Einstein relation and effective temperature for systems with quenched disorder

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(Received 24 March 2009; revised manuscript received 15 July 2009; published 9 September 2009)

According to the Einstein relation the ratio between independent measurements of fluctuations (e.g., diffusivity) and the response to a weak external field (e.g., mobility) is equal to the thermal temperature when the system is kept close to thermal equilibrium. For strongly disordered systems, which are not self-averaging this ratio is a random variable and hence in this sense the Einstein relation is not valid. Thus effective temperatures found using the fluctuation dissipation ratio are at least in some cases stochastic variables. This scenario is tested with the quenched trap model. An average over an ensemble of systems yields an averaged effective temperature, which is compared with results obtained from the mean-field continuous-time random-walk model.

DOI: 10.1103/PhysRevE.80.031108 PACS number(s): 05.40.−a, 02.50.Ey, 05.20.−y

I. INTRODUCTION

The Einstein relation teaches us that a measurement of the diffusion coefficient D of Brownian particles gives the response of these particles to a weak external field according to $D=\mu k_B T$, where μ is the mobility and T is the temperature. This profound relation is generalized by the fluctuation-dissipation theorem [1] which relates fluctuations of systems in thermal equilibrium to their response to weak external fields. More recently fluctuation dissipation ratios where used to characterize dynamics of systems far from equilibrium, for example, glassy systems and turbulence [2–10]. For usual Brownian motion, and for a system close to thermal equilibrium we may think of temperature as a ratio between fluctuation (D) and dissipation ($[1/\mu]$) $D/\mu=k_B T$. Even for a system far from equilibrium we can measure fluctuations and the response to external field and the ratio might be used as an effective temperature, T_{eff}. Such a concept of temperature does not generally have the same thermal meaning of ordinary temperature, and it can depend, for example, on the aging time [2,3], still it is a useful concept since it can be used to quantify fluctuation-dissipation relation in complex systems where standard meaning of thermal temperature is not valid.

We show that non-self-averaging can lead to fluctuations in the effective temperature and that the effective temperature depends sensitively on the initial conditions. In fact the usual Einstein relation itself is not valid in the following sense. In systems which are weakly disordered and self-averaging if we have two systems which are statistically identical the measurement of diffusivity in sample A gives a prediction of the mobility in sample B according to the Einstein relation. However, we argue below rather generally and in detail with regard to the quenched trap (QT) model that for systems which exhibit subdiffusion due to quenched disorder the Einstein relation does not hold in this sense. It does hold as we discuss below only after averaging over many systems however such an average does not necessarily exist in real measurements.

Previously Fielding and Sollich [4,5] investigated the fluctuation-dissipation ratio for the glassy phase of the annealed trap model, showing that the correlation function and response function of an arbitrary observable yield an effective temperature which depends on the observable (thus the effective temperature is specific to an observable and not general). They have used the annealed version of the trap model which has temporal fluctuations but does not have in it spatial disorder neither quenched disorder. Here we investigate the QT model which exhibits anomalous subdiffusion, and unlike the previous model [4,5] we consider a system with spatial quenched disorder which gives rise to the problem of self-averaging [11] (the same problem does not exist in annealed models). Usually, T_{eff} depends both on the experiment time t and the aging time [2–6] however here we do not consider aging effects at all since violations of Einstein relation are found already in the nonaging case.

II. QUENCHED TRAP MODEL

We consider an infinite one dimensional lattice whose spacing, a, is equal 1. The potential energy, E_x, of the x site is random and distributed identically and independently by the rule $\rho(E)=(1/T_g)e^{-E/T_g}$ [12,13], however, once the potential energy at some site x is raffled it stays constant in time (quenched disorder). The lattice is coupled to a heat bath with temperature T. This coupling has two results: the first a particle which is placed on the lattice undergoes a random walk between nearest neighbors. Specifically, with probability q $(1-q)$ the particle jumps to the right (left) and for the unbiased case with no external force $q=\frac{1}{2}$. Second the average time, τ_x, that the particle waits in any site x, is given by Arrhenius law $\tau_x=\exp[E_x/T]$. Notice that a small change in E_x leads to exponential change in τ_x. $\psi(\tau)$, the probability density function (PDF) of the waiting times can be easily calculated

