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# A far-from-equilibrium fluctuation-dissipation relation for Ising-Glauber-like models

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## Abstract

We derive an exact expression of the response function to an infinitesimal magnetic field for the Ising-Glauber model with arbitrary exchange couplings. The result is expressed in terms of thermodynamic averages and does not depend on the initial conditions or on the dimension of the space. The response function is related to time-derivatives of a complex correlation function and so the expression is a generalisation of the equilibrium fluctuation-dissipation theorem in the special case of the Ising-Glauber model. A discrete-time version of this relation is implemented in Monte Carlo simulations and then used to study the aging regime of the ferromagnetic two-dimensional Ising-Glauber model quenched from the paramagnetic phase to the ferromagnetic one. Our approach has the originality to give direct access to the response function and the violation ratio.

## 1 Introduction

The knowledge about out-of-equilibrium processes is far from being as advanced as for systems at equilibrium. In particular, the fluctuation-dissipation theorem (FDT) which holds at equilibrium is known to be violated out-of-equilibrium. This theorem states that at equilibrium the response function  $R^{\text{eq}}(t-s)$  at time  $t$  to an infinitesimal field applied to the system at time  $s < t$  is related to the time-derivative of the two-time autocorrelation function  $C^{\text{eq}}(t-s)$ :

$$R^{\text{eq}}(t-s) = \beta \frac{\partial}{\partial s} C^{\text{eq}}(t-s). \quad (1)$$

In the Ising case, the response function reads  $R_{ji}(t,s) = \frac{\delta \langle \sigma_j(t) \rangle}{\delta h_i(s)}$  and the correlation function  $C_{ji}(t,s) = \langle \sigma_j(t) \sigma_i(s) \rangle$ . Based on a mean-field study of spin-glasses, Cugliandolo *et al.* [1] have conjectured that for asymptotically large times the FDT can be generalised by adding a multiplicative factor  $X(t,s)$  which moreover depends on time only through the correlation function:

$$R(t,s) \underset{t \sim s \gg 1}{\sim} \beta X(C(t,s)) \frac{\partial}{\partial s} C(t,s). \quad (2)$$

The quantity  $\beta^{\text{eff}}(t, s) = \beta X(C(t, s))$  is interpreted as an effective temperature. Exact results have been obtained for the ferromagnetic Ising chain [2, 3] that confirm this conjecture. Unfortunately, the response function is rarely so easily accessible for more complex systems. Both numerically and experimentally, only the integrated response function is usually measured by applying a finite magnetic field to the system during a finite time. In the so-called TRM scheme, the magnetic field is applied between the times 0 and  $s$  and the magnetisation is measured at time  $t$ . Assuming the equation (2) valid for any times  $t$  and  $s$ , one can relate the integrated response function to the violation ratio:

$$\chi(t, s) = \int_0^s R(t, u) du \sim \beta \int_{C(t, 0)}^{C(t, s)} X(C) dC. \quad (3)$$

The violation ratio  $X(t, s)$  can thus be obtained as the slope of the integrated response function  $\chi(t, s)$  when plotted versus the correlation function  $C(t, s)$ . This method has been applied to the numerical study of many systems: 2d and 3d-Ising ferromagnets [4], 3d Edwards-Anderson model [5, 4], 3d and 4d-Gaussian Ising spin-glasses [6], 2d Ising ferromagnet with dipolar interactions [7], Heisenberg anti-ferromagnet on the Kagome lattice [8] ... The conjecture (2) has also recently been checked experimentally for a spin-glass [9]. More details may be found in the reviews [10, 11]. However, the integrated response function depends linearly on the violation ratio only if the conjecture (2) holds, which has not been demonstrated for any of the previously cited systems. We will see in the case of the homogeneous Ising model that this approach may lead to misinterpretations and erroneous values of  $X(t, s)$ . The generalisation of the equilibrium FDT has recently become an increasingly popular issue. During the writing of this paper, a long list of works have been dedicated to this subject. Let us mention two of them: an approximate generalisation of the FDT to metastable systems [12] (limited to dynamics having a transition rate  $W$  with only one negative eigenvalue) that has been successfully compared to numerical data for the 2D-Ising model and a generalisation of the FDT for two classes of trap models [13].

