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 behavior. 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.

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

Let us give a simple example of an *aging* behavior. 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 contrary 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 $\frac{t}{t_w} \neq 1$ $C(t_w,t)$ can be written as

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

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 being already present in the mean field approximation. It is obvious that we can have true, complete aging only in an infinite system. One should investigate the dynamics of an infinite system. In this 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, 4, 5, 6], although they give a coherent picture of aging, do not allow to study the time dependence of the different quantities. It is then highly desirable to have efficient methods to integrate the 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 non-linear integro-differential equations ([2, 3]), which are obtained by transforming eqs. (14,15) back to their constrained form (see the discussion in the following). 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 the time. The main problem is of the amount of information which needs to be stored, since if the discretization step in time is ϵ the number 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

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

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

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

For mainly technical purposes, and some extetical considerations, we find more suitable to switch to a formulation where the spins $s_i(t)$ are unconstrained. All what we have have done 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

$$\mathcal{N}(t) = e^{\int_0^t dt' \mu(t')} \ , \tag{6}$$

the dynamical equations become

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

Defining an effective time τ from the relation

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

we get that

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

where the ξ_i are a gaussian noise with zero mean and variance

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

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

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

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

From the previous equations (9,10) 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

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

and

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

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

$$
\begin{aligned}
\frac{1}{2}\frac{\partial}{\partial\tau}C(\tau,\tau) &= \frac{1}{2}p^2\int_0^{\tau} d\tau'' C^{p-1}(\tau,\tau'')R(\tau,\tau'') \\
&+ TC(\tau,\tau)^{\frac{p}{2}} \ ,
\end{aligned} \tag{16}
$$

where we used the fact that

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

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

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

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

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

In this note, 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 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-explaining formalism we will use in the following 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 at first computed the coefficients

$$\{\mathcal{N}(\tau)\}_k = \{C^{(d)}(\tau)^{\frac{1}{2}}\}_k = \{e^{\int_0^{t(\tau)} dt' \mu(t')}\}_k \ . \tag{22}$$

The coefficients of μ as a function of the *unconstrained time* τ are easily computed as

$$\{\mu(\tau)\}_k = \{\frac{1}{\mathcal{N}}\frac{d\mathcal{N}}{dt}\}_k = \{\frac{1}{\mathcal{N}}\frac{d\mathcal{N}}{d\tau}\frac{d\tau}{dt}\}_k = \{-\frac{d\mathcal{N}^{-1}}{d\tau}\}_k \ , \tag{23}$$

and for the *constrained time* t as a function of the *unconstrained time* τ

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

By inverting and composing these series expansions we eventually obtain

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

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

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

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 convenient to use Padè approximants. We have used the diagonal Padè approximants of order 48 to check this behavior[1]. We compute α from $\beta(\tilde{t})$, with an high enough value of $\tilde{t}$. having our best estimate for α 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].

[1] Lower order Padè approximants have been used to check stability.

