Exactly Solvable Model Glass with a Facilitated Dynamics

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Abstract. A model glass with fast and slow processes is studied. The statics is simple and the facilitated slow dynamics is exactly solvable. The main features of a fragile glass take place: Kauzmann transition, Vogel-Fulcher law, Adam-Gibbs relation and aging. The time evolution can be so slow that a quasi-equilibrium occur at a time dependent effective temperature. The same effective temperature is derived from the Fluctuation-Dissipation ratio, which supports the applicability of out of equilibrium thermodynamics.

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1. Introduction

We present the outcome of our investigation of an exactly solvable model glass that shows all of the basic features of much more complicated real glasses, such as aging \cite{1, 2}, diverging relaxation time to equilibrium (Vogel-Fulcher-Tammann-Hesse (VFTH) like \cite{3}), configurational entropy satisfying the Adam-Gibbs relation \cite{4}, Kauzmann transition \cite{5} and violation of Fluctuation-Dissipation Theorem \cite{6, 2}.

In studying the model we make use of a particular parallel Monte Carlo dynamics that retains the fundamental collective nature of the glassy dynamics and that can be carried out analytically on our model. We will see how this dynamics undergoes a huge slowing down as the system is cooled down and which kind of aging dynamics the system sets out. We can implement such dynamics even below the Kauzmann temperature, thus getting information in a regime where few analytic results are known.

The main motivations for this work are twofold. Firstly we want to get more insight in the glassy dynamics, in its various aspects, exploiting the analytical solvability of our model. Indeed, every detected feature of the glassy behaviour can be connected in a direct correspondence with given elements of the model, thanks to its simplicity. We can even switch on and off certain properties or certain dynamic behaviours, tuning the model parameters or implementing the facilitated dynamics in alternative ways. Furthermore, the configurational entropy is exactly computable (see section 2) as a function of the dynamic variables of the model.

The second goal is to check the generality of the concept of effective temperature, very often discussed in literature in many different approaches (see for instance in \cite{2, 6, 7, 8, 9, 10, 11, 12, 13}) and to see whether the possibility exists of inserting such a parameter in the construction of a consistent out of equilibrium thermodynamic theory. Even though the physics of our model is simple, we shall find general aspects of the results by formulating them in the thermodynamic language (see section 5).

In glasses, the exponential divergence of time-scales (as opposed to the algebraic divergence in standard continuous phase transitions), might induce an asymptotic decoupling of the time-decades \cite{14}. Exploiting this, we build the dynamics of our model on the reasonable assumption that, in a glassy system that has aged a long time \( t \), all processes with equilibration time much less than \( t \) (the \( \beta \) processes) are in equilibrium while those evolving on time scales much larger than \( t \) are still quenched, leaving the processes with time scale of order \( t \) (i.e., the \( \alpha \) processes), as the only interesting ones. To model this, we will introduce by hand two different kind of variables evolving on two very different (decoupled) time-scales.

Such an asymptotic decoupling of time scales, that is the input for the present model and for a set of other models of the same class \cite{10, 15, 16, 17, 18}, could be the basis for a generalization of equilibrium thermodynamics to systems out of equilibrium \cite{10}.

In section 2 we introduce the model and in section 3 the facilitated dynamics that we apply to it. The dynamical behaviour of the one-time observables will be shown in section 4. In section 5 an out of equilibrium formulation of thermodynamics is proposed. From the study of the two-time variables dynamics (in section 6) we show that, quite reasonably since we are not at equilibrium, the Fluctuation-Dissipation Theorem is not valid anymore. We will see in section 6 that from the Fluctuation-Dissipation Ratio we can derive an independent definition of effective temperature.
2. The model and its static properties

2.1. Hamiltonian and constraint on the configuration space

The model displaying a fragile glass behaviour was introduced in [20] and widely studied in [19]. It is described by the following local Hamiltonian:

\[ H[(x_i), (S_i)] = \frac{1}{2} K \sum_{i=1}^{N} x_i^2 - H \sum_{i=1}^{N} x_i - J \sum_{i=1}^{N} x_i S_i - L \sum_{i=1}^{N} S_i, \]

where \( N \) is the size of the system and \( \{x_i\} \) and \( \{S_i\} \) are continuous variables, the last satisfying a spherical constraint: \( \sum_i S_i^2 = N \). We will call them respectively harmonic oscillators and spherical spins. \( K \) is the Hooke elastic constant, \( H \) is an external field acting on the harmonic oscillators, \( J \) is the coupling constant between \( \{x_i\} \) and \( \{S_i\} \) on the same site \( i \), and \( L \) is the external field acting on the spherical spins. A separation of time scales is introduced by hand: the spins represent the fast modes and the harmonic oscillators the slow ones. We assume that the \( \{S_i\} \) relax to equilibrium on a time scale much shorter than the one of the harmonic oscillators. From the point of view of the motion of the \( \{x_i\} \), the spins are just a noise. To describe the long time regime of the \( \{x_i\} \), we can average over this noise by performing the computation of the \( \{S_i\} \) partition function, obtaining an effective Hamiltonian depending only on the \( \{x_i\} \), that determines the dynamics of these variables. Using the saddle point approximation for large \( N \) we find:

\[ Z_S(\{x_i\}) = \int \left( \prod_{i=1}^{N} ds_i \right) \exp \left\{ -\beta H[(x_i), (S_i)] \right\} \delta \left( \sum_{i=1}^{N} S_i^2 - N \right) \approx e^{-\beta H_{\text{eff}}(\{x_i\})} \]

where we introduce the effective Hamiltonian \( H_{\text{eff}}(\{x_i\}) \equiv -T \log Z_S(\{x_i\}) \), that is the free energy for a given configuration of \( \{x_i\} \), as

\[ H_{\text{eff}}(\{x_i\}) = \frac{K}{2} m_2^2 N - H m_1 N - w N + \frac{T N}{2} \log \frac{w + T}{T}. \]

