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Effective temperatures in an exactly solvable model for a fragile glass

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A model glass with facilitated dynamics is considered with one type of fast process (β type) and one type of slow process (α type). On time scales where the fast processes are in equilibrium, the slow ones have a dynamics that resembles that of facilitated spin models. The main features are the occurrence of a Kauzmann transition, a Vogel-Fulcher-Tammann-Hesse behavior for the relaxation time, an Adam-Gibbs relation between relaxation time and configurational entropy, and an aging regime. The model is such that its statics is simple and its (Monte Carlo type) dynamics is exactly solvable. The dynamics has been studied both on the approach to the Kauzmann transition and below it. In certain parameter regimes it is so slow that a quasiequilibrium occurs at a time dependent effective temperature. Correlation and response functions are also computed, as well as the out of equilibrium fluctuation-dissipation relation, showing the uniqueness of the effective temperature, thus giving support to the rephrasing of the problem within the framework of out of equilibrium thermodynamics.

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I. INTRODUCTION

A glass can be viewed as a liquid in which a huge slowing down of the diffusive motion of the particles has destroyed its ability to flow on experimental time scales. The slowing down can be expressed through the relaxation time, i.e., the characteristic time needed to have one interparticle diffusion process of a particle while it is rattling between its neighbor particles, which form a cage around it. This relaxation time is proportional to viscosity. Cooling down from the liquid phase, at some point the system falls out of equilibrium: the slow liquid degrees of freedom are no longer accessible and the relaxation time and the viscosity of the undercooled melt suddenly grow by several orders of magnitude. The temperature at which this happens is defined as the glass transition temperature T_g [1]. At T_g the heat capacity decreases in a clear way going from liquid to glassy phase, and on reheating an abrupt but different change shows up (some universal behavior in the cooling-heating process was pointed out by one of us [2,3]). Moreover, discontinuities of this kind occur also in the compressibility and the thermal expansivity. This looks similar to a continuous phase transition, even though the analogy is not perfect, because of the smeared nature of the discontinuities and because the smaller specific heat value occurs below the glass transition, rather than above, as would normally occur in mean field phase transitions.

The transition described above is not a true thermodynamic phase transition, but is strictly kinetic in origin: it takes place when the relaxation time becomes longer than the observation time and marks the transition from ergodic to nonergodic behavior. In general the location of this transition, the empirical glass transition temperature T_g, depends on the cooling rate, or more precisely on the cooling scheme. The glass transition temperature is commonly defined as the temperature where the viscosity equals 10^{13}, and the equilibration time is of the order of days. It is related to the slowest possible experiments one can realistically do. Cooling at higher rates induces a glass transition at a somewhat larger dynamical glass transition temperature.

The very slow relaxation of nonergodic systems evolving toward equilibrium structures on time scales longer than the characteristic time scales of the experiments, depending on the history of the system (e.g., on the phase space region in which the initial conditions are chosen and on the cooling rate), is the so called regime of aging dynamics [4,5].

Experimental data for the viscosity pattern of glass forming liquids are often fitted to a Vogel-Fulcher-Tammann-Hesse (VFTH) behavior [6–8], $\tau_{\text{eq}} \sim \exp[A^\gamma/(T-T_0)^\gamma]$, where the fitting parameter T_0 depends on the material and the range of temperatures in which the fit is performed. The exponent γ is usually set equal to 1, and an argument for this choice was given by Adam and Gibbs [9]. A correct explanation of this was given by Kirkpatrick, Thirumalai, and Wolynes [36], and further quantitative analysis has been recently presented in Ref. [37]. Their study, however, does not exclude an exponent $\gamma > 1$, also compatible with data, merely affecting the width of the fitting interval. Analytic approaches give $\gamma = 2$ in three dimensions [10,38]. Here we shall consider γ as a model parameter, which can be chosen below, equal to, or above unity, and investigate aspects of this standard picture.

Kauzmann [11] pointed out the paradox that the difference between the liquid entropy and the crystal entropy (i.e., the entropy of the most organized state for the system) if naively extrapolated to zero temperature would become negative at some point. To circumvent this unphysical result he proposed the occurrence of a thermodynamic phase transition at the temperature (commonly denoted by T_K) where this entropy difference vanishes. Such a thermodynamic transition would be characterized by a discontinuity of the specific heat and by the exponential divergence of the relaxation time (VFTH for fragile glasses or Arrhenius for strong ones). Connected to this last feature is the usual assumption that the fitting parameter T_0 of the VFTH law coincides with the Kauzmann temperature T_K. We note that at this phase transition the divergence of the relaxation time is not algebraic in temperature, as happens in ordinary continuous phase transitions, but is exponential, and no susceptibility diverges at the critical point.

The residual entropy, given by the difference between the entropy of the undercooled liquid and the entropy of the vibrational modes of the crystal that could in principle be formed, is usually called complexity or configurational entropy. According to standard knowledge, the Kauzmann transition should be characterized by a vanishing, or minimal, configurational entropy. This prediction is very difficult to test experimentally, since the relaxation time is too long. The existence of a Kauzmann transition was nevertheless recently supported by both analytical and numerical results [12–14]. The configurational entropy is the entropy determined by the number of states that the system at temperature $T_K < T < T_g$ can visit.

At a given dynamic critical temperature T_D, generally greater than T_g, the separation of the time scales of slow (α) and fast (β) processes starts to increase more rapidly than at higher temperature. Referring to the phase space, we can say that structures get organized at two levels: some minima of the free energy are separated by very small barriers and between them β processes take place; groups of those minima are contained in bigger basins separated by barriers requiring a much greater free energy variation to be crossed. To make the system go from a configuration in one of these basins to another configuration in another basin, i.e., to have an α process, a longer time is needed. The time scale on which these processes are happening is, however, at T_D and below (but above T_g) still very short in comparison with the observation time. In a cooling experiment the system is thus still in thermodynamic equilibrium. Going on with cooling, there is an increase in depth of the local and global minima appearing in the thermodynamic potential and corresponding to different metastable and stable states; barriers between them become higher and higher until, at the glass transition temperature T_g, some states become impossible to reach during the time scale we set for our system, i.e., the experimental time. The configurational entropy is the observable that counts the relevant states. As temperature decreases further the configurational entropy starts to decrease because there are fewer and fewer states available for the system. The Kauzmann temperature is reached when the system is stuck in one state and cannot move to any other, because, even asymptotically and even for short range systems where activated processes were present for $T_K < T < T_g$, the free energy barriers become infinite.

The configurational entropy density s_c is usually connected directly to the relaxation time through the Adam-Gibbs relation [9]: $\tau_{eq} \sim \exp(1/s_c)$.

To recapitulate we have been referring to the following different regimes for a glass former.

(1) For $T > T_D$ the system is in a disordered phase. Diffusion processes have a very short relaxation time. At very high temperature the free energy describing the system has only one global equilibrium minimum and on cooling toward the T_D temperature small local minima show up.

(2) Around T_D a dynamic transition takes place. The phase is still disordered but the number of minima of the free energy increases and some local minima become deeper: α-β bifurcation is qualitatively enhanced. In a simple mode coupling theory [15] this is the temperature T_{mc} at which a static transition is predicted with an algebraically diverging relaxation time. In the *p*-spin spin glass model [16,17] this corresponds to the dynamic critical temperature T_D at which the system goes to metastable states of energy higher than the minimum energy. For $T_g < T < T_D$ the dynamics of α processes has a huge slowing down but the temperature is high enough to reach equilibrium on the experimental time scales.

(3) Around T_g, which depends on the cooling rate, another transition takes place. Many other local minima of the free energy appear and the deepest of them, corresponding to metastable states, become ergodically separated on the time scales of the experiment. For $T_K < T < T_g$ the system has a very slow aging dynamics between the metastable states, proceeding by activated processes.

(4) At $T = T_K$ a thermodynamic phase transition shows up, with exponentially diverging relaxation time. The free energy barriers between deep local minima increase to infinity and the system gets stuck in one single minimum forever. Ergodicity is broken at any time scale. In the *p*-spin model this corresponds to the temperature at which the replica symmetry is broken [18]. The Kauzmann temperature T_K is usually assumed to coincide with the fitting parameter T_0 of the VFTH law. Below the Kauzmann temperature the system evolves only through the configurations belonging to the ergodic component of the phase space to which the dynamics brought it during the cooling.

(5) In a cooling experiment that goes below T_K, and in quenching experiments to a temperature below T_K, the aging dynamics visits only states with a free energy that is higher than the one in the static limit. The dynamics behaves as if occurring at a higher temperature.

The exponential divergence of time scale in glasses (as opposed to the algebraic divergence in standard continuous phase transitions) might induce an asymptotic decoupling of the time decades. The reasonable assumption can be made that, in a glassy system that has aged a long time *t*, all processes with equilibration time much less than *t* are in equilibrium (the β processes), 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 α processes) as the only interesting ones. Indeed, this assumption has already been tested successfully in models similar to, but even more idealized than, the one we are going to discuss in the present paper. Those models showed a glassy regime with an Arrhenius law (rather than VFTH), like the harmonic oscillator model [19,3] and the spherical spin model [2,3]. The asymptotic decoupling of time scales that is the input for the present set of models could be the basis for a generalization of equilibrium thermodynamics to systems out of equilibrium [3]. That approach involves systems where one extra variable is needed to describe the nonequilibrium physics, namely, the *effective temperature*. One of our aims will be to test this picture in an exactly solvable model glass; we shall see that there are domains where it does apply (namely, when the VFTH exponent γ exceeds unity) and where it does not apply (namely, when $\gamma \leqslant 1$). In this last case two extra variables will be needed, making compulsory the introduction of an *effective field*, in addition to the effective temperature.

In the present paper we are going to investigate an exactly solvable model with facilitated dynamics glass that shows all of the features that we recalled above for the much more complicated real glasses. For other examples of models built with a facilitated dynamics, see Refs. [23,24]. The model is introduced in Sec. II. It is built by processes evolving on two different, well separated time scales, representing the α and β processes taking place in real glassy materials. In Sec. III we introduce the dynamics that we apply to the model and we show the dynamic behavior in the aging regime. We can implement the dynamics even below the Kauzmann temperature, thus getting insight into a regime where few analytic results are known. Even though the physics of our model is simple, we shall find general aspects of the results by formulating them in the thermodynamic language. One of the most important points is that the configurational entropy, which we will denote by $\mathcal{I}$, is exactly computable (see Secs. II and IV) as a function of the dynamic variables of the model.

From the study of the dynamics (Secs. III and IV) it turns out that the system relaxes to equilibrium with a characteristic time that depends on temperature following a generalized VFTH law:

$$\tau_{eq} \sim \exp\left(\frac{A}{T-T_0}\right)^{\gamma}. \tag{1.1}$$

We will often refer to γ as the VFTH exponent.

As we show in Sec. IV, the parameter T_0 in the VFTH law is identified with the Kauzmann temperature, i.e., the temperature such that $\mathcal{I}(T_0) \equiv \mathcal{I}_0$ is the minimum of the configurational entropy [and for any $T<T_0$ $\mathcal{I}(T)=\mathcal{I}_0$]. Moreover, the specific heat displays a discontinuity at T_0; at that temperature the model thus indicates a real thermodynamic phase transition. In Sec. IV B the Adam-Gibbs relation between relaxation time and configurational entropy density is achieved, in the form

$$\tau_{eq} \sim \exp\left(\frac{N}{\mathcal{I}-\mathcal{I}_0}\right)^{\gamma}. \tag{1.2}$$

The study of single-time variable dynamics, in Sec. III, and of two-time variables, in Sec. V, reveals that the value of the VFTH exponent γ discriminates between different dynamics regimes. One of our results is indeed that three qualitatively different dynamic regimes arise, respectively, for $\gamma>1$, $0<\gamma<1$, and $\gamma=1$, the last of which is even model dependent. For $\gamma>1$ it is, however, possible to rephrase the asymptotic dynamics of the model into an out of equilibrium thermodynamics, using one extra thermodynamic parameter only, the effective temperature.

The phrasing of the dynamic properties in terms of a generalized out of equilibrium thermodynamic framework is carried out in Sec. IV, where we introduce effective parameters to take into account the history of the system.

In Sec. V we study two-time observables, such as correlation functions and response functions, and we look at the fluctuation-dissipation ratio out of equilibrium [20]. It coincides with the effective temperature independently found in Sec. IV.

II. MODEL

The model we study, introduced in [21], is described by the local Hamiltonian

$$\mathcal{H}[\{x_i\},\{S_i\}] = \frac{1}{2}K\sum_{i=1}^{N} x_i^2 - H\sum_{i=1}^{N} x_i - J\sum_{i=1}^{N} x_i S_i - L\sum_{i=1}^{N} S_i, \tag{2.1}$$

where N is the size of the system and $\{x_i\}$ and $\{S_i\}$ are continuous variables, the last satisfying a spherical constraint $\Sigma_i S_i^2 = N$. We will call them from now on harmonic oscillators and spherical spins, respectively. 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 $\{S_i\}$, and L is the external field acting on the spherical spins. As we will see in this paper the simple local form of Eq. (2.1) allows us to introduce an analytically solvable dynamics with glassy behavior.

In our simple model we introduce by hand a separation of time scales where the spins represent the fast modes and the harmonic oscillators the slow ones. Separation of time scales is one of the most important and most general characteristics that glasses are supposed to have. Indeed, we assume that the $\{S_i\}$ evolve with time on a much shorter time scale than that of the harmonic oscillators. From the point of view of the spins the $\{x_i\}$ are quenched random variables and the combination Jx_i can be seen as a random field exerted on spin i. On the other hand, 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 $\{x_i\}$ system we can average over this noise by performing the computation of the $\{S_i\}$ partition function, yielding an effective Hamiltonian depending only on the $\{x_i\}$, which will determine the dynamics of these variables.

Summing out fast variables is a standard technique in physics. For instance, in any Landau-Ginzburg-Wilson theory there occur coefficients of which the temperature dependence arises from summing out fast processes. We now do the same in our model.

We perform the spin integration in the partition function using the saddle point approximation for large N and we get

$$\begin{aligned} Z_S(\{x_i\}) &= \int \left(\prod_{i=1}^{N} dS_i\right) \exp\{-\beta\mathcal{H}[\{x_i\},\{S_i\}]\} \\ &\quad \times \delta\left(\sum_{i=1}^{N} S_i^2 - N\right) \\ &\simeq \exp\left[-\beta N\left(\frac{K}{2}m_2 - Hm_1 - w + \frac{T}{2}\ln\frac{w+T/2}{T}\right)\right] \end{aligned} \tag{2.2}$$

with $\beta = 1/T$ and where we introduced the short hand notations

$$m_1 \equiv \frac{1}{N}\sum_{i=1}^{N} x_i, \quad m_2 \equiv \frac{1}{N}\sum_{i=1}^{N} x_i^2, \tag{2.3}$$

and

$$w\equiv\sqrt{J^2m_2+2JLm_1+L^2+\frac{T^2}{4}}. \tag{2.4}$$

We can define the effective Hamiltonian

$$\mathcal{H}_{\rm eff}(\{x_i\})\equiv -T\ln Z_S(\{x_i\}),$$

obtaining

$$\mathcal{H}_{\rm eff}(\{x_i\})=\frac{K}{2}m_2N-Hm_1N-wN+\frac{TN}{2}\ln\frac{w+T/2}{T}. \tag{2.5}$$

This can also be written in terms of the internal energy $U(\{x_i\})$ and of the entropy of the equilibrium processes (i.e., the spins) $S_{\rm ep}(\{x_i\})$:

$$\mathcal{H}_{\rm eff}(\{x_i\})=U(\{x_i\})-TS_{\rm ep}(\{x_i\}), \tag{2.6}$$

$$U(\{x_i\})=N\left[\frac{K}{2}m_2-Hm_1-w+\frac{T}{2}\right], \tag{2.7}$$

$$S_{\rm ep}(\{x_i\})=\frac{N}{2}\left[1-\ln\frac{w+T/2}{T}\right], \tag{2.8}$$

and it can indeed be verified that U is the Hamiltonian averaged over the spins and that $S_{\rm ep}$ is the entropy of the spins.

