LOCALIZATION AS A MECHANISM FOR THE TRANSITION TO ANOMALOUS RELAXATION

S. Teitel

Department of Physics and Astronomy
University of Rochester
Rochester, NY 14627
USA

INTRODUCTION

Anomalously slow relaxation to equilibrium has been observed in a wide variety of disordered systems. These include spin glasses,[1] ionic glasses,[2] charge density waves,[3] amorphous semiconductors,[4] and plate glass.[5] A common feature of such glassy systems is generally believed to be a complex free energy surface consisting of many metastable local minima separated by barriers spanning a wide range of energy scales. Thermal activation over these barriers introduces a broad distribution of time scales leading to anomalously slow relaxation of correlations.

In a previous work,[6,7] a simple one-dimensional model with many of the above features was introduced. The model consists of a particle moving diffusively in a harmonic potential. Superimposed on this potential is a hierarchical barrier structure. As the barrier distribution is varied, an effective diffusion constant vanishes. For finite diffusion constant, the low lying eigenstates of the master equation, which determine the asymptotic decay to equilibrium, map onto to those of a

problem with all barriers replaced by an average effective barrier; decay is a simple exponential. When the diffusion constant vanishes however, the low lying eigenstates become localized at the most difficult barriers to cross; decay is anomalously slow.

In this work, I generalize this model by allowing the barriers to be placed in random positions, rather than in the ordered spatial hierarchy considered earlier. The low lying eigenstate structure, and relaxation to equilibrium, are investigated numerically. As in the ordered hierarchy, one finds that a vanishing of the effective diffusion constant produces a transition to localized eigenstates, resulting in anomalously slow decay.

DESCRIPTION OF THE MODEL

Consider the motion of a particle, hopping between discrete sites x on a one dimensional lattice. The dynamics is given by the classical master equation for the probability P(x,t) that the system is at position x at time t.

$$\frac{dP(x)}{dt} = W_{x+1,x}\ P(x+1)+W_{x-1,x}\ P(x-1)-(W_{x,x+1}+W_{x,x-1})P(x) \qquad (1)$$

The rates $W_{x,x+1}$ to hop from x to x+1 are given by[6]

$$W_{x,x+1} = R^{n(x)}\ e^{[\ E(x)\ -\ E(x+1)]\ /\ 2T} \qquad (2)$$

and describe diffusion in the potential E(x), where the factor $R^{n(x)} \equiv e^{-n(x)\Delta_o/T}$ represents a free energy barrier of height $n(x)\Delta_o$ separating sites x and x+1. The reverse hopping rates are given by detailed balance,

$$W_{x+1,x} = W_{x,x+1}\ e^{[\ E(x+1)\ -\ E(x)\ ]\ /\ T} \qquad (3)$$

The potential is taken to be harmonic

$$E(x) = \frac{1}{2}\ \kappa_o\ x^2 \qquad (4)$$

The energy barriers $n(x)\Delta_o$ are chosen to be symmetric about x=0, ie. n(x)=n(-x), but are otherwise selected at random from the probability distribution p(n),

$$p(n) = \frac{2}{3}\ \frac{1}{3^n} \qquad n = 0,\ 1,\ 2,\ \ldots \qquad (5)$$

p(n) above gives the same distribution of barrier hopping rates as studied in the earlier model[6] where barriers were placed in an ordered trifurcat-

ing spatial hierarchy. Here we retain the hierarchy of energy scales, but let the spatial structure be random.

For a flat potential, $\kappa_0 = 0$, and barriers parameterized by $R \equiv e^{-\Delta_0/T}$, the diffusion constant D(R) is given by the inverse of the average barrier hopping time[8,9]

$$\frac{1}{D} = \sum_{n=0}^{\infty} \frac{1}{R^n}\, p(n) = \frac{2}{3} \sum_{n=0}^{\infty} \frac{1}{(3R)^n}$$

$$D(R) = \begin{cases} \dfrac{3R-1}{2R}, & R > \dfrac{1}{3} \\ 0, & R < \dfrac{1}{3} \end{cases} \qquad (6)$$

