Spontaneous Relaxation in Generalized Oscillator Models with Glassy Dynamics†

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In this paper we introduce the generalized oscillator model (GOM) as a family of exactly solvable models useful to investigate theoretical aspects related to the statistical description of the aging state. GOMs are defined by a potential function $V(x)$ and characterized by a zero-temperature relaxation determined by entropy barriers and partial equilibration. Analytic expressions for the effective temperature can be derived using a fluctuation theorem valid in the aging regime without the need to solve the dynamical equations for correlations and responses. Two classes of models are investigated in detail: the homogeneous potential model with $V(x) = (k/2p)x^{2p}$ (p being a positive integer) and the wedge potential model ($V(x) = k|x|$ where $V(x)$ has a singularity at the ground-state coordinate $x = 0$). For the latter, we present some numerical simulations that reinforce the validity of the main analytical results. GOMs offer a conceptual framework to develop a statistical description of the spontaneous relaxation process that has been recently proposed[4] to be at the root of the intermittency phenomenon observed in glasses and colloids.

1. Introduction

Non-equilibrium phenomena is a field of research of much current interest. From turbulence in liquids to heat convection inside stars, a plethora of systems show a very rich and complex behavior, rarely describable in terms of few variables.[1] The opposite situation is encountered in equilibrium systems, where few parameters are needed to characterize the equilibrium state and its fluctuations. Entropy, a key concept in thermodynamics, admits a statistical interpretation in terms of the microscopic motion of molecules. Boltzmann established the bridge linking the microscopic and the macroscopic worlds, the central result in his theory being the relation $S = k_B \log(W)$ where W is the number of configurations available to the system. The extension of this approach to non-equilibrium systems and the characterization of their behavior in terms of a few number of parameters still represents a major theoretical challenge.

Two categories of non-equilibrium systems have received considerable attention in past years: systems in steady states and glassy systems. The first category encompasses all of those systems driven out of equilibrium to a stationary state by the action of an external perturbation. The most common example is a wire of metal with extremes in contact with two thermal sources at different temperatures. In this case, and if the temperature difference is not too large, the flow of heat from the hotter to the colder source is described by the Fourier law. The second category encompasses all systems that are not in a stationary state but which properties change very slowly with time. Structural glasses (such as ordinary window glass) are prototype examples.

The glass state is characterized by a very slow relaxation toward equilibrium and by a exceedingly low rate of the energy released from the system to the bath during the relaxation. A useful parameter to characterize the glass state is the age of the glass (also called waiting time in several experimental protocols), which is the time elapsed since the system was prepared in the non-equilibrium state. In the aging state correlation functions tend to decay in a time scale that is of the order of the age of the system. A statistical interpretation of the aging state has not yet been accomplished; however, our present understanding might not be far from resolving several of the most important clues. Recent experiments have observed the existence of intermittent fluctuations[2,3] that could be related to dissipative processes characteristic of the glass state.[4,5] A thermodynamic description of such processes could provide an important step in that direction.

Statistical models have been always an important source of inspiration and ideas to understand the glass transition. Many types of models have been considered in the past, from phenomenological two-state systems to spin glasses, passing through a wide range of family systems such as hard-sphere liquids, Lennard-Jones systems, lattice models, kinetically constrained models, among others. Most of these models have been investigated using approximate methods or numerical simulations.

To this list we should add exactly solvable models. From a historic point of view, these have played an important role in the early days of statistical mechanics. From the urn models introduced by the Ehrenfests aiming to understand concepts such as entropy and thermal equilibrium, to the Ising model that describes phase transitions and critical phenomena, solvable models offer conceptual frameworks to contrast ideas and check their consistency by evaluating specific predictions. In this way, exactly solvable models have also contributed to our current understanding of glassy systems.

The goal of this paper is to introduce a general family of exactly solvable models that might help to better understand the mechanisms behind the slow relaxation observed in glassy systems. We introduce the generalized oscillator model (GOM) as a generalized version of a previous model introduced by the author.[6] These share some properties with kinetically constrained models as statics is trivial but dynamics is not. Therefore they

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belong to a large category of models whose dynamics can be very rich despite the fact that the energy landscape has trivial properties. The main objective of this paper is to discuss a statistical approach to the aging state by emphasizing the relevance of the concept of effective temperature[19] as a useful way to quantify violations of the fluctuation−dissipation theorem.[7,8] In the framework of the GOM we stress the relevance of the effective temperature to quantify the spectrum of intermittent energy fluctuations in the aging regime that have been experimentally observed.[2,3] The link between intermittent effects in non-equilibrium systems and statistical effective temperatures has been recently proposed in the framework of simple models for the glass transition.[4,5] The present paper extends these considerations to the GOM.

2. The Generalized Oscillator Model (GOM)

Generalized oscillator models (GOMs) consist of a set of noninteracting oscillators each described by a continuous variable x_i and the energy function

$$E = \sum_{i=1}^{N} V(x_i) \tag{1}$$

where $V(x)$ is a real valued potential energy function that diverges to $+\infty$ in the limit $|x| \to \infty$. For instance, the potential can be of the type $V(x) = k/(2p)x^{2p}$ with p an integer value. This is called the homogeneous potential model, the case $p = 1$ corresponding to the harmonic case introduced in ref 6. Here we will only deal with potential energy functions such that the partition of an individual oscillator, $\mathcal{Z}_1$, remains finite at finite temperatures,

$$\mathcal{Z}_1 = \int_{-\infty}^{\infty} \exp(-\beta V(x)) \tag{2}$$

with $\beta = 1/k_B T$, k_B being the Boltzmann constant (that we will set equal to one) and T the temperature of the bath with which the system is put in contact.