We defined the short-hands

\[ m_1 = \frac{1}{N} \sum_{i=1}^{N} x_i, \quad m_2 = \frac{1}{N} \sum_{i=1}^{N} x_i^2, \quad w = \sqrt{J^2 m_2 + 2 J L m_1 + L^2 + \frac{T^2}{4}}. \]

The effective Hamiltonian, equation (3), can also be written in terms of the internal energy \( U(\{x_i\}) \) and of the entropy \( S_{\text{ep}}(\{x_i\}) \) of the equilibrium processes (i.e. the spins):

\[ H_{\text{eff}}(\{x_i\}) = U(\{x_i\}) - T S_{\text{ep}}(\{x_i\}) ; \]

\[ U(\{x_i\}) = \frac{K}{2} m_2^2 N - H m_1 N - w N + \frac{T N}{2}, \quad S_{\text{ep}}(\{x_i\}) = \frac{N}{2} - \frac{N}{2} \log \frac{w + T/2}{T}. \]

The model is also characterized by a constraint on the phase space, introduced to avoid the existence of the single global minimum, and implementing a large degeneracy of the allowable lowest states. The constraint is taken on the \( \{x_i\} \), thus concerning the long time regime. It reads:

\[ m_2 - m_1^2 \geq m_0, \]

where \( m_0 \) is a model parameter. It is a fixed, but arbitrary, strictly positive constant. This constraint, applied to the harmonic oscillator dynamics, is a way to reproduce...
the behavior of good glass formers, i.e., substances for which nucleation of the crystal phase is especially unlikely even at very slow cooling rates (e.g., network formers \( \text{B}_2\text{O}_3 \) and \( \text{SiO}_2 \), molecular organics such as glycerol and atactic polystyrene, and different multicomponent liquid mixtures). These are substances for which there are non-crystalline packing modes for the particles composing them, that have intrinsically low energy. The amorphous configurations are thus favored. In general the crystal state still exists, at lower energy, but the probability of nucleating a crystal instead of a glass is negligible. In specific cases (binary solutions) the glassy state can even be lower in energy than the crystalline one and is thermodynamically stable with respect to any crystal configuration \[21\].

In the next section we will impose a Monte Carlo dynamics \[15, 22\] satisfying this constraint and coupling the otherwise non-interacting \( \{x_i\} \) in a dynamic way. We will study such dynamics analytically.

To shorten the notation we define the modified “spring constant” \( \tilde{K} \) and “external field” \( \tilde{H} \):

\[
\tilde{K} = K - \frac{J^2}{w + T/2}, \quad \tilde{H} = H + \frac{JL}{w + T/2}
\]  

We stress that \( \tilde{K} \) and \( \tilde{H} \) are actually functions of the \( \{x_i\} \) themselves (through \( m_1 \) and \( m_2 \), occurring in \( w \)).

### 2.2. Statics at heat-bath temperature \( T \)

Before describing the facilitated dynamics employed we sketch very briefly the static of the model. The partition function of the whole system at equilibrium is:

\[
Z(T) = \int D\mathbf{x} D\mathbf{S} \exp \left[ -\beta \mathcal{H}(\{x_i\}, \{S_i\}) \right] \delta \left( \sum_i x_i^2 - N \right) = \int dm_1 dm_2 \exp \left\{ -\beta N \left[ \frac{K}{2} m_2 - H m_1 - w + \frac{T}{2} \log \left( \frac{w + T/2}{T} \right) - \frac{T}{2} \left( 1 + \log(m_2 - m_1^2) \right) \right] \right\}
\]  

The new object (with respect to equation (2)) appearing in the exponent of the above expression is the configurational entropy

\[
\mathcal{I} \equiv \frac{N}{2} \left[ 1 + \log(m_2 - m_1^2) \right] .
\]  

The saddle point equations are found minimizing the expression between square brackets in (3) with respect to \( m_1 \) and \( m_2 \). This yields

\[
\mathcal{H}(m_1, m_2) = \frac{T}{K(m_1, m_2)} m_1 \quad \text{and} \quad m_2 - m_1^2 = \frac{T}{K(m_1, m_2)} .
\]  

The form of the solutions \( m_1(T) \), \( m_2(T) \) is quite complicated because each of these equations is actually a fourth order equation, but they can be explicitly computed.

### 3. Facilitated Monte Carlo dynamics

We assume as dynamics a parallel Monte Carlo (MC) dynamics for the harmonic oscillators. This kind of analytic Monte Carlo approach was first introduced in \[22\], and later applied to the exactly solvable harmonic oscillator model \[15\] (which is just our model after setting \( J = L = 0 \)) and to the spherical spin model \[16, 10\].
(which is the present model after setting $H = K = 0$ and considering the $\{x_i\}$ as quenched random variables). The dynamical model thus obtained with a very simple Hamiltonian and a contrived dynamics has the benefit of being even solvable analytically, which yields a much deeper insight into its properties than numerical simulations. Moreover, in the long-time domain the dynamics looks quite reasonable in regard to what one might expect of any system with a VFTH-law in its approach to equilibrium.

