Anomalous relaxation in regular and fractal lattices

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Relaxation phenomena on disordered structures are studied by using a random walk model. The model is able to describe essential features of the relaxation process in terms of a one-body picture with geometrical restrictions on the particles' motion. Two cases are considered: relaxation on regular lattices with disordered variables taken from a power-law distribution (these variables have different updating rules), and on a fractal lattice which is a percolation cluster near criticality. Quantities such as the relaxation function, particle density, and complex susceptibility are evaluated. Different types of relaxation mechanisms are found as a function of frequency for regular and fractal lattices. Also for a regular lattice, we see an interesting dependence of the relaxation quantities as a function of a disorder parameter which describes the decay of the power-law distribution from which variables are drawn. The model is able to reproduce the relaxation behavior commonly observed in experiments and typically fitted to empirical laws. [S1063-651X(97)08202-0]

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I. INTRODUCTION

Relaxation phenomena occurring in many physical systems such as supercooled liquids, viscoelastic solids, and dielectric and magnetic relaxation in spin glasses and porous media [1–5] cannot be described by the classical exponential form in the time domain or a Debye function in the frequency domain. They are usually expressed in terms of more complicated mathematical forms such as stretched exponentials, power laws, Cole-Cole forms, etc. [6–10]. Even though these systems are relatively well known, the microscopic mechanisms for the occurrence of relaxation on them is not well established. These relaxation processes are called anomalous.

In general, relaxation processes are a consequence of many-body effects within a single system and interactions with its surroundings. However, some of their features can be described in terms of a one-body picture by applying geometrical restrictions to the motion of the particles relaxing in that medium, i.e., the motion of a particle affected by many-body effects is approximated by its motion in a restricted geometry [11–13]. Here we explore the ''limits'' of this approach by using a simple model based on the transport of random particles on a disordered structure. The effect of disorder is to trap temporarily the diffusing particles, thus representing the geometrical restriction to their motion. This same approach has been used in the literature to study relaxation phenomena in other systems [11–13].

We present a simple model to explain anomalous relaxation in disordered structures. The model is based on the properties of random walkers diffusing on a lattice, and is able to describe essential features of the relaxation process. Two types of disordered structures are considered, one with ''potential'' disorder, in which a regular lattice with a random variable attached to each site is used. The random variable ''behaves'' like a temporary trap for the motion of the random walker, and it may have the same value for the entire process as its value was frozen on the site (quenched case) or change its value with time as the transport process goes on (annealed case). These variables are drawn from a power-law distribution of the form $|\mu|\xi^{\mu-1}$. The second type of structure is a fractal structure, a percolation cluster at criticality.

Quantities related to the relaxation process such as the relaxation function, particle density, and complex susceptibility are calculated. For the case of regular lattices, an interesting behavior is observed as a function of the disorder parameter μ. Also, for the two types of structures, we find in the frequency domain two different relaxation mechanisms which are also seen in experiments. These are observed as a stretched exponential form of the relaxation function in the time domain, and the Cole-Cole form of the imaginary part of the complex susceptibility in the frequency domain. Thus this simple model is able to reproduce basic features of the relaxation process and allows one to quantify the effect of different types of disorder on such response functions. For the microscopic mechanisms of anomalous relaxation we are able to identify conditions for the occurrence of different types of relaxations.

II. MODEL AND SIMULATIONS

A particle released on a disordered structure cannot move freely since spatial irregularities of the structure will set restrictions on its motion. Frequently, the particle gets trapped temporarily in poorly connected regions, thus its diffusion is effectively reduced. In this section we present a simple model to simulate the relaxation of a localized ''signal'' on a disordered structure. Here the ''signal'' is represented by a bunch of particles initially localized at a given site of a lattice, and then allowed to diffuse on the structure. Two different disordered structures are considered. One is a regular lattice with random variables (which mimic disorder) attached to each site. This way of introducing disorder is called ''potential disorder.'' The second case is a fractal lattice, a

