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# Series expansion of the off-equilibrium mode coupling equations

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**Abstract.** We show that computing the coefficients of the Taylor expansion of the solution of the off-equilibrium dynamical equations characterizing models with quenched disorder is a very effective way to understand the long-time asymptotic behaviour. We study the $p = 3$ spherical spin-glass model, and we compute the asymptotic energy (in the critical region and down to $T = 0$) and the coefficients of the time decay of the energy.

It has been strongly stressed in recent years that the non-equilibrium dynamics of glassy systems displays very interesting phenomena. One of the most remarkable phenomena is *aging* [1]. The dependence on time of measurable quantities does not vanish when time goes to $\infty$, and a true equilibrium is never reached.

Let us give a simple example of an *aging* behaviour. In spin systems the spin–spin correlation function can be defined as

$$C(t_w, t) \equiv N^{-1} \sum_i \sigma_i(t_w)\sigma_i(t_w + t). \tag{1}$$

We can consider a system that has been kept at very high $T$ for times smaller than $t = 0$ and has been quenched to the measurement temperature $T_0$ at time $t = 0$. We wait a time $t_w$ after such a quenching, and we measure spin–spin correlations starting at $t_w$. The relevant point is that, in contrast to equilibrating systems, for large $t_w$ and $t$ the dependence of $C$ on the waiting time $t_w$ does not disappear. In the simplest cases it is found that for $t/t_w \neq 1$, $C(t_w, t)$ can be written as

$$C(t_w, t) = f\left(\frac{t}{t_w}\right) \tag{2}$$

where $f$ is not a constant function. Even for asymptotically large times the time translational invariance of the correlation functions is never recovered.

Aging is quite a widespread phenomenon in short-range models. Aging in disordered systems has the interesting peculiarity of already being present in the mean-field approximation. It is obvious that we can have true, complete aging only in an infinite

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system. In such a case one can write a closed set of dynamical equations [2, 3] which are the appropriate generalization of the famous mode–mode coupling equation for glasses. Unfortunately these equations are coupled integral equations in two variables and the analytic solutions found so far [3–6], although they give a coherent picture of aging, do not allow the study of the time dependence of the different quantities. Hence, it is highly desirable to have efficient methods to integrate these equations numerically.

An example of these equations for the spherical spin model with a $p$-spin interaction in the case $p = 3$ is given by a set of nonlinear integro-differential equations [2, 3], which are obtained by transforming equations (14) and (15) back to their constrained form (see the later discussion). The same equations also appear in the off-equilibrium dynamics of the Amit–Roginsky model [7] where, although quenched disorder is absent [8], the mode coupling approximation gives exact results.

It is possible to study such equations numerically [4], but it is rather difficult to study the solution for large values of time. The main problem is the amount of information which needs to be stored, since if the discretization step in time is $\epsilon$ the quantity of numbers needed to code the correlation function is $L^2$ where $L = t/\epsilon$.

The dynamical equations can be derived starting from the usual Langevin equation for the $p$-spin model:

$$\dot{\sigma}_i(t) = -\mu(t)\sigma_i(t) + \sum_{i_2<\cdots<i_p}^{1,N} J_{i,i_2,\ldots,i_p}\sigma_{i_2}(t)\cdots\sigma_{i_p}(t) + \eta_i(t) \tag{3}$$

where the $J$ couplings are quenched Gaussian random variables, and $\eta$ is a white noise with covariance $2T$. For all times $t$, the value of $\mu(t)$ is chosen so as to implement the spherical constraint

$$\sum_{i=1}^{N}\sigma_i(t)^2 = N. \tag{4}$$

For mainly technical purposes, and some aesthetic considerations, we find it more suitable to switch to a formulation where the spins $s_i(t)$ are unconstrained. All that we have performed here can be repeated, with essentially the same degree of complexity, in the formulation where the spins are the original constrained variables.

If we consider the transformation

$$s_i(t) = \mathcal{N}(t)\sigma_i(t) \tag{5}$$

with

$$\mathcal{N}(t) = \exp\left(\int_0^t \mathrm{d}t'\,\mu(t')\right) \tag{6}$$

the dynamical equations become

$$\mathcal{N}(t)^{p-2}\dot{s}_i(t) = \sum_{i_2<\cdots<i_p}^{1,N} J_{i,i_2,\ldots,i_p}s_{i_2}(t)\cdots s_{i_p}(t) + \mathcal{N}(t)^{p-1}\eta_i(t). \tag{7}$$

