Dynamical Phase Transitions in Hierarchical Structures

S. Teitel
Department of Nuclear Physics, Weizmann Institute of Science, Rehovot, Israel

and

Eytan Domany
Department of Electronics, Weizmann Institute of Science, Rehovot, Israel
(Received 15 July 1985)

We study diffusion in the presence of a hierarchical set of barriers. We find a phase transition in the dynamics from ordinary to anomalous diffusion as a parameter controlling the relative barrier heights is varied. Similar behavior is found in suitably defined random systems. Possible connections to glassy dynamics are discussed.

PACS numbers: 64.70.Ew, 05.40.+j, 61.40.Df

The problem of stochastic motion in the presence of a hierarchical array of barriers (and associated transition rates) is of considerable cross-disciplinary interest. Anomalous relaxation, observed in a wide range of physical phenomena,[1] can be explained in terms of hierarchically constrained dynamics. In particular, relaxation in spin-glasses can be interpreted in terms of stochastic motion (in phase space) with a hierarchical distribution of (free energy) barriers.[2] Random-field Ising magnets also exhibit anomalous relaxation.[3] Similar problems are encountered in the dynamics of macromolecules,[4] early evolutionary processes,[5] and possibly, computing architectures.[6]

Previous studies of stochastic motion in the presence of a hierarchical set of barriers concentrated on understanding the anomalous dynamics produced by various rules that determine the hierarchy.[1,7] In what follows we report observation of a *phase transition in the dynamics*,[8] from normal to anomalous behavior. Our model is that of hopping on a one-dimensional chain, with hierarchically placed barriers, as pictured in Fig. 1(a). Using a renormalization-group approach, we found that a transition occurs as a parameter R, the ratio between barriers that belong to two successive levels in the hierarchical structure, is varied. We find for the long-time autocorrelation function $P_0(t)$,

$$P_0(t) \sim \begin{cases} [D(R)t]^{1/2}, & 1 > R > R_c, \\ t^{-x(R)}, & 0 < R < R_c. \end{cases} \quad (1)$$

The diffusion constant[8] $D(R)$ vanishes linearly as $R \rightarrow R_c^+$. Anomalous diffusion, characterized by a continuously varying exponent $x(R)$, is associated with a line of fixed points of the renormalization group. We relate our work to previous studies of one-dimensional hopping in the presence of random barriers.[8,9] We find that for the two problems, of randomly and hierarchically distributed barriers, exactly the same results are obtained, provided that the distributions of barrier heights are the same.

Our model,[10] recently analyzed by Hubermann and Kerszberg,[7] consists of a linear chain of sites, $k = 1, 2, \ldots, 2^n$. A particle can hop from site k to sites $k \pm 1$ with transition rates $W_{k,k\pm 1} = W_{k\pm 1,k}$. The probability of finding the particle at time t at site k is $P_k(t)$. The Laplace-transformed function $\tilde{P}_k(\lambda)$ satisfies the eigenvalue equations

$$-\lambda \tilde{P}_k = W_{k,k+1}(\tilde{P}_{k+1} - \tilde{P}_k) + W_{k-1,k}(\tilde{P}_{k-1} - \tilde{P}_k), \quad (2)$$

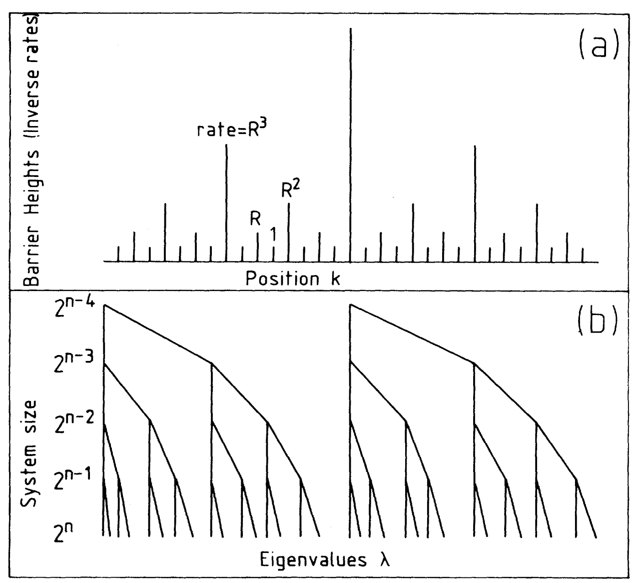

FIG. 1. (a) Hierarchical barrier structure. The height of a barrier is inversely proportional to the transition rate. The largest rate (smallest barrier) is equal to 1. The other rates are given by R^l ($0 \leq R \leq 1$, l integer), where l denotes the level of the hierarchy, as illustrated. (b) Schematic representation of eigenvalues of the master equation (2) for systems of size 2^n. All eigenvalues of a system of size 2^{n-1} remain eigenvalues of the system of size 2^n. An additional eigenvalue splits off from each of these old ones by an amount $O(R^{n-1}/2^{n-2})$.