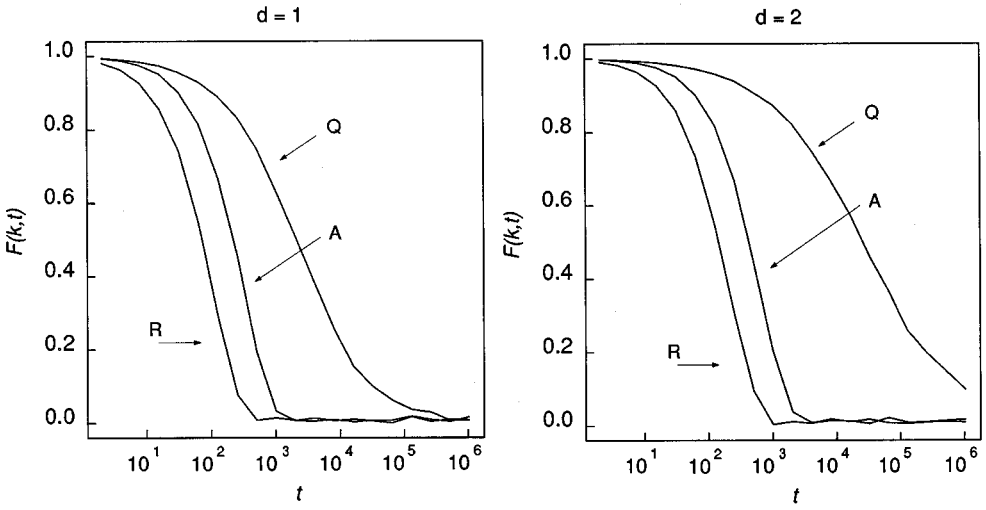

FIG. 1. Relaxation function $F(k,t)$ for regular lattices in $d=1,2$ with quenched (Q) and annealed disorder (A) for $\mu=0.5$. Also shown is $F(k,t)$ for a lattice without disorder (R). All curves are for $k=11\pi/250$.

percolation cluster near criticality. Disorder in this case is structural.

A. Potential disorder

We consider regular lattices in $d=1$ and 2. The first step is to assign a random variable to each lattice site. This variable is taken from a distribution with a power-law form $|\mu|\xi^{\mu-1}$, with $0\leqslant\mu\leqslant1$. Each variable is in the range between $0\leqslant\xi\leqslant1$. The parameter μ is called here the disorder exponent. Starting at a given site on the lattice, normally the origin, a walker is released. A random number is drawn from a uniform distribution and compared with the value of the disorder variable attached to its site. If this number is smaller, the particle can move to any of its neighbors with the same probability. Since the disorder variables are relatively small, most of the time the particles will not move. Thus the particle is temporarily trapped at its lattice site. This distribution and the motion rules for the particles induce a divergent waiting time distribution.

We consider two cases according to the updating rules of the disordered variables, one in which the variables are frozen on the lattice while the particles move around, called the ''quenched case,'' and the other is one where the variables are updated each time the particles attempt to move (annealed).

A sampling over many disorder configurations is done, typically for 10^4 realizations. The simulation is run for times up to 2^{20} units, in systems with sizes big enough to avoid situations where the particles reach the boundaries. For all cases we measure the position of the particles as a function of time.

B. Structural disorder

A percolating cluster near criticality is generated on a square lattice of dimensions 400×400. A random site on this structure is chosen and a walker is released from it. At each unit of time the particle attempts to move to any of its neighbors with equal probability. The motion occurs only if the selected neighbor site belongs to the cluster. The process is repeated for times up to 2^{20} and averages are taken over 20 different cluster realizations. For any realization of the percolation cluster, samples of about 10^4 particles were considered.

For the two types of disorder, a record of the particle's position $\vec{r}(t)$ is kept as a function of time t.

With the data obtained from the simulations we calculate several quantities related to the relaxation process as follows.

(1) Relaxation function $F(k,t)$, which is the characteristic function of the random variable $\vec{r}(t)-\vec{r}(0)$, i.e.,

$$F(k,t)=\langle e^{i\vec{k}\cdot[\vec{r}(t)-\vec{r}(0)]}\rangle,$$

where k is the wave vector number chosen as $\vec{k}=(1,1)$ for the two-dimensional (2D) lattice, and the angular brackets denote sample averaging.