In the present work, we study the Glauber dynamics of the Ising model. In the section 1, we describe the model and its dynamics which are studied analytically in the section 2. The response function to an infinitesimal magnetic field is exactly calculated far-from-equilibrium. It turns out that the response function is no more related to a time-derivative of the spin-spin correlation function but to time-derivatives of a more complex correlation function. The equilibrium limit is taken and an expression of the violation ratio is given. In the section 3, a discrete-time version of this expression is implemented in Monte Carlo simulations. Our approach presents several advantages: (i) we can compute directly the response function and not only the integrated response function, (ii) we obtain the response function to an infinitesimal magnetic field so that we avoid non-linear effects due to the use of a finite magnetic field, (iii) the violation ratio can be computed without resorting to Cugliandolo conjecture (2) and (iv) we can calculate the response function  $R(t, s)$  and the violation ratio  $X(t, s)$  for any time  $t$  and  $s < t$  during one single Monte Carlo simulation. We performed Monte Carlo simulations of the two-dimensional homogeneous Ising model quenched to and below the critical temperature  $T_c$ . In both cases, the expected scaling behaviour of the response function in the aging regime is well reproduced by the numerical data. The value of the exponent  $a$ , still controversial, is estimated and the violation ratio is computed. Our estimate of  $X_\infty$  at  $T_c$  turns out to be compatible with previous work and the scaling behaviour of  $X(t, s)$  below  $T_c$  is well reproduced. In both cases, the violation ratio depend on time not only through the correlation function.

## 2 The Ising-Glauber model

### 2.1 Useful relations on Markov processes

We consider a classical Ising model whose degrees of freedom are scalar variables  $\sigma_i = \pm 1$  located at the nodes of a  $d$ -dimensional lattice. Let us denote  $\wp(\{\sigma\}, t)$  the probability to observe the system in the state  $\{\sigma\}$  at time  $t$ . The dynamics of the system is supposed to be governed by the master equation:

$$\frac{\partial \wp(\{\sigma\}, t)}{\partial t} = \sum_{\{\sigma'\}} \left[ \wp(\{\sigma'\}, t) W(\{\sigma'\} \rightarrow \{\sigma\}) - \wp(\{\sigma\}, t) W(\{\sigma\} \rightarrow \{\sigma'\}) \right] \quad (4)$$

where  $W(\{\sigma\} \rightarrow \{\sigma'\})$  is the transition rate per unit time from the state  $\{\sigma\}$  to the state  $\{\sigma'\}$ . The normation is written  $\sum_{\{\sigma'\}} W(\{\sigma\} \rightarrow \{\sigma'\}) = 1$ . It is easily shown that the conditional probability,  $\wp(\{\sigma\}, t | \{\sigma'\}, s)$  with  $s < t$ , defined by the Bayes relation

$$\wp(\{\sigma\}, t) = \sum_{\{\sigma'\}} \wp(\{\sigma\}, t | \{\sigma'\}, s) \wp(\{\sigma'\}, s) \quad (5)$$

satisfies the master equation (4) too:

$$\left(1 + \frac{\partial}{\partial t}\right) \wp(\{\sigma\}, t | \{\sigma'\}, s) = \sum_{\{\sigma''\}} W(\{\sigma''\} \rightarrow \{\sigma\}) \wp(\{\sigma''\}, t | \{\sigma'\}, s). \quad (6)$$