where the rates $W_{k,k+1}$ are assigned hierarchically as shown in Fig. 1(a) (the transition rate is the inverse of the barrier height):

$$W_{k,k+1} = R^m, \quad R < 1,$$

if for all $l \leq m$,

$$k(\mathrm{mod} 2^l) = 0.$$

Our results will be stated in terms of the autocorrelation function $P_0(t)$ which measures the probability for a particle to be found at time t at the same site it started from at time $t=0$. In terms of the density of states [of eigenvalues of Eq. (2)], $g(\lambda)$, we have

$$P_0(t) = \int_0^\infty d\lambda\, e^{-\lambda t} g(\lambda). \qquad (3)$$

Since the problem involves a hierarchy of time scales and has a self-similar structure, one expects an interpretation within the renormalization-group context to be both possible and useful. Regarding R, the ratio of transition rates from one level of the hierarchy to the next, as the scaling parameter of our renormalization-group transformation, we compare a system S of size 2^n at ratio R to one S' of size 2^{n-1} at ratio R'. A matching condition, $R' = \beta(R)$, is determined by the requirement that the low-lying eigenvalues λ' of S' are related to those λ of S by a simple scale factor $\lambda'(R') = \alpha(R)\lambda(R)$. Such a condition assures that the density of states $g(\lambda)$ for the two systems S and S' will be proportional in the limit $n \to \infty$, and hence that $P_0(t)$ will have the same long-time behavior. Our results will be stated in terms of these two functions, $\alpha(R)$ and $\beta(R)$, which provide a complete determination of long-time properties. In terms of these functions, a recursion relation for the density of states[11] is determined,

$$g(\lambda,R) = [\alpha(R)/2] g(\alpha(R)\lambda, \beta(R)). \qquad (4)$$

We first consider a simple decimation scheme which can be implemented about the points $R=0$ and 1. These results will suffice to indicate the existence of a phase transition. We extend the results to higher order in R by perturbation theory. For general R, we use a numerical procedure similar to that introduced by Sarker[12] for quantum Hamiltonians. Within this numerical scheme, we will be able to check explicitly the consistency of our assumption that R is the only relevant scaling variable.

To perform the decimation calculation, we note that the master equation (2) couples only odd-numbered sites to even ones and vice versa. One can thus solve for the odd sites in terms of the even and write an effective master equation for the even sites alone.[11] The goal then is to recast this new master equation for half the number sites in the same form as the original problem. Normalizing the rates in the new effective master equation such that the largest is again 1, one finds to lowest order in R that the transition rates remain hierarchical with ratio $R' = R$, and that if λ is an eigenvalue of the original problem, $\lambda' = (2/R)\lambda$ is an eigenvalue of the decimated one. Thus $\beta(R) = R$, $\alpha(R) = 2/R$, and the decimation calculation yields a line of fixed points at small R. Using the recursion relation for the density of states (4), we find $g(\lambda,R) = (1/R) g((2/R)\lambda, R)$, which may be solved to give $g(\lambda,R) \sim \lambda^{-y}$, where $y = -\ln R/(\ln 2 - \ln R)$. The autocorrelation function is then

$$P_0(t) \sim t^{-x},$$

where

$$x = 1 - y = ln 2/(ln 2 - ln R). \qquad (5)$$

This is identical to the results of Huberman and Kerszberg.[7] A similar calculation, done to lowest order in $1-R$ yields the results $R' = \beta(R) = \sqrt{R}$ and $\alpha(R) = 4/\sqrt{R}$. In this case, under successive decimations R iterates to $R=1$, the equal-barrier model. Thus for R near 1 we expect $g(\lambda,R) \sim \lambda^{1/2}$ and $P_0(T) \sim t^{1/2}$, the ordinary diffusion result.