We consider a dynamics where all oscillators are updated in parallel according to the rule

$$x_i \to x_i + \frac{r_i}{\sqrt{N}} \tag{3}$$

where the r_i are uncorrelated Gaussian variables with $\overline{r_i} = 0$ and variance $\overline{r_i r_j} = \Delta^2 \delta_{ij}$. The updating of all oscillators is carried out in parallel in a single move. The move is accepted according to the Metropolis rule. We will focus our analysis on the zero-temperature dynamics, as this is the case where relaxation is fully determined by entropic effects. Indeed, at $T = 0$ activated jumps over energy barriers are suppressed and relaxation proceeds only through search of favorable directions in phase space where the energy decreases. As time goes on, dynamics slows down as most of the proposed moves tend to push the system away from the ground state by increasing its energy. Only those moves that decrease the energy are accepted. Glassy dynamics in the GOM is then consequence of the quick decrease with time of the acceptance rate.

The GOM shares with kinetically constrained models[9] the property that, while statics is trivial, dynamics is complicated. Oscillators in eq 1 are noninteracting and therefore the model has trivial static properties, the N-oscillator partition function being given by $\mathcal{Z}_N = (\mathcal{Z}_1)^N$. The thermodynamic properties are then derived by computing the integral in eq 2.

To solve the dynamics of the GOM we have to compute the probability distribution of energy changes $P(\Delta E)$. This is defined as the probability density that in a given move the energy changes by an amount ΔE. In general, this quantity shows a complicated dependence on the N-oscillator probability density $\mathcal{P}_t(\{x_i\})$ that the system occupies the configuration $\{x_i\}$ at time t. However, the GOM has the good property that the $P(\Delta E)$ depends on a finite number of observables rather than on the full configurational probability distribution. This property is characteristic of mean-field systems, the GOM being just another example. This makes the model amenable of analytical computations and a good laboratory to test many results regarding the glassy regime. To compute the probability $P(\Delta E)$ we consider the change of energy in an elementary move,

$$\Delta E = \sum_{i=1}^{N}\left[V\left(x_i + \frac{r_i}{\sqrt{N}}\right) - V(x_i)\right] = \sum_{k=1}^{\infty}\frac{1}{k!N^{k/2}}\sum_{i=1}^{N} V^{(k)}(x_i) r_i^k \tag{4}$$

As dynamics is stochastic, the quantity ΔE is a random variable whose distribution can be reconstructed from the moments $\overline{(\Delta E)^k}$. An explicit calculation of such moments shows that only the first two moments give a finite contribution in the large N limit. Therefore, in the thermodynamic limit, $P(\Delta E)$ is a Gaussian distribution

$$P(\Delta E) = (2\pi\sigma_{\Delta E}^2)^{-1/2} \exp\left[-\frac{(\Delta E - M_{\Delta E})^2}{2\sigma_{\Delta E}^2}\right] \tag{5}$$

with mean $M_{\Delta E}$ and variance $\sigma_{\Delta E}^2$ given by

$$M_{\Delta E} = \overline{\Delta E} = \frac{\Delta^2}{2}\overline{V''(x)} \tag{6}$$

$$\sigma_{\Delta E}^2 = \overline{(\Delta E)^2} - (\overline{\Delta E})^2 = \Delta^2 \overline{(V'(x))^2} \tag{7}$$

where $\overline{f(x)} = (1/N)\sum_{i=1}^{N} f(x_i)$. At $T = 0$ the equations for the acceptance a (i.e., the fraction of accepted moves) and the energy per oscillator $e = E/N = \overline{V(x)}$ can be written as

$$a = \int_{-\infty}^{0} P(y)\, dy \tag{8}$$

$$\frac{\partial e}{\partial t} = \int_{-\infty}^{0} yP(y)\, dy \tag{9}$$

Inserting eq 5 in eqs 8 and 9, we obtain

$$\frac{\partial e}{\partial t} = -\left(\frac{\sigma_{\Delta E}^2}{2\pi}\right)^{1/2} \exp\left(-\frac{M_{\Delta E}^2}{2\sigma_{\Delta E}^2}\right) + \frac{M_{\Delta E}}{2} Erfc\left(\frac{M_{\Delta E}}{(2\sigma_{\Delta E}^2)^{1/2}}\right) \tag{10}$$

$$a = \frac{1}{2} Erfc\left(\frac{M_{\Delta E}}{(2\sigma_{\Delta E}^2)^{1/2}}\right) \tag{11}$$

with $Erfc(x) = (2/\sqrt{\pi})\int_x^{\infty} \exp(-u^2)\, du$ the complementary error function. These equations are not generally solvable as they are not closed, and the time evolution for the mean $M_{\Delta E}$ and the variance $\sigma_{\Delta E}^2$ is unknown. Only for some types of potentials $V(x)$ can a closed solution be found. Oscillator models have the interesting property that relaxation at $T = 0$ gets steadily slower as the ground state is approached. In fact, the ground-state configuration $\{x_i^{GS}\}$ is characterized by the fact that the energy (eq 1) is an absolute minimum, therefore $x_i^{GS} =$

x^{GS}, with $V'(x^{GS}) = 0$. According to eq 7, the value of $\sigma^2_{\Delta E}$ steadily decreases as the ground state is approached. From eqs 10 and 11 this leads to a quick decrease of the decay rate of the energy and the acceptance rate. In such conditions the scenario of partial equilibration (as described in ref 5 and below in section 3) holds. A salient feature of eqs 10 and 11 is the dependence of the dynamical equations upon the following parameter:

$$\lambda = \frac{\sigma^2_{\Delta E}}{2M_{\Delta E}} \tag{12}$$

which has the dimensions of an energy (or temperature). Indeed, at $T = 0$ in the large-time limit, the quantity λ vanishes asymptotically. If we define $x = \sqrt{M_{\Delta E}/(4\lambda)}$ we can then expand the complementary error function in eqs 10 and 11 around $x = \infty$,

$$Erfc(x) = \frac{\exp(-x^2)}{\sqrt{\pi}x}\left(1 - \frac{1}{2x^2} + \mathcal{O}\left(\frac{1}{x^4}\right)\right) \tag{13}$$