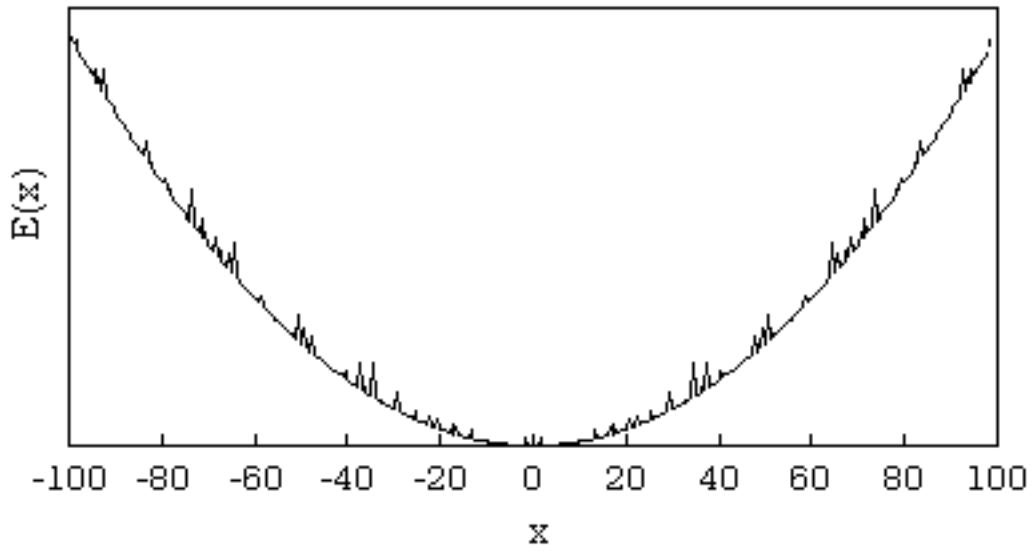


Fig. 1. A particular realization of hierarchical barriers placed randomly in a harmonic potential.

As R approaches $R_c = 1/3$ from above, D(R) vanishes.

For relaxation in a potential, ie. $\kappa_0 > 0$, I now show that $R>R_c$, ie. $D(R)>0$, corresponds to a "normal" regime. Relaxation to equilibrium in the harmonic potential is simple exponential, and the barriers may be replaced by the effective average barrier, in the limit κ_0 goes to zero. The regime $R<R_c$, ie. $D(R)=0$, is the "anomalous" regime. Low lying eigenstates of the master equation are localized at the most difficult barriers to cross, and relaxation is the sum of many exponentials.

NUMERICAL ANALYSIS OF THE MODEL

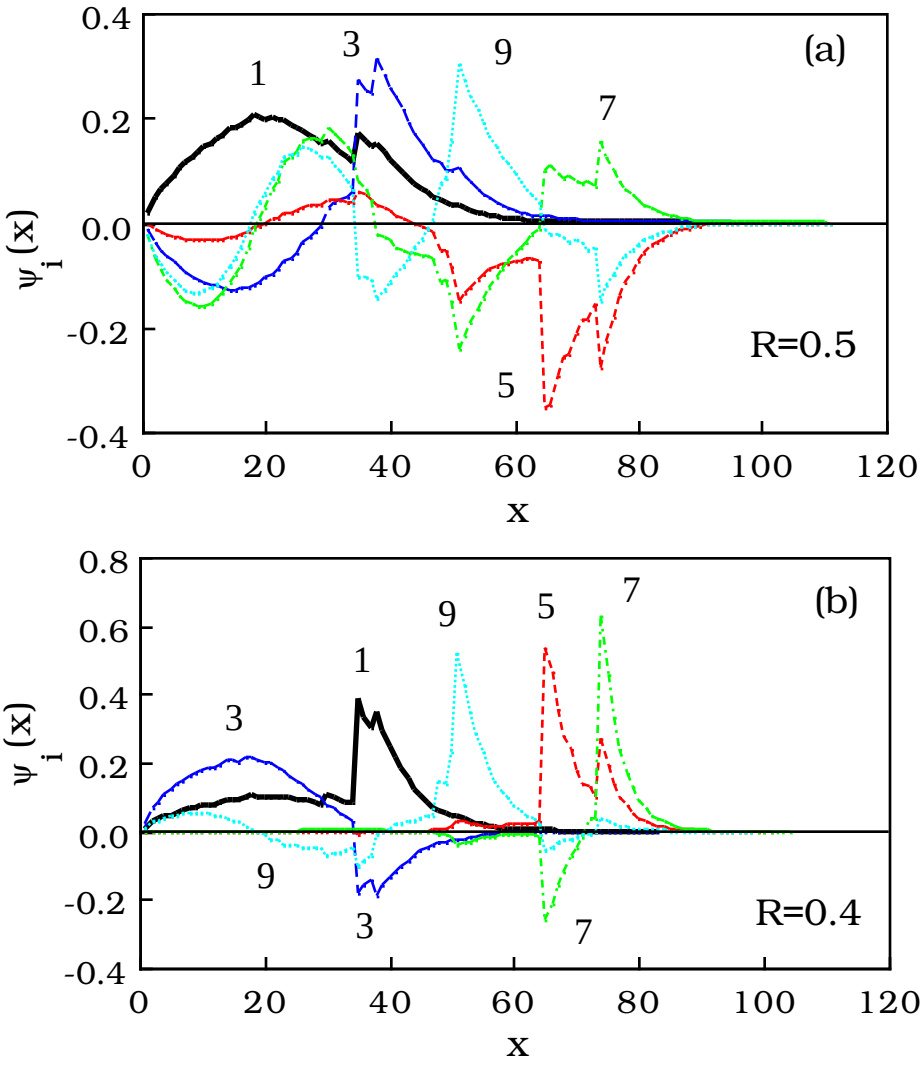
I have numerically studied the random hierarchical barrier model discussed above, on a finite lattice of size $N = 3^6$. A particular realization of the random potential, is shown in Fig. 1 above, for a finite interval of x about the global minimum at x=0.

