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Simulation of a toy model with constrained dynamics

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Abstract. We study a sliding block model incorporating constraints in an attempt to understand the slower than exponential relaxation observed in glassy systems. Blocks are free to slide along the axes of a regular lattice but cannot interpenetrate. We simulate two-dimensional $L \times L$ lattices with $L = 8$, 16, 32 and 64 and different number of vacancies. Three-dimensional $L \times L \times L$ lattices with $L = 4$, 8, 16 and 32 and one vacancy are also studied. We find the existence of three time regimes for relaxation towards complete disorder, in both two and three dimensions. In the short-time regime the relaxation follows a stretched exponential law; in the intermediate-time regime there is a $\sqrt{t}$ behaviour; and in the long-time regime the relaxation is exponential. In the intermediate- and long-time regimes the results agree well with the theoretical results of Brummelhuis and Hilhorst. The stretched exponential behaviour in the short-time regime is a natural consequence of the constrained dynamics.

1. Introduction

Glassy systems exhibit non-exponential relaxation. In a structural glass most atoms or groups of atoms are sterically hindered by their neighbours and cannot move far unless some of the neighbours move first. This is one form of *constrained dynamics*, in which some degrees of freedom are locked or suppressed unless other degrees of freedom are in particular states. Various idealised models using constrained dynamics produce slow relaxation and some other glassy properties. One class of examples is constrained kinetic Ising models, including the Fredrickson-Andersen [1-3] two-dimensional model, several one-dimensional models [4, 5], and the Cayley tree PSAA [6] model. Other models utilising constrained dynamics explicitly or implicitly are the tiling models of Stillinger and Weber [7] and the Gibbs-DiMarzio model [8]. Another closely related model by Ertel *et al* [9] treats diffusion of particles in a square-lattice gas; strong kinetic constraints exist at high concentration of particles.

We have examined another simple model which incorporates constrained dynamics. It is based on a child's puzzle which consists of labelled blocks sliding within a frame; see figure 1. Constraints exist because most blocks cannot move; motion is only possible if there is a neighbouring vacancy to move into. These particular constraints relate this model to free volume models [10] and also to vacancy diffusion models [11-13]. In free volume models each molecule is restricted to movement within a cell defined by its nearest neighbours and transport occurs only if the free volume is greater than the molecular volume. In vacancy diffusion models relaxation occurs at a site only when a defect has succeeded in diffusing to it.

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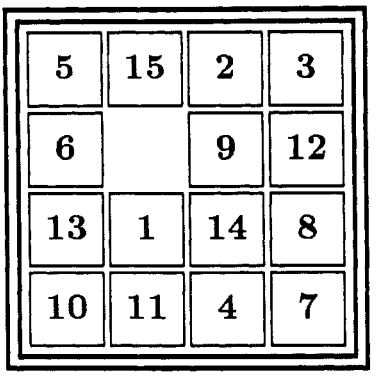

Figure 1. The toy model.

We simulate *random* motion of the blocks in two- and three-dimensional versions of this puzzle with one or more vacancies. The motion is thus that of a constrained random walk. The evolution of the system is followed as it relaxes from an initial configuration to the perfectly jumbled random equilibrium state. We find an approximately stretched exponential relaxation at short times, crossing over to a power law decay and finally to a pure exponential at long times. Brummelhuis and Hilhorst [14] have recently applied random walk theory to the two-dimensional model with one vacancy, and with a low vacancy density [15]. They make predictions for the appropriate decay function in the intermediate- and long-time regimes. Our results agree well with their theory.

In section 2 we describe the model and computational method in more detail. Our results are presented in section 3 with a conclusion in section 4.

2. The model

We consider a square or cubic frame of $N = L^2$ or $N = L^3$ sites. These sites are filled with $N - N_V$ labelled blocks able to slide along the rectangular axes. For convenience, we use periodic boundary conditions instead of rigid walls. A block can move only if it is adjacent to one of the N_V vacancies. The whole system has $N!/N_V!$ possible configurations. For the one-vacancy case though, only half of these configurations are accessible because returning the vacancy to its original position necessarily takes an even number of steps, and hence can only produce an even permutation of the remaining blocks; this applies for any position of the vacancy. Rearranging to a desired permutation can involve a very large number of steps; the path between states in configuration space is very tortuous.