Defining an effective time $\tau$ from the relation

$$\mathrm{d}t = \mathcal{N}^{p-2}\,\mathrm{d}\tau \tag{8}$$

we obtain

$$\frac{\partial s_i(\tau)}{\partial\tau} = \sum_{i_2<\cdots<i_p}^{1,N} J_{i,i_2,\ldots,i_p}s_{i_2}(\tau)\cdots s_{i_p}(\tau) + \xi_i(\tau) \tag{9}$$

where the $\xi_i$ are Gaussian noise with zero mean and variance:

$$\overline{\xi_i(\tau)\xi_j(\tau')} = 2T\mathcal{N}^p(\tau)\delta(\tau - \tau')\delta_{i,j}. \tag{10}$$

The unconstrained system of the $s$ variables is kept at a temperature

$$T_{\text{eff}}(\tau) \equiv T\mathcal{N}^p(\tau) \tag{11}$$

in order to keep the original constrained variables at a fixed, time-independent temperature $T$.

From equations (9) and (10), after standard manipulations we obtain a set of closed dynamical equations for the correlation function

$$C(\tau, \tau') \equiv \langle s_i(\tau)s_i(\tau')\rangle \tag{12}$$

and for the response function

$$R(\tau, \tau') \equiv \frac{\delta\langle s_i(\tau)\rangle}{\delta\xi_i(\tau')}. \tag{13}$$

For $\tau > \tau'$ they are, respectively,

$$\frac{\partial}{\partial\tau}C(\tau, \tau') = \tfrac{1}{2}p(p-1)\int_0^\tau \mathrm{d}\tau''\, C^{p-2}(\tau, \tau'')R(\tau, \tau'')C(\tau'', \tau')$$
$$+\tfrac{1}{2}p\int_0^{\tau'} \mathrm{d}\tau''\, C^{p-1}(\tau, \tau'')R(\tau', \tau'') \tag{14}$$

and

$$\frac{\partial}{\partial\tau}R(\tau, \tau') = \tfrac{1}{2}p(p-1)\int_{\tau'}^\tau \mathrm{d}\tau''\, C^{p-2}(\tau, \tau'')R(\tau, \tau'')R(\tau'', \tau'). \tag{15}$$

For equal times, $R = 1$, and $C$ verifies that

$$\frac{1}{2}\frac{\partial}{\partial\tau}C(\tau, \tau) = \tfrac{1}{2}p^2\int_0^\tau \mathrm{d}\tau''\, C^{p-1}(\tau, \tau'')R(\tau, \tau'') + TC(\tau, \tau)^{p/2} \tag{16}$$

where we have used the fact that

$$\mathcal{N}(\tau) = \sqrt{C(\tau, \tau)}. \tag{17}$$

We have rewritten our constrained system as an unconstrained system, kept at a time-dependent temperature $T_{\text{eff}}(\tau)$. We stress that this transformation has been allowed by the fact that our Hamiltonian is homogeneous. We will discuss the system in such an unconstrained formulation. We again remind the reader that all our results can also be easily obtained in the constrained formalism, where one can also deal with non-homogeneous Hamiltonians as in [4].

The method we suggest and employ here to study the asymptotic behaviour of the dynamic equations (14) and (15) is based on computing the coefficients of the Taylor expansion of $C$ and $R$, defined by

$$C(\tau_1, \tau_2) = \sum_{k,j} c_{k,j}\tau_1^k\tau_2^j \qquad R(\tau_1, \tau_2) = \sum_{k,j} r_{k,j}\tau_1^k\tau_2^j. \tag{18}$$

We always assume that $\tau_1 > \tau_2$. Equations (14) and (15) transform into two coupled iterative relations for the Taylor coefficients $c$ and $r$. Knowing the lower-order coefficients, we can determine the higher-order coefficients. The initial conditions are $c_{0,0} = 1$ and $r_{0,0} = 1$. We determine the coefficients $c_{k,j}$ and $r_{k,j}$ in turn with $i + j = \omega$ for $\omega = 2, 3, 4, \ldots$. It takes a few hours on a RISC workstation to go up to $\omega = 100$ (we analyse coefficients going up to order 48, see later). We repeat the procedure for different values of the temperature $T$; the complexity of the computation increases as $\omega^3$.

In this paper, as an example, we give the results of the computation of the energy, which happen to be in agreement with the theory [2,3]. In a forthcoming publication we will address the problem of verifying more striking issues of the theory, such as the asymptotic violation of time translation invariance and of the fluctuation dissipation theorem.