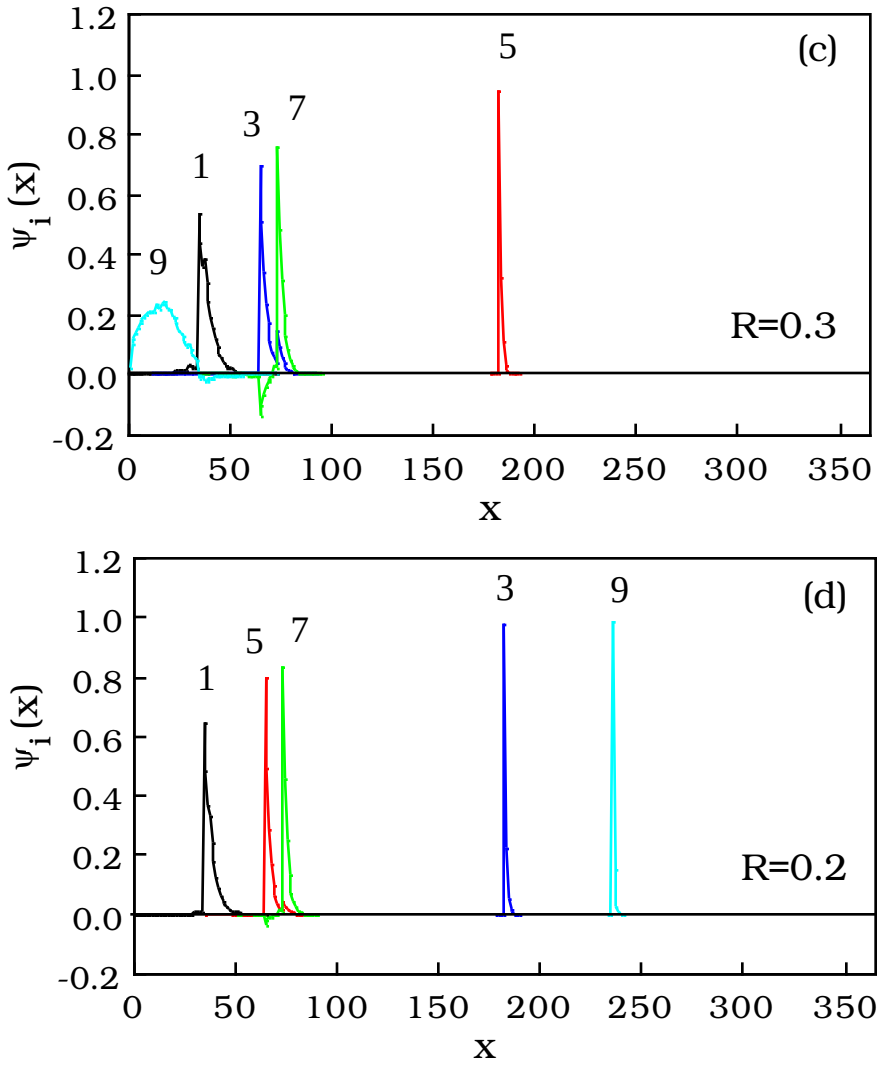
As the asymptotic relaxation of the system will be governed by the low lying eigenvalues and eigenstates of the master equation,[10] I have numerically computed the five lowest antisymmetric eigenstates, for varying values of the barrier parameter $R \equiv e^{-\Delta_0/T}$. The potential coupling κ_0 is fixed in the ratio $\kappa_0/\Delta_0 = 0.01$. (For symmetric barriers as chosen here, only antisymmetric states contribute to the correlation function $<x(t)x(0)>$.)[6] These eigenstates are shown in Fig. 2 below, for the particular barrier realization pictured in Fig. 1, at values of R=0.5, 0.4, 0.3, 0.2, and 0.1. Plotted are the functions $\psi_i(x) \equiv e^{E(x)/2T} P_i(x)$, where $P_i(x)$ is the i^{th} lowest right-handed eigenvector of the master equation matrix. For equal barriers, the ψ_i are just the eigenstates of the quantum harmonic oscillator[6] with frequency $\omega = \kappa_0/2$.