Substituting this expansion in eq 10, we get for the time evolution of the energy

$$\frac{\partial e}{\partial t} = -\left(\frac{\sigma^2_{\Delta E}}{8\pi}\right)^{1/2}\frac{\exp(-x^2)}{x^2} \tag{14}$$

This equation can be asymptotically solved for a quite broad family of models. In general, the asymptotic decay of the energy can be expressed in terms of the parameter λ (eq 12) by knowing the analytic behavior of $V(x)$ in the vicinity of $x = 0$. We show below how the parameter λ in eq 12 plays the role of an effective temperature that quantifies violations of the fluctuation−dissipation theorem.[8]

3. Partial Equilibration

To better understand what partial equilibration means, we will consider the case of an harmonic well $V(x) = (1/2)kx^2$, where k is the stiffness constant of the well. This case corresponds to the linear harmonic oscillator introduced in ref 6 and studied in detail in other works.[10,11] For the harmonic case the energy is quadratic in the variables x_i,

$$E = \frac{k}{2}\sum_{i=1}^{N} x_i^2 \tag{15}$$

Equations 6 and 7 give $M_{\Delta E} = k\Delta^2/2$, $\sigma^2_{\Delta E} = k^2\Delta^2\overline{x^2} = 2k\Delta^2E/N = 2k\Delta^2 e$, where $e = E/N$ is the energy per oscillator. We now follow the discussion presented in ref 11. The constant energy surface can be represented by an hypersurface centered around the origin $x_i = x^{GS} = 0$ (depicted as O) of radius $R = \sqrt{2E/k}$. In Figure 1 we depict a schematic representation of the motion of a representative configuration $\{x_i^0\}$ (depicted as P) of energy E in phase space. The smaller dashed circle represents the region of points accessible from $\{x_i^0\}$ according to the dynamics (eq 3). All accessible points $\{x_i\}$ satisfy $\sum_i(x_i - x_i^0)^2 = \Delta^2$, i.e., lie at a distance Δ from $\{x_i^0\}$ which is the radius of the smaller dashed circle. The accessible configurations in a single move lie in a spherical hypersurface of dimension $N - 2$ corresponding to the intersection of the hypersurface of energy E' and the smaller spherical hypersurface of radius Δ. We call this region the intersecting region I as shown in Figure 1. The final configurations contained in I lie at a distance $R' = \sqrt{2E'/K}$ to the origin O. The change in energy associated to this transition is $\Delta E = E' - E$. The probability of this jump is therefore proportional to the surface of the intersecting region, $P(\Delta E) \propto C^{N-2}$, where C is the radius of the intersecting region. The computation of C is quite straightforward as can be deduced from the triangle including the points P, O as vertexes and whose three sides are R, R', Δ. In terms of R, R', and Δ, the distance C is given by the relation $R = \sqrt{R'^2 - C^2} + \sqrt{\Delta^2 - C^2}$. Expressed in terms of E, ΔE, Δ we have

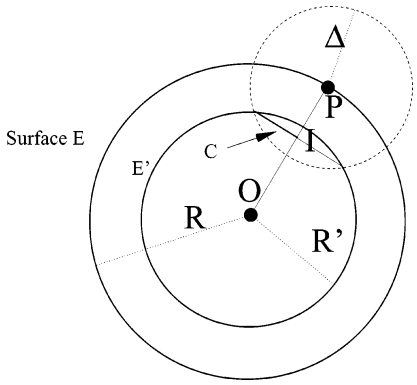

Figure 1. Geometrical construction to compute $P(\Delta E)$. The thick lines denote the departing and final energy hypersurfaces centered at O. The dashed circle indicates the hypersurface accessible from point P. The intersecting region between the accessible hypersphere centered at P and the final hypersurface of energy E' defines a hypersurface I of radius C (the radius is represented by a thick line). See the text for a more detailed explanation.

$$C^2 = \Delta^2 - \frac{k}{8E}\left(\frac{2\Delta E}{k} - \Delta^2\right)^2 \tag{16}$$

The surface $\Omega(E, \Delta E)$ corresponding to the region I of radius C, relative to the energy E of the reference configuration $\{x_i^0\}$ is

$$\Omega(E, \Delta E) \propto C^{N-2} = \left[\Delta^2 - \frac{k}{8E}\left(\frac{2\Delta E}{k} - \Delta^2\right)^2\right]^{(N-2)/2} \tag{17}$$

Using the fact that E is extensive with N, this expression can be rewritten as

$$\Omega(E, \Delta E) \propto \exp\left[-\frac{\left(\Delta E - \frac{K\Delta^2}{2}\right)^2}{4(E/N)K\Delta^2}\right] \tag{18}$$

which is then proportional to the probability distribution eq 5.

This construction then provides a geometric way to determine the Gaussian distribution (eq 5). From eq 16 we see that C (and therefore also $\Omega(E, \Delta E)$ or $P(\Delta E)$) has a maximum for $\Delta E = k\Delta^2/2$. The Gaussian distribution is depicted in Figure 2. Consider now a $T = 0$ dynamics where only moves with $\Delta E < 0$ are accepted. In this case, as the relative number of configurations that are accessible from P goes such as C^{N-2}, the largest number of accessible configurations lie in the vicinity of P. Because the radius of the small dashed hypersphere in Figure 1 is equal to Δ but the radius R of the hypersurface of energy E is proportional to $N^{1/2}$, dynamics constraints the system to move along the constant energy hypersurface in the thermodynamic limit. The system has then time to diffuse throughout a given energy shell of finite width before leaving that shell toward lower energy surfaces. This scenario was called partial equilibration in ref 5.