Another fundamental ingredient for the model is the introduction of a constraint on the phase space to avoid the existence of a single global minimum, thus 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

$$m_2-m_1^2\geqslant m_0, \tag{2.9}$$

where m_0 is a fixed, but arbitrary, strictly positive constant. The model glass now obtained has no crystalline state. 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 B_2O_3 and SiO_2, molecular organics such as glycerol and atactic polystyrene, and different multicomponent liquid mixtures). These are substances for which there are noncrystalline 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 [22].

As we will explain in detail in the next section, we impose a dynamics that satisfies this constraint and couples the otherwise noninteracting $\{x_i\}$ in a dynamic way.

To shorten the notation for later purposes we define here the modified ‘‘spring constant’’ $\widetilde{K}$ and ‘‘external field’’ $\widetilde{H}$:

$$\widetilde{K}=K-\frac{J^2}{w+T/2},\quad \widetilde{H}=H+\frac{JL}{w+T/2}. \tag{2.10}$$

We stress that $\widetilde{K}$ and $\widetilde{H}$ are actually functions of the $\{x_i\}$ themselves (through m_1 and m_2 which occur in w). We also define the constant

$$D\equiv HJ+KL. \tag{2.11}$$

Recalling the definitions (2.10) it is useful to note that

$$\widetilde{H}J+\widetilde{K}L=HJ+KL=D. \tag{2.12}$$

Statics

The partition function of the whole system at equilibrium is

$$\begin{aligned}Z(T)&=\int \mathcal{D}x\mathcal{D}S\,\exp[-\beta\mathcal{H}(\{x_i\},\{S_i\})]\,\delta\left(\sum_i S_i^2-N\right)\\ &=\int dm_1dm_2\,\exp\left\{-\beta N\left[\frac{K}{2}m_2-Hm_1-w\right.\right.\\ &\quad\left.\left.+\frac{T}{2}\ln\left(\frac{w+T/2}{T}\right)-\frac{T}{2}[1+\ln(m_2-m_1^2)]\right]\right\}.\end{aligned} \tag{2.13}$$

The additional object that appears in the exponent is the contribution to the entropy of the $\{x_i\}$ configurations:

$$\mathcal{I}\equiv\frac{N}{2}[1+\ln(m_2-m_1^2)]. \tag{2.14}$$

It is the expression for the configurational entropy, which will be widely discussed in Sec. IV after having introduced the dynamics. It comes from the Jacobian $e^{\mathcal{I}}$ of the transformation of variables $\mathcal{D}x\to dm_1dm_2$ [see Eq. (2.3)]. We can compute the large N limit of this partition using once again the saddle point approximation. The saddle point equations are found by minimizing with respect to m_1 and m_2 the function

$$\begin{aligned}\frac{\beta}{N}F(T,m_1,m_2)\equiv{}&\frac{1}{T}\left(\frac{K}{2}m_2-Hm_1-w\right)\\ &+\frac{1}{2}\left[\ln\frac{w+T/2}{T}-1-\ln(m_2-m_1^2)\right].\end{aligned} \tag{2.15}$$

Denoting the saddle point values of m_1 and m_2 as $\overline{m}_1$ and $\overline{m}_2$ the equations are

$$\overline{m}_1=\frac{\widetilde{H}(\overline{m}_1,\overline{m}_2)}{\widetilde{K}(\overline{m}_1,\overline{m}_2)}, \tag{2.16}$$

$$\overline{m}_2=\overline{m}_1^2+\frac{T}{\widetilde{K}(\overline{m}_1,\overline{m}_2)}. \tag{2.17}$$

The form of the solutions $\overline{m}_1(T)$, $\overline{m}_2(T)$ is quite complicated because each of these equations is actually a fourth order equation, but they can be explicitly computed. In terms of the equilibrium values $\overline{m}_k$ we find the following expression for the equilibrium free energy density:

$$
\begin{aligned}
F(T,\overline{m}_1(T),\overline{m}_2(T)) = {} & N\left[\frac{K}{2}\overline{m}_2 - H\overline{m}_1 - w(\overline{m}_1,\overline{m}_2)\right] \\
& + \frac{TN}{2}\left[\ln\frac{w(\overline{m}_1,\overline{m}_2)+T/2}{T} - 1 - \ln[\overline{m}_2 - (\overline{m}_1)^2]\right] \qquad (2.18) \\
= {} & U(T,\overline{m}_1,\overline{m}_2) - TS_{\text{ep}}(T,\overline{m}_1,\overline{m}_2) - T\mathcal{I}(T,\overline{m}_1,\overline{m}_2). \qquad (2.19)
\end{aligned}
$$

For the Hessian of $\beta F(T,m_1,m_2)/N$ we find the following expressions:

$$
\mathbf{H} \equiv \beta \begin{pmatrix} \dfrac{J^2L^2}{w(w+T/2)^2} + T\dfrac{m_2+m_1^2}{(m_2-m_1^2)^2} & \dfrac{J^3L}{2w(w+T/2)^2} - T\dfrac{m_1}{(m_2-m_1^2)^2} \\ \dfrac{J^3L}{2w(w+T/2)^2} - T\dfrac{m_1}{(m_2-m_1^2)^2} & \dfrac{J^4}{4w(w+T/2)^2} + \dfrac{T}{2}\dfrac{1}{(m_2-m_1^2)^2} \end{pmatrix} \qquad (2.20)
$$

$$
= \beta\frac{J^2}{2w(w+T/2)^2}\begin{pmatrix} 2L^2 & JL \\ JL & \dfrac{J^2}{2} \end{pmatrix} + \frac{1}{(m_2-m_1^2)^2}\begin{pmatrix} m_2+m_1^2 & -m_1 \\ -m_1 & \dfrac{1}{2} \end{pmatrix} \qquad (2.21)
$$

$$
= \text{Hessian of } \beta\mathcal{H}_{\text{eff}}(m_1,m_2) \; - \; \text{Hessian of } \mathcal{I}(m_1,m_2). \qquad (2.22)
$$

The determinant of the Hessian of $\beta F(T,m_1,m_2)/N$, computed at equilibrium, is

$$
\det(\mathbf{H}) = \frac{1}{2(\overline{m}_2 - \overline{m}_1^2)^3}(1 + Q_\infty D + P_\infty), \qquad (2.23)
$$

which is always positive. In the formula above we introduced the abbreviations

$$
Q \equiv \frac{J^2(HJ+KL)}{\tilde{K}^3 w(w+T/2)^2}, \quad Q_\infty \equiv Q(\overline{m}_1,\overline{m}_2), \qquad (2.24)
$$

$$
P \equiv \frac{J^4(m_2-m_1^2)}{2\tilde{K}w(w+T/2)^2}, \quad P_\infty \equiv P(\overline{m}_1,\overline{m}_2), \qquad (2.25)
$$

which we will often use in the following. The inverse matrix turns out to be

$$
\mathbf{C} \equiv \mathbf{H}^{-1} = -\frac{\overline{m}_2 - \overline{m}_1^2}{1 + Q_\infty D + P_\infty} \times \begin{pmatrix} 1 + P_\infty & 2\overline{m}_1 - 2\dfrac{L}{J}P_\infty \\ 2\overline{m}_1 - 2\dfrac{L}{J}P_\infty & 4\overline{m}_1^2 + 2(\overline{m}_2 - \overline{m}_1^2) + 4\dfrac{L^2}{J^2}P_\infty \end{pmatrix}. \qquad (2.26)
$$

The elements of this matrix are the thermodynamic averages of the fluctuations of m_1 and m_2 around their equilibrium values $\overline{m}_1$, $\overline{m}_2$, times a factor N, as we can immediately check by expanding F to the second order around $\overline{m}_1$ and $\overline{m}_2$ in Eq. (2.13). This holds for temperatures high enough that, asymptotically, the constraint (2.9) plays no role.

III. ANALYTICALLY SOLVABLE MONTE CARLO DYNAMICS WITH GLASSY ASPECTS

We assume as the dynamics a generalization of previously introduced parallel Monte Carlo dynamics for the harmonic oscillators. This kind of analytic Monte Carlo approach was first introduced in [23], and later applied in [19] to the simpler, exactly solvable harmonic oscillator model (which is just our model after setting $J=L=0$) and by one of us [2,3] also for a spherical spin model (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 not only programmable on a computer, but even solvable analytically, which yields a much deeper insight into its properties. 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 statics.

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 Δ^2. We indicate by x (without any subscript) the energy difference between the new and the old states, viz., $x \equiv \mathcal{H}(\{x_i'\}) - \mathcal{H}(\{x_i\})$. If the energy of the new configuration is higher than the energy of the initial configuration ($x>0$) the move is accepted with a probability $W(\beta x)\equiv\exp(-\beta x)$; if the new energy is lower or equal ($x\leqslant 0$) it is always accepted $[W(\beta x)=1]$.

The updating is parallel and it is this particular feature that gives the collective behavior leading to exponentially divergent time scales in a model with no interactions between particles such us ours. A sequential updating would not produce any glassy effect. In this sense there is an analogy with facilitated Ising models [24], and with the kinetic lattice-glass model with contrived dynamics of Kob and Andersen [25], where the transition probabilities depend on the neighboring configuration; this dynamics may induce glassy behavior in situations where ordinary Glauber dynamics [26] would not. Models of these types may give valuable insights into the long time dynamics, at least within a class that exhibits some long time universality.

In a Monte Carlo step the quantities $Nm_1=\Sigma_i x_i$ and $Nm_2=\Sigma_i x_i^2$ are updated. Let us denote their changes by y_1 and y_2, respectively. Following [3] we get the distribution function of y_1 and y_2, for given values of m_1 and m_2:

$$\begin{aligned}
p(y_1,y_2|m_1,m_2)\equiv&\int\prod_i\frac{dr_i}{\sqrt{2\pi\Delta^2}}\exp\left(-\frac{r_i^2}{2\Delta^2}\right)\\
&\times\delta\left(\sum_i x_i'-\sum_i x_i-y_1\right)\\
&\times\delta\left(\sum_i x'^2_i-\sum_i x_i^2-y_2\right)\\
=&\frac{1}{4\pi\Delta^2\sqrt{m_2-m_1^2}}\\
&\times\exp\left(-\frac{y_1^2}{2\Delta^2}-\frac{(y_2-\Delta^2-2y_1m_1)^2}{8\Delta^2(m_2-m_1^2)}\right).
\end{aligned}\tag{3.1}$$

We can express the energy difference as

$$x=\frac{\tilde{K}}{2}y_2-\tilde{H}y_1,\tag{3.2}$$

upon neglecting the variations of m_1 and m_2 that are of order $(y_k/N)^2\sim\Delta^2/N$.

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

$$\begin{aligned}
&p(y_1,y_2|m_1,m_2)dy_1dy_2\\
&\quad=p(x|m_1,m_2)p(y|x,m_1,m_2)dxdy\\
&\quad=\frac{1}{\sqrt{2\pi\Delta_x}}\exp\left(-\frac{(x-\overline{x})^2}{2\Delta_x}\right)\\
&\quad\quad\times\frac{1}{\sqrt{2\pi\Delta_y}}\exp\left(-\frac{[y-\overline{y}(x)]^2}{2\Delta_y}\right)dxdy,
\end{aligned}\tag{3.3}$$

where

$$\overline{x}=\Delta^2\tilde{K}/2,\tag{3.4a}$$

$$\Delta_x=\Delta^2\tilde{K}^2(m_2-m_1^2)+\Delta^2\tilde{K}^2(m_1-\tilde{H}/\tilde{K})^2,\tag{3.4b}$$

$$\overline{y}(x)=\frac{m_1-\tilde{H}/\tilde{K}}{m_2-m_1^2+(m_1-\tilde{H}/\tilde{K})^2}\,\frac{x-\overline{x}}{\tilde{K}},\tag{3.5a}$$

$$\Delta_y=\frac{\Delta^2(m_2-m_1^2)}{m_2-m_1^2+(m_1-\tilde{H}/\tilde{K})^2}.\tag{3.5b}$$

The variance of the randomly chosen updating $\{r_i\}$ of the slow variables was a constant in previous approaches [19,2,3,23]. That was enough to cause an Arrhenius relaxation of the glass. To find a VFTH-like relaxation, in the present model we let Δ^2 depend on the distance to the constraint, i.e., on the whole $\{x_i\}$ configuration before the Monte Carlo step:

$$\Delta^2(t)\equiv 8[m_2(t)-m_1^2(t)]\left(\frac{B}{m_2(t)-m_1^2(t)-m_0}\right)^{\gamma},\tag{3.6}$$

where B is a constant and γ is an exponent larger than zero that we discussed already as being used in practice to make the best VFTH-type fitting of the relaxation time in experiments [1,28]. In our model γ is a constant; it has no prescribed value since we do not make any connection with a microscopic system. In the standard VFTH law one would just take $\gamma=1$. One of our results will be to see that there are three qualitatively different regimes $\gamma>1$, $\gamma=1$, and $0<\gamma<1$, showing that the situation $\gamma=1$ is actually nongeneric.

We also define a quantity that we shall frequently encounter in the following:

$$\Gamma(t)\equiv\left(\frac{B}{m_2(t)-m_1^2(t)-m_0}\right)^{\gamma}.\tag{3.7}$$

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 becomes, thus 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 rare but very large moves, a thing that can be interpreted as activated dynamics. When the constraint is reached Γ becomes infinite and the system dynamics is stuck forever. The system no longer evolves toward equilibrium but is blocked in one single ergodic component of the configuration space. At large enough temperatures, the combination $m_2(t)-m_1^2(t)-m_0$ will remain strictly positive. The highest temperature T_0 at which it can vanish for $t\rightarrow\infty$ is identified with the Kauzmann temperature T_K (see Sec. IV A).

The question whether detailed balance is satisfied or not is also nontrivial 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

$$p(x|m_1,m_2)\exp(-\beta x)=p(-x|m_1,m_2) \tag{3.8}$$

but now, when we perform the inverse move $\{x_i'\}\rightarrow\{x_i\}$, the probability distribution also depends on the $\{r_i\}$ through Δ^2 as defined in Eq. (3.6). Thus the right hand side of the detailed balance consists of $p(-x|m_1',m_2';\Delta'^2)\neq p(-x|m_1,m_2;\Delta^2)$. Expanding this probability distribution in powers of $1/N$, however, we get that $p(-x|m_1',m_2';\Delta'^2) = p(-x|m_1,m_2;\Delta^2)+O(\Delta^2/N)$. Terms of $O(\Delta^2/N)$ were already neglected in the approximation of x done in Eq. (3.2). So, inasmuch as the whole approach is valid only for $N\rightarrow\infty$, detailed balance is also satisfied; it would be slightly violated in a finite N simulation. We work at very large N and, even though $\Delta^2\propto\Gamma(t)$ grows as the system approaches equilibrium (it even diverges at the Kauzmann temperature), we perform first the thermodynamic limit computing the dynamics equation and only eventually the limit $t\rightarrow\infty$. If we did the opposite there would be a region around the Kauzmann temperature where the detailed balance is violated and the dynamics is not the one discussed here. However, this is not our aim since we are interested in the ergodicity breaking that takes place in systems with a large number (Avogadro-like) of variables.

In the harmonic oscillator model and in the spherical spin model studied in [19,2,3], the dynamics was performed within this approach, but at fixed Δ. Both cases showed a relaxation time diverging at low temperature with an Arrhenius law, typical of *strong* glasses. We could also study enhanced Arrhenius law by setting $m_0=0$ in the present model (look at [27] for the study of such a model) but here we want, instead, to develop a model representing a *fragile* glass with a Kauzmann transition at a finite temperature.