Starting from an initial configuration, at each time step we select a vacancy and a direction independently at random, and move the vacancy in the selected direction unless there is already a vacancy there. This procedure generates a stochastic sequence of moves equivalent to that generated by selecting one block (i.e. non-vacant site) at random, selecting a direction at random, and moving the block if and only if the destination site is vacant. This latter procedure is more physical in that it involves atoms rather than vacancies being thermally excited, with a constant hopping attempt frequency per atom, but would be much slower since most attempts fail.

We monitor the configuration space distance $d(t)$ from the initial configuration to the configuration at time t. We define $d(t)$ as the sum of the individual displacements $d_i(t)$ of the $N - N_V$ blocks using the minimum Manhattan distance around the torus implied by the periodic boundary conditions:

$$d(t) = \sum_i d_i(t)$$

with

$$d_i(t) = |\Delta x_i| + |\Delta y_i| + \ldots$$

where

$$|\Delta x_i| \equiv \min(|x_i - x_{i0}|, |x_i - L + x_{i0}|).$$

Here the ith block has initial position $(x_{i0}, y_{i0}, \ldots)$, and position $(x_i, y_i, \ldots)$ at time t.

In the long-time limit $d(t)$ approaches d_∞ where

$$d_\infty = (N - N_V)LD/4$$

in D dimensions, since the average displacement of a block from its starting point tends to $L/4$ in each dimension. The approach to equilibrium is described by the relaxation function $q(t)$ defined by

$$q(t) = \frac{d_\infty - d(t)}{d_\infty}$$

which goes from 1 at $t = 0$ to 0 as $t \to \infty$. Our goal was to measure the average relaxation function $\langle q(t) \rangle$ for various values of the parameters D, L and N_V. For each case considered we performed at least 100 independent runs from random initial positions and averaged the resulting values of $q(t)$ at each time step.

Theoretically [14] we expect three distinct time regimes in the relaxation:

short:	$t \leqslant L^d \ln L$
intermediate:	$L^D \ln L \leqslant t \leqslant L^{D+2}$
long:	$t \geqslant L^{D+2}$.

In the short-time regime the constraints are crucial; there are strong correlations between steps, and vacancies still remember their initial positions. In the intermediate-time regime the vacancies have randomised (i.e. each has visited everywhere on average) and so the blocks move in uncorrelated random walks. In the long-time regime the blocks themselves have been everywhere and approach the perfectly randomised equilibrium state.

3. Results

Figure 2 shows typical results for $q(t)$ on linear-log axes for the $D = 2$ case with one vacancy and $L = 8$, 16, 32 and 64. The time axis is in units of a single jump attempt (selection of a vacancy and a direction), *not* normalised by any L-dependent factor. On these axes a pure exponential function $\exp(-t/\tau)$ has a fixed sigmoidal shape as exemplified by the broken curve; changing τ merely shifts the curve horizontally. The observed relaxation functions are clearly non-exponential, particularly at short times. In the long-time regime, when $q(t)$ has become small, an exponential *is* a good fit, with τ scaling as L^{D+2}, or as L^4 for the $D = 2$ results shown.