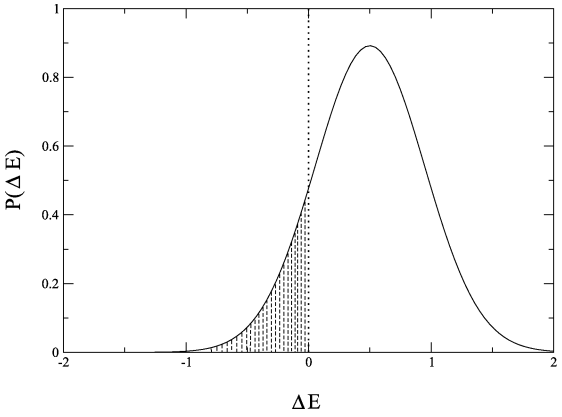

Figure 2. Probability distribution of energy changes for the GOM as derived from eqs 5 and 18. The major part of energy changes are with $\Delta E > 0$. At $T = 0$ the variance of distribution $\sigma^2_{\Delta E}$ decreases relative to the mean $M_{\Delta E}$ (i.e., the parameter λ in eq 12 decreases as the ground state is approached). The fraction of accepted moves (dashed area with $\Delta E < 0$) steadily decreases with time.

This derivation can be generalized to the GOM (eq 1) where the constant energy hypersurface is not necessarily a sphere. The crucial point in the argument is then the fact that Δ is a finite quantity while the typical spatial dimensions of the constant energy hypersurface are of the order $\sqrt{N}$. In the thermodynamic limit the hypersurface is locally a sphere and the length C (eq 16) can be mathematically expressed in terms of the mean energy curvature $\overline{V''(x)}$ and the modulus of the energy gradient vector given by $V'(x)^2$. The final result is again the most general expressions (eqs 5, 6, and 7).

4. The Fluctuation Theorem (FT) and Effective Temperatures

In the GOM a scenario of partial equilibration takes place in the constant energy hypersurface. This is exemplified in Figure 1 for the harmonic case where it is shown how the system is constrained to dwell in the constant energy hypersurface before moving to lower energy configurations. In this case, because dynamics is microscopically reversible and ergodic along the constant energy hypersurface, a quasi-stationary dynamics emerges with a probabilistic description that can be done in terms of a microcanonical measure. However, there are important differences between this dynamical measure and the usual microcanonical measure for equilibrium systems. While in the latter the energy is kept strictly constant and there is no time dependence of the microstate probability distribution, in the former the measure is dynamical and time dependent.

A key concept in such description is the notion of configurational entropy (sometimes also called complexity) $S(E)$, which counts the number of configurations with a given energy E. This quantity is precisely given by $P(\Delta E)$ except for the fact that $P(\Delta E)$ counts the number of configurations of energy E' that are accessible from a reference configuration of energy E. In a microcanonical description of the aging state, the probability to visit configurations with energy E' is then proportional to the number of configurations with that energy $\Omega(E')$,

$$P(\Delta E) \propto \Omega(E') = \exp(S(E')) \tag{19}$$

with $\Delta E = E' - E$, E' being the final energy and E the departure energy. It is important to emphasize that $P(\Delta E)$ in eq 19 (as well as in eq 5) is a probability rather than a rate. Transition rates are transition probabilities per unit of time and therefore have natural dimensions of frequency. We will denote them by $W(\Delta E)$. In general we can write

$$W(\Delta E) = \frac{P(\Delta E)}{\tau(E)} \tag{20}$$

where $\tau(E)$ denotes the average time to escape from a configuration of energy E. As these are microscopic transitions, the elementary escape process can be assumed to be a Poisson process described by its characteristic time $\tau(E)$. We can now imagine a situation where, in the large N limit, the average escape time is identical at both energies E, E' whenever the energy difference $\Delta E \sim \mathcal{O}(1)$. In this case, the time scale drops from the ratio between the forward ($E \rightarrow E'$) and reverse ($E' \rightarrow E$) transitions

$$\frac{W(\Delta E)}{W(-\Delta E)} = \frac{P(\Delta E)}{P(-\Delta E)} \tag{21}$$

Therefore, the rates W satisfy the same micorcanonical relation between the forward and the reverse paths as do the transition probabilities $P(\Delta E)$. Using eq 19 and expanding the term in the exponential up to the first-order term in ΔE we find

$$\frac{P(\Delta E)}{P(-\Delta E)} = \exp(S(E') - S(E)) = \exp\left[\left(\frac{\partial S(E)}{\partial E}\right)\Delta E\right] = \exp\left[\frac{\Delta E}{T^{\mathrm{FT}}_{\mathrm{eff}}(t_w)}\right] \tag{22}$$

where we have defined the time-dependent effective temperature

$$\frac{1}{T^{\mathrm{FT}}_{\mathrm{eff}}(t_w)} = \left(\frac{\partial S(E)}{\partial E}\right)_{E=E(t_w)} \tag{23}$$

The effective temperature is a quantity that depends on the age of the system t_w through the time-dependent value of the energy $E(t_w)$. A remark is now in place. The decomposition (eq 20) is reminiscent of the rates used in trap models.[12] However, there is an important difference between the GOM and trap models. In the latter the time scale $\tau(E)$ also depends on the energy of the trap but, contrarily to the present case, the rate is modified for energy changes $\Delta E \sim \mathcal{O}(1)$. Moreover, the partial equilibration scenario is difficult to visualize due to the absence of a proper configurational space. Although phenomenological trap models are very useful models to understand many aspects of the aging dynamics, several issues still remain controversial, especially regarding the physical significance of FD violations.[13−15]

Relations describing ratios between transition rates for forward and reverse processes in non-equilibrium systems are commonly known as fluctuation theorems (FTs). The relations in eqs 21 and 22 show a strong resemblance with some of these theorems; however, there are important differences that we want to highlight. There are two general classes of fluctuation theorems. In the first class there are the so-called entropy production FTs in stationary systems, where the relation between forward and reverse transitions is related to the entropy production in the asymptotic limit of large times.[16] In the second class there are exact non-equilibrium work relations valid at all times between the forward and reverse rates whenever the system is arbitrarily perturbed away from an initial equilibrium state along both the forward and reverse paths.[17,18] The most important difference between eqs 21 and 22 and these theorems concerns the fact that the aging state is not in a stationary state

(first class) and the system does not start from an initial equilibrium state (second class). Moreover, the relations in eqs 21 and 22 are not valid for energy changes ΔE arbitrarily separated in time as the effective temperature (eq 23) is age dependent.