As is plainly seen, for R=0.5, 0.4 $> R_c$, the low lying eigenstates resemble those of the equal barrier model. They are centered close to the origin, and extend over the equilibrium length scale $L_{eq} \sim 1/\sqrt{\kappa_0}$.

In particular, $\psi_1(x) \sim x\, e^{-\kappa_0 x^2/4}$, and as in the ordered hierarchical model,[6] decay approaches a simple exponential with rate given by the lowest non-zero eigenvalue $\lambda_1 \sim 1/\kappa_0$. For R=0.3, 0.2, 0.1 $< R_c$ however, the low lying eigenstates become localized at particular difficult barriers to cross. As in the ordered hierarchical model, decay will be a sum over

many exponentials, with rates determined by these difficult barriers. Relaxation will be anomalously slow.




(c)
R=0.3
5
7
3
1
9
$\psi_i(x)$
x
1.2
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
0
50
100
150
200
250
300
350
(d)
R=0.2
3
9
5
7
1
$\psi_i(x)$
x

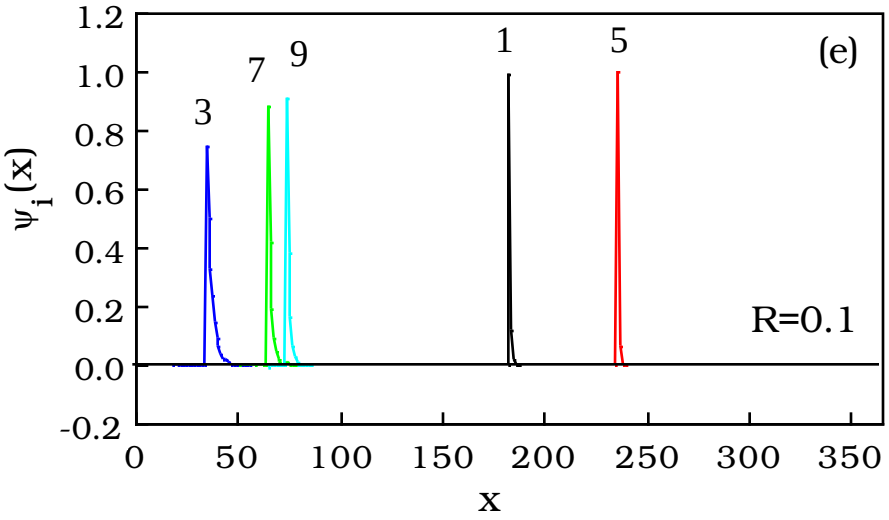


Fig. 2. The five lowest antisymmetric eigenstates for the master equation (1), $\psi_i(x)$, i=1, 3,...,9 (only the x>0 half is shown). For (a) and (b), $R > R_c$, and the states are similar to an equal barrier model, ie. extended about the origin on the equilibrium length scale. For (c) - (e), $R < R_c$, and the states are localized at the most difficult barriers to cross.