Moreover, one can work out a master equation for the time  $s$ :

$$\left(1 - \frac{\partial}{\partial s}\right) \wp(\{\sigma\}, t | \{\sigma'\}, s) = \sum_{\{\sigma''\}} \wp(\{\sigma\}, t | \{\sigma''\}, s) W(\{\sigma'\} \rightarrow \{\sigma''\}) \quad (7)$$

by using for example the identity  $\frac{\partial}{\partial s} \wp(\{\sigma\}, t) = 0$ . When the transition rates do not depend on time, the conditional probability  $\wp(\{\sigma\}, t | \{\sigma'\}, s)$  is a function only of  $t-s$ . This can be shown easily by introducing the matrix notation  $\wp(\{\sigma\}, t | \{\sigma'\}, s) = \langle \{\sigma\} | \hat{\wp}(t, s) | \{\sigma'\} \rangle$ . The master equation (6) reads then:

$$\frac{\partial}{\partial t} \hat{\wp}(t, s) = (\hat{W} - \mathbb{1}) \hat{\wp}(t, s) \quad (8)$$

where  $\langle \{\sigma\} | \hat{W} | \{\sigma'\} \rangle = W(\{\sigma\} \rightarrow \{\sigma'\})$ . This equation admits the formal solution

$$\begin{aligned} \wp(\{\sigma\}, t | \{\sigma'\}, s) &= \sum_{\{\sigma''\}} \langle \{\sigma\} | e^{\int_s^t (\hat{W} - \mathbb{1}) dt'} | \{\sigma''\} \rangle \wp(\{\sigma''\}, s | \{\sigma'\}, s) \\ &= \langle \{\sigma\} | e^{(\hat{W} - \mathbb{1})(t-s)} | \{\sigma'\} \rangle \end{aligned} \quad (9)$$

where the initial condition  $\wp(\{\sigma''\}, s | \{\sigma'\}, s) = \delta_{\{\sigma''\}, \{\sigma'\}}$  has been used. The dependence only on  $t-s$ , even far-from-equilibrium, will be used latter in the calculation of the response function.

### 2.2 The model and its dynamics

The Ising model is defined by its equilibrium probability distribution  $\wp_{\text{eq}}(\{\sigma\})$  which reads with general exchange couplings:

$$\wp_{\text{eq}}(\{\sigma\}) = \frac{1}{\mathcal{Z}} e^{-\beta \mathcal{H}(\{\sigma\})} = \frac{1}{\mathcal{Z}} e^{\beta \sum_{k,l < k} J_{kl} \sigma_k \sigma_l}. \quad (10)$$

where ferromagnetic couplings correspond to  $J_{kl} > 0$ . The condition of stationarity  $\frac{\partial}{\partial t} \wp_{\text{eq}}(\{\sigma\}) = 0$  leads according to the master equation (4) to a constrain on the transition rates:

$$\sum_{\{\sigma'\}} \left[ \wp_{\text{eq}}(\{\sigma'\}) W(\{\sigma'\} \rightarrow \{\sigma\}) - \wp_{\text{eq}}(\{\sigma\}) W(\{\sigma\} \rightarrow \{\sigma'\}) \right] = 0. \quad (11)$$

The equation (11) is satisfied when the detailed balance holds:

$$\wp_{\text{eq}}(\{\sigma'\}) W(\{\sigma'\} \rightarrow \{\sigma\}) = \wp_{\text{eq}}(\{\sigma\}) W(\{\sigma\} \rightarrow \{\sigma'\}). \quad (12)$$

This last unnecessary but sufficient condition is fulfilled by the heat-bath single-spin flip dynamics defined by the following transition rates:

$$W(\{\sigma\} \rightarrow \{\sigma'\}) = \left[ \prod_{l \neq k} \delta_{\sigma_l, \sigma'_l} \right] \frac{e^{\beta \sum_{l \neq k} J_{kl} \sigma'_k \sigma'_l}}{\sum_{\sigma = \pm 1} e^{\beta \sum_{l \neq k} J_{kl} \sigma \sigma'_l}}. \quad (13)$$

Only the single-spin flip  $\sigma_k \rightarrow \sigma'_k$  is allowed. The product of Kronecker deltas ensures that all other spins are not modified during the transition. After the transition, the spin  $\sigma_k$  takes the new value  $\sigma'_k$  chosen according to the equilibrium probability distribution  $\wp_{\text{eq}}(\{\sigma\})$ . All spins are successively updated during the evolution of the system. These transition rates reduce to Glauber's ones [14] in the case of the Ising chain.