$$\psi(\tau)=\alpha\tau^{-(1+\alpha)}, \tag{1}$$

where $\alpha=T/T_g$ and $\tau\geq 1$. Notice that for $\alpha<1$ $(T<T_g)$, all the moments of τ diverge, this leads to anomalous diffusion [12,14], aging [15], and nontrivial occupation times [16]. A constant weak external force applied to the system shifts q from $\frac{1}{2}$ to $\frac{1+h}{2}$, where $h=F/2k_B T$ [12].

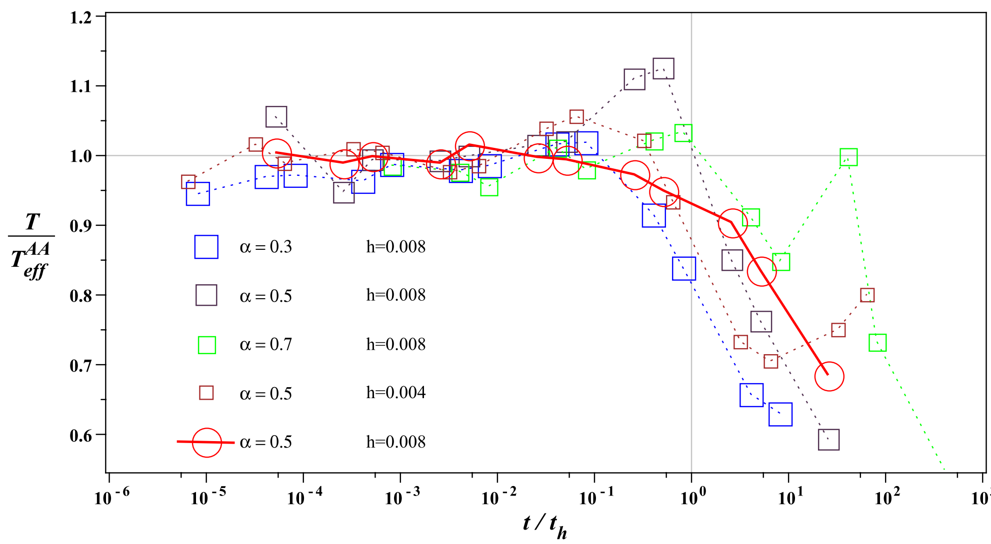

FIG. 1. (Color online) Simulation results of T/T_{eff}^{AA} versus $\log[t/t_h]$ in the glassy phase $T<T_g$. For various α and h we see $T_{eff}^{AA}\simeq T$ in the time regime of $t\ll t_h$ and without any averaging over the disorder. For longer times T_{eff}^{AA} is random as expected in this nonlinear-response regime. The averaged over disorder curve (solid line) is in agreement with Ref. [15]. The figure illustrates that $T_{eff}^{AA}\simeq T$ for $t<t_h$.

III. NON SELF AVERAGING FOR EINSTEIN RELATION

For particles exhibiting anomalous diffusion, transport properties such as D and μ are time dependent. Hence we investigate $\overline{x(t)}$ and $\overline{x^2(t)}$, the thermal mean and mean-square displacement of particles interacting with a thermal bath. The overline is a thermal average $\overline{\cdots}$ with fixed initial conditions and brackets $\langle\cdots\rangle$ are ensemble averages over the disorder. For unbiased diffusion $\langle\overline{x(t)}\rangle_0=0$ and $\langle\overline{x^2(t)}\rangle_0\sim t^{\delta}$, where the lower subscript $\ldots_0$ denotes that no external force is applied on the system. When $\delta=1$ the diffusion is called normal, whereas for anomalous diffusion $\delta\neq 1$. When external driving force, F, is applied on the system the symmetry is broken and then $\langle\overline{x(t)}\rangle_F\sim t^{\delta_F}$ [14,17].