The Monte Carlo equations for the dynamics of m_1 and m_2 can now be derived along the lines of [3]. They read

$$\begin{aligned}\dot{m}_1&=\int dy_1dy_2W(\beta x)y_1p(y_1,y_2|m_1,m_2)\\&=\int dxW(\beta x)\overline{y}(x)p(x|m_1,m_2),\end{aligned} \tag{3.9}$$

$$\begin{aligned}\dot{m}_2&=\int dy_1dy_2W(\beta x)y_2p(y_1,y_2|m_1,m_2)\\&=\frac{2}{\tilde{K}}\int dxW(\beta x)[x+\tilde{H}\overline{y}(x)]p(x|m_1,m_2).\end{aligned} \tag{3.10}$$

Before performing a study of the dynamics we define two new variables μ_1 and μ_2 depending on m_1 and m_2 and representing, respectively, the deviation from the equilibrium state and the distance from the constraint:

$$\mu_1\equiv\frac{\tilde{H}}{\tilde{K}}-m_1, \tag{3.11}$$

$$\mu_2\equiv m_2-m_1^2-m_0. \tag{3.12}$$

When $\mu_2=0$, the constraint is reached. This will happen if the temperature is low enough $(T\leqslant T_0)$. T_0 is the highest temperature at which the constraint is finally reached by the system. Above T_0 equilibrium will be achieved without reaching the constraint. The temperature is too high for the system to notice at all that there is a constraint on the configurations:

$$\lim_{t\rightarrow\infty}\mu_2(t)=\overline{\mu}_2(T)>0. \tag{3.13}$$

At and below T_0 the system goes to configurations that become arbitrarily close to the constraint, and then stays there for arbitrarily long times.

When $\mu_1=0$ equilibrium is obtained and the equilibrium values of m_1 and m_2 are given by the solution of the equations

$$\frac{\tilde{H}(\overline{m}_1,\overline{m}_2)}{\tilde{K}(\overline{m}_1,\overline{m}_2)}=\overline{m}_1, \tag{3.14}$$

$$\overline{m}_2-\overline{m}_2^2=\frac{T}{\tilde{K}(\overline{m}_1,\overline{m}_2)}\,\theta(T-T_0)+m_0\theta(T_0-T). \tag{3.15}$$

$\theta(T)$ is the Heaviside step function.

For $T\geqslant T_0$, these are the saddle point equations (2.16),(2.17), with $\overline{m}_k$ denoting the equilibrium value of m_k. When T reaches the value $T_0=m_0\tilde{K}(T_0)$, set by the constraint (2.9), the combination $\overline{m}_2-\overline{m}_2^2$ becomes, for $t\rightarrow\infty$, independent of temperature: it remains equal to m_0 for all $T<T_0$.

When all system parameters are fixed (aging setup) the equations of motion (3.9),(3.10) become, in terms of μ_1 and μ_2,

$$\begin{aligned}\dot{\mu}_1=&-JQ\int dxW(\beta x)xp(x|m_1,m_2)\\&-(1+QD)\int dxW(\beta x)\overline{y}(x)p(x|m_1,m_2),\end{aligned} \tag{3.16}$$

$$\begin{aligned}\dot{\mu}_2=&\frac{2}{\tilde{K}}\int dxW(\beta x)xp(x|m_1,m_2)\\&+2\mu_1\int dxW(\beta x)\overline{y}(x)p(x|m_1,m_2),\end{aligned} \tag{3.17}$$

where we have used D and Q defined, respectively, in Eqs. (2.11) and (2.24).

We also shorten the expression $\tilde{K}(m_2-m_1^2)$ by the parameter

$$T_e\equiv\tilde{K}(m_2-m_1^2), \tag{3.18}$$

possibly depending on time through $m_1(t)$ and $m_2(t)$. For the moment this is just an abbreviation but in the next section we will show that an alternative description of the dynamics is possible where $T_e(t)$ turns out to be a mapping of the history of the system into an effective thermodynamic parameter. This effective temperature would be the temperature of a system at equilibrium visiting with the same frequency the same states that the actual—out of equilibrium—system at temperature T visits on a given time scale during its dynamics.

In the time regime where $\Gamma \gg x^2/T_e^2 \sim O(1)$ [i.e., $\mu_2(t) \ll 1$], the Gaussian distribution of the x can be approximated by

$$p(x|m_1,m_2) \simeq \frac{\exp(-\Gamma)}{4T_e\sqrt{\Gamma\pi}}\exp\left(\frac{x}{2T_e}\right)\times\left(1-\frac{x^2}{16T_e^2\Gamma}+\frac{x^4}{512T_e^4\Gamma^2}\right) \quad (3.19)$$

and Eqs. (3.16) and (3.17) become

$$\dot{\mu}_1 = 4\Upsilon\left[JQ\tilde{K}(m_0+\mu_2)r\left(1-\frac{3(1-2r+2r^2)}{\Gamma}\right) - \mu_1(1+QD)[\Gamma-(1-3r+4r^2)]\right], \quad (3.20)$$

$$\dot{\mu}_2 = -4\Upsilon\left[2(m_0+\mu_2)r\left(1-\frac{3(1-2r+2r^2)}{\Gamma}\right) - \mu_1^2[\Gamma-(1-3r+4r^2)]\right], \quad (3.21)$$

where r is the normalized difference between the parameter T_e and the heat-bath temperature T,

$$r \equiv \frac{T_e-T}{2T_e-T}, \quad (3.22)$$

and

$$\Upsilon \equiv \frac{\exp(-\Gamma)}{\sqrt{\pi\Gamma}}(1-r). \quad (3.23)$$

Υ is the leading term of the expansion of the integral representing the acceptance rate of the Monte Carlo dynamics,

$$\int dxW(\beta x)p(x|m_1,m_2) \simeq \frac{\exp(-\Gamma)}{\sqrt{\pi\Gamma}}(1-r)\times\left[1-\frac{1}{2\Gamma}(1-2r+4r^2)+O(\mu_2^{2\gamma})\right]. \quad (3.24)$$

The solutions to Eqs. (3.20) and (3.21) depend on the relative sizes of μ_1 and μ_2, and thus also on γ, as well as on r, which has a different behavior above T_0, where T_e tends to T in the infinite time limit, and below, where T_e never equals the heat-bath temperature (see Sec. IV A).

The solution to Eq. (3.21) can be easily found by neglecting the second term, proportional to μ_1^2. It is expressed in the implicit form

$$2\pi\frac{\text{erf}[i\sqrt{\Gamma(t)}]}{i}-2\frac{\exp[\Gamma(t)]}{\Gamma(t)^{1/\gamma}}=\frac{8r_1m_0\gamma}{\pi}t+\text{const}, \quad (3.25)$$

where

$$\text{erf}(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{-t^2}dt. \quad (3.26)$$

To second order approximation this can be written as

$$\mu_2(t) \simeq \frac{1}{\{\ln(t/t_0)+c\ln[\ln(t/t_0)]\}^{1/\gamma}}. \quad (3.27)$$

The constants t_0 and c depend on the temperature phase as will be clarified in the following.

To study the case above T_0, we also introduce the variable

$$\delta\mu_2(t) \equiv \mu_2(t)-\overline{\mu_2} \quad (3.28)$$

where $\overline{\mu_2}$ is defined in Eq. (3.13). Since in this range of temperature $T_e(t)-T\sim\delta\mu_2(t)$, the first order expansion of r is

$$r \simeq \frac{\delta\mu_2(t)}{m_0+\overline{\mu_2}(T)}\left(1+\frac{P_\infty}{1+Q_\infty D}\right) - \mu_1(t)\frac{2P_\infty D}{J\tilde{K}_{eq}[m_0+\overline{\mu_2}(T)](1+Q_\infty D)}, \quad (3.29)$$

where P_∞ and Q_∞ were introduced, together with P and Q, in Eqs. (2.25) and (2.24) and, from a dynamical point of view, they are nothing other than

$$Q_\infty = \lim_{t\to\infty}Q, \quad P_\infty = \lim_{t\to\infty}P. \quad (3.30)$$

In this case in Eq. (3.27) c is equal to 1/2 and the expression for t_0 in terms of the parameters of the model is

$$t_0 \equiv \frac{\sqrt{\pi}(1+Q_\infty D)}{8\gamma(1+P_\infty+Q_\infty D)}. \quad (3.31)$$

Below T_0 the qualitative behavior of $\mu_2(t)$ (in this case the $\overline{\mu_2}$ part is zero) is the same, but T is never reached. This implies that r goes to some asymptotic constant r_∞. Concerning the solution (3.27) the only difference is in the values

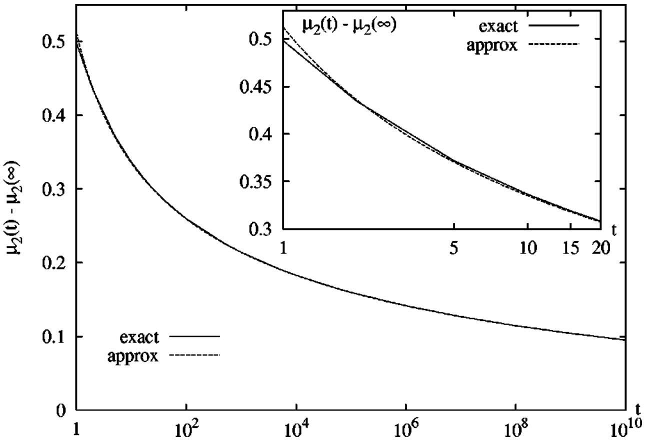

FIG. 1. The difference between $\mu_2(t)$ and its asymptotic value $\overline{\mu_2}$ is plotted for heat-bath temperature $T=0.41$, slightly above the Kauzmann temperature $T_0=4.002\,48$. At this temperature $\overline{\mu_2}=0.097\,63$. The case is plotted with $K=J=1$, $H=L=0.1$, $m_0=5$, $B=1$, and $\gamma=2$. The ‘‘exact’’ curve represents the exact solution (3.25), with initial condition $\Gamma(0)=1$. The ‘‘approx’’ curve is a plot of the approximated solution (3.27). In the inset the initial behavior is shown: clearly the approximation (3.27) is very good already after two decades of the dynamics.

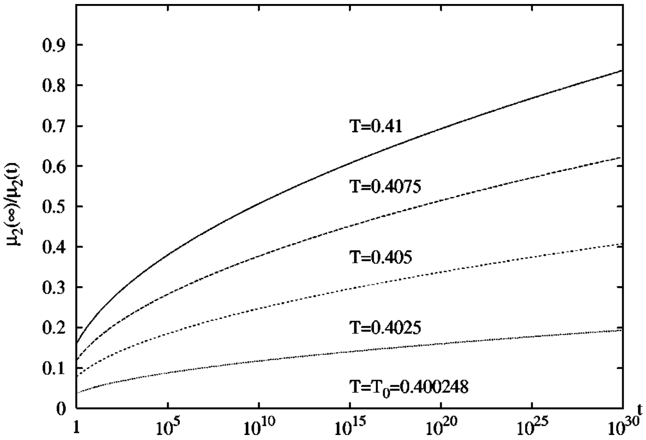

FIG. 2. Ratio of $\overline{\mu_2}/\mu_2(t)$ at different temperatures, at and above the Kauzmann temperature. Too far away from T_0 the contribution of $\overline{\mu_2}$ to $\mu_2(t)$ becomes relevant at shorter time decades. The case is plotted with $K=J=1$, $H=L=0.1$, $m_0=5$, and with a VFTH exponent $\gamma=2$. For this set of parameters the Kauzmann temperature turns out to be $T_0=4.002\,48$.

$$c=\frac{2+\gamma}{2\gamma},\quad t_0\equiv\frac{B\sqrt{\pi}}{8m_0\gamma r_\infty(1-r_\infty)}. \tag{3.32}$$

In Fig. 1 we show the exact solution, numerically computed, of Eq. (3.21) for a particular choice of the parameter values, $K=J=1$, $H=L=0.1$, $m_0=5$, $B=1$, $\gamma=2$. We can see that after a couple of decades the behavior is that given in Eq. (3.27).

The ratio of Eqs. (3.20) and (3.21) gives the equation

$$\frac{d\mu_1}{d\mu_2}=\frac{\mu_1(1+QD)(\Gamma+2-3r+2r^2)-JQT_e r}{2r(m_0+\mu_2)-\mu_1^2(\Gamma+2-3r+2r^2)}. \tag{3.33}$$

With respect to the relative weights of μ_1 and μ_2 we can identify different regimes, where the solution has different behaviors.

(1) $T>T_0$. The leading term of the solution is given by the stationary solution. We can also neglect the term of $O(\mu_1^2\Gamma)$ in the denominator. Using the expansion (3.29) for r we get

$$r\simeq\frac{1}{m_0+\overline{\mu_2}}\,\frac{1+P_\infty+Q_\infty D}{1+Q_\infty D}\,\delta\mu_2 \tag{3.34}$$

and

$$\mu_1(t)=\frac{TJQ_\infty(1+P_\infty+Q_\infty D)}{(m_0+\overline{\mu_2})(1+Q_\infty D)^2}\,\frac{\delta\mu_2(t)}{\overline{\Gamma}}+O(\delta\mu_2^2)+O(\delta\mu_2^{2\gamma+1}). \tag{3.35}$$

Here we have also expanded $\Gamma(t)$ as

$$\Gamma(t)=\overline{\Gamma}-\gamma\overline{\Gamma}\frac{\delta\mu_2(t)}{\overline{\mu_2}} \tag{3.36}$$

with $\overline{\Gamma}\equiv\lim_{t\to\infty}\Gamma(t)$. We are most interested in what happens next to the Kauzmann temperature, i.e., for very big $\overline{\Gamma}$, at long but not extremely long times, which means $\delta\mu_2(t)$ is small but not vanishing. A more detailed treatment, including an expansion in $T-T_0$ of $\overline{\mu_2}$ appearing in P_∞ and Q_∞, can also be done, examining carefully to what extent $\overline{\mu_2}$ can be approximately neglected with respect to $\delta\mu_2(t)$. We can neglect $\overline{\mu_2}$ with respect to $\delta\mu_2(t)$ at temperatures very close to the Kauzmann temperature and for times that are not extremely long, so that we are far from thermalization and the dynamics still has aging behavior. In Fig. 2 we show the relative weight of $\overline{\mu_2}$ in $\mu_2(t)$ for a specific case. As is clear from the figure, as soon as we go too far from T_0 we cannot neglect in $\mu_2(t)$ its asymptotic value $\overline{\mu_2}$.

(2) $T<T_0$, $\gamma>1$. In this and in the following cases the asymptotic value of $\mu_2(t)$ is $\overline{\mu_2}=0$ so that $\delta\mu_2(t)=\mu_2(t)$. In this dynamic regime also the adiabatic approximation can be carried out and the second term in the denominator of Eq. (3.33) is again negligible. In this case the leading term of r in its expansion in powers of μ_2, r_∞, is of $O(1)$. Therefore we get

$$\mu_1(t)=\frac{J\overline{T_e}r_\infty Q_\infty}{1+Q_\infty D}\,\frac{1}{\Gamma(t)}+O(\mu_2^{1+\gamma}), \tag{3.37}$$

where

$$\overline{T_e}\equiv\lim_{t\to\infty}\tilde{K}(m_1(t),m_2(t))[m_0+\mu_2(t)]=\tilde{K}_\infty m_0, \tag{3.38}$$

$$\widetilde{K}_\infty \equiv \lim_{t\to\infty} \widetilde{K}(m_1(t), m_2(t)), \tag{3.39}$$

$$r_\infty = \frac{\overline{T}_e - T}{2\overline{T}_e - T}. \tag{3.40}$$

(3) $T<T_0$, $\gamma=1$. In this case the adiabatic expansion is no longer consistent. We have to solve Eq. (3.33) taking $d\mu_1/d\mu_2$ into account. To leading order the equation takes the form

$$\frac{d\mu_1}{d\mu_2} = \frac{\mu_1\Gamma(1+Q_\infty D) - JQ_\infty \overline{T}_e r_\infty}{2 r_\infty m_0} + O(\mu_1) + O(\mu_2) + O(\Gamma\mu_1^2) + cO(\Gamma\mu_1\mu_2). \tag{3.41}$$

Defining the quantity $\epsilon \equiv B(1+Q_\infty D)/2r_\infty m_0$ we identify other five subregimes in the case $\gamma=1$.