In a Monte Carlo step a random updating of the variables is performed $(x_i \rightarrow x_i' = x_i + r_i/\sqrt{N})$ where the $\{r_i\}$ have a Gaussian distribution with zero mean and variance $\Delta^2$. We define $x = H(\{x_i\}) - H(\{x_i\})$ as the energy difference between the new and the old state. If $x > 0$ the move is accepted with a probability $W(\beta x) \equiv \exp(-\beta x)$; else it is always accepted ($W(\beta x) = 1$). The updating is made in parallel. It is the parallel nature of the updating that allows the collective behavior leading to exponentially divergent time scales in models with no interactions between particles such as ours. A sequential updating would not produce any glassy effect. This dynamics may induce glassy behavior in situations where ordinary Glauber dynamics [24] would not. In our model the parallel dynamics mimics the presence of interactions between atoms in realistic glasses, where a large internal cooperativeness occur. In this respect the constraint is not essential. A parallel MC dynamics that does not take into account the constraint on the $\{x_i\}$ still maintains glassy behaviour (see [17] for the study of such dynamical version of our model). Here, however, we will only look at the dynamics with a built-in constraint. For different examples of dynamics implying non trivial collective behavior the reader can look, for instance, at the $n$-spin facilitated kinetic Ising model [24, 25] or at the kinetic lattice-gas model [21, 26].

In this section we will show the basic steps leading to dynamical equations. For further details refer to [11, 13, 17, 19]. In a Monte Carlo step the quantities $\sum_i x_i = N m_1$ and $\sum_i x_i^2 = N m_2$ are updated. We denote their change by $y_1$ and $y_2$, respectively. Their distribution function is, for given values of $m_1$ and $m_2$,

$$p(y_1, y_2|m_1, m_2) = \int \prod_i \frac{dy_i}{\sqrt{2\pi\Delta^2}} e^{-r_i^2/(2\Delta^2)} \delta \left(\sum_i x_i' - \sum_i x_i - y_i\right) \delta \left(\sum_i x_i'^2 - \sum_i x_i^2 - y_2\right)$$

$$= \frac{1}{4\pi\Delta^2 \sqrt{m_2 - m_1^2}} \exp\left(\frac{y_1^2}{2\Delta^2} - \frac{(y_2 - \Delta^2 - 2y_1m_1)^2}{8\Delta^2(m_2 - m_1^2)}\right).$$

Neglecting the variations of $m_1$ and $m_2$ of order $\Delta^2/N$ we can express the energy difference as

$$x = \frac{\tilde{K}}{2} y_2 - \tilde{H} y_1,$$

In terms of $x$ and $y = y_1$ the distribution function can be formally written as the product of two Gaussian distributions:

$$p(y_1, y_2|m_1, m_2) dy_1 dy_2 = \frac{dx}{\sqrt{2\pi\Delta^2_x}} p(x|m_1, m_2) \frac{dy}{\sqrt{2\pi\Delta^2_y}} p(y|x, m_1, m_2)$$

where

$$\pi = \Delta^2 \tilde{K}/2,$$

$$\Delta_x = \Delta^2 \tilde{K}^2 (m_2 - m_1^2) + \Delta^2 \tilde{K}^2 \left(1 - \tilde{H}/\tilde{K}\right)^2,$$

$$\pi(x) = \frac{m_1 - \tilde{H}/\tilde{K}}{m_2 - m_1^2 + \left(1 - \tilde{H}/\tilde{K}\right)^2} \frac{x - \pi}{\tilde{K}},$$

$$\Delta_y = \frac{\Delta^2 (m_2 - m_1^2)}{m_2 - m_1^2 + \left(1 - \tilde{H}/\tilde{K}\right)^2}.$$
To represent a fragile glass the dynamics that we apply to the system is a generalization of the analytic treatment of Monte Carlo dynamics introduced in [22]. Also in this generalized case the dynamical model with a contrived dynamics can be analytically solved.

We let \( \Delta^2 \), the variance of the random updating \( \{ r_i \} \), depend on the distance from the constraint, i.e., on the whole \( \{ x_i \} \) configuration before the Monte Carlo update:

\[
\Delta^2(t) \equiv 8\left[ m_2(t) - m_1^2(t) \right] \left[ \frac{B}{m_2(t) - m_1^2(t) - m_0} \right] \gamma
\]

where \( B, m_0 \) and \( \gamma \) are constants. The exponent \( \gamma \) also enter the VFTH relaxation law, as we will see later on. In literature it is usually set equal to 1, and an argument for this choice was given by Adam and Gibbs [4]. An exact explanation for it was provided by Kirkpatrick, Thirumalai and Wolynes in [27] and a further quantitative analysis is also reported in [28]. However, their studies do not exclude exponents \( \gamma > 1 \), always compatible with data, merely affecting the width of the fitting interval. Analytic approaches [29, 30] give \( \gamma = 2 \) in three dimensions. Here we consider \( \gamma \) as a model parameter, which can be chosen below, equal to, or above unity, and investigate aspects of this standard picture.

The VFTH law that we obtain is a direct consequence of the special choice (17) for the MC update. In the harmonic oscillator model and in the spherical spin model studied in [10, 15, 16], the dynamics was performed within this approach, but at fixed \( \Delta \). Both cases showed a relaxation time diverging at low temperature with an Arrhenius law, typical of strong glasses. The same is found by setting \( m_0 = 0 \) and \( \gamma = 1 \) in the present model [17] but here we want, instead, to develop a model representing a fragile glass with a Kauzmann transition at a finite temperature.