(2) Non-Gaussian parameter (NGP) X_{NGP}, which is a convenient parameter that describes how the distribution deviates from a Gaussian. In d dimensions it is defined by

$$X_{\mathrm{NGP}}\equiv\frac{\langle[\vec{r}(t)-\vec{r}(0)]^4\rangle}{[(d+2/2)]\{\langle[\vec{r}(t)-\vec{r}(0)]^2\rangle\}^2}-1.$$

(3) Complex susceptibility

$$\chi(k,\omega)=1+i\omega\int_0^\infty e^{i\omega t}F(k,t)dt.$$

The results are compared with the corresponding quantities associated to the same process on a nondisordered structure.

III. RELAXATION RESULTS. REGULAR AND FRACTAL LATTICES

Figure 1 shows a plot of the relaxation function $F(k,t)$ for different wave number values and lattices in $d=1$ and 2. For comparison, the curve for the case without disorder is also shown. All curves are for fixed $k=11\pi/250$. It is clear that the decay is faster on the nondisordered lattice.

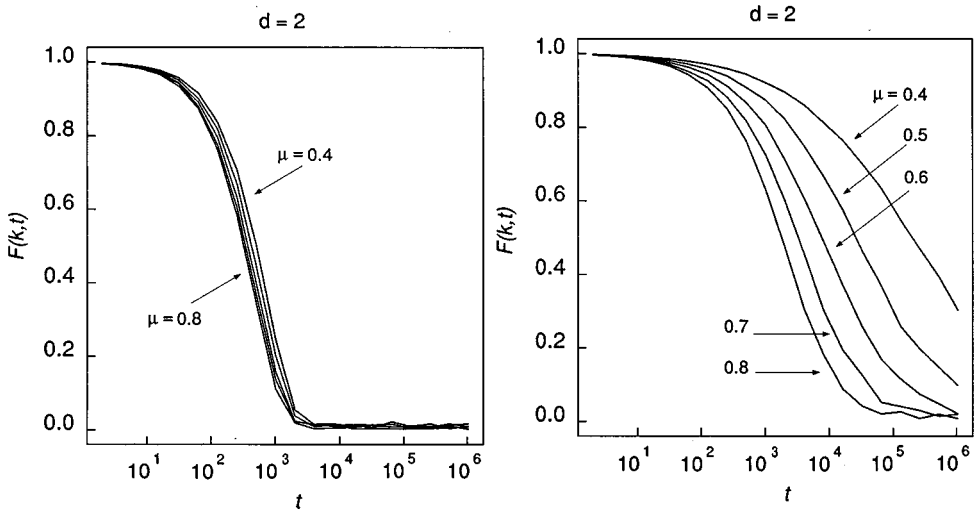

FIG. 2. Relaxation function $F(k,t)$ for regular lattices with annealed and quenched disorder in $d=2$. Curves are for different values of disorder exponent μ as indicated in figure. On the left is shown the plot for the annealed variables; the corresponding curve for quenched variables is shown on the right. All curves are for $k=11\pi/250$.

We study the effect of disorder on the relaxation function by varying the value of parameter μ. In Fig. 2 we plot the decay of $F(k,t)$ for several μ values and the same wave number value k. For the quenched case, the relaxation is slower for small values of this parameter. As μ increases, disorder is weaker, making the relaxation faster. For the ''annealed'' case, in which the disorder variables are updated each time the particles attempt to move, there is almost no sensitivity to the μ value. The decay is faster for the annealed case for any k value and disorder strength.

The relaxation data for a fixed μ value and several wave number values (the $\vec{k}$ direction is not changed) are shown in Fig. 3 where it is observed that the relaxation is faster for larger k. The same qualitative behavior is observed for lattices in one and two dimensions. Thus we find the following tendencies for the two types of disorder variables in regular lattices: faster decay for fixed μ when increasing the wave number value k, faster decay for fixed k when increasing the value of μ, and qualitatively the same behavior for lattices in one and two dimensions.

We have also calculated the relaxation time τ, and found a power-law relation between this quantity and the wave number value, i.e., $\tau\sim k^{-\gamma}$. For the quenched case, exponent γ is a function of parameter μ. When μ decreases, γ increases. For the annealed case $\gamma=2$ for any μ value regardless of the value of spatial dimensionality. This is similar to the case without disorder. Table I summarizes the values of these exponents for lattices in one and two dimensions.