The effective temperature is

$$\frac{1}{k_B T_{eff}^{AB}}=\frac{2}{F}\frac{\overline{x_A(t)}_F}{\overline{x_B^2(t)}_0}, \tag{2}$$

where the indices AB mean that we measure the response $\overline{x_A(t)}_F$ and fluctuations $\overline{x_B^2(t)}_0$ over two independent systems [18]. Similarly $1/k_B T_{eff}^{AA}$ is the effective temperature measured on the same sample with *identical initial conditions* (see precise definition below) for the two measurements of response and diffusion. Usual Einstein relation implies $1/T_{eff}^{AA}=1/T_{eff}^{AB}=1/T$, at least when the measurement time is long. In the first part of this paper we investigate cases where T_{eff}^{AB} is random and then we consider its average.

The response of particles to an external field in a disordered quenched system exhibits linear response with respect to the field only for short times. For any finite external field there exists a time we call t_h where the response is nonlinear with respect to the field. This time was estimated in Ref. [15], and it was shown $t_h\sim h^{-(1+\alpha)/\alpha}$. When $h\to 0$ we have $t_h\to\infty$ however in any measurement or simulation h is finite and this time scale must be taken into consideration.

In Fig. 1 simulation results for T/T_{eff}^{AA} versus $\log[t/t_h]$ (for scaling we take $t_h=h^{-(1+\alpha)/\alpha}$) show that if we prepare the particles in the same sample and with the same initial conditions and then measure separately the diffusion and mobility the effective temperature is equal to the thermal temperature even in the anomalous diffusion phase of the model $T<T_g$. This however happens only for times shorter than t_h, once usual linear response breaks down we see an effective temperature T_{eff}^{AA} which depends on measurement time, and it fluctuates from sample to sample [20].

In contrast if we calculate T/T_{eff}^{AB} (Fig. 2) we see that T_{eff}^{AB} is not equal to the temperature when $T<T_g$. In fact T/T_{eff}^{AB} is a random function of time which depends on the particular realization of disorder which is evident from the scatter of data. We will soon discuss the average over disorder of T/T_{eff}^{AB}. Notice that in Fig. 2, in the phase of normal diffusion $T>T_g$ (the case $\alpha=2$), we find $T_{eff}^{AB}\approx T$ for long enough times and the sample to sample fluctuations are absent. Deviations of the effective temperature from thermal temperature are found for short times even in the ordered phase $T>T_g$ which is expected since the particles must have enough time to sample the system. Namely, only in the glassy phase $T<T_g$ we have deviations from usual meaning of temperature when we investigate systems with no ensemble averaging. This is clearly related to the divergence of the average waiting time in Eq. (1): if the average waiting time is infinite we can never average for long enough times so that fluctuations and response become identical, in complete contrast to the usual meaning of the Einstein relation.

Since we observe for $T<T_g$ deviations from usual Einstein relation, in the sense that $T_{eff}^{AB}\neq T$, we see that the Einstein relation is valid only in the following two ways. The first is when we make ensemble averages. Then as well known the Einstein relation holds after thermal and ensemble averaging [12]