The question whether detailed balance is satisfied is also non-trivial in our model. Indeed, it happens to be satisfied for this kind of dynamics only for large \( N \). For exact detailed balance we should have

\[
p(x|m_1, m_2) \exp(-\beta x) = p(-x|m_1, m_2)
\]

but now, when we perform the inverse move \( \{ x_i' \} \rightarrow \{ x_i \} \), the probability distribution also depends on the \( \{ r_i \} \) through \( \Delta^2 \) as defined in equation (17). It can be verified that the violation is of order \( 1/N \).

The Monte Carlo equations for the dynamics of \( m_1 \) and \( m_2 \) derived from this construction read

\[
\dot{m}_1 = \int dy_1 dy_2 W(\beta x) y_1 p(y_1, y_2|m_1, m_2) = \int dx W(\beta x) \overline{\gamma}(x) p(x|m_1, m_2),
\]

\[
\dot{m}_2 = \int dy_1 dy_2 W(\beta x) y_2 p(y_1, y_2|m_1, m_2) = \frac{2}{K} \int dx W(\beta x) (x + \overline{\text{H}}(x)) p(x|m_1, m_2)
\]

4. Single-time dynamical observables

The dynamics of the system can be expressed in terms of two combinations of \( m_1 \) and \( m_2 \). The first one, defined as

\[
\mu_1 \equiv \frac{\overline{\text{H}}}{K} - m_1.
\]

represents the distance from the instantaneous equilibrium state. By instantaneous equilibrium state we mean that \( \overline{\text{H}} \) and \( K \) depend on the values of \( m_1 \) and \( m_2 \) at a given time \( t \). For \( t \rightarrow \infty \), at the true equilibrium, one has \( \mu_1 = 0 \).
The second dynamical variable is defined as the distance from the constraint (22):
\[ \mu_2 \equiv m_2 - m_1^2 - m_0. \]
When \( \mu_2 = 0 \) the constraint is reached. This will happen if the temperature is low enough (\( T \leq T_0 \)) and the time large enough. \( T_0 \) is the highest temperature at which the constraint is asymptotically (\( t \to \infty \)) reached by the system, it is identified with the Kauzmann temperature [19].

The nearer the system goes to the constraint (i.e. the smaller the value of \( m_2 - m_1^2 - m_0 \)), the larger the variance \( \Delta^2 \), implying almost always a refusal of the proposed updating. In this way, in the neighborhood of the constraint, the dynamics is very slow and goes on through very seldom but very large moves, which can be interpreted as activated processes. When the constraint is reached the variance \( \Delta^2 \) becomes infinite and the system dynamics gets stuck. The system does not evolve anymore towards equilibrium but it is blocked in one single ergodic component of the configuration space.

In terms of \( \mu_1 \) and \( \mu_2 \), the equations of motion (19), (20) become
\[
\dot{\mu}_1 = -JQ \int dx \, W(\beta x) \, x \, p(x|m_1, m_2) -(1 + QD) \int dx \, W(\beta x) \, \overline{p}(x) \, p(x|m_1, m_2),
\]
\[
\dot{\mu}_2 = \frac{2}{K} \int dx \, W(\beta x) \, xp(x|m_1, m_2) + 2\mu_1 \int dx \, W(\beta x) \, \overline{p}(x) \, p(x|m_1, m_2),
\]
where \( D \) and \( Q \) are given by
\[
D \equiv HJ + KL = \tilde{H}J + \tilde{K}L, \quad Q \equiv \frac{J^2 D}{K^3 w(w + T/2)^2}.
\]

Above \( T_0 \) ordinary equilibrium will be achieved without reaching the constraint. The temperature is, then, too high for the system to notice that there is a constraint at all on the configurations (we are speaking about the asymptotic time regime), and this implies
\[
\lim_{t \to \infty} \mu_2(t) = \overline{\mu}_2(T) = \frac{T}{K_\infty(T)} - m_0 > 0,
\]
where
\[
K_\infty(T) \equiv \lim_{t \to \infty} \tilde{K}(m_1(t), m_2(t); T) = \tilde{K}(\overline{m}_1(T), \overline{m}_2(T)).
\]

\( \overline{m}_1 \) and \( \overline{m}_2 \) are the solutions of the static self-consistent equations (11), if \( T \geq T_0 \). For \( T < T_0 \) the second equation in (11) should be replaced by
\[
\overline{m}_2 - \overline{m}_1^2 = m_0 \quad \forall T < T_0.
\]
Below \( T_0 \) the system goes to configurations arbitrarily close to the constraint, and then stay there arbitrarily long. By definition of \( T_0 \), we can write
\[
m_0 = \frac{T_0}{K_\infty(T_0)}.
\]

The equations of motion 23 and 24 can be solved in the long time regime, for fixed parameters (aging setup). We notice that the value of the VFTH exponent \( \gamma \) discriminates between different dynamic regimes if \( \gamma > 1, \gamma = 1 \) or \( 0 < \gamma < 1 \) [19] (the situation \( \gamma = 1 \) remains model dependent even in the long time limit). We find,
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to the leading orders of approximation for large times, the following behavior for \( \mu_2 \):

\[
\mu_2(t) \simeq \frac{B}{[\log(t/t_0) + c \log(\log(t/t_0))]^{1/\gamma}}.
\]  

(30)

For \( T \geq T_0 \) the parameters \( c \) and \( t_0 \) are

\[
c = \frac{1}{2}; \quad t_0 \equiv \frac{\sqrt{\pi}(1 + Q_\infty D)}{8\gamma(1 + P_\infty + Q_\infty D)}.
\]  

(31)

\( t_0 \) is of \( O(1) \) for a large range of parameters values and \( Q_\infty \) is given by equation (25) computed at \( m_1 = \overline{m}_1(T) \) and \( m_2 = \overline{m}_2(T) \). The other function of temperature appearing in the above expression, \( P_\infty \), is defined as the infinite time limit of

\[
P \equiv \frac{J^4(m_2 - m_1^2)}{2Kw(w + T/2)^2}.
\]  

(32)

That means \( P \) computed at \( m_1 = \overline{m}_1(T) \) and \( m_2 = \overline{m}_2(T) \). The solution (30) is valid in the aging regime, when \( t_0 \ll t \ll \tau_{eq}(T) \).