### 3 Fluctuation-dissipation relation

#### 3.1 Far-from-equilibrium fluctuation-dissipation relation

A magnetic field  $h_i$  is coupled to the spin  $\sigma_i$  between the times  $s$  and  $s + \Delta s$  where  $\Delta s$  is supposed to be small. During the interval  $\Delta s$ , the transition rates are changed to  $W_h(\{\sigma\} \rightarrow \{\sigma'\})$  satisfying equation (13) with an additional Zeeman term  $\beta h_i \sigma_i$  in the Hamiltonian of the equilibrium probability distribution (10):

$$W_h(\{\sigma\} \rightarrow \{\sigma'\}) = \left[ \prod_{l \neq k} \delta_{\sigma_l, \sigma'_l} \right] \frac{e^{\beta [\sum_{l \neq k} J_{kl} \sigma'_k \sigma'_l + h_i \sigma'_k \delta_{k,i}]}}{\sum_{\sigma = \pm 1} e^{\beta [\sum_{l \neq k} J_{kl} \sigma \sigma'_l + h_i \sigma \delta_{k,i}]}}. \quad (14)$$

The transition rates are identical to the case  $h_i = 0$  apart from the single-spin flip involving the spin  $\sigma_i$ . Using the Bayes relation and the master equation (4), the average of the spin  $\sigma_j$  at time  $t > s$  can be expanded to lowest order in  $\Delta s$  under the following form:

$$\begin{aligned} \langle \sigma_j(t) \rangle &= \sum_{\{\sigma\}} \sigma_j \wp(\{\sigma\}, t) \\ &= \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s + \Delta s) \wp(\{\sigma'\}, s + \Delta s) \\ &= \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s + \Delta s) \left[ (1 - \Delta s) \wp(\{\sigma'\}, s) \right. \\ &\quad \left. + \Delta s \sum_{\{\sigma''\}} \wp(\{\sigma''\}, s) W_h(\{\sigma''\} \rightarrow \{\sigma'\}) \right] + \mathcal{O}(\Delta s^2). \end{aligned} \quad (15)$$

$W_h$  being the only quantity depending on the magnetic field in equation (15), the first term disappears after a derivative with respect to the magnetic field. In the last

term, the single-spin flip involving the spin  $\sigma_i$ , i.e. the one coupled to the magnetic field, is the only one giving a non-vanishing contribution. The integrated response function between the time  $s$  and  $s + \Delta s$  is  $\left[ \frac{\partial \langle \sigma_j(t) \rangle}{\partial h_i} \right]_{h_i \rightarrow 0}$  and the limit  $\Delta s \rightarrow 0$  leads to the response function:

$$\lim_{\Delta s \rightarrow 0} \frac{1}{\Delta s} \left[ \frac{\partial \langle \sigma_j(t) \rangle}{\partial h_i} \right]_{h_i \rightarrow 0} = \lim_{\Delta s \rightarrow 0} \frac{1}{\Delta s} \int_s^{s+\Delta s} R_{ji}(t, u) du = R_{ji}(t, s). \quad (16)$$

The calculation can be limited to the lowest order in  $\Delta s$ . As a consequence, the conditional probability in equation (15) can be replaced by  $\wp(\{\sigma\}, t | \{\sigma'\}, s)$ . The integrated response function between the time  $s$  and  $s + \Delta s$  is to lowest order in  $\Delta s$

$$\left[ \frac{\partial \langle \sigma_j(t) \rangle}{\partial h_i} \right]_{h_i \rightarrow 0} = \Delta s \sum_{\substack{\{\sigma\}, \{\sigma'\}, \\ \{\sigma''\}}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s) \left[ \frac{\partial W_h}{\partial h_i}(\{\sigma''\} \rightarrow \{\sigma'\}) \right]_{h_i \rightarrow 0} \wp(\{\sigma''\}, s). \quad (17)$$

