define a uniformly distributed random variable x by $\mathrm{d}x = \rho(W)\mathrm{d}W$ or

$$x = KW^{1-\alpha} \tag{8}$$

where K is a normalisation constant. Since the expected value of the average of the minimum of cN uniformly distributed random variables is proportional to $(cN)^{-1}$ it follows from (8) that $W_{\min}$ is proportional to $(cN)^{-1/(1-\alpha)}$ where $0 \leq \alpha < 1$. Thus, in the limit $N \to \infty$, $c \neq 0$ the first term on the right-hand side of (5) is the dominant one and D is then related to c and N by

$$D \sim 1/(cN^\alpha)^{1/(1-\alpha)}. \tag{9}$$

In one dimension we can identify N with the displacement x, with the result that

$$\begin{aligned} D^{-1} = \lim_{t,x^2\to\infty} t/x^2 &\sim (cN^\alpha)^{1/(1-\alpha)} \\ &\sim (cx^\alpha)^{1/(1-\alpha)}. \end{aligned} \tag{10}$$

We will interpret this in terms of the mean square displacement by

$$\langle x^2\rangle^{(2-\alpha)/(2(1-\alpha))} \sim t/c^{1/(1-\alpha)}. \tag{11}$$

The exponent appearing in the LHS of (11) has been found earlier by Alexander *et al* [18]. In two dimensions we can identify N, the number of sites sampled, as being proportional to $\langle r^2\rangle$ with the possibility of a logarithmic correction. Although the validity of (4) has not been established in dimensions greater than one we will assume its validity in all dimensions. Since our simulation results are in good agreement with the theory developed on the basis of (4) we believe it to be true although so far unproven. We find, by a similar argument,

$$\langle r^2\rangle^{1/(1-\alpha)} \sim t/c^{1/(1-\alpha)}. \tag{12}$$

Diffusion is normal when $\alpha = 1 - T/T_c$ is negative, i.e. when $T > T_c$. When $T < T_c$ the diffusion exponent, d_w, is

$$d_w = \begin{cases} \dfrac{2-\alpha}{1-\alpha} = (T+T_c)/T & d=1 \\ & \qquad T < T_c. \\ \dfrac{2}{1-\alpha} = 2T_c/T & d=2 \end{cases} \tag{13}$$

In both cases $d_w \to \infty$, as $T \to 0$, as in the limit of pure trapping.

The results, (11)-(13), were tested in one and two dimensions by simulation using the exact enumeration method [8, 9]. The agreement between numerical and theoretical results is shown in figures 1-4 and appears to confirm our theoretical predictions.

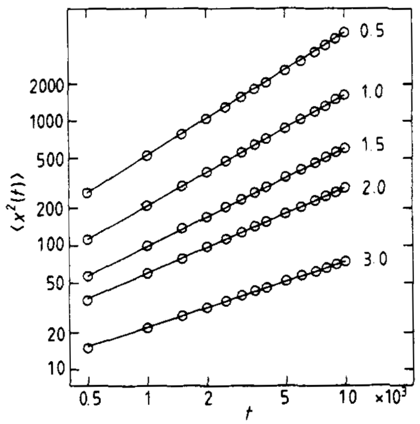

Figure 1. A log-log plot of $\langle x^2(t)\rangle$ as a function of the number of steps t for a one-dimensional lattice and concentration of traps $c = 1.0$. The different values of T_c/T used are indicated on the RHS of the figure. The slopes in this plot represent $2/d_w$ and their values are given in figure 4. We used lattices with up to 200 sites and averages were made over 100 configurations.