Below \( T_0 \) the qualitative behavior of \( \mu_2(t) \) is the same, but \( T \) is never reached. Concerning the solution (30) the only difference is in the values

\[
c = \frac{2 + \gamma}{2\gamma}; \quad t_0 \equiv \frac{B\sqrt{\pi}}{8\gamma \overline{m}_1(T) \left( \overline{K}_\infty(T) m_0 - T \right)}.
\]  

(33)

The dynamical behavior of \( \mu_1 \) depends not only on the temperature (above or below \( T_0 \)) but also on \( \gamma \) being greater, equal to or less than one. With respect to the relative weight of \( \mu_1 \) and \( \mu_2 \) we can identify different regimes\[19\]. In this presentation we just state that for the regime with \( T \geq T_0 \) and for the one with \( T < T_0 \) and \( \gamma > 1 \), \( \mu_1(t) \ll \mu_2(t) \) and a unique effective thermodynamic parameter can be properly defined in various independent ways (see next section).

What we said up to now concerns the aging regime, but, when time grows on even larger time scales, finally approaching equilibrium in the temperature regime \( T \geq T_0 \), the equations of motion for any one-time observable \( o(t) \) (magnetization, energy, distance from the constraint, etc.) take the form

\[
\dot{o}(t) \simeq -\frac{o(t)}{\tau_{eq}}.
\]  

(34)

From the study of the dynamics for very large times \[13\ 21\] we get a characteristic relaxation time to equilibrium that depends on temperature following a generalized VFTH law:

\[
\tau_{eq} \sim \exp \left( \frac{A}{T - T_0} \right)^\gamma.
\]  

(35)

When \( t \sim \tau_{eq}(T) \sim \exp [A/(T - T_0)]^\gamma \) the “distance” \( \mu_2 \) becomes,

\[
\overline{\mu}_2(T) \simeq \frac{B}{\left( \frac{A}{T - T_0} \right)^{1/\gamma}} \propto T - T_0.
\]  

(36)

The parameter \( T_0 \) in the VFTH law is identified with the Kauzmann temperature, i.e. the temperature such that \( I(T_0) \equiv I_0 \) is the minimum of the configurational entropy [and for any \( T < T_0 \) remains \( I(T) = I_0 \)]. Moreover, the specific heat
5. Effective temperature and out of equilibrium thermodynamics

In this section we introduce effective parameters in order to rephrase the dynamics of the system out of equilibrium into a thermodynamic description (for a complete derivation see [10]).

In [19] we got, through different methods, various expressions for the effective temperature $T_e$ as function of the interaction parameters of the model and of the time evolution of its observables. All of them were coinciding in the regime for $T > T_0$ and $\gamma > 1$.

We want to shortly recall one particular derivation of $T_e$. Knowing the solution of the dynamics at a given time $t$ a quasi-static approach can be followed by computing the partition function $Z_e$ of all the macroscopically equivalent states at the time $t$. In order to generalize the equilibrium thermodynamics we assume an effective temperature $T_e$ and an effective field $H_e$, and substitute the Boltzmann-Gibbs equilibrium measure by $\exp(-\mathcal{H}_{\text{eff}}\{\{x_i\}, T, H_e\}/T_e)$, where $\mathcal{H}_{\text{eff}}$ is given in (37) and the true external field $H$ has been substituted by the effective field $H_e$. As we get the expression of the “thermodynamic” potential $F_e = -T_e \log Z_e$ as a function of macroscopic variables $m_{1,2}$ and effective parameters, we can determine $T_e$ and $H_e$ minimizing $F_e$ with respect to $m_1$ and $m_2$ and evaluating the resulting analytic expressions at $m_{1,2} = m_{1,2}(t)$.

The partition function of the macroscopically equivalent states is:

$$Z_e \equiv \int \mathcal{D}x \exp \left(-\frac{1}{T_e} \mathcal{H}_{\text{eff}}\{\{x_i\}, T, H_e\} \right) \delta(Nm_1 - \sum_i x_i) \delta(Nm_2 - \sum_i x_i^2).$$

From this we build the effective thermodynamic potential as a function of $T_e$ and $H_e$, besides of $T$ and $H$, where the effective parameters depend on time through the time dependent values of $m_1$ and $m_2$, solutions of the dynamics:

$$F_e(t) = U - TS_{\text{ep}} - T_e(t)I + \left[H - H_e(t)\right]Nm_1(t),$$

with

$$T_e(t) = \tilde{K}(m_1(t), m_2(t)) [m_0 + \mu_2(t)],$$

$$H_e(t) = H - \tilde{K}(m_1(t), m_2(t)) \mu_1(t).$$

$T_e$ and $H_e$ are actually a way of describing the evolution in time of the system out of equilibrium. $U$ is the internal energy of the whole system, $S_{\text{ep}}$ is the entropy of the fast or equilibrium processes (the spherical spins) (see equation (11)) while $I$ is the entropy of the slow, ”configurational”, processes (the harmonic oscillators, see equation (13)). The last term of $F_e$ replaces the $-HNm_1$ occurring in $U$ by $-H_eNm_1$. $U$, $S_{\text{ep}}$ and $I$ are ‘state’ functions, in the sense that they depend on the state described by $T$, $T_e$, $H$ and, if needed, $H_e$. In the case where only one relevant effective parameter $T_e$ remains, these functions do not depend on the path along which its value has been reached.
As we already mentioned, for our VFTH relaxing model at $T \geq T_0$, and at $T < T_0$ with $\gamma > 1$, the effective temperature alone is enough for a complete thermodynamic description of the dominant physical phenomena ($H_e = H$).