There is another important feature of eq 21 that must be emphasized. Standard FTs allow for transitions to occur in both directions, and certainly this is what the identity in eq 21 seems to imply. Because no work is exerted upon the system during the relaxation, the energy change is related to the heat transferred between system and bath. Therefore, eq 21 relates transition rates between identical amounts of heat that are absorbed and released between the system and bath. However, we face the problem that at zero temperature no heat can be absorbed by the system (i.e., the energy can never increase), and therefore eq 21 cannot hold. The resolution of this issue concerns the true meaning of the effective temperature discussed in the next section.

4.1. Spontaneous Relaxation and Effective Temperatures. Developments during recent years in the theory of spin glasses and glasses have shown that aging systems show violations of the fluctuation−dissipation theorem[8] that can be quantified in terms of an effective temperature. This is usually defined in terms of the fluctuation−dissipation ratio (FDR),[19]

$$T_{\mathrm{eff}}^{\mathrm{FDR}}(t, t_w) = \frac{1}{R(t, t_w)} \frac{\partial C(t, t_w)}{\partial t_w} \quad t > t_w \tag{24}$$

where we assume that $(t - t_w)/t_w \sim \mathcal{O}(1)$. In general the effective temperature is a quantity that depends on the measured observable and the probed frequency $\omega \sim 1/(t - t_w)$ relative to the age, $\omega t_w = t_w/(t - t_w)$. The interesting meaning of eq 24 is found in the low-frequency regime $\omega t_w \ll 1$ where violations are expected to be strong. The effective temperature defined in this way requires the measure of the response function, i.e., the application of an external perturbation or field that shifts the energy levels and exerts mechanical work upon the system. In this case, the exerted work might account for part of the energy transferred from the system to the bath, making zero-field transitions with $\Delta E > 0$ accessible. Therefore, eqs 21 and 22 have to be understood as the proper way of quantifying forward and reverse transitions in a configurational space that has been perturbed by the action of an external field. This establishes a way to evaluate the effective temperature from the rate of heat exchange between system and bath *without the explicit need to introduce an applied external field*. Note that an external field is usually required to evaluate the response function $R(t, t_w)$. (In another context, numerical methods to compute the response function have been recently proposed.[20,21])

The existence of the effective temperature is then related to the presence of a heat exchange process between system and bath that we call spontaneous, as it is determined by the fact that the system has been prepared in a non-equilibrium state. The spontanoeus relaxation is different from the heat exchange process (that we call stimulated) between system and bath typical of equilibrium systems. In particular, the stimulated process is a high-frequency process characterized by a Gaussian distribution of exchange events, while the spontaneous process is a low-frequency process that manifests in the form of some tails in the heat-exhanged distribution, which width is age dependent. (The words "spontaneous" and "stimulated" make explicit reference to the problem of light emission by atoms in a bath of photons. In that case, the spontaneous process is the emission of radiation by atoms in an excited state independently of the presence of the bath. The stimulated process, though, is the emission and absorption of energy by atoms induced by the bath of photons.) For a recent discussion of these ideas, see refs 4 and 5. The existence of these two heat exchange processes is at the root of the intermittency phenomenon recently observed in glasses and colloids.[2,3]

The effective temperature can be computed in the GOM by using eqs 22 and 23. Indeed, from eqs 22 and 5 we get

$$\frac{P(\Delta E)}{P(-\Delta E)} = \exp\left(\frac{2M_{\Delta E}\Delta E}{\sigma_{\Delta E}^2}\right) \tag{25}$$

and therefore,

$$T_{\mathrm{eff}}^{\mathrm{FT}}(t_w) = \lambda(t_w) = \frac{\overline{(V'(x))^2}}{\overline{V''(x)}} \tag{26}$$

where λ is an age-dependent quantity that has been defined in eq 12 and where we have substituted eqs 6 and 7. In equilibrium it is straightforward to check that eq 26 coincides with the bath temperature by integrating by parts twice the integral in the denominator of eq 26,

$$\overline{V''(x)} = \int_{-\infty}^{\infty} \mathrm{d}x V''(x) \exp(-\beta V(x)) = \beta \int_{-\infty}^{\infty} \mathrm{d}x (V'(x))^2 \exp(-\beta V(x)) \tag{27}$$

In the aging regime in a partial equilibration scenario, the effective temperature eq 26 is related to the energy at time t_w through the relation eq 23.

5. The Homogeneous Potential Model

An example of the GOM where many quantities can be easily worked out is the case of an homogeneous potential of the type

$$V_p(x) = \frac{k}{2p} x^{2p} \tag{28}$$

with p a positive integer. The probability distribution (eq 5) is given by

$$P(\Delta E) = (2\pi k^2 \Delta^2 h_{2p})^{-1/2} \exp\left(-\frac{\left(\Delta E - \frac{k(2p-1)}{2}\Delta^2 h_p\right)^2}{2k^2\Delta^2 h_{2p}}\right) \tag{29}$$

with $h_k = \overline{x^{2(k-1)}}$. By definition, $E = N\bar{V}_p = N(k/2p)h_{p+1}$. Results similar to to eq 29 can then be obtained for the distribution of changes $P(\Delta h_k)$ for generic observables h_k, which lead to a hierarchy of coupled dynamical equations similar to eq 10. These equations can then be studied using generating functional techniques similar to those developed in other solvable spin-glass models.[22] Only for the harmonic case $p = 1$ is the equation for the energy (eq 10) closed and Markovian as its time evolution depends only on the energy.