We start the analysis from the Taylor expansion for $C(\tau,\tau)$. If we define

$$c_k^{(d)} \equiv \sum_{j=0}^{k} c_{k-j,k} \tag{19}$$

we have that

$$C(\tau,\tau) = \sum_{l=0}^{\infty} c_l^{(d)} \tau^l. \tag{20}$$

In the self-explanatory formalism that we use later, we will be working on the Taylor coefficients

$$\{C^{(d)}(\tau)\}_k. \tag{21}$$

We have computed the coefficients of the series expansions which follow by using a simple program written in C-language. We have first computed the coefficients

$$\{\mathcal{N}(\tau)\}_k = \{C^{(d)}(\tau)^{1/2}\}_k = \left\{ \exp\left( \int_0^{t(\tau)} \mathrm{d}t' \, \mu(t') \right) \right\}_k. \tag{22}$$

The coefficients of $\mu$ as a function of the *unconstrained time* $\tau$ are easily computed as

$$\{\mu(\tau)\}_k = \left\{ \frac{1}{\mathcal{N}} \frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} \right\}_k = \left\{ \frac{1}{\mathcal{N}} \frac{\mathrm{d}\mathcal{N}}{\mathrm{d}\tau} \frac{\mathrm{d}\tau}{\mathrm{d}t} \right\}_k = \left\{ -\frac{\mathrm{d}\mathcal{N}^{-1}}{\mathrm{d}\tau} \right\}_k \tag{23}$$

and for the *constrained time* $t$ as a function of the *unconstrained time* $\tau$

$$\{t(\tau)\}_k = \left\{ \int_0^t \mathrm{d}\tau \, \mathcal{N}(\tau) \right\}_k = \frac{\mathcal{N}_{k-1}}{k}. \tag{24}$$

By inverting and composing these series expansions, we eventually obtain

$$\{\mu(t)\}_k \tag{25}$$

which is basically the energy as a function of the *constrained time* $t$. It is useful to define the Taylor expansion of the function

$$\{\beta(t)\}_k \equiv \left\{ t \frac{\mu''(t)}{\mu'(t)} \right\}_k. \tag{26}$$

Under the assumption that, for $t \to \infty$,

$$\mu(t) \to \mu_\infty - At^{-\alpha} \tag{27}$$

one has that

$$\beta(t) \to -(\alpha + 1). \tag{28}$$

Different techniques may be used to extrapolate the function $\beta(t)$ to $t = \infty$. After a series of tests we have found it convenient to use Padè approximants. We have used the diagonal Padè approximants of order 48 to check this behaviour†. We compute $\alpha$ from $\beta(\tilde{t})$, with a high enough value of $\tilde{t}$. Using our best estimate for $\alpha$, we compute $\mu(\tilde{t})$ and the extrapolated value $\mu(\tilde{t} = \infty)$. Once $\mu(t)$ is known, the energy $E(t)$ is obtained by the simple relation $\mu(t) = T - 3E(t)$ [2].

† Lower-order Padé approximants have been used to check stability.

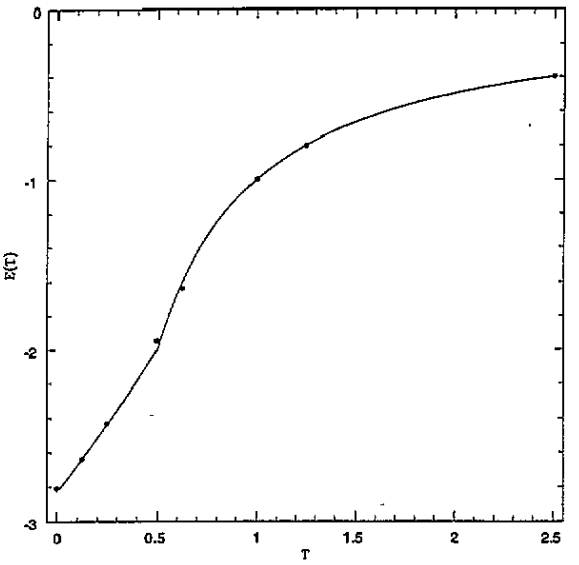


**Figure 1.** Theoretical result for the asymptotic dynamic energy $E(T)$ (solid curve) and our values (full circles). The dynamic critical temperature is $T_D = \frac{1}{2}$. In the high $T$ region $E(T) = 1/T$.