6. Two-time variables: breaking of time-translation invariance and the fluctuation-dissipation relation

In this section we compute the correlation and response functions which, unlike the energy and the quantities $m_1(t)$ and $m_2(t)$, depend in a non-trivial way on two times, when the system is out of equilibrium, thus showing directly the loss of time translation invariance with respect to the case at equilibrium. The aim of computing such quantities is also to build a Fluctuation Dissipation relation and look at the meaning of the Fluctuation-Dissipation Ratio (FDR), $\frac{\partial_t C(t, t')}{G(t, t')}$, far from equilibrium, and to compare it with the effective temperature derived in other ways, e.g., as in [10].

The correlation functions between the thermodynamic fluctuation of a quantity $m_a(t)$ at time $t$ and that of a quantity $m_b(t')$ at a different time $t'$ are defined as

$$C_{ab}(t, t') \equiv N \langle \delta m_a(t) \delta m_b(t') \rangle, \quad a, b = 1, 2$$

where $\langle \ldots \rangle$ is the average over the dynamic processes, i.e., the harmonic oscillators.

The response of an observable $m_a$ at time $t$ to a perturbation in a conjugate field $H_b$ at some previous time $t'$ takes the form

$$G_{ab}(t, t') \equiv \frac{\delta \langle m_a(t) \rangle}{\delta H_b(t')}, \quad a, b = 1, 2$$

In our model $H_1 = H$ and $H_2 = -K/2$.

In order to be concise, in the following we will only give results without derivation; moreover, we will concentrate on the FDR for fluctuations of $\sum_i x_i = Nm_1$, coupled to the external field $H$, i.e., we only consider $a = b = 1$. For the complete derivation refer to [10].

Knowing the evolution of the two-time observables we can generalize the Fluctuation Dissipation Theorem defining another effective temperature, $T^{FD}_e$, by means of the ratio between the derivative with respect to the initial time (also called “waiting” time) $t'$ of the correlation function $C_{11}$ and the response function $G_{11}$:

$$T^{FD}_e(t, t') = \frac{\partial_t C_{11}(t, t')}{G_{11}(t, t')}.$$  

Dynamics varies strongly if $T$ is above or below the Kauzmann temperature and this difference produces different equations for the leading terms in the correlation and response functions. Therefore, we present results for the two cases separately.

6.1. High temperature case: $T > T_0$, $\forall \gamma$

First of all we define the time evolution function for the considered time-scale sector as

$$\tilde{h}(\tau) = \exp \left(-\int_0^\tau \tilde{f}(t)dt\right)$$

and the acceptance rate of the MC dynamics

$$\Upsilon = \frac{\exp (-\Gamma)}{\sqrt{2\pi T}} \frac{T_e}{2T_e - T}.$$
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In the above expression, just an abbreviation for \( \tilde{K}(m_0 + \mu_2) \), as given in equation (34). We will look at its relation with \( T_e^{FD}(t, t') \). The function \( \tilde{f} \) in equation (45) is, in this regime,

\[
\tilde{f} = -4\Upsilon \left\{ (1 + QD)\Gamma - \left[ 1 + QD - \frac{2DQ\Gamma P(1 + QD)}{1 + QD} - \frac{\Gamma P(1 + QD)}{\gamma(1 + P + QD)} \right] + O\left( \frac{1}{T} \right) \right\} \tag{47}
\]

with \( D, Q \) and \( P \) given respectively by (25) and (32).

The correlation function comes out to be

\[
C_{11}(t, t') = C_{11}(t', t) \frac{\tilde{h}(t')}{\tilde{h}(t)} + O(\mu_2^{1+\gamma} \Upsilon), \tag{48}
\]

with

\[
C_{11}(t', t') \approx \frac{m_0 + \mu_2(t')}{1 + Q(t')D}. \tag{49}
\]

Following the approach of [10] we also derive the response function:

\[
G_{11}(t, t') = G_{11}(t', t) \frac{\tilde{h}(t')}{\tilde{h}(t)} + O(\mu_2^{1+\gamma} \Upsilon), \tag{50}
\]

with

\[
G_{11}(t', t') = -\beta \int dy_1 dy_2 W'(\beta x) y_1^2 p(y_1, y_2|m_1, m_2) \tag{51}
\]

\[
= -\beta \int dx W'(\beta x) \Delta p(x|m_1, m_2) + O(\mu_2^{1+\gamma} \Upsilon)
\]

\[
= \frac{4\Upsilon(t')\Gamma(t')}{K(t')} - \frac{2\Upsilon(t')}{K(t')} + O(\mu_2 \Upsilon). \tag{52}
\]

Eventually we get

\[
T_e^{FD}(t, t') \simeq T_e(t') \left[ 1 + O(\mu_2(t')^{1+\gamma}) + O(\mu_2(t')^2) \right]. \tag{53}
\]

For \( \gamma > 1 \) this is equal to \( T_e \) in the aging regime \( (\mu_2(t')^\gamma \) goes to zero faster than \( \mu_2(t') \sim T_e(t') - T \), while as soon as the VFTH exponent equals one, the correspondence breaks down and only the asymptotic limits of the two effective temperature will be equal to each other (and to the heat bath temperature).