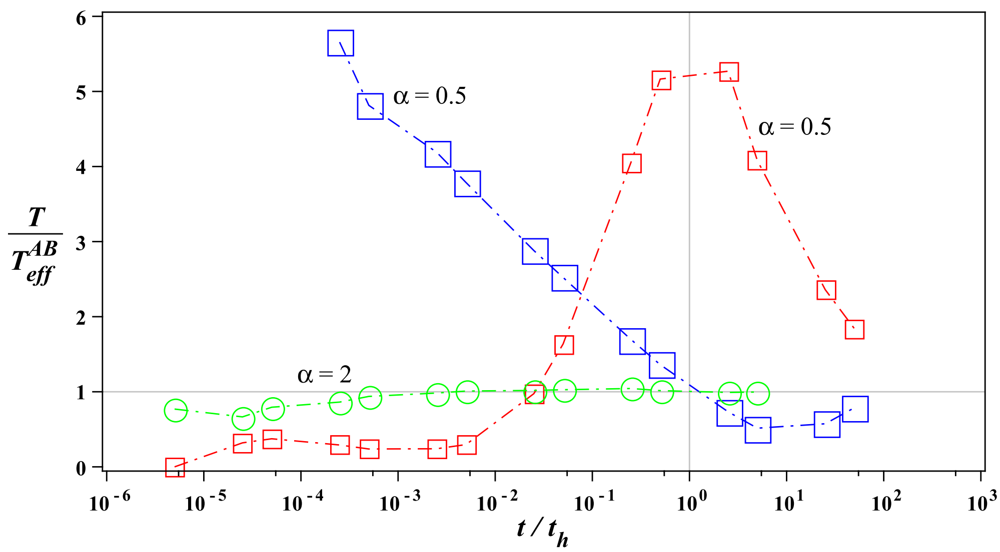

FIG. 2. (Color online) Simulation results of T/T_{eff}^{AB} versus $\log[t/t_h]$ with $h=0.008$. Two examples of the invalidity of the Einstein relation for $\alpha<1$ and an additional example for $\alpha=2$ where $T_{eff}^{AB}\simeq T$. Deviation of T_{eff}^{AB} from T can be seen even for $\alpha=2$ when t is small [19].

$$\langle\bar{x}(t)\rangle_F = \frac{F}{2k_BT}\langle\overline{x^2}(t)\rangle_0 \qquad t \ll t_h. \tag{3}$$

However in experiments we might not always be averaging over many samples hence this relation must be used with care. The second case is as mentioned when we do not use ensemble average but use the same initial conditions for both the response and the diffusion measurements that is we must be able to prepare the system in the same state with respect to the disorder which might be very difficult in practice. In contrast the validity of Einstein relation for $T>T_g$ is general in the long time limit and does not dependent on the way we prepare the system.

IV. AVERAGE EFFECTIVE TEMPERATURE

We now investigate the average inverse effective temperature $\langle 1/T_{eff}^{AB}\rangle$ in the glassy phase. Is this average equal to the inverse thermal temperature or do we find that the average inverse effective temperature is different from the thermal one? Does it depend on the measurement time? Is the average effective temperature finite? To begin with the analysis we consider a mean-field (MF) approach. In this approach we replace the disordered system with an ordered one, however using the averaged waiting time PDF Eq. (1) to describe sojourn times. The particles then perform a continuous-time random walk (CTRW) [12], where a particle waits between jumps, with waiting times distributed according to Eq. (1). Within this annealed approach $x_F \sim hN_F$ and $x_0^2 \sim N_0$, where N_F and N_0 are independent random numbers of jumps in