(a) $\epsilon>1$. The solution is

$$\mu_1(t) = \frac{JQ_\infty \overline{T}_e r_\infty}{2r_\infty m_0(\epsilon-1)}\mu_2(t) - c_1\frac{1}{\epsilon-1}\mu_2^\epsilon(t). \tag{3.42}$$

The exponent ϵ is always positive, at least in cooling, because $\overline{T}_e > T$, making r_∞ and Q_∞ positive. c_1 is also positive because it is the exponential of the integration constant (the value of which depends on the initial conditions). Since $\epsilon > 1$, the second term in the right hand side can be neglected and $\mu_1 \sim \mu_2$.

(b) $\epsilon=1$. We find

$$\mu_1(t) = -\frac{J\overline{T}_e r_\infty Q_\infty}{1+Q_\infty D}\frac{\ln\mu_2(t)}{\Gamma(t)} + c_2\mu_2, \tag{3.43}$$

where c_2 is the integration constant and can take any value. In the long time dynamics the logarithmic term will take over and, independently of the initial conditions, $\mu_1>\mu_2$ and will be positive.

(c) $1/2<\epsilon<1$. The second term in Eq. (3.42) is leading and the solution is

$$\mu_1(t) = c_1\frac{1}{1-\epsilon}\mu_2^\epsilon(t). \tag{3.44}$$

c_1 is a positive constant and $\mu_1 \gg \mu_2$ and positive.

(d) $\epsilon=1/2$. When $\epsilon\leqslant 1/2$ the second term in the denominator, always neglected up to now, has to be taken into account. In this case the leading term in the denominator goes to zero and $J\overline{T}_e r_\infty Q_\infty$ can be neglected with respect to $\mu_1\Gamma(1+Q_\infty D)$ in the numerator. We can thus easily solve the equation

$$\frac{d\mu_2}{d\mu_1} = \frac{2r_\infty m_0 - 2\mu_1^2\Gamma}{\mu_1\Gamma(1+Q_\infty D)}. \tag{3.45}$$

For $\epsilon=1/2$ we get

$$\mu_2(t) = -\frac{2}{1+Q_\infty D}\mu_1^2(t)\ln\mu_1(t) + c_2\mu_1^2(t), \tag{3.46}$$

which is not invertible analytically. It is clear anyway that in this subregime $\mu_1 \gg \mu_2$. c_2 can take any value.

(e) $\epsilon<1/2$. The solution is

$$\mu_1(t) = \sqrt{\frac{m_0 r_\infty(1-2\epsilon)}{\Gamma(t)}} \times \left[1 + \frac{c_1}{2}\left(\frac{1+Q_\infty D}{2}\right)^{1/\epsilon}\left(\frac{1-2\epsilon}{\epsilon}\right)^{1/\epsilon-1}\mu_2(t)^{1/2\epsilon-1}\right] \tag{3.47}$$

where $c_1>0$. Still $\mu_1 \gg \mu_2$.

(4) $T<T_0$, $\gamma<1$. Considering also the term $\mu_1^2\Gamma$ in the denominator of Eq. (3.33), the solution is now

$$\mu_1(t) = \sqrt{\frac{r_\infty m_0}{\Gamma(t)}}\left(1 - \frac{1+Q_\infty D}{2m_0 r_\infty \gamma}\mu_2(t)\Gamma(t)\right). \tag{3.48}$$

In this low temperature regime $\mu_1 \gg \mu_2$ once again.

For $\gamma=1$, $\epsilon\leqslant 1/2$ and for $\gamma<1$ the solution to Eq. (3.45) involves only the absolute value of μ_1, thus giving two possible choices for the sign of the function $\mu_1(\mu_2)$. In order to guarantee continuity of μ_1 at the parameter values at which the dynamics changes regime, we require μ_1 to have the same sign in two contiguous regimes. That means that in Eqs. (3.46), (3.47), and (3.48) we chose the plus sign.

The time dependent variables $\mu_1(t)$ and $\mu_2(t)$ give the dynamic behavior of every observable in the long, but not extremely long, time regime, i.e., in the aging regime. When the time increases further the dynamics will exponentially relax to equilibrium as $\exp(-t/\tau_{eq})$. We will see what τ_{eq} is in the next section.

IV. OUT OF EQUILIBRIUM THERMODYNAMICS

The history of a system that is far from equilibrium can be expressed by a number of effective parameters, like the effective temperature or other effective fields, in order to recast the out of equilibrium dynamics in a thermodynamic approach [3]. The number of effective parameters needed to make such a translation is, in principle, equal to the number of independent observables considered. For a certain class of system, however, there is some effective thermalization and the effective parameters pertaining to processes having the same time scale become asymptotically equal to each other in time. Examples of out of equilibrium regimes governed by a single effective temperature have been considered in [3,29]. In computer glasses the approach has been applied with some success [30,31].

Given the solution of the dynamics [and thus the form of the functions $m_1(t)$ and $m_2(t)$] a quasistatic approach can be followed by computing the partition function Z_e of all the macroscopically equivalent states (those having the same values for $m_{1,2}$) at the given time t. The measure on which this out of equilibrium partition function is evaluated is not the Gibbs measure. In order to generalize the equilibrium thermodynamics we assume an effective temperature T_e and an effective field H_e, and substitute the equilibrium measure by $\exp[-\mathcal{H}_{\rm eff}(\{x_i\},T,H_e)/T_e]$, where $\mathcal{H}_{\rm eff}$ was introduced in Eq. (2.6) and the true external field H in it has been substituted by an effective field H_e. T_e and H_e are at this step of the computation just fictitious parameters. However, as soon as we get the expression of the ‘‘thermodynamic’’ potential $F_e \equiv -T_e \ln Z_e$ as a function of macroscopic variables $m_{1,2}$ and effective parameters, we can fix T_e and H_e as taking those values that make the potential as small as possible. We thus have to minimize F_e with respect to m_1 and m_2 to determine T_e and H_e and evaluate the resulting analytic expressions at $m_1 = m_1(t)$ and $m_2 = m_2(t)$ given by the dynamics at the considered time *t*. Counting all the macroscopically equivalent states at the time t at which the dynamical variables take values m_1 and m_2, we get

$$\begin{aligned} Z_e(m_1,m_2;T_e,H_e) &\equiv \int \mathcal{D}x \exp\left[-\frac{1}{T_e}\mathcal{H}_{\rm eff}(\{x_i\},T,H_e)\right] \\ &\quad \times \delta\left(Nm_1 - \sum_i x_i\right)\delta\left(Nm_2 - \sum_i x_i^2\right). \end{aligned} \tag{4.1}$$

From this partition function we can build an effective thermodynamic potential as a function of T_e and H_e, as well as of *T* and *H*, where the effective parameters depend on time through the time dependent values of the m_1 and m_2 solutions of the dynamics. They actually are a way of describing the evolution in time of the system out of equilibrium. The effective free energy takes the form

$$\begin{aligned} F_e(t) &= U(m_1(t),m_2(t)) - TS_{ep}(m_1(t),m_2(t)) \\ &\quad - T_e(t)\mathcal{I}(m_1(t),m_2(t)) + [H - H_e(t)]Nm_1(t), \end{aligned} \tag{4.2}$$

with

$$T_e(t) = \tilde{K}(m_1(t),m_2(t))[m_0 + \mu_2(t)], \tag{4.3}$$

$$H_e(t) = H - \tilde{K}(m_1(t),m_2(t))\mu_1(t), \tag{4.4}$$

where the last term of F_e replaces the $-HNm_1$ occurring in U [see Eq. (2.7)] by $-H_eNm_1$. The quantity

$$\mathcal{I}(t) = \frac{N}{2}\{1 + \ln[m_0 + \mu_2(t)]\} \tag{4.5}$$

is the configurational entropy (2.14) and the expressions for U and S_{ep} are given in Eqs. (2.7) and (2.8).

As we see from Eqs. (4.3) and (4.4) in the dynamic regimes 1 and 2, reported in Sec. III, where $\mu_1 \ll \mu_2$, the effective temperature alone is enough for a complete thermodynamic description of the dominant physic phenomena ($H_e = H$), while in the regimes 3a and 3b ($\mu_1 \sim \mu_2$) and in 3c, 3d, 3e, and 4 ($\mu_1 \gg \mu_2$), when μ_1 is no longer negligible, the effective field H_e is also needed.

Effective temperature from generalized first law. Letting $M \equiv Nm_1$, and using Eqs. (2.7), (2.8), and (2.14), the differential of the free energy (4.2) turns out to be

$$dF = -S_{ep}dT - \mathcal{I}dT_e - MdH_e, \tag{4.6}$$

thus implying

$$dU = TdS_{ep} + T_e d\mathcal{I} + (H_e - H)dM - MdH. \tag{4.7}$$

Using this expression we are able to write down the first law of thermodynamics $dU = \bar{d}Q + \bar{d}W$, in the two-temperature–two-field case, where the change in work done on the system is $\bar{d}W = -MdH$. In order for the conservation of energy to be satisfied the heat variation has, then, to take the form

$$\bar{d}Q = TdS_{ep} + T_e d\mathcal{I} + (H_e - H)dM. \tag{4.8}$$

This is the same expression obtained in the two-temperature picture of [29] where the fields where absent. At equilibrium, where $H_e = H$ and $T_e = T$, this reduces to the usual expression for ideal reversible quasistatic transformations $\bar{d}Q = TdS$, with the total entropy $S = S_{ep} + \mathcal{I}$.

From Eq. (4.8) the complete expression for the rate of change of the heat of the system turns out to be

$$\begin{aligned} \dot{Q} &= N\dot{\mu}_1 \frac{T\tilde{K}^2(w + T/2)}{2DJ} + N\dot{\mu}_2 \frac{\tilde{K}}{2} \\ &\quad + N\mu_1 \frac{\tilde{K}}{2(1 + QD - \tilde{K}JQ\mu_1)}(\dot{\mu}_1 + \dot{\mu}_2\tilde{K}JQ). \end{aligned} \tag{4.9}$$

The heat flowing out of the system is $-\dot{Q}$. Referring to the aging regimes described in Sec. III the quantity $\dot{Q}$ turns out to be proportional to $\dot{\mu}_2$ in the regimes 1 ($T > T_0$) and 2 ($T < T_0, \gamma > 1$). In the dynamic regimes 3a and 3b ($T < T_0, \gamma = 1, \epsilon \geqslant 1$) $\dot{Q} \propto \dot{\mu}_1 + \dot{\mu}_2$. For regimes 3c, 3d, and 3e ($T < T_0, \gamma = 1,\ \epsilon \leqslant 1$) and for regime 4 ($T < T_0, \gamma < 1$) $\dot{Q} \propto \dot{\mu}_1$.

In every dynamic regime $\dot{\mu}_1$ and $\dot{\mu}_2$ are negative and this implies that the heat flow of the out of equilibrium system is positive in its approach to equilibrium, as it should be, no matter the values of the parameters of the model.

Starting from the first law of thermodynamics, we can derive the effective temperature in yet another way, through a generalization of the Maxwell relation $T = \partial U/\partial S$ valid at equilibrium for a system of internal energy U and entropy S, with the derivative taken at constant magnetization (or volume). We put for simplicity $H_e = H$ in the rest of this subsection. Out of equilibrium, together with the previous Maxwell relation for equilibrium processes (where S has to be substituted by S_{ep}) the following generalization also holds:

$$T_e = \left.\frac{\partial U}{\partial \mathcal{I}}\right|_{S_{ep}}. \tag{4.10}$$

A more feasible identity, where the variable to be kept constant during the transformation is the bath temperature, rather than the entropy of the fast processes, can be obtained [32,33,12]. Let us introduce, with this aim, the function Φ:

$$\Phi \equiv F_e + T_e \mathcal{I}, \tag{4.11}$$

inducing $d\Phi = T_e d\mathcal{I} - S_{ep} dT$. Through this auxiliary potential function Φ we can then rewrite the effective temperature as

$$T_e(t) = \left.\frac{\partial \Phi}{\partial \mathcal{I}}\right|_T . \tag{4.12}$$

This result is a firm prediction for systems that satisfy the assumption of a two-temperature thermodynamics. For underlying mechanisms in specific cases see [32,33,12]. Writing Eq. (4.12) as $\dot{\Phi}/\dot{\mathcal{I}}$ and using Eqs. (3.9) and (3.10) we get [neglecting terms of $O(\mu_1)$]

$$T_e(t) = \tilde{K}(m_1(t), m_2(t))[m_2(t) - m_1^2(t)] \tag{4.13}$$

in agreement with Eq. (4.3).

A. Statics

T_0 is defined as the temperature at which the constraint is reached from above: some configurations become infeasible and the valleys of the free energy landscape are divided by infinite barriers. The breaking of ergodicity in a landscape with many minima gives rise to a real thermodynamic phase transition [11].

When the constraint (2.9) on the phase space of the $\{x_i\}$ is first reached, at T_0, in the infinite time limit, $\mathcal{I}$ goes to its minimal value $\mathcal{I}_0 \equiv \mathcal{I}(T_0) = 1 + \ln m_0$. Coming from high temperature there would thus be a transition from a many (metastable) states phase to a phase in which the system is stuck forever in one single minimum. This transition is what is thought to happen in real glasses, at the so called Kauzmann temperature. Since we are using the continuous variable $\{x_i\}$, the entropy $\mathcal{I}$ (as well as S_{ep}) is, in our case, ill defined at low temperature: it would diverge like $\ln T$ at zero temperature if no constraint were present. Our value $\mathcal{I}(T_0)$ is greater than zero, because this entropy counts all the multiple ways in which the continuous harmonic oscillators can arrange themselves in order to satisfy the constraint (2.9). Since we are dealing with classical variables we can bypass this inconvenience by just subtracting from $\mathcal{I}$ the constant $\mathcal{I}_0$ to make $\mathcal{I}(T = T_0) = 0$. The entropy value $\mathcal{I}_0$ is related to the dynamics on time scales where all the degenerate minima are sampled. These are much longer than the scales of our interest, and for our purposes the constant $\mathcal{I}_0$ plays no role.

To see how the transition takes place we first look at the asymptotic behavior of the effective temperature. When $T \geqslant T_0$ and $t \to \infty$, T_e becomes the heat-bath temperature T. When $T < T_0$, instead, T_e never reaches such a temperature. It rather goes toward some limiting value $\overline{T_e}(T)$ that we can get from Eq. (4.3), which may be rewritten for clarity in the explicit form

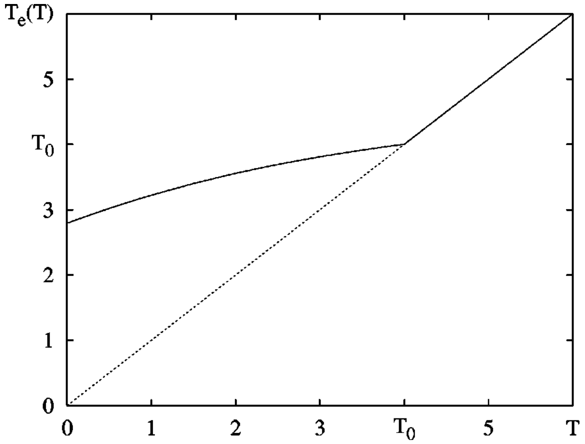

FIG. 3. In the static regime the effective temperature is shown as a function of the heat-bath temperature. At high temperature they coincide but below the Kauzmann transition $\overline{T_e}$ does not reach T, not even in the infinite time limit. The system remains out of equilibrium for ever. Values of the constants are $K = J = 1$, $H = L = 0.1$, $m_0 = 5$.

$$(Km_0 - \overline{T_e} + T)(Km_0 - \overline{T_e})(J\overline{T_e})^2 + D^2 m_0 (Km_0 - \overline{T_e})^2 - J^4 m_0 (\overline{T_e})^2 = 0, \tag{4.14}$$

a quartic equation for the effective temperature in the infinite time limit. The same equation evaluated at $T_e = T = T_0$ gives us the value of the Kauzmann temperature T_0 as a function of the parameter of the model. In Fig. 3 we plot $\overline{T_e}$ versus T for a choice of parameter values.