The mean square displacement behaves asymptotically as $\langle r^2(t)\rangle\sim t^{\theta}$, with θ a disorder dependent exponent for the quenched case, whereas for the annealed variables we get essentially the same results as for the nondisordered structure. The value of θ decreases as μ decreases. This dependence of θ with the disorder parameter μ has been reported previously [14]. For the annealed case $\theta=1$ as in regular diffusion (only a renormalized diffusion constant). The data

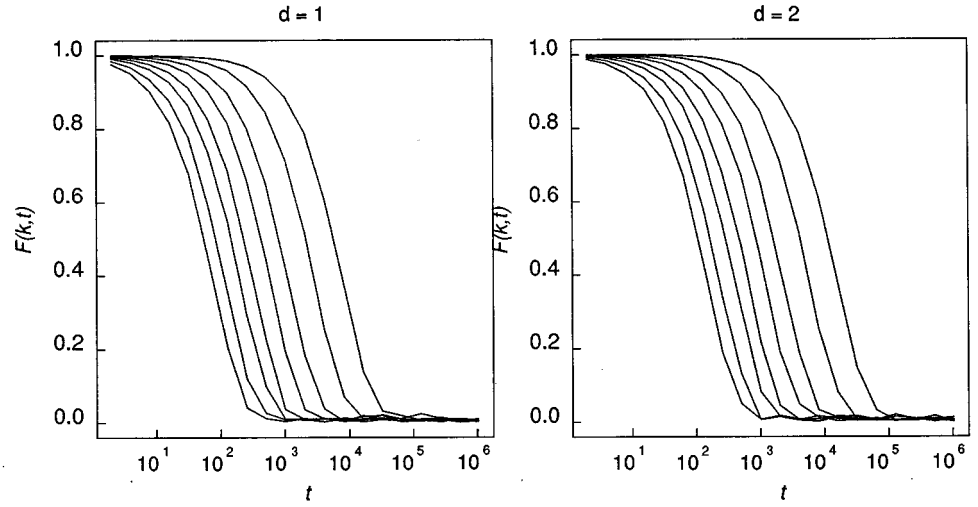

FIG. 3. Typical behavior of $F(k,t)$ for lattices in $d=1$ and 2 with quenched disorder for $\mu=0.2$. Different curves are for various wave number values $k=n\pi/250$. From right to left $n=1,3,5,8,11,19,25,33$.

TABLE I. Relaxation exponents γ for regular lattices in $d=1$ and 2. Subindex in γ exponent refers to type of disorder variable: Q (quenched), A (annealed).

μ	$d=1$		$d=2$	
	γ_Q	γ_A	γ_Q	γ_A
0.4	3.45±0.02	2.00±0.02	4.96±0.02	2.00±0.02
0.5	2.97±0.02	2.00±0.02	3.97±0.02	2.00±0.02
0.6	2.69±0.02	2.00±0.02	3.34±0.02	2.00±0.02
0.7	2.44±0.02	2.00±0.02	2.84±0.02	2.00±0.02
0.8	2.28±0.02	2.00±0.02	2.51±0.02	2.00±0.02

TABLE II. Exponent θ associated to scaling of mean square displacement, i.e., $\langle r^2(t)\rangle \sim t^\theta$, for regular lattices with quenched (θ_Q) and annealed (θ_A) disorder variables in $d=1$ and 2.

μ	$d=1$		$d=2$	
	θ_Q	θ_A	θ_Q	θ_A
0.2	0.34±0.02	1.00±0.01	0.21±0.02	1.00±0.01
0.4	0.58±0.02	1.00±0.01	0.41±0.02	1.00±0.01
0.6	0.75±0.02	1.00±0.01	0.61±0.02	1.00±0.01
0.8	0.89±0.02	1.00±0.01	0.80±0.02	1.00±0.01

for various disorder values appear in Table II. It is interesting to note that the product of the exponents $\theta(\gamma/2)=1$. This result (justifiable by straightforward dimensional analysis) seems to be valid for lattices in $d=1$ and 2, and for any type of disorder, and does not depend on the disorder parameter μ. For quenched disorder we were able to fit the numerical data to empirical relations $\gamma=(1+\mu)/\mu$ for $d=1$ and $\gamma=2/\mu$ for $d=2$ with an error less than 3% and 5% for $d=1$ and 2, respectively.