These simple decimation calculations indicate that the line of fixed points, responsible for the anomalous diffusion found by Huberman and Kerszbert[7] at small R, ends at some $0 < R_c < 1$, above which ordinary diffusion occurs. However, an alternative scenario is also possible; the $R << 1$ calculation could indicate that $R=0$ is marginally unstable, with no line of fixed points and no transition. To resolve this, a higher than first-order calculation is needed. However, to next order in R or $1-R$, the decimation calculation produces nonhierarchical couplings. Thus to extend the results to higher order, another procedure is necessary. If $\lambda_0 = 0$, λ_1, and λ_2 are the lowest eigenvalues of a system of size 2^n and $\lambda_0' = 0$, λ_1', and λ_2' are the lowest eigenvalues of a system of size 2^{n-1}, then the matching condition $\lambda'(R') = \alpha(R)\lambda(R)$ can be rephrased in terms of the ratio $\gamma = \lambda_1/\lambda_2$ as $\gamma'(R') = \gamma(R)$. Thus we can construct a β function by matching γ for finite systems, 2^n to 2^{n-1}. If the scaling assumption is correct, β should approach a unique function as $n \to \infty$, and the same β which is constructed by comparison of λ_1/λ_2 should also lead to matching for all low-lying ratios λ_1/λ_i. We have first implemented this procedure by calculating the lowest eigenvalues of (2) with ordinary Rayleigh-Schrödinger perturbation theory in R. The structure of the eigenvalue spectrum is indicated in Fig. 1(b). Here we will state the main results; details of the calculation will be presented elsewhere.[13] In going from a matrix of size 2^{n-1} to 2^n, all the eigenvalues of the 2^{n-1} system remain eigenvalues of the 2^n system, and new eigenvalues are created which are split off from the old by a positive amount $O(R^{n-1}/2^{n-2})$. Thus the lowest nonzero eigenvalue λ_1' of size 2^{n-1} is the second lowest nonzero eigenvalue λ_2 of size 2^n. In matching γ we find $R' = R$ and

$\alpha(R)=2/R$ to all orders in perturbation, as $n\rightarrow\infty$. Thus the simple decimation procedure produced the exact answer to all orders in R.

The ending of the line of fixed points at small R is caused by the breakdown of perturbation theory, and one must go to numerical methods. We have numerically computed the low-lying eigenvalues of systems with up to 2^{15} sites, and in Fig. 2 we plot the results for $\gamma=\lambda_1/\lambda_2$ for $n=9,\ldots,15$. Our computational algorithm consists of a combination of the negative eigenvalue theorem[14] with bisection and was found to be very efficient and stable. The limiting $(n\rightarrow\infty)$ curve (dashed lines in Fig. 2) for γ is the line $\gamma(R)=R/2$ for $0\leqslant R\leqslant\frac{1}{2}$ which joins continuously onto the line $\gamma(R)=\frac{1}{4}$ for $\frac{1}{2}\leqslant R\leqslant 1$. Thus the transition between anomalous and ordinary diffusion is seen to occur at $R_c=\frac{1}{2}$. For $R\leqslant\frac{1}{2}$, we expect perturbation theory to hold and give a line of fixed points. In this case we know that λ_1' of the system of size 2^{n-1} is equal to λ_2 of the system with size 2^n, and since $R=R'$, we see that $\gamma=\lambda_1/\lambda_2=\lambda_1/\lambda_1'=1/\alpha(R)=R/2$ as expected. For $\frac{1}{2}\leqslant R\leqslant 1$, the ratio γ is just that of the equal-barrier $R=1$ model, and so we expect the long-time behavior to be ordinary diffusion. From comparing curves of γ_n to γ_{n-1} for finite n, we can construct the β function $R'=\beta(R)$ by matching $\gamma_n(R)=\gamma_{n-1}(R')$ as discussed above. In Fig. 3 we plot $R'-R=\bar{\beta}(R)$ from various sizes. As expected, as $n\rightarrow\infty$, the $\bar{\beta}$ function is converging to zero for $0\leqslant R\leqslant\frac{1}{2}$, while giving a flow to $R=1$ for $R\geqslant\frac{1}{2}$. Agreement with the decimation result $R'=\sqrt{R}$ near $R=1$ is found. We have checked the $\bar{\beta}$ functions of Fig. 3 for consistency by matching the other low-lying eigenvalue ratios λ_1/λ_i between systems of size 2^n and 2^{n-1}, and find good agreement. This verifies the validity of our one-parameter scaling assumption. A straightforward extension of the above analysis to hierarchical barrier structures in arbitrary dimension d will be presented elsewhere[13]; again we find $R_c=\frac{1}{2}$ with $x(R)$ in Eq. (1) being replaced by $dx(R)$.