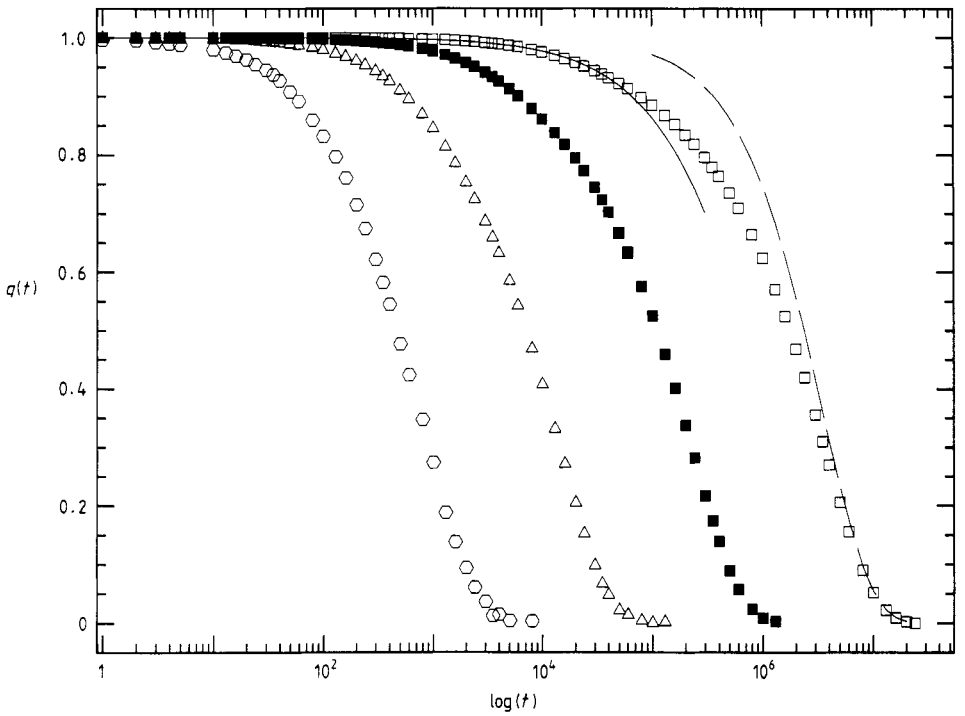

Figure 2. Plot of $q(t)$ against $\log t$ for the two-dimensional model. The full curve is a fit of a stretched-exponential function, and the broken curve is a simple exponential function. The fitting parameters are given in table 1. The error bars for the points are smaller than the point size used in this and other figures. □, 64×64; ■, 32×32; △, 16×16; ○, 8×8.

In the short-time regime, where $q(t)$ is close to 1, a stretched exponential function $q(t)=\exp(-(t/\tau_{se})^{\beta})$ provides a good fit to the data. The fit is much better than that obtainable with an enhanced power law ($A\exp[-B(\log(t/\tau))^{\alpha}]$). The stretched exponential fit is exemplified by the full curve in figure 2. Figure 3 shows this more clearly on log–log against log axes, chosen to produce a straight line for a true stretched exponential. Results are shown for the largest two-dimensional one-vacancy case ($L=64$) from figure 1, for a three-dimensional $L=32$ case with one vacancy, and for a two-dimensional case with many vacancies. For few vacancies, the fit is good for almost four decades in time. As the vacancies increase in number, implying a smaller degree of constraint (i.e. paths in configuration space are much less tortuous) the fit is good for only around two decades in time. Table 1 gives the values of the various parameters for the straight line fits of the figures. The value of the exponent β is not closely related to that expected for a physical system like a glass, since this model is so simplistic.

In the intermediate-time regime, a power law function $q(t)=1-kt^{n}$ yields points lying on a straight line for two decades of time. Figure 4 shows this on log axes, with the time axis normalised by L^{D+2}. The near coincidence of the lines shows that $k\sim L^{-(D/2)-1}$ for the two- and three-dimensional versions of the model. As indicated by the theory [14, 16] this is the regime where the atoms perform an uncorrelated walk, and we do not expect a stretched exponential decay. The results are in accord with the theory of Brummelhuis and Hilhorst [14, 15, 17] who predict a power law with