The expression for the effective temperature (eq 26) for the homogeneous potential model is given by

$$T_{\mathrm{eff}}^{\mathrm{FT}}(t_w) = \frac{k h_{2p}(t_w)}{(2p-1)h_p(t_w)} \tag{30}$$

In the partial equilibration scenario, all observables are functions of the energy E of the hypersurface over which the system

partially equilibrates. The relation between the value of $T_{\rm eff}^{\rm FT}(t_w)$ and the energy $E(t_w)$ can be easily derived from eq 23. Introducing eq 28 in eq 2 we get

$$\mathcal{Z}_1 = \int_{-\infty}^{\infty} \exp(-\beta V_p(x)) = \left(\frac{2p}{\beta k}\right)^{1/2p} \int_{-\infty}^{\infty} dy \exp(-y^{2p}) \quad (31)$$

yielding the free energy $F = \text{const} - NT \log(\mathcal{Z}_1) = \text{const} - (NT/2p) \log(T)$ and the following expressions for the energy and entropy,

$$E = \frac{\partial \beta F}{\partial \beta} = \frac{NT}{2p} \quad (32)$$

$$S = -\frac{\partial F}{\partial T} = \frac{N}{2p} + \frac{N \log(T)}{2p} = \frac{N \log(E)}{2p} + \text{const} \quad (33)$$

giving

$$\frac{1}{T_{\rm eff}^{\rm FT}(t_w)} = \left(\frac{\partial S(E)}{\partial E}\right)_{E=E(t_w)} = \frac{N}{2pE(t_w)} \quad (34)$$

The case $p = 1$ corresponds to the harmonic oscillator and gives the well-known equipartition relation $T_{\rm eff}^{\rm FT}(t_w) = 2E(t_w)$. As remarked in the paragraph following eq 14, the dynamical evolution of the energy can be solved in general by knowing the relation (eq 34) between the energy $e = E/N$ and the effective temperature $T_{\rm eff}^{\rm FT}(t_w) = \lambda(t_w)$. In this case it is possible to derive the following asymptotic behavior for the energy:

$$e(t) \sim \frac{1}{(\log(t))^p} + (\text{subleading logarithmic corrections}) \quad (35)$$

The effective temperatures (eq 30) can be also derived using the fluctuation−dissipation relation (eq 24) or a set of microcanonical relations describing observable changes. The possibility to obtain the same value of the effective temperature by using three different approaches (the FDR (eq 24), the FT (eq 25), and the microcanonical rates for observables) has been explicitly shown for the harmonic case $p = 1$.[5] In ref 5 the main assumption was the validity of the partial equilibration scenario. Because the partial equilibration scenario also holds for the GOM, the main conclusions of ref 5 are expected to hold also for the present more general case.

The procedure to derive the FDR (eq 24) entails the computation of the correlation and response functions for the magnetization M defined as $M(t) = \sum_i x_i(t)$

$$C(t, t_w) = \frac{1}{N}\sum_{i=1}^{N} \overline{x_i(t) x_i(t_w)} \quad (36)$$

$$R(t, t_w) = \overline{\frac{\delta x(t)}{\delta h(t_w)}} \quad (37)$$

where $h(t_w)$ is an impulse field coupled to the magnetization M at time t_w. At $T = 0$ the response (eq 37) is finite due to the shift of the energy levels induced by the field. For the harmonic case $p = 1$, dynamics is closed and a simple expression can be derived for the effective temperature (eq 24),

$$T_{\rm eff}^{\rm FDR}(t, t_w) = 2e(t_w) + \frac{1}{f(t_w)} \frac{\partial e(t_w)}{\partial t_w} \quad (38)$$

where $f(t_w)$ is a function that asymptotically decays as $1/t_w$. Two remarkable facts emerge from eq 38: (1) eq 38 depends only on the age t_w at all times $t > t_w$, therefore $T_{\rm eff}^{\rm FDR}(t, t_w) \equiv T_{\rm eff}^{\rm FDR}(t_w)$ characterizes the aging state of the system at time t_w; and (2) the second term in the r.h.s of eq 38 is subdominant with respect to the first term. Using eq 34, this leads to $T_{\rm eff}^{\rm FDR}(t_w) \to T_{\rm eff}^{\rm FT}(t_w) \to 2e(s)$, so both the effective temperature derived from the FDR and the FT coincide.

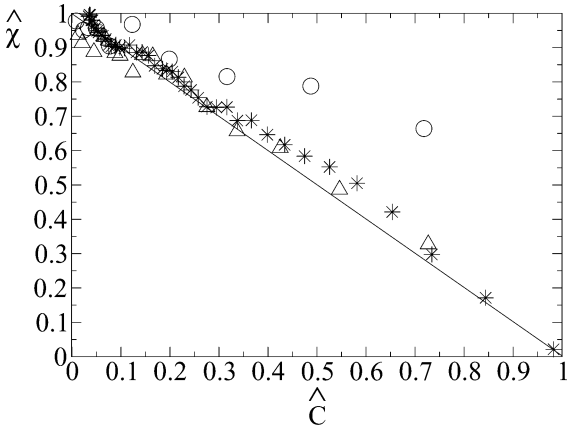

Figure 3. FD plot for the harmonic model ($p = 1$) obtained from Monte Carlo simulations at $T = 0$ with $N = 1000$ oscillators, $k = \Delta = 1$, magnetic field intensity equal to 0.01 and $t_w = 1$, 10, 100 (circles, triangles up, and stars, respectively). It represents $\hat{\chi}(\hat{C})$ and the straight line is the theoretical asymptotic prediction for large values of t_w. Data were averaged over 200 dynamical histories.