6.2. Low temperature case: \( T < T_0, \gamma > 1 \)

Our approach also allows us to study the regime below the Kauzmann temperature. In this last case, though, we have qualitatively different behaviors depending on the value of \( \gamma \), i.e., on the relative weight of \( \mu_1 \) and \( \mu_2 \). We describe here the case \( \gamma > 1 \), where \( \mu_1 \ll \mu_2 \).

We find the solutions of the equations for the two-time correlation functions with the following expressions for the function \( \tilde{f} \):

\[
\tilde{f} = -4\Upsilon \left\{ (1 + QD) - 8\Upsilon \frac{QDP}{1 + QD} (1 - 3r + 2r^2) \right\} + O(\mu_2 \Upsilon) \tag{54}
\]

where \( r \) is an abbreviation for the normalized difference between the effective temperature \( \tilde{h}(t') \) and the heat bath temperature

\[
r \equiv \frac{T_e - T}{2T_e - T}. \tag{55}
\]
The two-time correlation function turns out to be:

\[
C_{11}(t, t') \simeq \frac{1}{1 + Q(t')D \left[m_0 + \mu_2(t') + O(\mu_2^2(t'))\right]} \frac{\tilde{h}(t')}{\tilde{h}(t)} \quad (56)
\]

For the response function, we have

\[
G_{11}(t, t') \simeq \left[\frac{4\Upsilon(t')\Gamma(t')}{K(t')} - \frac{2\Upsilon(t')(1 - 2r(t'))^2}{K(t')} + 8\Upsilon(t')T_e(t') \left(\frac{Jr(t')Q(t')}{1 + Q(t')D}\right)^2\right] \frac{\tilde{h}(t')}{\tilde{h}(t)} \quad (57)
\]

It follows that

\[
T_e^{FD}(t, t') \simeq T_e(t') \left[1 + O(\mu_2(t')^\gamma) + O(\mu_2(t')^{1+\gamma})\right] \quad (58)
\]

In this case \(O(\mu_2^3)\) is always smaller than \(O(\mu_2)\): in the long time regime \(T_e^{FD}(t)\) coincides with \(T_e(t)\).

With this outcome we demonstrate that it is possible to identify an effective temperature that, coupled to the configurational entropy, is able to map the dynamics of a system out of equilibrium into a thermodynamic frame. In our model, either above and below the Kauzmann transition, such a construction seems to be well founded, provided that the VFTH exponent \(\gamma\) is bigger than one. In this case the time evolution is so slow that a quasi-equilibrium occur at a time dependent effective temperature. For \(\gamma\) below one, instead, the time evolution is too fast to allow for such a straightforward translation into thermodynamics.

7. Conclusions

In the present work we have been studying a particular model glass, that has all the basic attributes of a real glass and the dynamics of which can be analytically solved.

An important assumption for our study has been the decoupling of time-scales of the processes taking place in the glassy dynamics. The decoupling of time scales is also fundamental for a generalization of equilibrium thermodynamics to systems far from equilibrium.

From the temporal behavior of the slowly varying observables in the aging regime we found a VFTH relaxation time above the Kauzmann transition and we derived the Adam-Gibbs relation between the relaxation time and the configurational entropy, which can be explicitly computed for our model. It is also possible to study the dynamics of the system quenched to a temperature below the Kauzmann temperature. For such an analysis we refer to [19].

We proposed an out of equilibrium thermodynamic formulation and we tested on our exactly solvable model whether or not such a generalized approach holds, having one extra variable, namely the effective temperature, for the description of the nonequilibrium thermodynamics. By effective temperature we mean a thermodynamic quantity that would be the temperature of a system at equilibrium visiting with the same frequency the same states that the real - out of equilibrium - system at temperature \(T\) visits on a given time-scale during its dynamics. This kind of parameter appears in the thermodynamic functions together with the heat-bath temperature and the fields coupled to the system’s observables and is coupled to the configurational entropy.

Generally speaking, in order to recast the out of equilibrium dynamics into a thermodynamic frame, the history of a system that is far from equilibrium can be expressed by more than one effective parameter. This happens when more than one
long time-scale is involved in the dynamic evolution of a system. In those cases
to every time-sector there will correspond an effective temperature \( \mu_1(t) \). Moreover,
in a given time-sector, the number of effective parameters needed to make such a
translation into a thermodynamic frame can, in principle, be equal to the number of
relevant observables considered. In our model, however, for certain dynamic regimes
determined by the temperature and by the VFTH exponent \( \gamma \), the effective parameters
pertaining to processes having the same time scale become equal to each other for large
times. When the distance \( \mu_1(t) \) from equilibrium is much smaller than the distance
from the constraint, \( \mu_2(t) \), a single effective temperature alone is enough for a complete
thermodynamic description of the dominant physical phenomena; this happens when
\( \gamma > 1 \).

In many models the concept of effective temperature is used in an attempt to give
a thermodynamic description of the glassy phase. There are several analytical and
numerical works defining the effective temperature as the fluctuation dissipation ratio
(among others \([32, 33, 34]\)) and also glassy models in which the effective temperature
is measured coupling the system to a slow relaxing thermometer \([18, 35]\). Even
in granular systems such an approach is followed with some success \([36]\). However,
as far as we know, either no comparison is made between alternative (equally well
based) definitions of effective temperature or, when such a comparison is carried out,
very often no coincidence is found \([34, 37, 35]\). Nevertheless, in the \( p \)-spin model
the fluctuation-dissipation effective temperature coincides with the thermodynamic
effective temperature; both are equal to \( T/x \) where \( x \) is the break point of the Parisi
function \([38, 39]\).