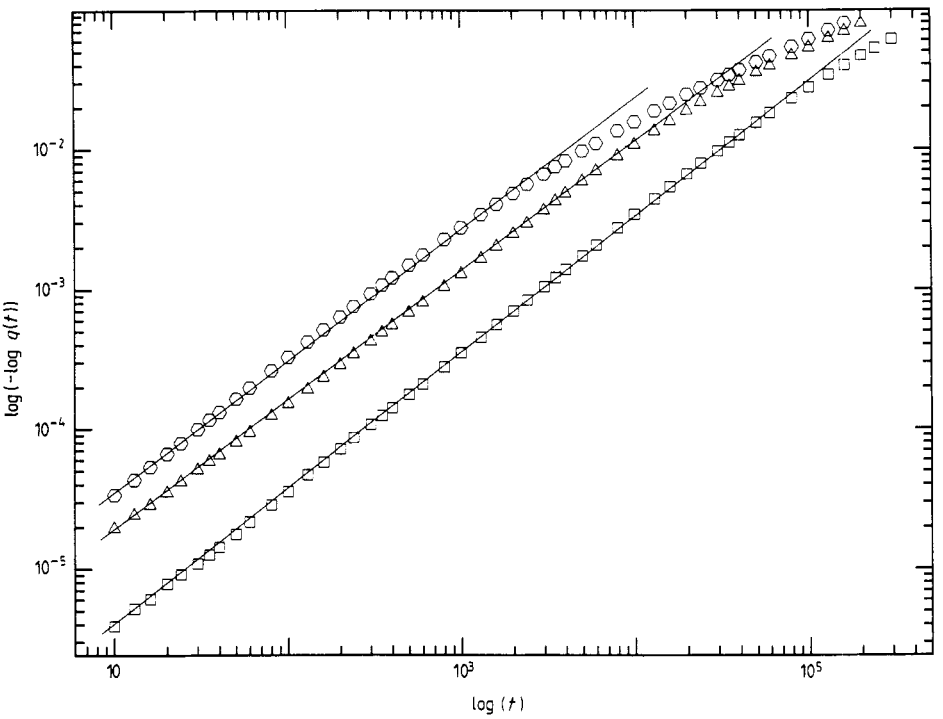

Figure 3. Plot of $\log(-\log q(t))$ against $\log(t)$ for three examples in the short-time regime. The straight-line fits are stretched exponential functions. □, $32\times32\times32$, one vacancy; △, 64×64, one vacancy; ○, 64×64, 1000 vacancies.

Table 1. Table showing a representative sample of the results obtained.

			Short		Intermediate		Long
Dimension	Size	Vacancies	β	$\tau_{se}\times10^{-6}$	n	$k\times10^{-4}$	$\tau_{exp}\times10^{6}$
2	64	1	0.73 ± 0.01	2.51 ± 0.2	0.51 ± 0.01	3.7 ± 0.1	8.06 ± 0.02
2	64	1000	0.78 ± 0.01	5.01 ± 0.2	0.52 ± 0.01	3.4 ± 0.1	6.77 ± 0.02
3	32	1	0.76 ± 0.01	0.39 ± 0.02	0.51 ± 0.01	5.7 ± 0.1	18.2 ± 0.2

$n=0.5$. There is a simple relationship between our $q(t)$ and their $\langle|y_1|+|y_2|+\ldots\rangle$:

$$\left\langle\sum_{i=1}^{D}|y_i|^2\right\rangle=[(L/D)(1-q(t))]^2$$

for D dimensions. Brummelhuis and Hilhorst predict the following relation for the intermediate-time regime:

$$\left\langle\sum_{i=1}^{D}|y_i|^2\right\rangle=\alpha_D(t/L^D)$$

for two and three dimensions with $\alpha_2=0.5945\ldots$ and $\alpha_3=1.2473\ldots$. In our simulations we find $\alpha_2=0.57\pm0.01$ and $\alpha_3=1.21\pm0.01$ with $n=0.5$ in both the cases, showing that our results are compatible with the theory. Note that the table gives results in