To explicitly verify this transition to anomalously slow relaxation, I have numerically simulated a particle taking a one-dimensional random walk with hopping rates given by Eq. (2) and (3). The initial position of the particle is selected at random from the equilibrium distribution. At each update of the particles position, the particle moves one step to the right with probability $p = W_{x,x+1}/(W_{x,x+1}+W_{x,x-1})$, or one step left with probability q = 1 - p. After each update the time is advanced by $\Delta t = 1/W_{x,x\pm1}$ according to whether the particle moved left or right. In this way a trajectory $x(t_i)$ is generated. The decay of the correlation function $\langle\langle x(t)x(0)\rangle\rangle$, where the double brackets indicate a combined thermal average and average over the random barrier configurations, was computed by averaging $x(t_i)x(0)$ over 1000 independent walks for each fixed barrier configuration, and then averaging over 50 different configurations. The results are shown in Fig. 3 for the same parameter values as in Fig. 2 ($R= e^{-\Delta_o/T}$, $\kappa_o/\Delta_o = 0.01$).

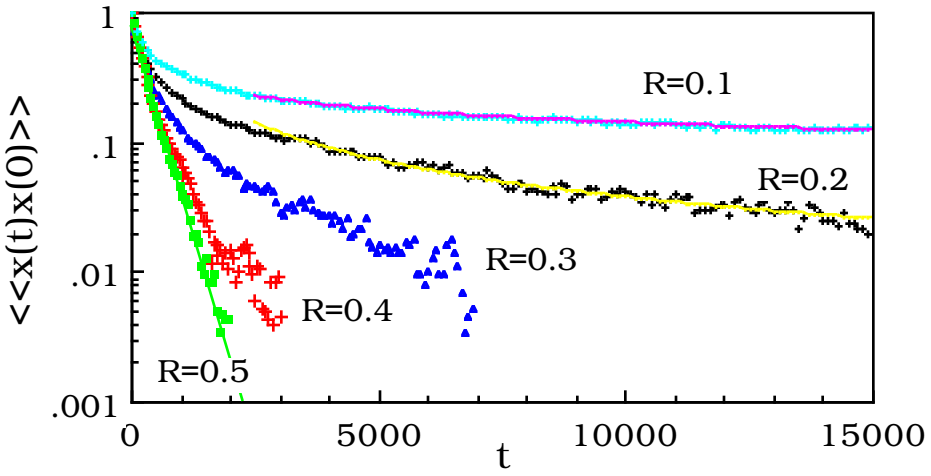


Fig. 3. The decay of the position correlation function versus time. For R=0.5 > R_c, the decay is a exponential. For R=0.1, 0.2 < R_c, the decay is algebraic. For R=0.3, 0.4 ≈ R_c=1/3 the decay is intermediate between these two limits, for the times simulated.

For R=0.5 > R_c =1/3, the decay is reasonably well approximated by a simple exponential (solid line in Fig.3). For R=0.1, 0.2 < R_c, the correlation function decays more slowly than exponential. In contrast to what was found in the ordered hierarchical barrier structure,[6] the anomalous decays here are not particularly well fit by the stretched exponential form. An algebraic decay law (~$t^{-.34}$ for R=0.1, ~$t^{-.95}$ for R=0.2) fits better at long times (solid lines in Fig. 3 for R=0.2, and 0.1). For R=0.3, 0.4, which are close to R_c, the asymptotic behavior takes a longer time to reach. The decays for the times simulated, appear intermediate between exponential and algebraic.

CONCLUSIONS

In this paper I have considered a simple one-dimensional model of classical diffusive relaxation in a harmonic potential, in the presence of a randomly positioned hierarchy of energy barriers. As in a previous

model, in which the barriers were placed in an ordered hierarchical spatial structure, there is a critical value of the barrier parameter R_c which marks a transition in the dynamic behavior. For $R>R_c$, the low lying eigenstates of the master equation resemble those of a model in which all barriers have been replaced by an effective average barrier. Relaxation to equilibrium is well approximated by a simple exponential. For $R<R_c$, the low lying eigenstates of the master equation become sharply localized at the most difficult barriers to cross. Relaxation to equilibrium is slower than exponential, and at long times seems well approximated by an algebraic law.

The transition to anomalously slow relaxation, in both the present random model as well as the spatially ordered model, is signalled by the vanishing of an effective diffusion constant. The vanishing of the diffusion constant may thus be the general indicator for such transitions to anomalous relaxation via localization, and one can hope that this idea may be extended to the multi-dimensional configuration space of more realistic glassy systems.

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