From Eq. (4.14) or Fig. 3 we observe that $dT_e/dT|_{T_0^-} < 1$ whereas, coming from above the Kauzmann temperature, one has, of course, $dT_e/dT|_{T_0^+} = 1$. The derivative of $T_e(T)$ thus shows a discontinuity at $T = T_0$.

Any thermodynamic function, like U and m_1, will depend on the heat-bath temperature both explicitly and through this effective temperature. For the specific heat we will have, for instance,

$$C \equiv \frac{1}{N}\left.\frac{dU}{dT}\right|_H = \frac{1}{N}\left.\frac{\partial U}{\partial T}\right|_H + \frac{1}{N}\left.\frac{\partial U}{\partial T_e}\right|_{H,T}\left.\frac{dT_e}{dT}\right|_H . \tag{4.15}$$

This is of the same form $C = c_1 + c_2(\partial T_e/\partial T)_p$ assumed originally by Tool [34] for the study of caloric behavior in the glass formation region.

The discontinuity in $dT_e/dT|_H$ causes a discontinuity in the specific heat and also in the quantity $-\partial m_1/\partial T|_H$, called magnetizability in [2,3] (it is the analog of a thermal expansivity for the model here described), because both of these quantities contain terms proportional to $\partial T_e/\partial T|_H$. One could now discuss the Ehrenfest relations between these discontinuities, and the Prigogine-Defay ratio, as was done for related models by one of us [29,2,3]. Because of the close analogy between all these cases, we shall not go deeper into this at the present moment.

B. Dynamics

The relaxation time is the characteristic time scale on which the system initially out of equilibrium (because, for example, of a sudden quench to low temperature) relaxes toward equilibrium. It can be defined, for instance, from the dynamical equations of the internal energy per harmonic oscillator $u \equiv U/N$,

$$\dot{u} = -\frac{u}{\tau_{eq}}, \tag{4.16}$$

or, equivalently, from the equations of motion for m_1, m_2 as the time at which the quantity of interest goes to $1/e$ of its initial value. In any temperature regime it turns out that the relaxation time has an exponential behavior in Γ:

$$\tau_{eq} \sim e^{\Gamma} = \exp\left(\frac{B}{\mu_2}\right)^{\gamma}. \tag{4.17}$$

Making use of the solution (3.27) we find the following behavior for the relaxation time versus the heat-bath temperature.

(1) $T > T_0$. $\mu_2(t) \to \overline{\mu}_2(T)$ and near enough to the Kauzmann temperature we can linearize the latter in $T - T_0$. For $t \to \infty$ we get an exponential decay with relaxation time

$$\tau_{eq} \propto \exp\left(\frac{A_0}{T - T_0}\right)^{\gamma}, \tag{4.18}$$

$$A_0 = B\left(\left.\frac{\partial \overline{\mu}_2(T)}{\partial T}\right|_{T_0}\right)^{-1} = \left.\frac{B\tilde{K}_\infty (K - \tilde{K}_\infty)(1 + DQ_\infty + P_\infty)}{(K - \tilde{K}_\infty)(1 + DQ_\infty) - \tilde{K}_\infty P_\infty}\right|_{T_0}. \tag{4.19}$$

This behavior is a generalized Vogel-Fulcher-Tammann-Hesse law [6–8], where γ can have any value and in particular $\gamma = 1$.

Looking at the configurational entropy, since at the first order expansion in μ_2 we have $\mathcal{I} - \mathcal{I}_0 \simeq (N/2m_0)\mu_2$, we also find from Eq. (4.17) the Adam-Gibbs relation [9]

$$\tau_{eq} \propto \exp\left[\frac{NB}{2m_0(\mathcal{I} - \mathcal{I}_0)}\right]^{\gamma}. \tag{4.20}$$

Far from equilibrium, in the aging regime where the relaxation is very slow, we can still define a time dependent ‘‘relaxation time’’ giving the characteristic time scale on which the α processes are taking place. Always for T very near to T_0, in the aging regime, $\overline{\mu}_2$, the static part of μ_2, is negligible with respect to the dynamic part $\delta\mu_2$ so that for the effective temperature we have the following expansion:

$$T_e(t) \simeq T_0 + \frac{1 + DQ_\infty + P_\infty}{1 + Q_\infty D}\tilde{K}_\infty \delta\mu_2(t) + O(T - T_0). \tag{4.21}$$

We get

$$\tau(t) \propto \exp\left(\frac{A(T)}{T_e(t) - T}\right)^{\gamma} \simeq \exp\left(\frac{A(T_0)}{T_e(t) - T_0}\right)^{\gamma}, \tag{4.22}$$

$$A(T) \equiv \frac{B(1 + DQ_\infty + P_\infty)}{1 + Q_\infty D}\tilde{K}_\infty, \tag{4.23}$$

where $A(T_0) < A_0$, meaning that in the static regime τ is more divergent.

(1) $T < T_0, \gamma > 1$. For $T < T_0$ the relaxation time always diverges for $t \to \infty$. However, as was done in the case above T_0 for the relaxation in the aging regime, an instantaneous relaxation time can be considered and expressed in terms of the effective temperature using the first order expansion of T_e in μ_2:

$$T_e(t) = \overline{T}_e + \frac{1 + DQ_\infty + P_\infty}{1 + Q_\infty D}\tilde{K}_\infty \mu_2(t). \tag{4.24}$$

We find

$$\tau(t) = \tau(T, T_e(t)) \propto \exp\left(\frac{A(T)}{T_e(t) - \overline{T}_e(T)}\right)^{\gamma}, \tag{4.25}$$

where $A(T)$ is the one given in Eq. (4.23). The aging behavior just above and well below T_0 are thus intimately related. The expression (4.25) resembles a VFTH law where the heat-bath temperature has been substituted by a time dependent effective temperature $T_e(t)$ and the Kauzmann temperature by the asymptotic value $\overline{T}_e$. Such a relation for the time scale of the aging dynamics could hold very well in more general systems.

(3) $T < T_0, \gamma \leqslant 1$. In these regimes, where μ_1 cannot be neglected with respect to μ_2, there is no simple expression for τ.

V. 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 nontrivial 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) $\partial_{t'}C(t,t')/G(t,t')$ far from equilibrium.

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

$$C_{ab}(t,t') \equiv N\langle \delta m_a(t)\,\delta m_b(t')\rangle, \quad a,b = 1,2, \tag{5.1}$$

where $\langle \cdots \rangle$ 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

$$G_{ab}(t,t') \equiv \frac{\delta\langle m_a(t)\rangle}{\delta H_b(t')}, \quad a,b=1,2. \tag{5.2}$$

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

Since we will very often make use of the derivatives with respect to m_1 and m_2 of the integrals given by the Monte Carlo dynamics introduced in Sec. III, we show them in the Appendix explicitly computed and we shorten the notation by defining the variables f_k and g_k, $k=0,1,2,3$, in Eqs. (A11)–(A18).

A. High temperature case: $T > T_0$

First we analyze the case above the Kauzmann temperature. In this case the expansion of Eqs. (A11)–(A18) in powers of $\mu_2(t)$ becomes an expansion both in $\delta\mu_2(t)$ and in $\overline{\mu}_2$ [or equivalently in $1/\overline{\Gamma} = (\overline{\mu}_2/B)^\gamma$], because we are interested in studying what happens for large times and near the Kauzmann temperature T_0, i.e., for small values of $\delta\mu_2(t)$ and for small values of $\overline{\mu}_2$ (or large values of $\overline{\Gamma}$). In the f_k and g_k written in the Appendix we leave the notation without the overbar meaning that an expansion for long times, i.e., an expansion in $\delta\mu_2(t)$, or an expansion in $\overline{\mu}_2$, has still to be done, depending on the kind of approximation that we need. For the sake of clarity we repeat here the expansion of $\Gamma(t)$ in the aging regime:

$$\mu_2(t) = \overline{\mu}_2 + \delta\mu_2(t), \quad \Gamma(t) = \overline{\Gamma} - \gamma\overline{\Gamma}\frac{\delta\mu_2(t)}{\overline{\mu}_2}. \tag{5.3}$$

The following exact relations hold:

$$\partial_{m_1}\mu_1 = -1 - LQ\tilde{K}, \quad \partial_{m_2}\mu_1 = -\frac{J}{2}Q\tilde{K}. \tag{5.4}$$

We stress that $\partial_{m_1}\mu_1$ and $\partial_{m_2}\mu_1$ are still functions of μ_2, through Q and $\tilde{K}$, and that they can thus be expanded in powers of $\delta\mu_2$, leading to corrections to the f_k and g_k. Since in the end they will appear only in the combinations $\partial_{m_1}\mu_1 + 2m_1\partial_{m_2}\mu_1$ and $\partial_{m_1}\mu_1 - 2L/J\,\partial_{m_2}\mu_1$ we just give the expressions of these combinations:

$$\begin{aligned}\partial_{m_1}\mu_1 + 2m_1\partial_{m_2}\mu_1 &= -(1+QD)\\ &\simeq -(1+Q_\infty D) - \delta\mu_2 Q_1 D,\end{aligned} \tag{5.5}$$

$$\partial_{m_1}\mu_1 - 2\frac{L}{J}\partial_{m_2}\mu_1 = -1, \tag{5.6}$$

where

$$Q_1 = \frac{Q_\infty}{(1+Q_\infty D)(m_0+\overline{\mu}_2)}\left[\frac{J^2(m_0+\overline{\mu}_2)(3\overline{w}+T/2)}{2\overline{w}^2(\overline{w}+T/2)} - 3P_\infty\right] \tag{5.7}$$

is the coefficient of $\delta\mu_2(t)$ in the first order expansion of Q,

$$Q(t) = Q_\infty + Q_1\delta\mu_2(t), \tag{5.8}$$

and

$$\overline{w} \equiv \sqrt{J^2\overline{m}_2 + 2JL\overline{m}_1 + L^2 + T^2/4}. \tag{5.9}$$

In the following formulas the derivatives of μ_1, as well as μ_1 itself, have to be considered as general, regular functions of μ_2.

In addition to the expansion (5.8) of Q we also give the expansions to first order in $\delta\mu_2(t)$ of the quantities r [defined in Eq. (3.22)], m_1, $\tilde{K}$ [Eq. (2.10)], P [Eq. (2.25)], and Q [Eq. (2.24)]:

$$r(t) = \frac{1}{m_0+\overline{\mu}_2}\left(\frac{1+Q_\infty D + P_\infty}{1+Q_\infty D}\right)\delta\mu_2(t), \tag{5.10}$$

$$\tilde{K}(t) = \tilde{K}_\infty + \frac{\tilde{K}_\infty P_\infty}{(1+Q_\infty D)(m_0+\overline{\mu}_2)}\delta\mu_2(t), \tag{5.11}$$

$$m_1(t) = \overline{m}_1 - \frac{P_\infty D}{\tilde{K}_\infty J(1+Q_\infty D)(m_0+\overline{\mu}_2)}\delta\mu_2(t), \tag{5.12}$$

$$\begin{aligned}P(t) = P_\infty &+ \frac{P_\infty}{(1+Q_\infty D)(m_0+\overline{\mu}_2)}\\ &\times\left[1+Q_\infty D - P_\infty + \frac{J^2(m_0+\overline{\mu}_2)(3\overline{w}+T/2)}{2\overline{w}^2(\overline{w}+T/2)}\right]\delta\mu_2(t).\end{aligned} \tag{5.13}$$

For the terms containing $\Gamma\mu_1$, from Eq. (3.35) we see that in this dynamic regime

$$\Gamma\mu_1 = \frac{JQ_\infty T}{m_0+\overline{\mu}_2}\,\frac{1+Q_\infty D+P_\infty}{(1+Q_\infty D)^2}\,\delta\mu_2 + O(\delta\mu_2^2). \tag{5.14}$$

In [3] equations of motion for simpler models were obtained. Our present model share the basic attributes that are needed to get those equations, namely, the possibility of writing the transition probability (3.1) of the Monte Carlo dynamics as the product of two Gaussian probability distributions (3.3), functions, respectively, of the energy variation x and of the variation y of the magnetizationlike quantity $\sum_i x_i$.

We thus recall here the following equations holding for the equal time correlation functions:

$$\frac{d}{dt}C_{ab}(t,t)=\int W(\beta x)\Bigg\{\overline{y}_a(x)\overline{y}_b(x)+\Delta_y\left(-\frac{H_1}{H_2}\right)^{a+b-2} + \sum_{c=1}^{2}\frac{\partial}{\partial m_c}[\overline{y}_a(x)C_{cb}(t,t) + \overline{y}_b(x)C_{ca}(t,t)]\Bigg\}p(x|m_1,m_2)dx, \quad a,b=1,2, \tag{5.15}$$

where [recalling Eqs. (3.2) and (3.5) and using Eqs. (3.6) and (4.3)]

$$\overline{y}_1(x)=\frac{\mu_1}{m_2-m_1^2+\mu_1^2}\,\frac{\overline{x}-x}{\tilde{K}}=\left(4\Gamma\mu_1-\mu_1\frac{x}{T_e}\right)+O(\mu_1^3), \tag{5.16}$$

$$\overline{y}_2(x)=\frac{2}{\tilde{K}}[x+\tilde{H}\overline{y}_1(x)], \tag{5.17}$$

$$\overline{x}=\frac{\Delta^2\tilde{K}}{2}=4T_e\Gamma, \tag{5.18}$$

$$\Delta_y=\frac{\Delta^2(m_2-m_2)}{m_2-m_1^2+\mu_1^2}=8(m_0+\mu_2)\Gamma+O(\Gamma\mu_1^2). \tag{5.19}$$

Expanding the integrals $\int W(\beta x)\overline{y}_a(x)\overline{y}_b(x)p(x|m_1,m_2)dx$ and $\Delta_y\int W(\beta x)p(x|m_1,m_2)dx$ up to order Υ, Eqs. (5.15) become

$$\dot{C}_{11}(t,t)=8[m_0+\mu_2(t)]\Gamma(t)\left(1-\frac{1-2r+4r^2}{\Gamma(t)}\right)\Upsilon(t) + 2f_1(t)C_{11}(t,t)+2g_1(t)C_{12}(t,t), \tag{5.20}$$

$$\dot{C}_{12}(t,t)=16m_1(t)[m_0+\mu_2(t)]\Gamma(t)\left(1-\frac{1-2r+4r^2}{\Gamma(t)}\right)\Upsilon(t) + f_2(t)C_{11}(t,t)+[f_1(t)+g_2(t)]C_{12}(t,t) + g_1(t)C_{22}(t,t), \tag{5.21}$$

$$\dot{C}_{22}(t,t)=32m_1(t)^2[m_0+\mu_2(t)]\Gamma(t) \times\left(1-\frac{1-2r+4r^2}{\Gamma(t)}\right)\Upsilon(t)+32[m_0+\mu_2(t)]^2\Upsilon(t) + 2f_2(t)C_{12}(t,t)+2g_2(t)C_{22}(t,t). \tag{5.22}$$

The functions f_1, g_1, f_2, and g_2 are given in the Appendix. Due to the complicated form of the equations we are not able to find solutions valid at every time. We are obliged to find approximate solutions valid on given time scales. First we will study the solutions in the aging regime, for times that are long but not longer than some given time scale t_g, after which the system begins to thermalize. Afterward we will study the dynamics of correlation and response functions for times longer than t_g, when the system approaches equilibrium.

1. Dynamics in the aging regime

In the aging regime, for temperature just above the Kauzmann temperature T_0, we can neglect $\overline{\mu}_2$ with respect to $\delta\mu_2(t)$. This means that in expressions (5.8)–(5.13) we have to put $\overline{\mu}_2$ equal to zero everywhere, including the constants Q_∞, P_∞, and $\tilde{K}_\infty$ [defined, respectively, in Eqs. (2.24), (2.25), and (3.39)], and we can write $\delta\mu_2(t)=\mu_2(t)$.