This coincidence of effective temperatures for the present model (in those
parameter regions where it does take place) appears to be connected to a slow enough
relaxation dynamics. In order to understand what could happen in other models a
very general analysis should be done to identify what are the minimal requirements
to produce a thermalization of different degrees of freedom within a single time-scale
(for a contribution in this direction see, for instance, \([40]\)).

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[1] A. Barrat, R. Burioni, M. Mezard, J. Phys. A: Math. Gen. 29 (1996) 1311.
[2] J. P. Bouchaud, L. Cugliandolo, J. Kurchan, M. Mezard, in Spin Glasses and Random Fields,
A. P. Young, ed. (World Scientific, Singapore, 1998), p. 161.
[3] H. Vogel, Physik. Z. 22 (1921) 645. G.S. Fulcher, J. Am. Ceram. Soc. 8 (1925) 339. G. Tammann
and G. Hesse, Z. Anorg. Allgem. Chem. 156 (1926) 245.
[4] G. Adam and J.H. Gibbs, J. Chem. Phys. 43 (1965) 139.
[5] W. Kauzmann, Chem. Rev. 43 (1948) 219.
[6] L. F. Cugliandolo, J. Kurchan, Phys. Rev. Lett. 71 (1993) 173.
[7] A. Q. Tool, J. Am. Ceram. Soc. 29 (1946) 240.
[8] F. Sciortino, W. Kob, P. Tartaglia, Phys. Rev. Lett. 83 (1999) 3214; W. Kob, F. Sciortino, P.
Tartaglia, Europhys. Lett. 49 (1999) 590.
[9] A. Crisanti, F. Ritort, Physica A 280 (2000) 155; Europhys. Lett. 51 (2000) 147.
[10] Th.M. Nieuwenhuizen, Phys. Rev. E 61 (2000) 267
[11] Th.M. Nieuwenhuizen, J. Phys. A 31 (1998) L201; Phys. Rev. Lett. 79 (1997) 1317.
[12] S. Franz, M. A. Virasoro, J. Phys. A 33 (2000) 891.
[13] G.W. Scherer, Relaxation in Glass and Composites (Wiley, New York, 1986). S.A. Brawer,
Relaxation in Viscous Liquids and Glasses (American Ceramic Society, Columbus, OH, 1985).
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G.W. Scherer, J. Non-Cryst. Solids 123, 75 (1990). A. Prados, J. J. Brey, e-print cond-mat/0103325.

14 C.A. Angell, Science 267 (1995) 1924.
15 L.L. Bonilla, F.G. Padilla, and F. Ritort, Physica A 250 (1998) 315.
16 Th.M. Nieuwenhuizen, Phys. Rev. Lett. 80 (1998) 5580.
17 L. Leuzzi, T.M. Nieuwenhuizen, e-print cond-mat/0103147.
18 A. Garriga, F. Ritort, Eur. Phys. J. B 20 (2001) 105.
19 L. Leuzzi, T.M. Nieuwenhuizen, Phys. Rev. E 64 011508 (2001).
20 Th.M. Nieuwenhuizen, e-print cond-mat/9911052.
21 W. Kob, H.C. Andersen, Phys. Rev. E 47 (1993) 3281.
22 L.L. Bonilla, F.G. Padilla, G. Parisi, F. Ritort, Phys. Rev. B 54 (1996) 4170.
23 R. J. Glauber, J. Math. Phys., 4 (1963) 294.
24 G.H. Fredrickson and H.C. Andersen, Phys. Rev. Lett 53 (1984) 1244; J. Jackle and S. Eisinger
   Z. Phys. B 84 (1991) 115; M. Schulz, S. Trimper, Phys. Rev. B 53 (1996) 8421.
25 E. Follana, F. Ritort, Phys. Rev. B, 54 (1996) 930.
26 J. Kurchan, L. Peliti, M. Sellitto, Europhys. Lett. 39 (1997) 365.
27 T.R. Kirkpatrick, D. Thirumalai, P.G. Wolynes, Phys. Rev. A 40 (1989) 1045.
28 X. Xia and P.G. Wolynes, Proc. Natl. Acad. Sci. 97 (2000) 2990.
29 T.R. Kirkpatrick and P.G. Wolynes, Phys. Rev. B 36 (1987) 8552.
30 G. Parisi, in The Oscar Klein Centenary, U. Lindström ed., (World Scientific, Singapore, 1995);
   e-print cond-mat/9411115.
31 L. Cugliandolo, J. Kurchan, P. Le Doussal, Phys. Rev. Lett. 76 (1996) 2390.
32 R. di Leonardo, L. Angelani, G. Parisi and G. Ruocco, Phys. Rev. Lett. 84 (2000) 6054.
33 D. Alvarez, S. Franz and F. Ritort, Phys. Rev. B 54 (1996) 9756.
34 S. Franz and F. Ritort, J. Phys. A 30 (1997) L359.
35 R. Exartier and L. Peliti Eur. Phys. J. 16 (2000) 119.
36 L. Berthier, L.F. Cugliandolo and J.L. Iguain, Phys. Rev. E 63 (2001) 051302.
37 S. Fielding and P. Sollich, e-print cond-mat/0107627.
38 Th. M. Nieuwenhuizen, Phys. Rev. Lett. 79 (1997) 1317.
39 Th.M. Nieuwenhuizen, J. Phys. A 31 (1998) L201.
40 L.F. Cugliandolo, J. Kurchan and L. Peliti, Phys. Rev. E 55 (1997) 3898.