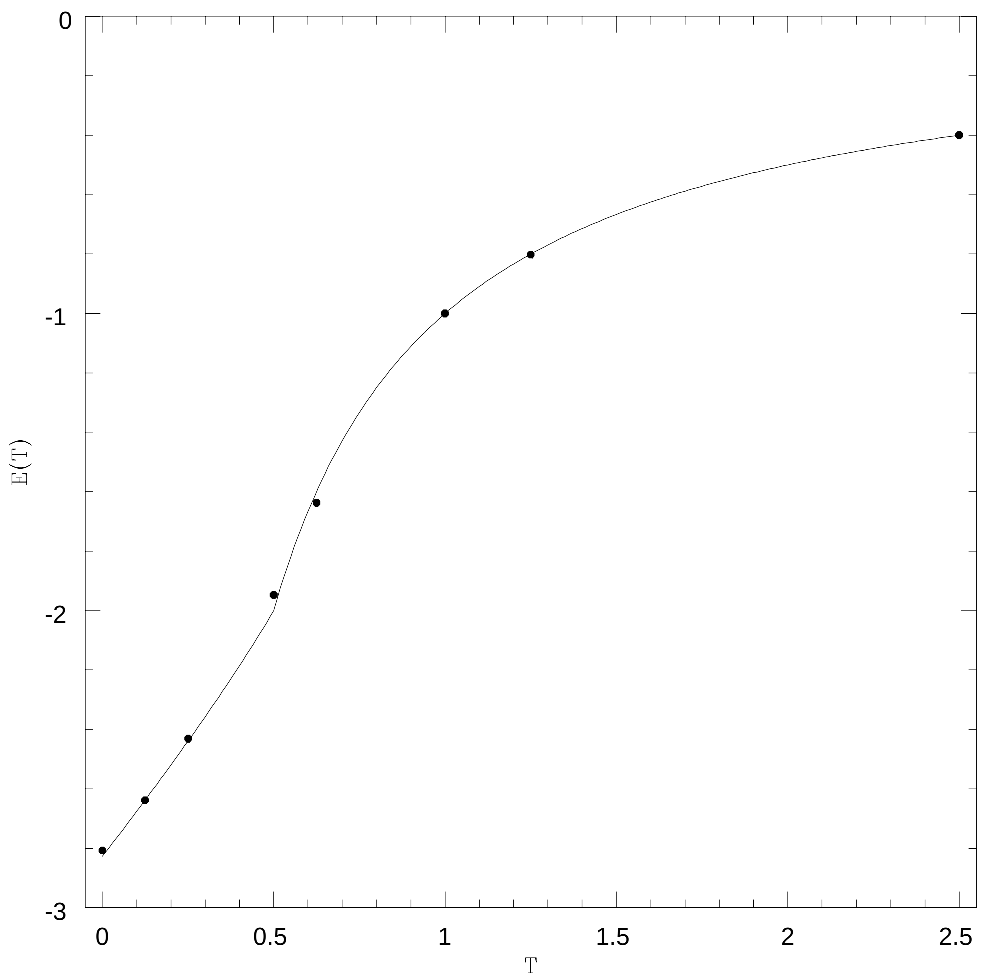

Figure 1: Theoretical result for the asymptotic dynamic energy $E(T)$ (solid curve) and our values (filled dots). The dynamic critical temperature is $T_D = \frac{1}{2}$. In the high T region $E(T) = \frac{1}{T}$.

Let us start with a brief summary of our results. Our method confirms that the asymptotic dynamic energy, $E(T)$ is correctely 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 get a very good estimate for the exponent α 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