To find the solutions to Eqs. (5.20)–(5.22) we can first perform an adiabatic expansion neglecting the time derivatives of the correlation functions. Indeed, to first order of approximation $\dot{C}_{ab}$ is proportional to $\dot{\mu}_2$: they are of $O(\delta\mu_2\Upsilon)$, negligible with respect to the right hand side terms. We then compute the second order corrections. The solutions for the case $T>T_0$, in the aging regime with negligible $\overline{\mu}_2$ and r proportional to $\mu_2(t)$, turn out to be

$$C_{11}(t,t)=\frac{1}{1+Q_\infty D}\left\{m_0+\mu_2(t)\left[1-\frac{m_0Q_1D}{1+Q_\infty D}\right]+O\left(\frac{1}{\Gamma}\right) + O(\mu_2^2(t))\right\}, \tag{5.23}$$

$$C_{12}(t,t)=\frac{1}{1+Q_\infty D}\left\{2m_1(t)m_0+\mu_2(t) \times\left[2m_1(t)\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)-m_0Q_\infty D\right]+O\left(\frac{1}{\Gamma}\right) + O(\mu_2^2(t))\right\}, \tag{5.24}$$

$$C_{22}(t,t)=\frac{1}{1+Q_\infty D}\left\{4m_1(t)^2m_0+\mu_2(t) \times\left[4m_1(t)^2\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)-4m_0m_1Q_\infty D\right] + O\left(\frac{1}{\Gamma}\right)+O(\mu_2^2(t))\right\}. \tag{5.25}$$

To get these expressions it is enough to keep in f_1, g_1, f_2, and g_2 [defined in Eqs. (A13)–(A16)] only terms up to $O(\Upsilon)$.

Once we have the equal time solutions we can solve the equations for the two-time functions. Always following the approach of [3] we get the equations

$$\partial_t C_{ab}(t,t')=f_a(t)C_{1b}(t,t')+g_a(t)C_{2b}(t,t'), \quad a,b=1,2, \tag{5.26}$$

where f_a and g_a are defined in Eqs. (A13)–(A16). We introduce the function

$$\tilde{f} \equiv f_1 + \frac{2\dot{m}_1 g_1}{g_2 - 2m_1 g_1} - g_1 \frac{f_2 - 2m_1 f_1}{g_2 - 2m_1 g_1}$$
$$= -4\Upsilon \left\{ (1+QD)\Gamma - \left[1 + QD - \frac{2DQP}{1+QD} - \frac{DP(1+QD)}{\gamma(1+P+QD)} \right] + O\left(\frac{1}{\Gamma}\right) \right\} \tag{5.27}$$

where $\dot{m}_1$ is obtained from Eq. (3.9) as

$$\dot{m}_1 \simeq 4\mu_1 \Upsilon \Gamma - 4\mu_1 \Upsilon (1 - 3r + 4r^2) = O(\mu_2 \Upsilon) \tag{5.28}$$

and is negligible with respect to the leading orders.

The decoupled equations for C_{11} and C_{12} are, in this notation,

$$\partial_t C_{1b}(t,t') = \tilde{f}(t) C_{1b}(t,t'), \quad b = 1,2. \tag{5.29}$$

To the leading order the two correlation functions above are connected to C_{21} and C_{22} in the following way:

$$C_{2b}(t,t') \simeq 2m_1(t) C_{1b}(t,t'), \quad b = 1,2. \tag{5.30}$$

Defining the time evolution function for the considered time scale sector as

$$\tilde{h}(\tau) \equiv \exp\left(-\int_0^\tau \tilde{f}(t) dt \right), \tag{5.31}$$

the solution of Eq. (5.29) comes out to be

$$C_{1b}(t,t') = C_{1b}(t',t') \frac{\tilde{h}(t')}{\tilde{h}(t)} + O(\mu_1 \Upsilon). \tag{5.32}$$

Following the approach of [3] we also derive the response function. Neglecting the terms of $O(\Upsilon^2)$ (called *switch terms* in [3]) they are

$$G_{11}(t,t^+) = -\beta \int dy_1 dy_2 W'(\beta x) y_1^2 p(y_1,y_2|m_1,m_2) = -\beta \int dx W'(\beta x) [\overline{y_1}(x)^2 + \Delta_y] p(x|m_1,m_2)$$
$$= -\beta \int dx W'(\beta x) \Delta_y p(x|m_1,m_2) + O(\mu_2^2 \Upsilon) = \frac{4\Upsilon\Gamma}{\tilde{K}} - \frac{2\Upsilon}{\tilde{K}} + O(\mu_2 \Upsilon), \tag{5.33}$$

$$G_{12}(t,t^+) = -\beta \int dy_1 dy_2 W'(\beta x) y_1 y_2 p(y_1,y_2|m_1,m_2) = -\beta \frac{2}{\tilde{K}} \int dx W'(\beta x) \{x \overline{y_1}(x) + \tilde{H}[\overline{y_1}(x)^2 + \Delta_y]\} p(x|m_1,m_2)$$
$$= -2\beta \frac{\tilde{H}}{\tilde{K}} \int dx W'(\beta x) \Delta_y p(x|m_1,m_2) + O\left(\frac{\mu_2}{\Gamma}\Upsilon\right) = \frac{8m_1}{\tilde{K}} \Upsilon\Gamma - \frac{4m_1\Upsilon}{\tilde{K}} + O(\mu_2 \Upsilon), \tag{5.34}$$

$$G_{22}(t,t^+) = -\beta \int dy_1 dy_2 W'(\beta x) y_2^2 p(y_1,y_2|m_1,m_2)$$
$$= -\beta \frac{4}{\tilde{K}^2} \int dx W'(\beta x) \{x^2 + 2\tilde{H} x \overline{y_1}(x) + \tilde{H}^2 [\overline{y_1}(x)^2 + \Delta_y]\} p(x|m_1,m_2) = -4\beta \frac{1}{\tilde{K}^2} \int dx W'(\beta x)(x^2$$
$$+ \tilde{H}^2 \Delta_y) p(x|m_1,m_2) + O\left(\frac{\mu_2}{\overline{\Gamma}}\Upsilon\right)$$
$$= \frac{16m_1^2}{\tilde{K}} \Upsilon\Gamma - \frac{8m_1^2 \Upsilon}{\tilde{K}} - 32\Upsilon m_0^2 + O(\mu_2 \Upsilon). \tag{5.35}$$

The equations describing the evolution in t of the response to a perturbation at t' have the same shape as those for the correlation functions (5.26). The solutions are then

$$G_{ab}(t,t') = G_{ab}(t',t') \frac{\tilde{h}(t')}{\tilde{h}(t)}. \tag{5.36}$$

With these results we can generalize the fluctuation-dissipation theorem defining another effective temperature T_e^{FD} by means of the ratio between the derivative with respect to the initial time (also called the ‘‘waiting’’ time) t' of the correlation function C_{11} and the response function G_{11}:

$$T_e^{FD}(t,t') \equiv \frac{\partial_{t'} C_{11}(t,t')}{G_{11}(t,t')}. \tag{5.37}$$

To compute it we need

$$
\begin{aligned}
\partial_{t'}C_{11}(t,t')&=(\partial_{t'}C_{11}(t',t'))\frac{\tilde{h}(t')}{\tilde{h}(t)}-\tilde{f}(t')\frac{\tilde{h}(t')}{\tilde{h}(t)}C_{11}(t',t')\\
&\simeq-\tilde{f}(t')\frac{\tilde{h}(t')}{\tilde{h}(t)}C_{11}(t',t')\\
&\simeq-4\Upsilon(t')\\
&\quad\times\{[1+Q_\infty D+Q_1D\mu_2(t')]\Gamma(t')\\
&\quad+O(1)\}\frac{1}{1+Q_\infty D}\\
&\quad\times\left[m_0+\mu_2(t)\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)\right]\frac{\tilde{h}(t')}{\tilde{h}(t)}\\
&\simeq-4\Upsilon(t')\{[m_0+\mu_2(t')]\Gamma(t')+O(1)\}\frac{\tilde{h}(t')}{\tilde{h}(t)}.
\end{aligned}
\tag{5.38}
$$

Eventually we get

$$
\begin{aligned}
T_e^{FD}(t,t')&\simeq T_e(t')\left[1+O\left(\frac{1}{\Gamma(t')}\right)+O(\mu_2(t')^2)\right]\\
&=T_e^{FD}(t'),
\end{aligned}
\tag{5.39}
$$

where T_e was first introduced in Sec. III and later on derived in Eq. (4.3). We recall that $\Gamma^{-1}\propto\mu_2^\gamma$. As we see here the above defined fluctuation-dissipation effective temperature coincides, on the time scale of our interest, with the effective temperature T_e that we got by the quasistatic approach only if $1/\Gamma$ is negligible with respect to μ_2. This is true only if γ, the exponent of the generalized VFTH law (4.18), is greater than 1. Otherwise the last correction is no longer subleading: already for $\gamma=1$, $T_e^{FD}\to T_e$ only in the infinite time limit, i.e., for time scales longer than those of the considered aging regime. As already discussed in Sec. III, where we presented the results of the dynamics of the one-time observables, the value of the exponent γ discriminates between different regimes. For $\gamma>1$ an out of equilibrium thermodynamics can be built in terms of a single additional effective parameter (the effective temperature T_e). For $\gamma\leqslant1$, T_e alone does not give consistent results in the generalization of the equilibrium properties to the nonequilibrium case and in order to cure this inconsistency more effective parameters are probably needed. This discrepancy was clear, from Sec. III, for the regimes below T_0 where already the one-time variables had different behaviors depending on the value of γ being greater, equal to, or less than 1. For $T>T_0$ there was not such a difference at the one-time observable level. As we just saw, it shows up, instead, at the level of two-time observables.

2. Approach to equilibrium

For times longer than the aging regime time scales the terms that are relevant in Eqs. (5.20)–(5.22) for the correlation functions and in the expressions (5.34)–(5.36) for the response functions are different. When $t\gg t_g$ the equilibrium value $\overline{\mu_2}$ of the variable μ_2 is no longer negligible with respect to its time dependent part $\delta\mu_2(t)$ (which eventually goes to zero as $t\to\infty$). We are in a regime where $r\simeq0$ ($T_e\simeq T$). In the solution of Eqs. (5.20)–(5.22) this means that all the terms of $O(\Upsilon r\Gamma/\mu_2)=O(\delta\mu_2\Upsilon)$ are now subdominant with respect to those of $O(\Upsilon\Gamma)$ and of $O(\Upsilon)$. To solve Eqs. (5.20)–(5.22) we use the adiabatic expansion, as in the previous case.

The solutions for very large time, with finite though small $\overline{\mu_2}$ and a vanishing r, are

$$
\begin{aligned}
C_{11}(t,t)&=\frac{m_0+\mu_2(t)}{1+QD+P}(1+P)+c_{11,r}r\\
&=\frac{m_0+\overline{\mu_2}}{1+Q_\infty D+P_\infty}(1+P_\infty)+c_{11,\delta\mu_2}\delta\mu_2(t),
\end{aligned}
\tag{5.40}
$$

$$
\begin{aligned}
C_{12}(t,t)=C_{21}(t,t)&\simeq\frac{m_0+\mu_2(t)}{1+QD+P}\left(2\tilde{m}_1(t)-2\frac{L}{J}P\right)+c_{12,r}r\\
&=\frac{m_0+\overline{\mu_2}}{1+Q_\infty D+P_\infty}\left(2\overline{m}_1-2\frac{L}{J}P_\infty\right)+c_{12,\delta\mu_2}\delta\mu_2(t),
\end{aligned}
\tag{5.41}
$$

$$
\begin{aligned}
C_{22}(t,t)&\simeq\frac{m_0+\mu_2(t)}{1+QD+P}\left[4m_1(t)^2+2(m_0+\mu_2(t))+4\frac{L^2}{J^2}P\right]\\
&\quad+c_{22,r}r\\
&=\frac{m_0+\overline{\mu_2}}{1+Q_\infty D+P_\infty}\\
&\quad\times\left[4\overline{m}_1^2+2(m_0+\overline{\mu_2})+4\frac{L^2}{J^2}P_\infty\right]+c_{22,\delta\mu_2}\delta\mu_2(t).
\end{aligned}
\tag{5.42}
$$

Here

$$
c_{11,r}\equiv-\frac{4\gamma[m_0+\mu_2(t)]^3\tilde{K}^2J^2Q^2}{\mu_2(t)(1+DQ)(1+P+DQ)^2}(1+P),
\tag{5.43}
$$

$$
\begin{aligned}
c_{12,r}&\equiv\frac{4\gamma[m_0+\mu_2(t)]^3\tilde{K}JQ}{\mu_2(1+DQ)(1+P+DQ)^2}\\
&\quad\times\left[(1+P)(1+\tilde{K}LQ)+\tilde{K}JQ\left(P\frac{L}{J}-m_1\right)\right],
\end{aligned}
\tag{5.44}
$$

$$
\begin{aligned}
c_{22,r}&\equiv\frac{16\gamma[m_0+\mu_2(t)]^3\tilde{K}JQ}{\mu_2(t)(1+DQ)(1+P+DQ)^2}\left(P\frac{L}{J}-m_1\right)\\
&\quad\times(1+\tilde{K}LQ),
\end{aligned}
\tag{5.45}
$$

and

$$c_{11,\delta\mu_2} \equiv \frac{1}{1+DQ_\infty+P_\infty}\left\{1+P_\infty-(m_0+\overline{\mu}_2)\frac{P_1 DQ_\infty+Q_1 D(1+P_\infty)}{1+P_\infty+DQ_\infty}-\frac{8\gamma DQ_\infty P_\infty(1+P_\infty)(m_0+\overline{\mu}_2)}{\overline{\mu}_2(1+DQ_\infty)^2}\right\}, \tag{5.46}$$

$$\begin{aligned}c_{12,\delta\mu_2} \equiv \frac{2}{1+DQ_\infty+P_\infty}&\left\{\left[\overline{m}_1-\frac{L}{J}P_\infty\left(1+\frac{D}{L\tilde{K}_\infty(1+DQ_\infty)}\right)\right]-\frac{(m_0+\overline{\mu}_2)\{P_1[\overline{m}_1+(L/J)(1+DQ_\infty)]+DQ_1(\overline{m}_1-L/J)\}}{1+P_\infty+DQ_\infty}\right.\\ &\left.+\frac{4\gamma DP_\infty[(1+P_\infty)(1+\tilde{K}_\infty LQ_\infty)+\tilde{K}_\infty JQ_\infty(L/JP_\infty-\overline{m}_1)]}{J\tilde{K}_\infty\overline{\mu}_2(1+DQ_\infty)^2}\right\},\end{aligned} \tag{5.47}$$

$$\begin{aligned}c_{22,\delta\mu_2} \equiv \frac{2}{1+DQ_\infty+P_\infty}&\left\{2(m_0+\overline{\mu}_2)+2\overline{m}_1^2+2\frac{L^2}{J^2}P_\infty-\frac{4\overline{m}_1P_\infty D}{\tilde{K}_\infty J(1+DQ_\infty)}\right.\\ &-\frac{(m_0+\overline{\mu}_2)\{P_1[2\overline{m}_1^2+2L^2/J^2(P_\infty-1)+m_0+\overline{\mu}_2]+DQ_1(2\overline{m}_1^2+2L^2/J^2P_\infty+m_0+\overline{\mu}_2)\}}{1+P_\infty+DQ_\infty}\\ &\left.-\frac{8\gamma DP_\infty(\overline{m}_1-L/JP_\infty)(1+\tilde{K}_\infty LQ_\infty)}{J\tilde{K}_\infty\overline{\mu}_2(1+DQ_\infty)^2}\right\},\end{aligned} \tag{5.48}$$

where Q_1 is defined in Eq. (5.7) and P_1 in the first order coefficient of P in its expansion in $\delta\mu_2$ [see Eq. (5.13)].