The probability density shows deviations from the Gaussian form as described by the values of NGP for the quenched case. For a nondisordered lattice the probability density is a Gaussian, hence the NGP is zero. On the other hand, when the strength of disorder increases (by reducing the μ value) the NGP increases monotonically, shifting its value from zero. This behavior is almost independent of time. For the annealed case the distribution is Gaussian and the NGP is zero after a short transient period. Figure 4 shows the time evolution of the NGP for lattices in $d=2$ with quenched disorder, and for annealed variables data are shown in Fig. 5.

Regarding the complex susceptibility, we have computed its imaginary part for the two types of disorder variables. As a function of frequency we find curves $\chi''(k,\omega)$ which are increasing monotonically up to a maximum at a particular frequency $\omega_{\max}$; beyond that value, the curves decrease monotonically. The data are slightly scattered due to the approximations carried out to evaluate the integral in the definition of χ. Around the maximum, the curves have the Cole-Cole form $(\chi(\omega)=[1+(-i\omega/\omega_{\max})^\alpha]^{-1}, 0\leqslant\alpha\leqslant 1)$ and for small and high frequencies linear regimes are observed in a log-log plot (see Fig. 6). The slopes of the lines are different, suggesting different relaxation mechanisms as a function of frequency. This linear behavior is associated to stretched exponential relaxation since the slopes of the lines are smaller than one.

For the transport on the substrate with structural disorder, we observed a similar decay of the relaxation function as a function of the wave number value. The relaxation time τ also shows a power-law dependence with k, $\tau\sim k^{-\gamma}$ with $\gamma=3.06\pm0.09$. The mean square displacement also scales with time as $\langle r^2(t)\rangle\sim t^\theta$, with $\theta=0.72\pm0.02$. Again, the product of the exponents $\theta(\gamma/2)=1.10\pm0.06$.

The NGP also deviates from its value for a Gaussian distribution. This parameter increases from zero for short times and remains almost constant up to $t_c\approx 10^5$; beyond this time we started to notice finite size effects.

The imaginary part of the complex susceptibility has qualitatively a similar form to the one observed for regular lattices (see Fig. 6). Around the maximum, $\chi''(k,\omega)$ has the Cole-Cole form whereas for low and high frequencies a similar linear regime with different slopes is observed. These two linear regimes are associated to stretched exponential relaxation.

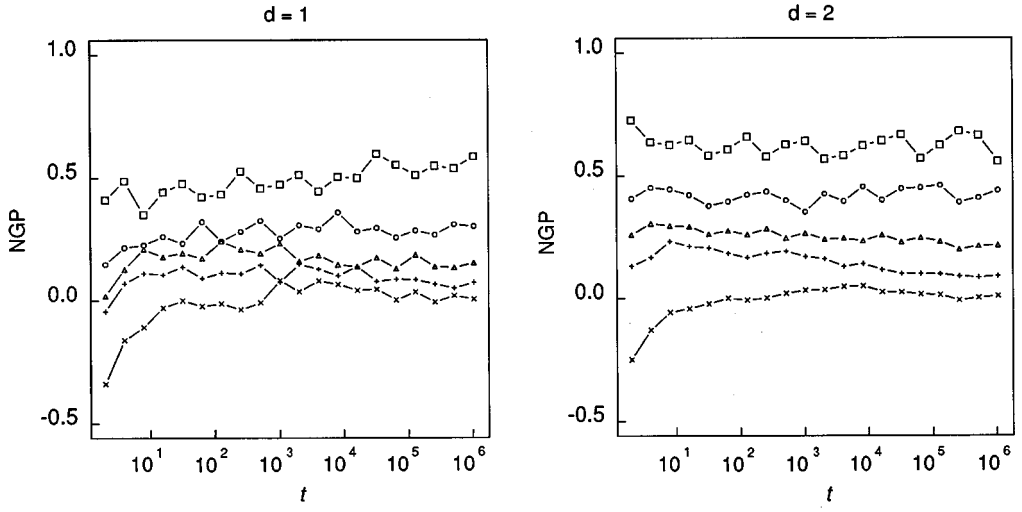

FIG. 4. Non-Gaussian parameter (NGP) for lattices in $d=1$ and 2 with quenched disorder for $\mu=0.4$ (□); 0.6 (○); 0.8 (△); 1.0 (+). The curve with (×) is for a nondisordered lattice.