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

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

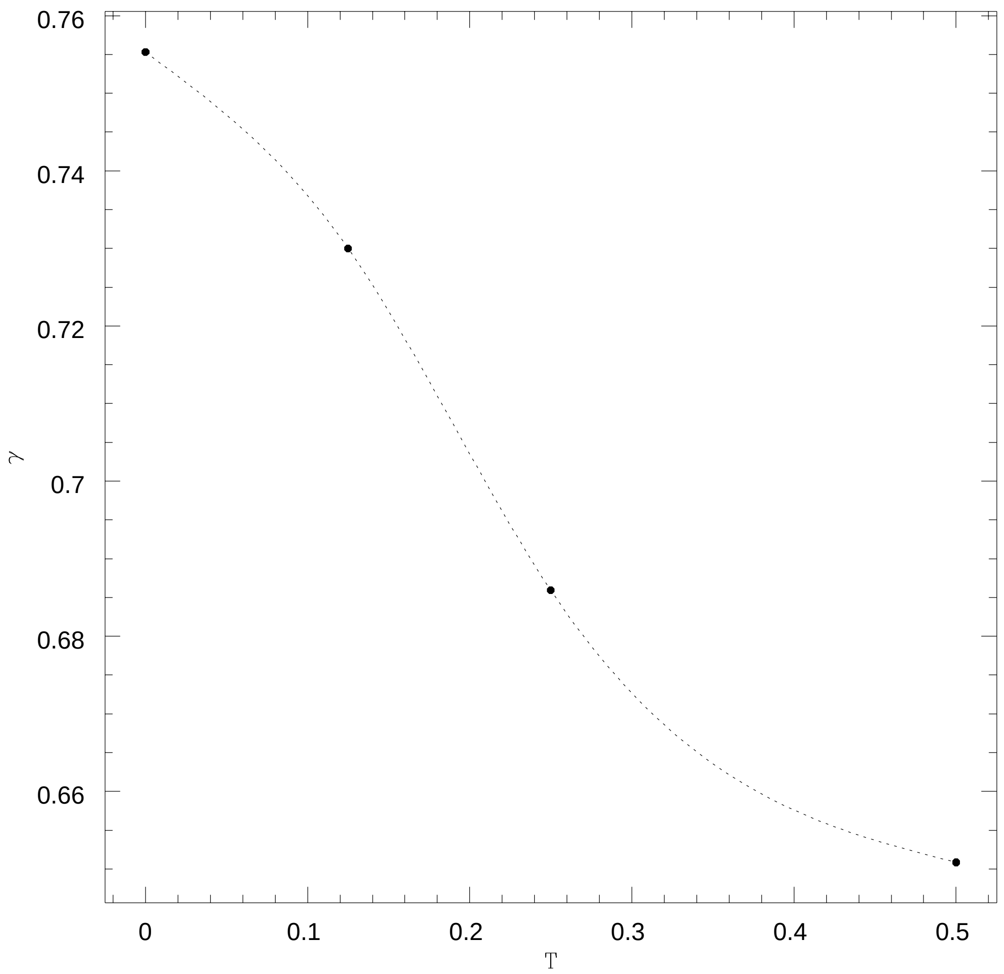

Figure 2: α as a function of T. In these units the dynamic transition temperature $T_D = \frac{1}{2}$. The smooth curve is just used for presenting the data, and does not have any physical meaning of a best fit.

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

The agreement is very good at low T. The convergence (in time) becomes slower when approaching the critical point, and exactly at T_D we have the higher 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 α 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 percent. If we try to estimate α 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

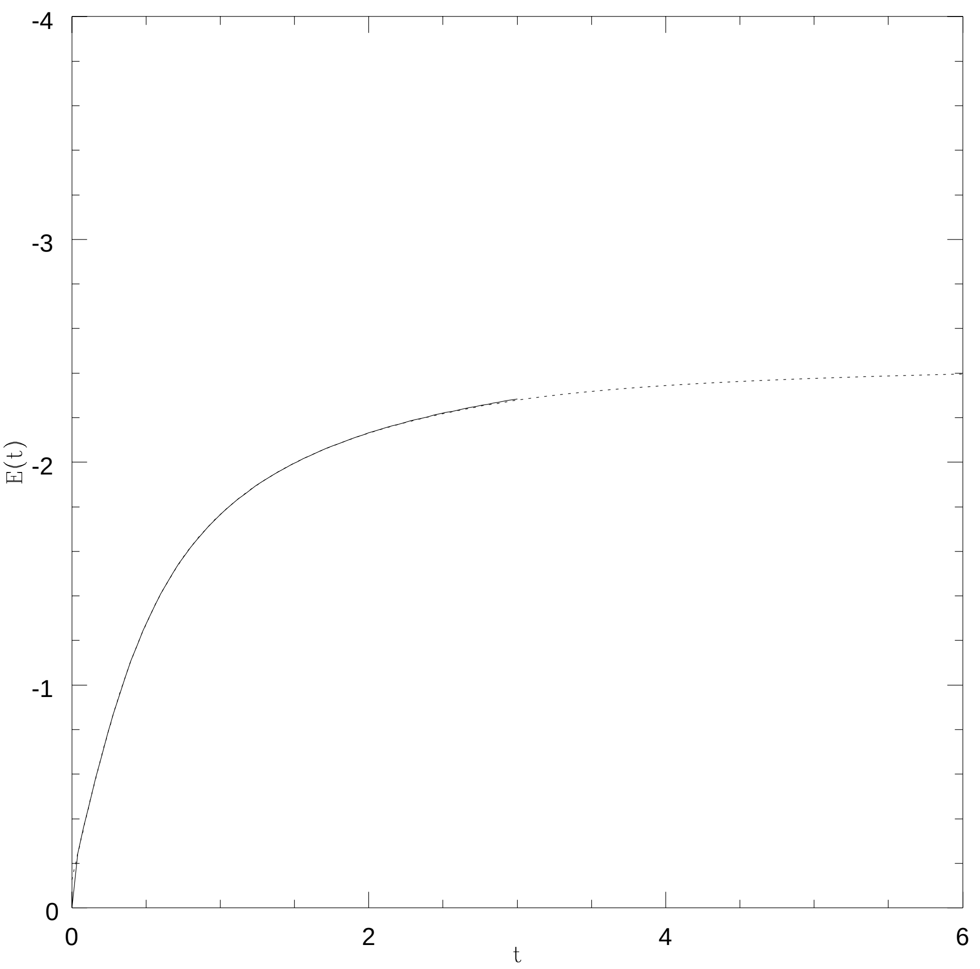

Figure 3: Result for the asymptotic dynamic energy $E(t)$ from the direct numerical integration of the dynamical equations (solid curve) and our result as a function of time (dotted line). here $T = \frac{T_D}{4}$, i.e. $T = 0.125$ with our normalization.

such a problem would reflect itself in the value we are estimating for α.

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 from there 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 computing the coefficients of the Taylor expantion of the correlation and the response functions. As an example of 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 power law decay to the value predicted by the mean field theory.

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