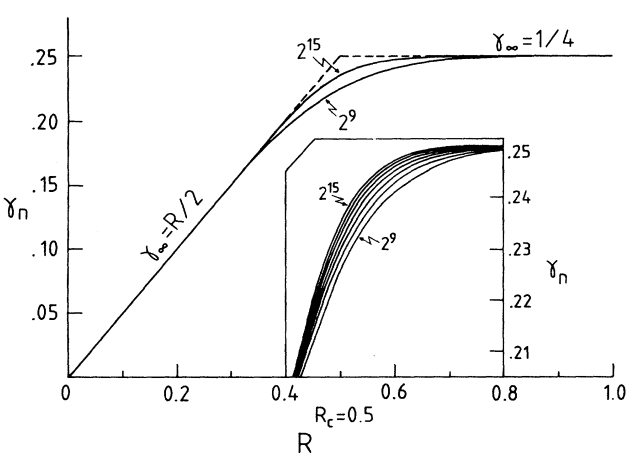

FIG. 2. Ratio of lowest two nonzero eigenvalues $\lambda_n=\lambda_1/\lambda_2$ vs R for systems of size 2^n. Full graph shows results for sizes 2^{15} and 2^9. As $n\rightarrow\infty$ the limiting curve (dashed lines) is $\gamma_\infty=R/2$ for $R<R_c=\frac{1}{2}$ and $\gamma_\infty=\frac{1}{4}$ for $R>R_c$. Inset shows curves for sizes 2^n, $n=9,\ldots,15$, on an expanded vertical scale.

In principle we can use the recursion relation for the density of states to derive how the diffusion constant goes to zero as $R\rightarrow\frac{1}{2}^+$ and how the anomalous diffusion region is approached from above. Combining Eqs. (3) and (4), we get a recursion relation for $P_0(t)$, and using the fact that for $R\geqslant\frac{1}{2}$, $\lim_{n\rightarrow\infty}P_0(t,\beta^{(n)}(R))=P_0(t,1)\approx t^{-1/2}$ we find

$$D=\prod_{n=0}^{\infty}\frac{4}{\alpha(R_n)},$$

where $R_n=\beta^{(n)}(R)$. However, for the problem at hand, D can be calculated directly as discussed below.

We turn to the related problem of one-dimensional hopping in the presence of random barriers.[8,9] Now

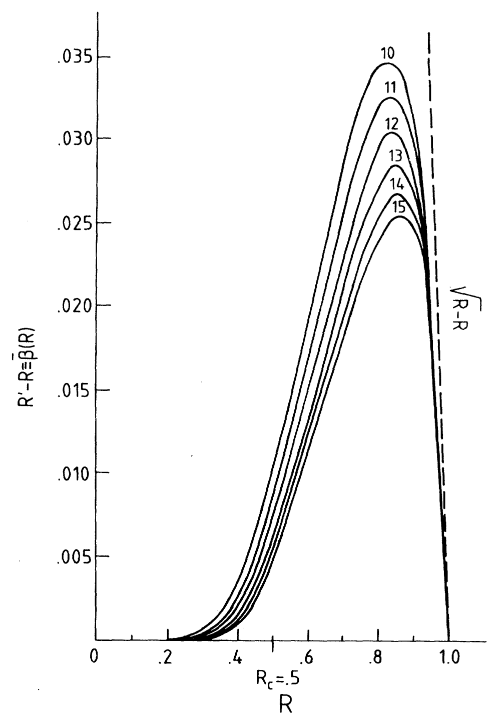

FIG. 3. Scaling functions $\bar{\beta}(R)$ between systems of size 2^n and 2^{n-1}, i.e., $R'(2^{n-1})=R(2^n)+\bar{\beta}(R)$, as obtained by matching $\gamma_{n-1}(R')=\gamma_n(R)$ from the curves of Fig. 2. Curve 15, for example, results from comparison of the system of size 2^{15} to one of size 2^{14}. For $R<R_c=0.5$, the curves converge to zero as $n\rightarrow\infty$, and one has a line of fixed points. For $R_c<R\leqslant 1$, R flows to $R=1$ under successive iterations. Near $R=1$, the decimation result $R'=\sqrt{R}$ is found.