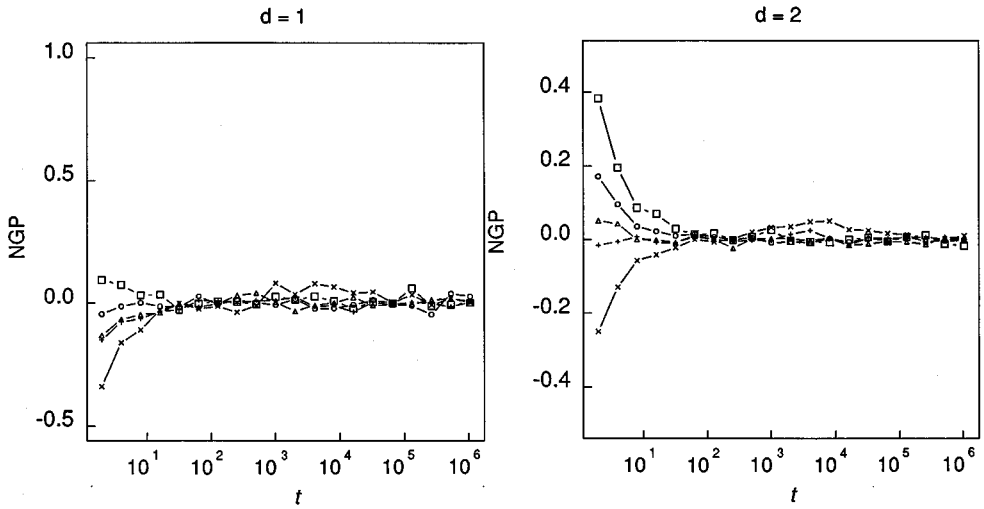

FIG. 5. Non-Gaussian parameter (NGP) for lattices in $d=1$ and 2 with annealed disorder variables for $\mu=0.4$ (□); 0.6 (○); 0.8 (△); 1.0 (+). The curve with (×) is for a regular lattice without disorder.

IV. DISCUSSION AND CONCLUSIONS

We have found that anomalous relaxation could be modeled by diffusive effects in a restricted geometry. Thus a one-body picture is able to reproduce features observed in experiments and previously fitted to empirical laws. Anomalous behavior is observed in regular disordered lattices and fractal lattices. Even though our simulations were done for lattices in one and two dimensions, similar results are expected for higher dimensions since it is known that the critical dimension for the anomalous diffusion on those systems is $d_c=2$ [14]. We can summarize the main results as follows.

(1) The relaxation function in the time domain for a fixed wave vector magnitude depends strongly on the value of the disorder parameter μ for quenched variables, whereas for the annealed case the results are clearly described by the current relaxation theory.

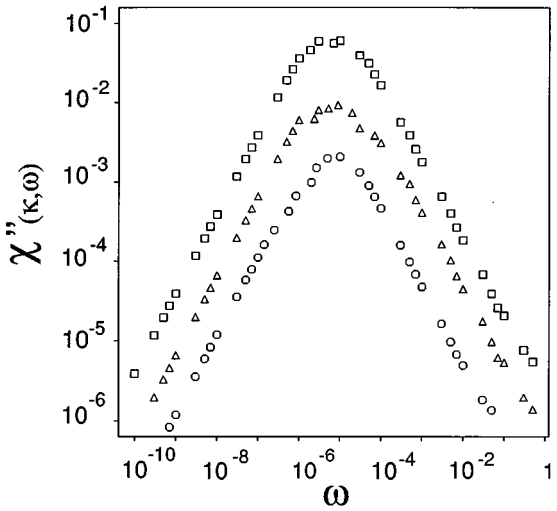

FIG. 6. Imaginary part of complex susceptibility $\chi''(k,\omega)$ as a function of frequency for two-dimensional lattices with quenched disorder, $\mu=0.8$, $k=3\pi/250$ (□); annealed disorder, $\mu=0.5$, $k=3\pi/250$ (○), and percolation cluster at criticality for $k=3\pi/125$ (△).