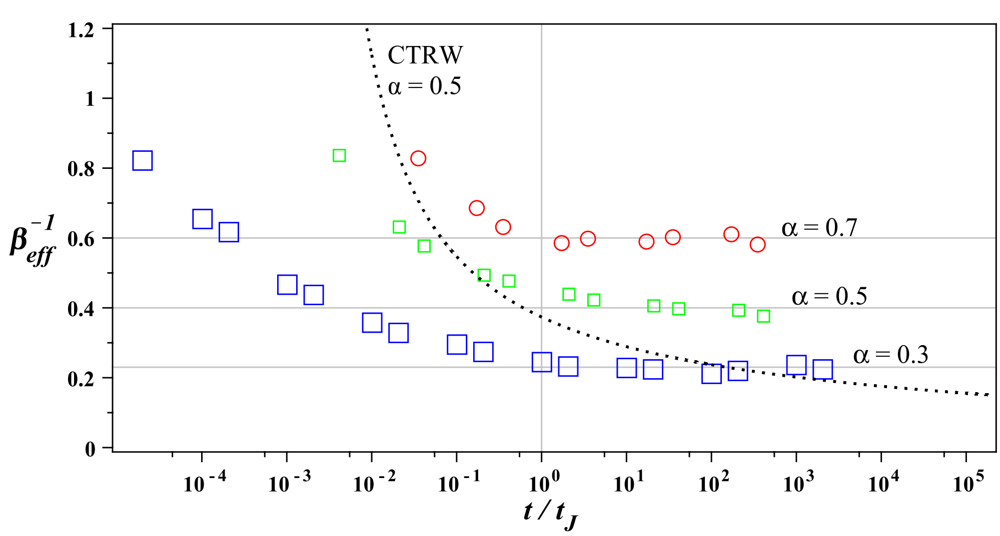

FIG. 3. (Color online) Simulation results of β_{eff}^{-1} versus $\log[t/t_J]$. In the QT model, for different α-**s** with h=0.008 $-\beta_{eff}^{-1}$ attains a constant value when $t>t_J$. In the CTRW approach an inverse logarithmic decrease to zero of T_{eff}^{MF} is shown (dashed line).

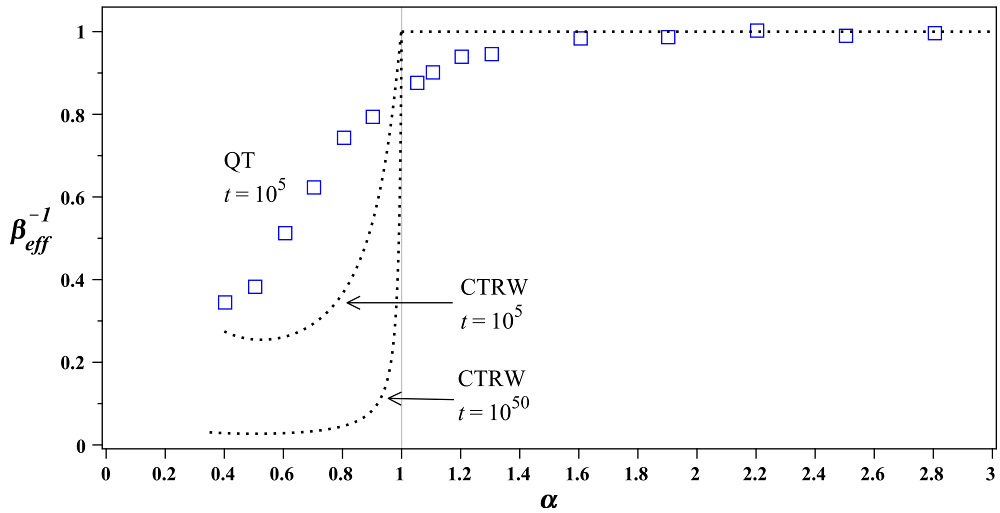

FIG. 4. (Color online) Results of β_{eff}^{-1} versus α for $t=10^5$. In the QT model a phase transition is seen around $\alpha=1$ in the slope of β_{eff}^{-1}: For $\alpha>1$, $\beta_{eff}^{-1}\approx 1$ whereas for $\alpha<1$, β_{eff}^{-1} has some finite value. The MF CTRW theory predicts a phase transition at $\alpha=1$. In addition an analytical result for $t=10^{50}$ illustrates that T_{eff}^{MF} is a step function for $t\to\infty$ although convergence to $t\to\infty$ limit is extremely slow.