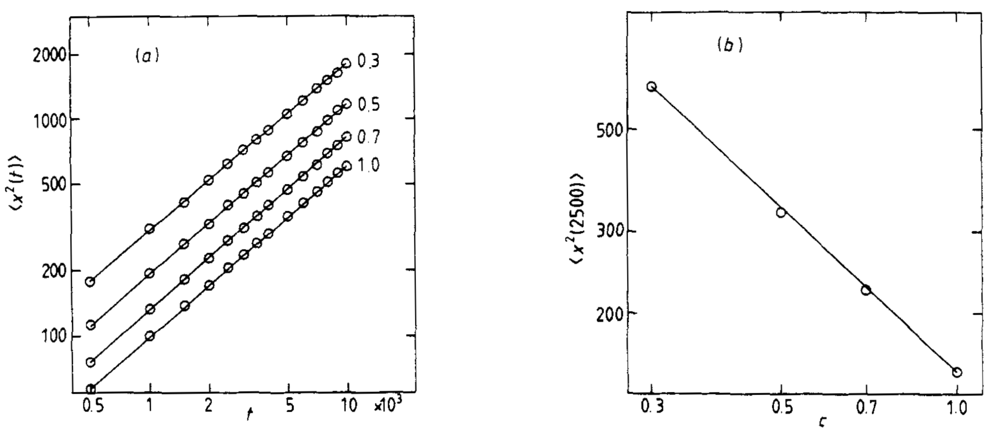

Figure 2. (a) A log-log plot of $\langle x^2(t)\rangle$ in one dimension as a function of the number of steps t, with $T_c/T = \frac{3}{2}$. The different trap concentrations are indicated by the numbers to the right of the lines. (b) Results for $\langle x^2(2500)\rangle$ for the concentrations given in figure 2(a). The circles represent the numerical data and the line represents the theoretical prediction, equation (11).

It is noted that although the relation $d_w = 2T_c/T$ has been checked by simulation in two dimensions, we believe it to be valid in higher dimensions as well. The argument is a consequence of the relation between the mean number of distinct sites visited by an ordinary random walker and the mean square displacement $\langle r^2\rangle$. The relation in

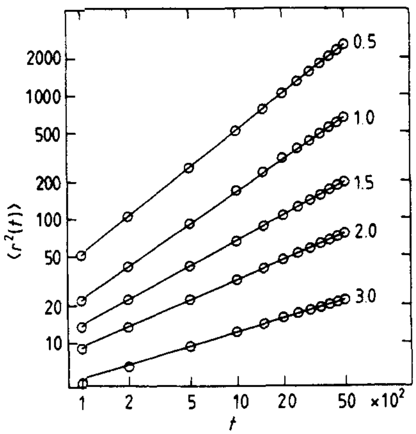

Figure 3. A log-log plot of $\langle r^2(t)\rangle$ against t for a two-dimensional lattice and concentration of traps $c = 1.0$. The different values of T_c/T used are indicated on the right-hand side of the figure. Lattices with up to 200×200 sites were used and averages were taken over 100 configurations. The values of d_w derived from the slopes of this figure are given in figure 4.

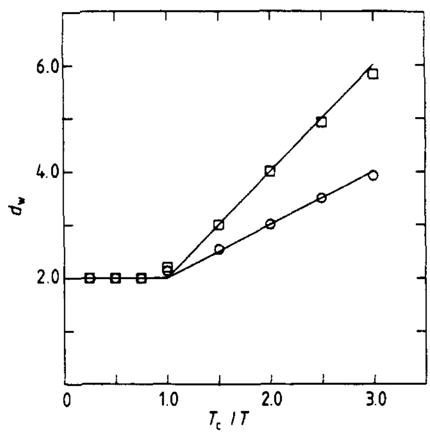

Figure 4. Plot of d_w as a function of T_c/T for one (○) and two (□) dimensions. The points represent the numerical data obtained from plots in figures 1 and 3, and the lines are theoretically predicted values from equation (12). The deviation at $T = T_c$ from the theoretical values may be due to logarithmic corrections appearing in equation (12) when $\alpha = 0$.

greater than or equal to three dimensions is $\langle S_n\rangle \sim \langle r^2\rangle$ which is implicitly the result needed to prove equation (12).

An important consequence of (13) is that the upper critical dimension of the present system is $d_c = 2$. This follows from comparing our result (13) to studies of CTRW or mean-field theory [19-21], which obtain $d_w = 2/(1-\alpha)$ independent of dimension. That is for $d \geqslant d_c = 2$, we obtain the mean-field result independent of dimension.

Several interesting further results and conjectures are raised by the present analysis.

(i) Our results given in (13) are for the particular probability density $P(V)$ given in (1). This raises the question of what is to be expected for other forms of $P(V)$. Using similar heuristic arguments we suggest that there are forms for $P(V)$ which ensure that a phase transition will not occur. It is possible, however, that more complicated relations between $\langle r^2 \rangle$ and t may be valid. For example, when a power law distribution is assumed, $P(V) \sim V^{-(1+\gamma)}$, we expect that the one-dimensional asymptotic relation will be $\langle x^2 \rangle \sim (\log t)^{2\gamma}$ with γ a constant.

(ii) In the presence of a field, the time spent in N sites is of the order of $t \sim \Sigma_{j=1}^{N} (1/W_j)$. This implies, by using similar arguments, that in any dimension $d_w = T_c/T$ for $T < T_c$ and $d_w = 1$ for $T \geq T_c$. This argument is independent of (4) whose validity is still conjectural in dimensions greater than one.

(iii) It is interesting to note that if the system consists of barriers with a power law distribution of heights of barriers (not traps as in the present model) a dynamical phase transition above one dimension is not expected [22]. This is due to the fact that the random walker will always find an 'easy' way to travel in the system and regular diffusion is expected for each value of α.

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