To find the solutions to first order approximation in $\delta\mu_2(t)$ it is enough to keep in each of Eqs. (A13)–(A16) only terms up to $O(r\Upsilon)$ and $O(r\Upsilon/(\Gamma\mu_2))$. Whether or not the terms of $O(r\Upsilon)$ or those of $O(r\Upsilon/(\Gamma^n\mu_2))$, with $n=1,2,\ldots,$ are the most important depends on the value of the VFTH exponent γ: if $\gamma>1$, $O(r\Upsilon/(\Gamma\mu_2))\ll O(r\Upsilon)$ for large times; they are of the same order at $\gamma=1$; while if $1/2<\gamma<1$ $O(r\Upsilon/(\Gamma\mu_2))\gg O(r\Upsilon)$. Furthermore, if $\gamma\leq 1/2$ terms of order $O(r\Upsilon/(\Gamma^2\mu_2))$ will also be more important or as important as those of $O(\Upsilon)$. For yet smaller values of γ more and more terms of the kind $r\Upsilon/(\Gamma^n\mu_2)$ will be much greater than $O(r\Upsilon)$ in the aging regime.

As $t\to\infty$ the solutions (5.40)–(5.42) coincide with the elements of the matrix (2.26), the inverse of the Hessian of the free energy of the model, i.e., they coincide with the average squared fluctuations at equilibrium.

Once we have the equal time solutions we can solve Eqs. (5.26) for the two-time functions.

The function $\tilde{f}$ is now

$$\begin{aligned}\tilde{f}&\equiv f_1+\frac{2\dot{m}_1g_1}{g_2-2m_1g_1}-g_1\frac{f_2-2m_1f_1}{g_2-2m_1g_1}\\ &=-4\Upsilon(\Gamma-1)\frac{1+QD+P}{1+P}-4\Upsilon\frac{\Gamma^2}{\mu_2}r\gamma(m_0+\mu_2)\frac{QDP}{(1+P)^2}\\ &\quad+O\left(\frac{\Upsilon\Gamma r}{\mu_2}\right).\end{aligned} \tag{5.49}$$

The decoupled equations for $C_{11}(t,t')$ and $C_{12}(t,t')$ are always Eq. (5.29). From them we can compute $C_{21}(t,t')$ and $C_{22}(t,t')$ as follows:

$$C_{21}(t,t')\simeq 2\frac{m_1(t)-P(t)L/J}{1+P}C_{11}(t,t'), \tag{5.50}$$

$$C_{22}(t,t')\simeq\frac{2m_1(t)^2+2P(t)L^2/J^2+m_0+\mu_2(t)}{m_1(t)-P(t)L/J}C_{12}(t,t'). \tag{5.51}$$

Using the time evolution function $\tilde{h}$ [Eq. (5.31)] for the time scale sector considered, the solution of Eq. (5.29) comes out to be

$$C_{1b}(t,t')=C_{1b}(t',t')\frac{\tilde{h}(t')}{\tilde{h}(t)}+O(\mu_1\Upsilon),\quad b=1,2. \tag{5.52}$$

In the leading terms of our expansion in $\delta\mu_2(t)$ and $\overline{\mu}_2$ the expressions for the f's and g's are given, for the case $T>T_0$, by Eqs. (A13)–(A16).

Using Eqs. (5.40), (5.41), and (5.49), we get

$$\begin{aligned}C_{11}(t,t')\simeq&\frac{1+P_\infty}{1+Q_\infty D+P_\infty}[m_0+\overline{\mu}_2+O(\delta\mu_2(t))]\\ &\times\exp\left\{-4\int_{t'}^{t}\Upsilon(t'')[\Gamma(t'')-1]\right.\\ &\left.\times\frac{1+Q(t'')D+P(t'')}{1+P(t'')}dt''\right\},\end{aligned} \tag{5.53}$$

$$C_{12}(t,t')\simeq\frac{2P_\infty L/J-\overline{m_1}}{1+Q_\infty D+P_\infty}[m_0+\overline{\mu_2}+O(\delta\mu_2(t))]\times\exp\left\{-4\int_{t'}^{t}\Upsilon(t'')[\Gamma(t'')-1]\times\frac{1+Q(t'')D+P(t'')}{1+P(t'')}dt''\right\}. \tag{5.54}$$

B. Low temperature case: $T<T_0$

Our approach also allows us to study the regime below the Kauzmann temperature T_0. In this last case, though, we have qualitatively different behaviors depending on the value of γ, i.e., on the relative weights of μ_1 and μ_2. We describe here the case $\gamma>1$, where $\mu_1\ll\mu_2$ [see Eq. (3.35)]. For $\gamma>1$, according to the results shown in Sec. IV, it is indeed not necessary to introduce any effective thermodynamic parameter other than the effective temperature, and the analysis can be carried out in a way similar to that of the previous case (Sec. V A). In expanding the time dependent coefficients of C_{ab} in the equations of motion [$f_{1,2}$ and $g_{1,2}$ given in Eqs. (A13)–(A16)] we have now to take into account that r never vanishes, while on the contrary the asymptotic value of $\mu_2(t)$, denoted by $\overline{\mu_2}$, is zero. The leading terms in f_k and g_k ($k=0,1,2,3$) are in this case those of $O(\Upsilon\Gamma/\mu_2)$. The subleading terms are those of order $\Gamma\Upsilon$ and $\Gamma\mu_2\Upsilon$ (coming always with r as a multiplicative factor). All these terms are diverging terms, in the limit $t\to\infty$, and hence terms of $O(1)$ are now negligible with respect to them. They lead to corrections to the FDR of order $1/\Gamma\ll\mu_2$.

The equations of motions for the equal time correlation functions are identical to Eqs. (5.20)–(5.22). What change are the time dependent coefficients $f_{1,2}$ and $g_{1,2}$ and $r=r_\infty+O(\delta\mu_2(t))$, where r_∞ is defined in Eq. (3.40).

Solutions to these equations are obtained, as before, in the adiabatic approximation and expanding all the functions in powers of $\mu_2(t)$,

$$C_{ab}(t)=[2m_1(t)]^{a+b-2}\times\left\{\frac{1}{1+Q_\infty D}\left[m_0+\mu_2(t)\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)\right]-\frac{m_0}{\Gamma}\left[\frac{\alpha_1 r+\alpha_2 r^2}{(1+Q_\infty D)^4}+\gamma r\,\delta_{a,2}\delta_{b,2}\alpha_3\right]\right\}+O(\mu_2^2(t)), \tag{5.55}$$

where Q_1 is the coefficient of the first order expansion of Q given in Eq. (5.8), with $\overline{\mu_2}=0$ in this case and $\overline{w}\to w_\infty\equiv\sqrt{J^2m_0+(D/\widetilde{K}_\infty)^2+T^2/4}$,

$$Q_1\equiv\frac{Q_\infty}{(1+Q_\infty D)m_0}\left[\frac{J^2m_0(3w_\infty+T/2)}{2w_\infty^2(w_\infty+T/2)}-3P_\infty\right], \tag{5.56}$$

and

$$\alpha_1\equiv 1+3DQ(1-2P)+(DQ)^2(3-4P)+(DQ)^3, \tag{5.57}$$

$$\alpha_2\equiv 4(1+DQ)[\widetilde{K}LQ(1+P)-DQ(1-P)], \tag{5.58}$$

$$\alpha_3\equiv\frac{Jm_1}{\widetilde{K}}Q(1+DQ-m_0)(1+\widetilde{K}LQ)(5-12r+12r^2). \tag{5.59}$$

In the asymptotic limit these solutions do not coincide with Eqs. (5.40)–(5.42). That means that they are also different from the static limit of the correlation functions found in Sec. II from the inverse of the Hessian matrix (2.26). This is due to the fact that the static limit does not take into account the constraint (2.9) on the configuration space. Above the Kauzmann temperature the dynamics never reaches this constraint so that, even if it is slowed down by the existence of the constraint, it arrives the same static results. But as soon as we perform the dynamics at T_0 or below it, the asymptotic regime will never coincide with the equilibrium one. The system will be stuck forever in one ergodic component of the phase space, artificially created by imposing the constraint in the dynamics of the model, but not in the Hamiltonian. The implementation of the constraint in the dynamics makes the variance Δ^2 of the distribution of the random variables giving the updating of Monte Carlo dynamics [see Eq. (3.6)] diverging, when $T\leq T_0$. The divergent factor of Δ^2 is the quantity $\Gamma(t)$ [Eq. (3.7)], appearing in the equations of motion so far discussed. Going from a regime where the contributions of $O(1)$ are relevant ($T>T_0$) to another where they are not even subleading, with respect to $O(\Gamma)$, we lose the static limit.

We find the solutions of Eqs. (5.26) for the two-time correlation functions by following exactly the approach shown in the preceding section, with the following expressions for the functions $\dot{m}_1$ and $\tilde{f}$:

$$\dot{m}_1=4\Gamma\mu_1\Upsilon+O(\mu_2^\gamma\Upsilon), \tag{5.60}$$

$$\tilde{f}=-4\Upsilon\Gamma(1+QD)-8\Upsilon\frac{QDP}{1+QD}(1-3r+2r^2)+O(\mu_2\Upsilon), \tag{5.61}$$

The two-time correlation functions turn out to be

$$C_{1b}(t,t')\simeq\frac{[2m_1(t')]^{b-1}}{1+Q_\infty D}\times\left[m_0+\mu_2(t')\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)+O(\mu_1(t'))\right]\times\left\{4\int_{t'}^{t}[1+Q(t'')D]\Upsilon(t'')\Gamma(t'')dt''\right\},\qquad b=1,2, \tag{5.62}$$

$$C_{2b}(t,t')\simeq 2[m_1(t)]^{b-1}C_{1b}(t,t'),\quad b=1,2. \tag{5.63}$$

For the response functions, from Eqs. (5.34)–(5.36) we get

$$G_{11}(t,t^+)\simeq \frac{4\Upsilon\Gamma}{\tilde{K}}-\frac{2\Upsilon(1-2r)^2}{\tilde{K}}+\frac{8\Upsilon(\Gamma\mu_1)^2}{T_e}, \tag{5.64}$$

$$G_{12}(t,t^+)\simeq \frac{8m_1\Upsilon\Gamma}{\tilde{K}}-\frac{4m_1\Upsilon(1-2r)^2}{\tilde{K}}+\frac{16m_1\Upsilon(\Gamma\mu_1)^2}{T_e}+\frac{16r\Gamma\mu_1\Upsilon}{\tilde{K}}, \tag{5.65}$$

$$G_{22}(t,t^+)\simeq \frac{16m_1^2\Upsilon\Gamma}{\tilde{K}}-\frac{8m_1^2\Upsilon(1-2r)^2}{\tilde{K}}+\frac{32m_1^2\Upsilon(\Gamma\mu_1)^2}{T_e}+\frac{64m_1r\Gamma\mu_1\Upsilon}{\tilde{K}}+\frac{8m_0(1-2r)^2\Upsilon}{\tilde{K}}, \tag{5.66}$$

where this time the contributions $\Gamma\mu_1$ and $(\Gamma\mu_1)^2$ are both of order Υ and we take them into account.

The two-time behavior of the response functions is as in Eq. (5.36) with $\tilde{f}$ given by Eq. (5.61).

The last thing that we need, before computing T_e^{FD}, is the derivative

$$\begin{aligned}\partial_{t'}C_{11}(t,t')&=\frac{\tilde{h}(t')}{\tilde{h}(t)}\partial_{t'}C_{11}(t',t')-\tilde{f}(t')\frac{\tilde{h}(t')}{\tilde{h}(t)}C_{11}(t,t')\\&\simeq 4\Upsilon(t')\frac{1}{1+Q_\infty D}\left[m_0+\mu_2(t')\left(1-\frac{m_0Q_1D}{1+Q_\infty D}\right)\right]\\&\quad\times[1+Q(t')D]\Gamma(t')\\&\quad\times\exp\left\{4\int_{t'}^{t}[1+Q(t)D]\Upsilon(t'')\Gamma(t'')dt''\right\}.\end{aligned} \tag{5.67}$$

It follows that

$$T_e^{FD}(t,t')\simeq T_e(t')\left[1+O\left(\frac{1}{\Gamma}\right)+O(\mu_2^{1+\gamma})\right]=T_e^{FD}(t'). \tag{5.68}$$

In this case $O(1/\Gamma)=O(\mu_1)$ is always smaller than $O(\mu_2)$, because $\gamma>1$: in the long time regime $T_e^{FD}(t)$ coincides with $T_e(t)$.

C. Effective temperature from the fluctuation formula

A self-consistent picture with an effective temperature should also imply that the same effective temperature also governs other physical variables. From the expression of $m_1(t;T)$ as a function of H we can compute the quantity $\chi^{(fl)}\equiv(\partial m_1/\partial H)|_{T,t}$ that is the contribution to susceptibility in a cooling-heating setup caused by a change in the field H at fixed time (also called the *fluctuation susceptibility*). In a cooling experiment the whole susceptibility can, indeed, be written as [3]

$$\chi_{ab}\equiv\left.\frac{\partial m_a}{\partial H_b}\right|_T=\left.\frac{\partial m_a}{\partial H_b}\right|_{T,T_e}+\left.\frac{\partial m_a}{\partial T_e}\right|_{T,H_b}\left.\frac{\partial T_e}{\partial H_b}\right|_T \tag{5.69}$$

$$=\left.\frac{\partial m_a}{\partial H_b}\right|_{T,t}-\left.\frac{\partial m_a}{\partial T_e}\right|_{T,H_b}\left.\frac{\partial T_e}{\partial H_b}\right|_{T,t}+\left.\frac{\partial m_a}{\partial T_e}\right|_{T,H_b}\left.\frac{\partial T_e}{\partial H_b}\right|_T \tag{5.70}$$

$$\equiv\chi_{ab}^{fluct}(t)+\chi_{ab}^{loss}(t)+\chi_{ab}^{conf}(t). \tag{5.71}$$

Here we are considering an aging situation, so only the first term is relevant. We can reasonably assume that $\chi_{ab}^{fluct}(t)$ can take the form

$$\chi_{ab}^{fluct}(t)=\left.\frac{\partial m_a}{\partial H_b}\right|_{T,t}=N\frac{\langle\delta m_a(t)\,\delta m_b(t)\rangle_{fast}}{T}+N\frac{\langle\delta m_a(t)\,\delta m_b(t)\rangle_{slow}}{T_e^{(fl)}(t)}, \tag{5.72}$$

where $\langle\cdots\rangle_{fast/slow}$ is the average, respectively, over fast and slow processes. The fast ones are governed by the heat-bath temperature, and the slow ones by some effective temperature $T_e^{(fl)}$ depending on the time scale t. Through $\chi_{ab}^{fluct}(t)$ one can look at the connection between the fluctuation effective temperature $T_e^{(fl)}$, introduced in [2], and the other effective temperatures so far defined. To work it out we start from

$$\chi_{11}^{fluct}(t)\equiv\left.\frac{\partial m_1}{\partial H}\right|_{T,t}=N\frac{\langle\delta m_1(t)\,\delta m_1(t)\rangle}{T_e^{(fl)}}=\frac{C_{11}(t,t)}{T_e^{(fl)}}. \tag{5.73}$$

Using the following expression for m_1, obtained from Eq. (3.14):

$$m_1(t;T,H)=-\frac{L}{J}+\frac{D}{J\tilde{K}(m_1(t;T,H),m_2(t;T,H);T)}, \tag{5.74}$$

the fluctuation susceptibility $\chi_{11}^{(fl)}$ turns out to be

$$\left.\frac{\partial m_1}{\partial H}\right|_{T,t}=\frac{1}{\tilde{K}(1+QD)}+O(\mu_1). \tag{5.75}$$

Here we are neglecting terms like $\partial\mu_1/\partial H$ and $\partial\mu_2/\partial H$, of order μ_1 or higher (we deal with the regimes $[T>T_0,\forall\gamma]$ and $[T<T_0,\gamma>1]$ where $\mu_1\ll\mu_2$). Taking the expressions (5.23) and (5.55) we see that in both dynamic regimes that we are considering the leading term of C_{11} can be written as

$$C_{11}(t,t)=\frac{m_0+\mu_2}{1+QD}+O(\mu_2^\gamma), \tag{5.76}$$

and this leads to

$$T_e^{(fl)}=\tilde{K}(m_0+\mu_2)+O(\mu_2^\gamma), \tag{5.77}$$

thus coinciding with Eq. (4.3) to the order of our interest, i.e., $O(\mu_2)$. At higher orders there will be nonuniversalities. If $\gamma\leqslant 1$ the terms of $O(\mu_2^\gamma)$ become dominant with respect to $O(\mu_2)$, leading to the same situation that we had for T_e^{FD} in Eq. (5.39), namely, the thermodynamic description does not lead to a unique effective parameter.