CTRW. To calculate the MF effective temperature we use

$$\frac{T}{T_{eff}^{MF}} = \overline{\left(\frac{x_F}{hx_0^2}\right)} = \bar{N}\overline{\left(\frac{1}{N}\right)}, \tag{4}$$

where $\bar{N}$ and $\overline{(N^{-1})}$ are calculated with CTRW theory (see details below). Even for normal CTRW ($T>T_g$) the average $\overline{(N^{-1})}$ diverges since there is always a finite probability of not making a jump. In practice (i.e., in simulation or experiment) the probability to encounter dynamics with no jumps is very small, in fact if the particle does not move at all clearly there is no sense discussing mobility or diffusivity. Certainly, measurements for very long times will solve this problem if we take first time to be long and only then the number of systems in our ensemble to be large. To estimate the minimum time for simulation (which should be much smaller then t_h), we note that the average number of systems n which did not make any jump (particles stuck in place) is $\langle n\rangle=[1-\int_1^t\psi(\tau)d\tau]m$, where m is the total number of systems in our ensemble. Hence $\langle n\rangle\sim mt^{-\alpha}$. Now, we must have $\langle n\rangle/m\ll 1$. If we take $\langle n\rangle/m=\epsilon$ to be a small number we find that the measurement time should be larger then $t_J=\epsilon^{-1/\alpha}$. To summarize we must have $t_J<t<t_h$ to investigate a meaningful effective temperature.

The probability of making N jumps [21] in Laplace $t\to s$ space is $P_N(s)=[1-\psi(s)]\psi(s)^N/s$, where $\psi(s)$ is the Laplace transform of the waiting time PDF Eq. (1). For $0<\alpha<1$ $\psi(s)\sim 1-\gamma s^{\alpha}$, with $\gamma=\Gamma(1-\alpha)$ and $s\to 0$. It is easy to show that $\bar{N}(t)\sim t_\gamma^{\alpha}/\Gamma(1+\alpha)$, where $t_\gamma=\Gamma^{-1/\alpha}(1-\alpha)t$. In general $\overline{N^{-1}}$ diverges because of the probability to $N=0$, however, $N>0$ is assured by the condition $t>t_J$, as already explained. By definition $\overline{N^{-1}}$ is

$$\overline{N^{-1}}(t) = \sum_{N=0}^{\infty}\frac{P_N(t)}{N} = \left.\frac{P_N(t)}{N}\right|_{N=0} + \sum_{N=1}^{\infty}\frac{P_N(t)}{N}, \tag{5}$$

neglecting the $P_N(t)|_{N=0}$ term

$$\overline{N^{-1}}(s) \approx \frac{1-\psi}{s}\sum_{N=1}^{\infty}\frac{\psi^N}{N} = -\frac{1-\psi}{s}\ln[1-\psi]. \tag{6}$$

Substituting $\psi(s)$ in Eq. (6) and using Tauberian theorem [21,22], the final result is

$$\overline{N^{-1}}(t) \sim \frac{1-\alpha}{\Gamma(2-\alpha)}t_\gamma^{-\alpha}\ln[t_\gamma^{\alpha}] \tag{7}$$

for $t\to\infty$. Using Eq. (7) and $\bar{N}(t)$ gives

$$\frac{T}{T_{eff}^{MF}} \sim \frac{1-\alpha}{\Gamma(1+\alpha)\Gamma(2-\alpha)}\ln[t_\gamma^{\alpha}]. \tag{8}$$

We see that according to this MF approach the effective temperature depends on measurement time and goes to zero as $1/\ln[t]$ for long times.

To investigate the averaged effective temperature, beyond MF, we numerically calculated $\langle 1/T_{eff}^{AB}\rangle$, using Eq. (2), i.e., $(F/2k_BT)\beta_{eff}=\langle\overline{x_A}\rangle_F\langle\overline{x_B^{2}}^{-1}\rangle_0$, where $\beta_{eff}\equiv\langle T/T_{eff}^{AB}\rangle$ is a dimensionless effective inverse temperature. Figure 3 presents the behavior of β_{eff}^{-1} versus $\log[t/t_J]$. Analytical results are shown for the CTRW model with $\alpha=0.5$ and simulation results for the QT model with $\alpha=0.3$, 0.5, 0.7, and $h=0.008$. From Fig. 3 we see that for long enough times β_{eff}^{-1} reaches a constant value, namely, our results converge and the average effective temperature attains a finite value [23]. This behavior is different from the MF theory where $T_{eff}^{MF}\sim 1/\ln[t]$. Since when $t>t_h$ nonlinear effect appears, the results are shown for $t<t_h$. The simulations were made over 10^4 realizations with 10^3 particles on each realization. In our simulation we choose to scale our time with t_J to obtain data collapse on a reasonable scale. We choose $\epsilon=0.02$ and we have 10^4 realizations. For $t=t_J$ we find 200 frozen realizations (that we had to remove from the average), and for $t=100t_J$ we find only around 15 frozen ones (corresponding to