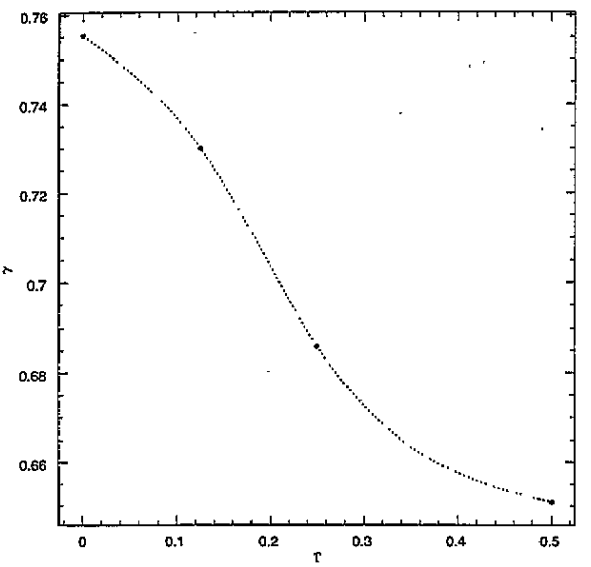


**Figure 2.** $\alpha$ as a function of $T$. In these units the dynamic transition temperature is $T_D = \frac{1}{2}$. The curve is used for presenting the data, and does not have any physical meaning such as a best fit.

Let us start with a brief summary of our results. Our method confirms that the asymptotic dynamic energy $E(T)$ is correctly predicted by the theory. We find, in addition, the remarkable result that the value of the asymptotic dynamic energy of the dynamics at zero temperature is the smooth limit of the values for $T \neq 0$. This does not seem to be true

in other spin-glass systems, as for example the SK model [9]. We also obtain a very good estimate for the exponent $\alpha$ for $T < T_D = 0.5$. These results have been obtained with very small computational effort.

In figure 1 we compare the theoretical result for the asymptotic value of the dynamic energy to our findings. Here the critical temperature is obtained by solving the equation

$$\frac{2}{T_D^2} q_D (1 - q_D)^2 = 1 \qquad q_D \equiv q(T_D) = \tfrac{1}{2} \tag{29}$$

which gives $T_D = \frac{1}{2}$, and the dynamic energy is defined as

$$-\frac{1}{T}(1 + q^2(1 - 2q)). \tag{30}$$

The agreement is very good at low $T$. The convergence (in time) becomes slower when approaching the critical point; exactly at $T_D$ we have the highest discrepancy from the exact value (of more or less 2%). In the high $T$ phase the convergence to the asymptotic result becomes very fast again.

In figure 2 we plot the exponent $\alpha$ that we have estimated from Padè approximants as a function of $T$. We do not have a precise estimate of the errors (this is a known drawback of the Padè approach), but judging from the dispersion of different diagonal approximants they appear to be of the order of magnitude of a few per cent. If we try to estimate $\alpha$ for $T > T_D$, in the high-temperature phase, where we expect the correlations to decay exponentially, we find a value that starts to increase with $T$ and dramatically explodes for high $T$. The relatively large discrepancy of the extrapolated energy value close to $T_D$ makes us suspicious about the possible presence of tricky confluent singularities. Obviously such a problem would reflect itself in the value we are estimating for $\alpha$.

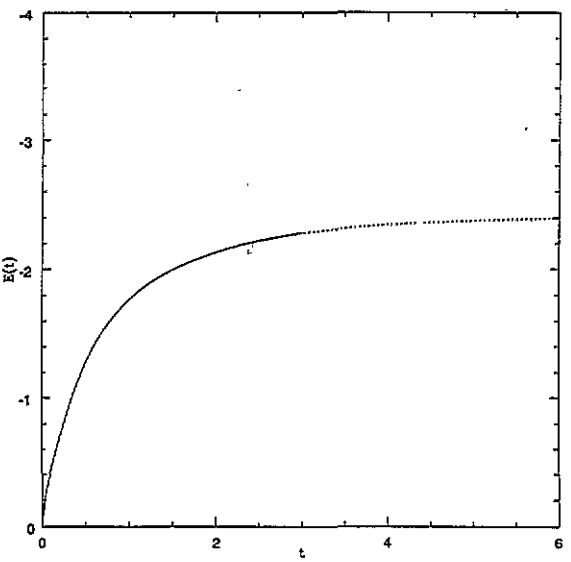


**Figure 3.** Result for the asymptotic dynamic energy $E(t)$ from the direct numerical integration of the dynamical equations (solid curve) and our result as a function of time (dotted curve). Here $T = T_D/4$, i.e. $T = 0.125$ with our normalization.

The fact that our method works very well is also clear from figure 3, where we compare the results of our expansion to the result from the direct numerical integration of the

dynamical equations. We have a perfect matching, but, as we discussed, the numerical integration is limited to small times, and it is difficult to extract reliable asymptotic values for the coefficients.

Summing up, we have seen that the numerical integration of the off-equilibrium mode coupling equations can effectively be performed by computing the coefficients of the Taylor expansion of the correlation and the response functions. As an example of an application we have computed the energy as a function of time and temperature. In the low-temperature phase (and down to zero temperature) we find a power-law decay to the value predicted by mean-field theory.

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