(2) Power-law dependence of the relaxation time with the wave number value $\tau\sim k^{-\gamma}$. Exponent γ depends on the strength of disorder for quenched variables on regular lattices whereas for the annealed case γ remains fixed to 2. Without disorder, this relation is given by $\tau\sim k^{-2}$, also a power law but with a fixed exponent. We have quantified the relation between exponents γ and μ and found that for $d=1$, $\gamma=(1+\mu)/\mu$ and for $d=2$, $\gamma=2/\mu$ [15].

(3) Universal values of product of exponents $\theta(\gamma/2)=1$ [θ describes the scaling in time of the mean square displacement $\langle r^2(t)\rangle\sim t^{\theta}$]. This relation holds for potential and structural disorder, and is independent of spatial dimensionality. For systems without disorder, this relation is obtained by straightforward dimensional analysis using the expressions $P(r,t)=[1/(2\pi)^d]\int F(k,t)e^{-i\vec{k}\cdot\vec{r}}d\vec{k}$ (d stands for spatial dimension) and $\langle r^2(t)\rangle=\int r^2P(r,t)d\vec{r}$. Here, it is shown that the relation also holds for relaxation on disordered structures. Our findings are also consistent with numerical data previously reported in Ref. [11] for relaxation on fractal structures; in this sense, they reconfirm the theory.

(4) Non-Gaussian behavior of the probability density $P(r,t)$ demonstrated by using a parameter that measures deviations of this function from a Gaussian. For regular lattices with annealed variables the distribution was found to be asymptotically Gaussian.

(5) With respect to the imaginary part of the complex susceptibility we observed different relaxation mechanisms in the frequency domain: A stretched exponential relaxation for low and high frequencies, whereas for the intermediate range we observe in all cases a Cole-Cole form, associated with a symmetric maximum for a given frequency $\omega_{\max}$, which depends on the dimensionality and type of disorder.

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[1] W. Götze, in *Liquids, Freezing and Glass Transition*, edited by J.P. Hansen, D. Levesque, and J. Zinn-Justin (North-Holland, Amsterdam, 1991).
[2] J.-P. Hansen, Phys. World **4**, 32 (1991).
[3] K. Binder and A.P. Young, Rev. Mod. Phys. **58**, 801 (1986).
[4] K.H. Fisher and J.A. Hertz, *Spin Glasses* (Cambridge University Press, Cambridge, England, 1991).
[5] W.P. Halperin, F. D'Orazio, S. Bhattacharja, and J.C. Tarczon, in *Molecular Dynamics in Restricted Geometries*, edited by J. Klafter and J.M. Drake (Wiley InterScience, New York, 1989).
[6] H. Scher, M. Shlesinger, and J.T. Bendler, Phys. Today **44**, 26 (1991).
[7] K.S. Cole and R.H. Cole, J. Chem. Phys. **9**, 639 (1941).
[8] G. Williams and D.C. Watts, Trans. Faraday Soc. **66**, 80 (1970).
[9] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
[10] P. Debye, *Polar Molecules* (Chemical Catalog Company, New York, 1929).
[11] S. Fujiwara and F. Yonezawa, Phys. Rev. Lett. **74**, 4229 (1995).
[12] S. Fujiwara and F. Yonezawa, Phys. Rev. E **51**, 2277 (1995).
[13] S. Gomi and F. Yonezawa, Phys. Rev. Lett. **74**, 4125 (1995).
[14] S. Havlin and D. Ben-Avraham, Adv. Phys. **36**, 695 (1987).
[15] Based on the definition of the relaxation function, it is easily shown that $F(k,t)$ depends on k and t only through the product $t^{\theta/2}k$ (θ being the exponent which describes the scaling of the mean square displacement), and that it shows scaling for various k which allows one to write its argument in terms of a single scaled variable t/τ.