α). At such long times our simulations converge (see Fig. 3). Hence, roughly speaking, convergence is controlled by the condition that particles make many jumps.

The simulations shown in Fig. 4 present results of β_{eff}^{-1} versus α on the background of the analytical results for T_{eff}^{MF}/T (dotted curves). The results are for $t=10^5$ with $h=0.001$. This time is in the range of $t_J<t<t_h$ for $\alpha>0.34$. For QT model β_{eff}^{-1} is continuous and finite; however, the slope of β_{eff}^{-1} seems not continuous around $T\simeq T_g$. Also the analytical result for CTRW model with $t=10^{50}$ is shown, which illustrates that T_{eff}^{MF} is a step function for $t\to\infty$, where $T_{eff}^{MF}\to 0$ for $\alpha<1$ and $T_{eff}^{MF}\simeq T$ for $\alpha>1$ with phase transition at $\alpha=1$. For finite time (here $t=10^5$) still a phase transition appears near $\alpha=1$. However this MF theory fails to give a quantitative agreement with QT model, indicating that quenched and annealed approaches are fundamentally different. For Fig. 4 the simulations were made over 10^3 realizations with 10^3 particles on each realization.

V. DISCUSSION

Similar effects are expected to be found for other models of anomalous diffusion in quenched disordered systems. Models of anomalous diffusion on comb structures (models of loopless random fractal) or models of anomalous diffusion of a particle on structures with distributed dangling bonds in the presence of bias [12] are also characterized by a waiting time distribution with an infinite mean similar to Eq. (1). Generally, aging, non-self-averaging, and anomalous diffusion are found in these systems, hence the basic violation of Einstein relation $T_{eff}^{AB}\neq T$ is expected to be general within the anomalous phase of these models.

In ordinary statistical mechanics temperature, T, describes equilibrium properties of a system and also the ratio of fluctuation and dissipation. Does the effective temperature we found here have a similar dual meaning? Our finding in Fig. 4 indicates $\beta_{eff}^{-1}\simeq\alpha$ using the definitions of β and α one gets $\langle 1/T_{eff}^{AB}\rangle\simeq T_g^{-1}$, thus the effective temperature is T_g. This effective temperature characterizes the fluctuation dissipation ratio. Previous work [16] investigated the occupation time statistics of a particle in a binding potential $U(x)$, the relevant Boltzmann factor describing equilibrium properties was $\exp[-U(x)/T_g]$. Thus both for thermal equilibrium [16] and for the fluctuation dissipation ratio found here the relevant temperature is T_g. In this sense the effective temperature has a broad meaning, similar to the ordinary temperature, T.

ACKNOWLEDGMENT

This work was supported by the Israel Science foundation.

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[18] A and B presents two independent samples or equivalently the same sample but with different initial conditions. We consider sample with free boundary condition and assume measurements are made at large enough distances (or not too long times).
[19] In the normal phase t_h is not defined, just for comparison with the results of $T<T_g$ we scale our results in Fig. 2 with $t_h=2\times 10^6$.
[20] In Fig. 1 a thermal average over 10^6 particles was made. In Fig. 2 the number of particles simulated for the thermal average is 10^6 for $\alpha<1$ and 10^5 for $\alpha>1$. In simulations E_x at each site is raffled from $\rho(E)$, the waiting time in each site is taken as τ_x.
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[23] We also measured the variance of β_{eff}^{-1} and found it to be finite. Details in future work.