the transition rates $W_{k,k+1}$ are independent random variables taken from a probability distribution $f(W)$. If we take for $f(W)$ the same density of rates as in the hierarchical model [but now the rates are distributed randomly along the chain, rather than in the ordered structure of Fig. 1(a)] we have $f(W) \sim W^{-\alpha}$, where $\alpha = 1 - \ln 2/|\ln R|$. For such a distribution, Dyson[8,9] computes the autocorrelation function $P_0(t)$ and obtains exactly the same results as in our hierarchical model. Thus the transition from ordinary to anomalous diffusion appears to be a more general property, dependent on the distribution of transition rates, rather than on the particular hierarchical ordering.

Finally, one can compute the diffusion constant $D(R)$ of Eq. (1) for the region of normal diffusion, i.e., $\frac{1}{2} \leqslant R \leqslant 1$, and in particular, how it vanishes as $R \rightarrow R_c^+$. A very general result[15] yields

$$\frac{1}{D} = \frac{1}{N} \sum_{k=1}^{N} \frac{1}{W_{k,k+1}}, \tag{6}$$

for *any* arrangement of N barriers. For the hierarchical case, this is just the geometric series $1/D = \frac{1}{2}\sum_{n=0}^{\infty}(1/2R)^n$. For $R > \frac{1}{2}$, the series diverges, and so $D = 0$. This is the region of anomalous diffusion. For $R \leqslant \frac{1}{2}$, the series converges, and $D = (2/R)(R - \frac{1}{2})$, going linearly to zero at $R_c = \frac{1}{2}$.

To conclude, we have demonstrated that a model with hierarchical barriers undergoes a phase transition from anomalous to normal diffusion, as a parameter R is varied. R measures the relative transition rates associated with successive levels of the hierarchy. Thus one expects R to be controlled, in systems such as glasses, by variation of the temperature. Since the main results depend only on the average inverse transition rate, the existence of such a transition in the dynamics does not require a hierarchical spatial arrangement of the barriers. We believe that various models of statistical mechanics will provide examples of such a transition and hope that experimental realizations can also be found.

We thank J. Gubernatis, M. Kerszberg, W. Kinzel, and D. Mukamel for most helpful suggestions. One of us (S.T.) would like to acknowledge partial support from the Bantrell Foundation, and the other (E.D.) partial support from the Israel Academy of Sciences and Humanities.

[1]R. G. Palmer, D. L. Stein, E. Abrahams, and P. W. Anderson, Phys. Rev. Lett. **53**, 958 (1984).

[2]Vik. S. Dotsenko, Landau Institute Report No. 1984-22 (to be published).

[3]G. Grinstein and J. F. Fernandez, Phys. Rev. B **29**, 6389 (1984); R. J. Birgenau, R. A. Cowley, G. Shirane, and H. Yoshizawa, Phys. Rev. Lett. **54**, 2147 (1985).

[4]M. Levitt, Ann. Rev. Biophys. Bioeng. **11**, 251 (1982); A. Ansari *et al.*, University of Illinois Report No. ILL-(EX)-85 No. 16 (to be published).

[5]D. L. Stein, D. Rokhsar, and P. W. Anderson, unpublished.

[6]B. A. Huberman and T. Hogg, Phys. Rev. Lett. **52**, 1048 (1984).

[7]B. A. Huberman and M. Kerszberg, J. Phys. A **18**, L331 (1985).

[8]S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. **53**, 175 (1981).

[9]F. J. Dyson, Phys. Rev. **92**, 1331 (1953).

[10]H. A. Simon and A. Ando, Econometrica **29**, 111 (1961).

[11]E. Domany, S. Alexander, D. Bensimon, and L. P. Kadanoff, Phys. Rev. B **28**, 3110 (1983).

[12]S. Sarker, Phys. Rev. B **30**, 2752 (1984).

[13]S. Teitel and E. Domany, to be published.

[14]P. Dean, Rev. Mod. Phys. **44**, 127 (1972).

[15]R. Zwanzig, J. Stat. Phys. **28**, 127 (1982).