VI. CONCLUSIONS

In this paper we consider a model that has all the basic properties of a fragile glass, built by processes evolving on two well separated time scales, representing the α and β processes taking place in real glassy materials. Also, the model is provided with a constraint applied to the harmonic oscillator dynamics, i.e., to the slow process dynamics, in order to reproduce the behavior of a good glass former.

Introducing a facilitated Monte Carlo dynamics [19,23,3] and developing it analytically, thus having the opportunity of probing it in more detail than in a numerical study, we found equations of motion that are in all respects those typical of glass relaxation. By means of the constrained dynamics we identified the Kauzmann temperature T_0 as the one at which the constraint is reached, asymptotically, for the first time in a cooling experiment from high temperature. There we showed how the real thermodynamic phase transition [11], taking place due to the breaking of ergodicity in the landscape of our model, rich in degenerate minima, is characterized. A detailed study of the dynamics was performed both above and below the Kauzmann temperature and for arbitrary values of the exponent γ generalizing the typical VFTH behavior, usually assumed for glasses, to $\tau_{eq}=\exp[A/(T-T_0)]^\gamma$. The dynamics in the aging regime of both one-time and two-time variables was carefully analyzed, including the corrections to this regime, relevant at shorter times.

The decoupling of time scales is fundamental for a generalization of equilibrium thermodynamics to systems far from equilibrium. We tested on our exactly solvable model whether or not the generalized approach holds, involving one extra variable, namely, the effective temperature, in 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. In our work it was derived as a function of time (for given values of the heat-bath temperature and of all the other parameters of the model) such that the evolving system out of equilibrium can be characterized by a probability measure of the configurations having a Boltzmann-Gibbs form with a factor $1/T_e$ instead of $1/T$ in front of the Hamiltonian.

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 time scale is involved in the dynamic evolution of a system. In those cases to every time sector will correspond an effective temperature [35]. Moreover, in a given time sector, the number of effective parameters needed to make such a translation into a thermodynamic viewpoint can, in principle, be equal to the number of relevant observables considered in every time sector. For certain dynamic regimes, however, determined by the temperature and by the VFTH exponent γ, the effective parameters pertaining to processes having the same time scale become equal to each other in time, for large times.

As we saw in Sec. IV, in the dynamic regimes reported in Sec. III, when the distance $\mu_1(t)$ from equilibrium is much smaller than the distance from the constraint, $\mu_2(t)$, the effective temperature alone is enough for a complete thermodynamic description of the dominant physical phenomena (the effective field $H_e=H$), while in the regimes where $\mu_1(t)$ is no longer negligible with respect to $\mu_2(t)$ the effective field $H_e(t)$ is also needed to map the dynamics on long time scales into a thermodynamic frame. From the time behavior of the slowly varying observables in the aging regime we found in Sec. IV a VFTH relaxation time dependence on temperature above the Kauzmann transition and we derived the Adam-Gibbs relation between the relaxation time and the configurational entropy, which we can explicitly compute for our model.

We have also been able to study the dynamics of the system quenched to a temperature below the Kauzmann temperature. At long, finite time t we see that it is possible to introduce an instantaneous relaxation time depending on the heat-bath temperature in a nontrivial way but expressible in terms of the effective temperature. What we got in this way is actually a VFTH law where the heat-bath temperature has been substituted by a time dependent effective temperature $T_e(t)$ and its asymptotic value $\overline{T_e}$ takes the place of the Kauzmann temperature T_0. Such a relation for the time scale of the aging dynamics below T_0 could hold very well in more general systems.

At equilibrium the heat-bath temperature enters many relations that can be rigorously proved and connected to each other in the framework of thermodynamics. Out of equilibrium we miss first principles to start with in the generalization of such a construction. We do not have any guaranty, for instance, that a given definition of effective temperature, made by generalizing a given equilibrium formula, will match any other definition coming from the generalization of another equilibrium formula. At equilibrium the heat-bath temperature enters the Boltzmann-Gibbs measure, the laws of thermodynamics, the fluctuation-dissipation theorem, and different Maxwell relations. However, out of equilibrium we have to check whether a single definition of effective temperature is compatible with any other. Since all effective temperatures have definite limits for long times, in our model we verify that these limits are identical (which happens always) and that the leading approaches to these limits coincide (which happens only for $\gamma > 1$). When that works out we find a way to completely recast the long time domain of the out of equilibrium dynamics into the language of thermodynamics in a given time sector, of course, well separated from the other time sectors of the glassy dynamics. This behavior may occur if the aging is so slow that the system has time enough to clearly demonstrate an effective temperature before going to a lower value of it.

With this aim we also rederived the effective temperature from the fluctuation-dissipation ratio and from the fluctuation formula connecting the susceptibility with the fluctuations of the slow variables of the system. In Sec. V we showed that the effective temperature T_e^{FD} defined as the fluctuation-dissipation ratio tends to the effective temperature T_e that we obtained by the quasistatic approach in Sec. IV only if μ_2^γ is negligible with respect to μ_2. This is true if γ is greater than 1. Otherwise the corrections of order μ_2^γ are no longer subleading and significantly change the time evolution of T_e^{FD}. Already for $\gamma = 1$, $T_e^{FD} \to T_e$ only in the infinite time limit, i.e., for time scales longer than those of the aging regime considered. Even above the Kauzmann temperature the value of the exponent γ discriminates between different regimes. For $\gamma > 1$ an out of equilibrium thermodynamics can be built in terms of the single additional effective parameter T_e. For $\gamma \leqslant 1$, T_e alone does not give consistent results in the generalization of the equilibrium properties to the nonequilibrium case. In those cases one also needs an effective field H_e. However, no universal behavior for the T_e, H_e combination has been found. Even within the solvable model of this paper, the applicability of the thermodynamic picture depends on how fast the relaxation time diverges.

We already mentioned that in the case $\gamma > 1$, for temperatures above the Kauzmann temperature, both the statics and the dynamics in the aging regime can be described by Vogel-Fulcher-Tammann-Hesse laws; see Eqs. (4.20) and (4.22). Notice that these laws are not identical, the static one diverging more strongly, due to a larger prefactor of the divergent term in the exponent. We also notice that in this situation $\gamma > 1$ the aging (well) below the Kauzmann temperature can be described in a form very similar to the aging above it. For this reason it is meaningful to compare experiments in those two aging regimes, and, in particular, to test whether the decay of measurable quantities, like the energy or the magnetization, has a common temporal law in the full aging regime.

Finally we checked the consistency of the widely mentioned thermodynamic picture by writing the first and second laws using the effective temperature, and we verified that it can also be computed from the generalization of the Maxwell relation at equilibrium giving the heat-bath temperature as the derivative of internal energy with respect to the entropy [see Eq. (4.12)]. We found the same results we got from the other derivations in the same validity limits.

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APPENDIX: MONTE CARLO INTEGRALS

Here we present the expressions of the integrals that we use in computing the dynamics of the observables following the Monte Carlo method explained in Sec. III. We recall that x, defined in Eq. (3.2), is the energy difference between the current configuration of the system and the one proposed for the updating. The variable r [defined in Eq. (3.22)] is the distance of the effective temperature T_e from the heat-bath temperature (which is also the equilibrium value of T_e in the dynamic regime above the Kauzmann temperature). First we define the abbreviation

$$\Upsilon \equiv \frac{e^{-\Gamma}(1-r)}{\sqrt{\pi\Gamma}}, \tag{A1}$$

which is the leading term of the acceptance ratio of the Monte Carlo dynamics given by

$$\int dx W(\beta x) p(x|m_1,m_2) = \Upsilon\Bigg[1 - \frac{1-2r+4r^2}{\Gamma} + \frac{3}{4\Gamma^2}(1-4r+16r^2-24r^3 + 16r^4) + O\left(\frac{1}{\Gamma^3}\right)\Bigg]. \tag{A2}$$

Then we give the behavior of the derivative with respect to time of the energy

$$\int dx W(\beta x) x p(x|m_1,m_2) = -4rT_e\Upsilon\Bigg[1 - \frac{3(1-2r+2r^2)}{\Gamma} + \frac{15}{4\Gamma^2}(3-12r+28r^2 - 32r^3+16r^4) + O\left(\frac{1}{\Gamma^2}\right)\Bigg] \tag{A3}$$

and of the variable m_1 [defined in Eq. (2.3)]

$$\int dx W(\beta x) \overline{y_1}(x) p(x|m_1,m_2) = 4\mu_1\Upsilon\left[\Gamma - (1-3r+4r^2) + O\left(\frac{1}{\Gamma}\right)\right]. \tag{A4}$$

In Sec. V we compute the correlation and the response functions. In order to find their time dependence we need the following derivatives. In these formulas we show the derivatives with respect to m_1 and m_2, taken as independent variables, of the effective temperature T_e, the variable r, and the leading term of the Monte Carlo acceptance ratio Υ. They are

$$\frac{\partial T_e}{\partial m_1} = 2\tilde{K}\left(P\frac{L}{J} - m_1\right), \tag{A5}$$

$$\frac{\partial T_e}{\partial m_2}=\tilde{K}(P+1), \tag{A6}$$

$$\frac{\partial r}{\partial m_1}=2\frac{1-3r+2r^2}{m_0+\mu_2}\left(P\frac{L}{J}-m_1\right), \tag{A7}$$

$$\frac{\partial r}{\partial m_2}=\frac{1-3r+2r^2}{m_0+\mu_2}(P+1), \tag{A8}$$

and

$$\frac{\partial \Upsilon}{\partial m_1}=-\Upsilon\left[\frac{m_1\gamma}{\mu_2}(2\Gamma+1)+2\frac{1-2r}{m_0+\mu_2}\left(P\frac{L}{J}-m_1\right)\right], \tag{A9}$$

$$\frac{\partial \Upsilon}{\partial m_2}=\Upsilon\left[\frac{\gamma}{2\mu_2}(2\Gamma+1)-\frac{1-2r}{m_0+\mu_2}(P+1)\right]. \tag{A10}$$

Furthermore, we show the extensive computation of the coefficients of Eqs. (5.20)–(5.22) and (5.26) for the dynamics of the two-time observables:

$$\begin{aligned}f_0&\equiv\partial_{m_1}\int dx W(\beta x)p(x|m_1,m_2)\\&\simeq -m_1\gamma\frac{\Upsilon}{\mu_2}\bigg[2\Gamma-1+4r-8r^2+\frac{3}{2\Gamma}(13-56r\\&\quad+136r^2-160r^3+80r^4)\bigg]+O\left(\frac{\Upsilon}{\mu_2\Gamma^2}\right)\\&\quad-2\frac{\Upsilon}{m_0+\mu_2}\left(P\frac{L}{J}-m_1\right)\left[1-2r+\frac{3-20r+40r^2-32r^3}{\Gamma}\right]\\&\quad+O\left(\frac{\Upsilon}{\Gamma^2}\right),\end{aligned} \tag{A11}$$

$$\begin{aligned}g_0&\equiv\partial_{m_2}\int dx W(\beta x)p(x|m_1,m_2)\\&\simeq \gamma\frac{\Upsilon}{2\mu_2}\bigg[2\Gamma-1+4r-8r^2+\frac{3}{2\Gamma}(13-56r+136r^2\\&\quad-160r^3+80r^4)\bigg]+O\left(\frac{\Upsilon}{\mu_2\Gamma^2}\right)-\Upsilon\frac{1}{m_0+\mu_2}(P+1)\\&\quad\times\left[1-2r+\frac{3-20r+40r^2-32r^3}{\Gamma}\right]+O\left(\frac{\Upsilon}{\Gamma^2}\right),\end{aligned} \tag{A12}$$

$$\begin{aligned}f_1&\equiv\partial_{m_1}\int dx W(\beta x)\overline{y_1}(x)p(x|m_1,m_2)\\&\simeq -4m_1\gamma\Upsilon\frac{\Gamma\mu_1}{\mu_2}[2\Gamma-3+6r-8r^2]+O\left(\frac{\Upsilon\mu_1}{\mu_2}\right)\\&\quad-16\Upsilon\frac{\Gamma\mu_1}{m_0+\mu_2}\left(\frac{L}{J}P-m_1\right)\\&\quad+4\Upsilon\partial_{m_1}\mu_1(\Gamma-1+3r-4r^2)+O(\mu_1\Upsilon),\end{aligned} \tag{A13}$$

$$\begin{aligned}g_1&\equiv\partial_{m_2}\int dx W(\beta x)\overline{y_1}(x)p(x|m_1,m_2)\\&\simeq 2\gamma\Upsilon\frac{\Gamma\mu_1}{\mu_2}[2\Gamma-3+6r-8r^2]+O\left(\frac{\Upsilon\mu_1}{\mu_2}\right)\\&\quad-8\Upsilon\frac{\Gamma\mu_1}{m_0+\mu_2}(P+1)+4\Upsilon\partial_{m_2}\mu_1(\Gamma-1+3r-4r^2)\\&\quad+O(\mu_1\Upsilon),\end{aligned} \tag{A14}$$

$$\begin{aligned}f_2&\equiv\partial_{m_1}\int dx W(\beta x)\overline{y_2}(x)p(x|m_1,m_2)\\&\simeq 2m_1f_1+\frac{2}{\tilde{K}}f_3+16\Upsilon r\frac{L}{J}\frac{P}{1+QD}+O(\mu_1\Upsilon),\end{aligned} \tag{A15}$$

$$\begin{aligned}g_2&\equiv\partial_{m_2}\int dx W(\beta x)\overline{y_2}(x)p(x|m_1,m_2)\\&\simeq 2m_1g_1+\frac{2}{\tilde{K}}g_3+8\Upsilon r\frac{P}{1+QD}+O(\mu_1\Upsilon),\end{aligned} \tag{A16}$$

$$\begin{aligned}f_3&\equiv\partial_{m_2}\int dx W(\beta x)xp(x|m_1,m_2)\\&\simeq 4m_1\gamma\Upsilon T_e\frac{r}{\mu_2}\bigg[2\Gamma-5+12r-12r^2-\frac{3}{\Gamma}(3+9r-54r^2\\&\quad+140r^3-160r^4+80r^5)\bigg]+O\left(\frac{\Upsilon r}{\mu_2\Gamma^2}\right)\\&\quad-8\Upsilon\tilde{K}\left(\frac{L}{J}P-m_1\right)\bigg[1-3r+4r^2\\&\quad-\frac{3}{\Gamma}(1-5r+12r^2-14r^3+8r^4)\bigg]+O\left(\frac{\Upsilon}{\Gamma^2}\right),\end{aligned} \tag{A17}$$

$$\begin{aligned}g_3&\equiv\partial_{m_2}\int dx W(\beta x)xp(x|m_1,m_2)\\&\simeq -2\gamma\Upsilon T_e\frac{r}{\mu_2}\bigg[2\Gamma-5+12r-12r^2\\&\quad-\frac{3}{\Gamma}(3+9r-54r^2+140r^3-160r^4+80r^5)\bigg]\\&\quad+O\left(\frac{\Upsilon r}{\mu_2\Gamma^2}\right)-4\Upsilon\tilde{K}(P+1)\\&\quad\times\left[1-3r+2r^2-\frac{3}{\Gamma}(1-5r+12r^2-14r^3+8r^4)\right]\\&\quad+O\left(\frac{\Upsilon}{\Gamma^2}\right).\end{aligned} \tag{A18}$$

All partial derivatives with respect to m_1 have been computed keeping m_2 fixed and vice versa. At this stage time has not yet been introduced. Introducing it, we are able to make an expansion of Eqs. (A11)–(A18) in powers of $\mu_2(t)$. In the formulas we already performed such an expansion, breaking it at $O(\Upsilon/(\Gamma\mu_2))$, which is more than sufficiently refined to derive the dynamics of the correlation and response functions in all the regimes of our interest.

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