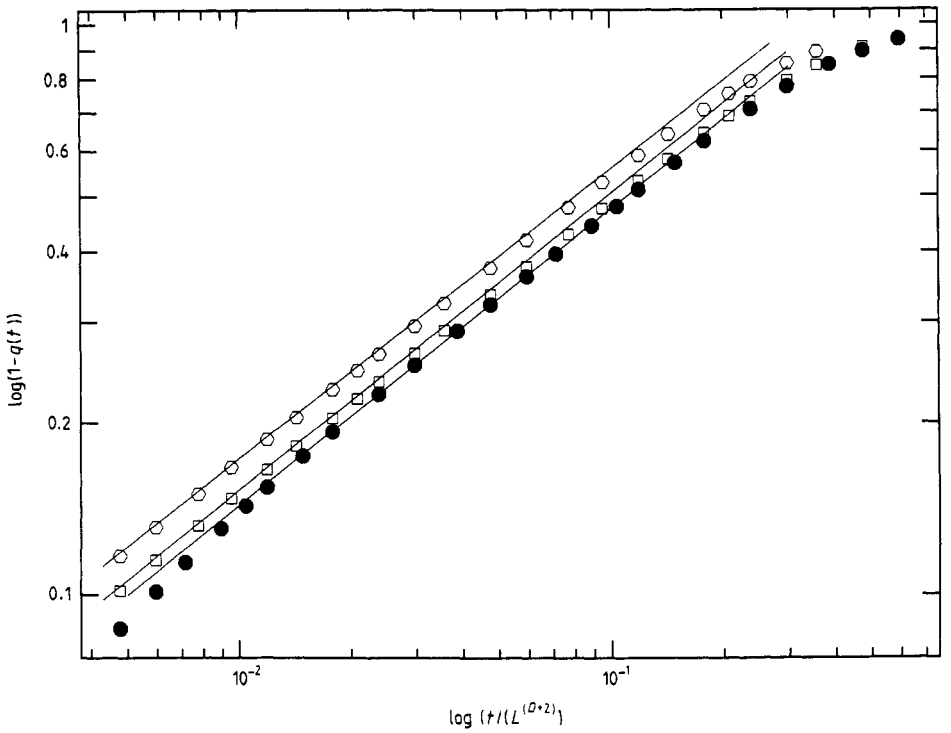

Figure 4. Plot of $\log(1-q(t))$ against $\log(t/L^{D+2})$ in the intermediate-time regime. The straight-line fits are of the form $q(t)=1-kt^n$ with $n=0.5$. ●, $32\times32\times32$, one vacancy; □, 64×64, one vacancy; ○, 64×64, 1000 vacancies.

terms of the equation $q(t)=1-kt^n$ rather than the Brummelhuis and Hilhorst equation. For $N_V \ll N$, we find that α_D scales with the number of vacancies, as predicted by Brummelhuis and Hilhorst. However, this breaks down before the 1000 vacancy case shown for which $N_V/N=0.24$. The exponent does not depend appreciably on the number of vacancies or the dimension.

For the long-time regime the decay is pure exponential with $q(t)\sim\exp(-t/\tau_{exp})$, as is seen in the broken curve in figure 2. Values of τ_{exp} are given in the table. The exponential behaviour is seen for any N_V/N.

4. Conclusion

We have studied a simple toy model of sliding blocks to examine the consequences of constraints on the relaxation. We obtain good agreement with the results of Brummelhuis and Hilhorst in the intermediate- and long-time regimes where their analytical results are applicable. We also see that going from two to three dimensions does not change the qualitative behaviour of our results for the whole relaxation regime.

In the short-time regime, where our model is highly constrained, we obtain stretched exponential relaxation. The constraints give rise to a correlated walk for any particular atom. The walk is correlated, in two dimensions, up to times of the order of $L^2 \ln L$; the direction from which a vacancy next returns to a site is correlated with that from which it last left. For longer times the directional correlation is lost. The correlated

walk, a consequence of the constraints, gives rise to a relaxation function for which a stretched exponential is a good fit. This indicates, as do other models mentioned in the introduction that strong constraints which imply a correlated motion [18, 19] for the atoms lead to approximately stretched exponential relaxation in glassy systems. In three dimensions, we expect that the atoms should exhibit a correlated motion for times of the order of $L^3 \ln L$, and again a stretched exponential is observed in this time regime. As the vacancies increase in number the stretched exponential behaviour is a good fit only in a smaller and smaller region of $\log t$, extablishing further the relationship between constraints and the stretched exponential relaxation.

Acknowledgments

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