To obtain the effective temperature it is sometimes useful to construct the so-called fluctuation−dissipation (FD) plots.[8,23−25] The FD plots for the homogeneous model can be worked out as follows (the same construction holds for the GOM). As $C(t_w, t_w) = \overline{x^2(t_w)} = h_2(t_w)$ is time dependent, then it is convenient to normalize the correlation $C(t, t_w)$ by the autocorrelation value taken at the lowest time $\hat{C}(t, t_w) = C(t, t_w)/C(t_w, t_w)$ and plotting the integrated response $\chi(t, t_w) = \int_{t_w}^{t} ds R(t, s)$ as a function of $\hat{C}$ for t_w fixed and varying t. The resulting asymptotic curve is then expected to have a the form of a straight line, $\hat{\chi}(\hat{C}) = \hat{\chi}_0(1 - \hat{C})$, where χ_0 is the equilibrium susceptibility at zero temperature $\hat{\chi}_0 \propto \beta^{(p-1)/p}$. These straight FD plots are characteristic of the one-step behavior observed in structural glasses. Figure 3 shows the resulting FD plot for the $p = 1$ case as obtained from numerical simulations of the model.

6. The Wedge Potential Model

An interesting example of the GOM is the case where the first derivative of the potential $V'(x)$ is not continuous at the ground-state configuration $x = 0$. In this case the eqs 6 and 7 need to be reconsidered. The classical example for a potential of this type is the wedge potential model defined by

$$V(x) = k|x| \quad (39)$$

This potential is depicted in Figure 4. The statics for this model is straightforward and the partition function is given by $\mathcal{Z}_1 = 2/(\beta k)$. The internal energy and entropy are given by eqs 32 and 33, with $p = 1/2$. At equilibrium the one-oscillator probability density $q^{\rm eq}(x)$ is given by

$$q^{\rm eq}(x) = \frac{k\beta}{2} \exp(-\beta k|x|) \quad (40)$$

To solve the off-equilibrium dynamics of this model, we proceed similarly as was done in section 2 for a general function $V(x)$. The main difference now is that the potential (eq 39) is not

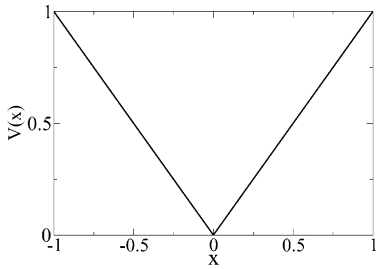

Figure 4. Wedge potential model (eq 39) with $k = 1$. It can be seen as a special case of the homogeneous model of section 5 with $p = 1/2$.

differentiable at $x = 0$. While the expression for $\sigma^2_{\Delta E}$ is well defined, $\overline{(V'(x))^2} = k^2$ is continuous for all x), the expression for $M_{\Delta E}$ is not because the second derivative $\overline{V''(x)}$ is discontinuous at $x = 0$. The expression, however, can be guessed by noticing that $V''(x) = a\delta(x)$ and using the relation

$$\int_{-\infty}^{\infty} dx V''(x) = a = V'(\infty) - V'(-\infty) = 2k \qquad (41)$$

From eqs 6 and 7, this gives

$$M_{\Delta E} = k\Delta^2\overline{\delta(x)} = k\Delta^2 q_t(0) \qquad (42)$$

where $q_t(x)$ is the one-oscillator probability density,

$$q_t(x) = \frac{1}{N}\sum_{i=1}^{N}\delta(x - x_i(t)) \qquad (43)$$

The result of eq 42 together with the relation

$$\sigma^2_{\Delta E} = k^2\Delta^2 \qquad (44)$$

gives the final probability distribution

$$P(\Delta E) = (2\pi k^2\Delta^2)^{-1/2}\exp\left[-\frac{(\Delta E - k\Delta^2 q_t(0))^2}{2k^2\Delta^2}\right] \qquad (45)$$

This result can be alternatively derived doing a more elaborated but better controlled calculation that we do not consider interesting enough to reproduce here in detail. The effective temperature (eq 24) can be obtained using the FT (eqs 25,26):

$$T^{\mathrm{FT}}_{\mathrm{eff}}(t_w) = \frac{k}{2q_{t_w}(0)} \qquad (46)$$

Using the thermodynamic relation of eq 32 with $p = 1/2$, we get $e = E/N = k\overline{|x|} = T$. If we now assume that eq 40 holds in the aging regime by replacing β with $\beta_{\mathrm{eff}}(t_w) = 1/T_{\mathrm{eff}}(t_w)$ then, in a partial equilibration scenario, we get

$$q_{t_w}(x) = \frac{k\beta_{\mathrm{eff}}(t_w)}{2}\exp(-\beta_{\mathrm{eff}}(t_w)k|x|) \qquad (47)$$

which gives $q_{t_w}(0) = (k\beta_{\mathrm{eff}}(t_w))/2 = k/(2e(t_w))$. Substituting this last result in eq 46 we obtain

$$T^{\mathrm{FT}}_{\mathrm{eff}}(t_w) = \frac{k}{2q_{t_w}(0)} = e(t_w) \qquad (48)$$

which coincides with the result derived using the thermodynamic relations of eqs 23 and 33, with $p = 1/2$. Finally, we mention

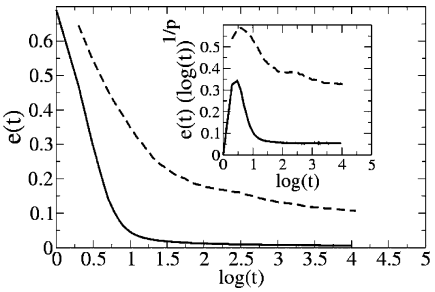

Figure 5. Monte Carlo studies of the harmonic model (continuous line) and the wedge model (dashed line). Simulations have been done at $T = 0$ with $N = 1000$ oscillators and $k = \Delta = 1$. Main: Energy decay $e(t)$ in both models. Inset: $e(t)$ multiplied by $(\log(t))^{1/p}$ (harmonic model with $p = 1$, wedge model with $p = 1/2$) as a function of $\log(t)$. In the large t limit, both curves converge to a constant value.

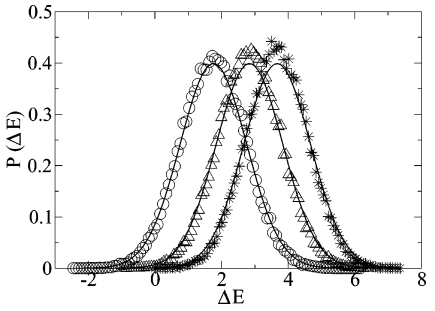

Figure 6. Probability distribution $P(\Delta E)$ (eq 45) for the wedge model numerically evaluated at $T = 0$, $N = 1000$, $k = \Delta = 1$ for $t_w = 10$, 100, 1000 (circles, triangles up and stars respectively). The continuous lines are the fitted Gaussians with $M_{\Delta E} = q_{t_w}(0)$ as fitting parameter. The effective temperature (eq 46) is then compared with that obtained from the energy in Table 1.

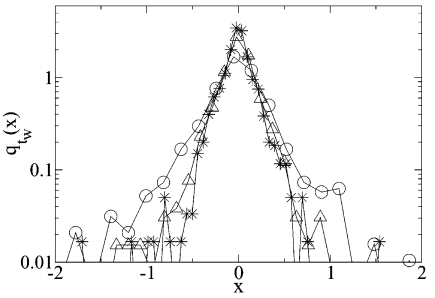

Figure 7. One-oscillator probability distribution $q_{t_w}(x)$. The same parameters and symbols as in Figure 6. Note the presence of the exponential tails in the distribution as expected from (47).

that the asymptotic decay for the energy derived for the homogeneous potential model (eq 35) also holds in the wedge model, substituting $p = 1/2$, i.e., $e(t) \sim 1/\sqrt{\log(t)}$. In Figures 5, 6, and 7 we show some numerical results for the wedge model obtained by doing Monte Carlo calculations. These have been done at zero temperature for $N = 1000$ oscillators with parameters $k = \Delta = 1$ and starting from a random initial configuration with initial coordinates x_i chosen from a Gaussian distribution of zero mean and unit variance. These simulations are useful to verify the main predictions. Figure 5 shows the time decay of the energy for the wedge model compared to the harmonic model. Figure 6 is a test of the main result (eq 45). The energy change distributions have been evaluated at three different waiting times $t_w = 10$, 100, and 1000 and fitted to a Gaussian distribution of variance $k^2\Delta^2 = 1$ where the mean $q_{t_w}(0)$ is the fitting parameter. This value is then compared with the value of the energy $e(t_w)$ to check the identity (eq 48). The results are shown in Table 1. Figure 7 shows the one-oscillator

TABLE 1: Effective Temperature in the Wedge Model (eq 48) Obtained in Two Independent Ways

t_w	$T_{eff}^{FT}(t_w) = e(t_w)$ [a]	$T_{eff}^{FT}(t_w) = k/(2q_{t_w}(0))$ [b]
10	0.335	0.28
100	0.180	0.178
1000	0.132	0.136

[a] Second column: from the value of the energy $e(t_w)$ shown in Figure 6. [b] Third column: from the value of $q_{tw}(0)$ obtained by fitting eq 45 to the numerical distribution $P(\Delta E)$ shown in Figure 5. [c] Both values asymptotically coincide for large values of t_w.

probability density in the aging regime $q_{t_w}(x)$ at three different waiting times compared to the expected result (eq 47).

7. Conclusions

In this paper we have introduced a new family of exactly solvable models characterized by zero-temperature relaxation determined by entropy barriers and partial equilibration. Generalized oscillator models (GOMs) offer a conceptual framework to develop a statistical description of the aging state. The interesting property of this class of models stems from the validity of the partial equilibration scenario:[5] dynamics is ergodic and microscopically reversible when the system is constrained to move along the constant energy hypersurface. We have then computed the probability distribution of energy changes $P(\Delta E)$ that characterizes the spontaneous relaxation process at zero temperature. The spontaneous process is not thermally activated but determined by the fact that the system has been prepared in a non-equilibrium aging state. Using a fluctuation theorem for the aging state, it is then possible to derive analytic expressions for the effective temperature (eq 26) without the need to solve the dynamical equations for correlations and responses (eq 24). The quantitative description of the spontaneous process in terms of a fluctuation theorem valid in the aging state has been recently proposed[4] to be at the root of the intermittency phenomenon observed in glasses and colloids.[2,3]

Two classes of models have been studied in detail. The homogeneous potential model in section 5 and the wedge potential model in section 6. Particularly interesting is the latter where the first derivative of the potential is singular at the ground-state configuration. In this case, the effective temperature (eq 46) depends on the value of the one-oscillator probability distribution at the value of the singularity of the potential. The present studies can be extended to other interesting potential functions, and some results will be presented in the future.

A salient feature of the GOM is the Gaussian shape of the distribution $P(\Delta E)$ in large N limit. This is a direct consequence of the dynamics of the model (eq 3) which is of the mean-field type, as oscillator correlations do not enter the analytical expression of $P(\Delta E)$. In this regard, the validity of the partial equilibration scenario in the GOM is a consequence of the mean-field character of the dynamics. The extension of these ideas to non mean-field dynamical models is an open problem. Nevertheless, despite the fact that the present ideas have been derived from the study of mean-field systems, we do not foresee conceptual limitations in their adaptation to spatially correlated dynamics. A conceptual description of the aging state in terms of heat exchange processes[4,5] could be achieved in terms of a spatially fluctuating effective temperature that would describe local fluctuations in the rate of energy relaxation in the system. At difference with bath temperatures, effective temperatures should be considered as fluctuating intensive variables, as they describe energy exchange processes, either heat releasing or work releasing (through mechanical stresses), occurring over nanoscale spatial regions where energies are not macroscopic but of the order of few k_BT. It would be very interesting to explore the possible connection between these ideas and the existence of spatial heterogeneities that have received considerable attention during the past years (see for instance refs 26 and 27). Establishing a thermodynamic description of these heterogeneous excitations is probably an important step toward their understanding.

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