The derivative of the transition rate  $W_h$  defined by equation (14) is easily taken and reads

$$\left[ \frac{\partial W_h}{\partial h_i}(\{\sigma''\} \rightarrow \{\sigma'\}) \right]_{h_i \rightarrow 0} = \beta W(\{\sigma''\} \rightarrow \{\sigma'\}) \left[ \sigma'_i - \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma'_k \right) \right]. \quad (18)$$

Combining (17) and (18), the integrated response function is rewritten as

$$\begin{aligned} \left[ \frac{\partial \langle \sigma_j(t) \rangle}{\partial h_i} \right]_{h_i \rightarrow 0} &= \Delta s \beta \sum_{\substack{\{\sigma\}, \{\sigma'\}, \\ \{\sigma''\}}} \sigma_j \sigma'_i \wp(\{\sigma\}, t | \{\sigma'\}, s) W(\{\sigma''\} \rightarrow \{\sigma'\}) \wp(\{\sigma''\}, s) \\ &\quad - \Delta s \beta \sum_{\substack{\{\sigma\}, \{\sigma'\}, \\ \{\sigma''\}}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s) W(\{\sigma''\} \rightarrow \{\sigma'\}) \\ &\quad \times \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma'_k \right) \wp(\{\sigma''\}, s). \end{aligned} \quad (19)$$

In the first term of (19), the sum over  $\{\sigma''\}$  can be performed using the master equation (4) and the expression reorganised using the fact that after the limit  $h_i \rightarrow 0$ , the conditional probability becomes invariant under a time-translation (see equation (9)) and depends only on the difference  $t - s$ . One obtains

$$\begin{aligned} &\sum_{\substack{\{\sigma\}, \{\sigma'\}, \\ \{\sigma''\}}} \sigma_j \sigma'_i \wp(\{\sigma\}, t | \{\sigma'\}, s) W(\{\sigma''\} \rightarrow \{\sigma'\}) \wp(\{\sigma''\}, s) \\ &= \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \sigma'_i \wp(\{\sigma\}, t | \{\sigma'\}, s) \left( 1 + \frac{\partial}{\partial s} \right) \wp(\{\sigma'\}, s) \\ &= C_{ji}(t, s) + \frac{\partial}{\partial s} C_{ji}(t, s) - \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \sigma'_i \frac{\partial \wp}{\partial s}(\{\sigma\}, t | \{\sigma'\}, s) \wp(\{\sigma'\}, s) \\ &= C_{ji}(t, s) + \frac{\partial}{\partial s} C_{ji}(t, s) + \frac{\partial}{\partial t} C_{ji}(t, s). \end{aligned} \quad (20)$$

Similarly, in the second term of equation (19) the sum over  $\{\sigma''\}$  can be performed using the master equation (4) and leads to

$$\sum_{\substack{\{\sigma\}, \{\sigma'\}, \\ \{\sigma''\}}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s) \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma'_k \right) W(\{\sigma''\} \rightarrow \{\sigma'\}) \wp(\{\sigma''\}, s)$$

$$\begin{aligned}
&= \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s) \tanh\left(\beta \sum_{k \neq i} J_{ik} \sigma'_k\right) \left(1 + \frac{\partial}{\partial s}\right) \wp(\{\sigma'\}, s) \quad (21) \\
&= \left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s) \tanh\left(\beta \sum_{k \neq i} J_{ik} \sigma'_k\right) \wp(\{\sigma'\}, s).
\end{aligned}$$

Putting together equations (20) and (22) into (19), one can then evaluate the response function (16):

$$R_{ji}(t, s) = \beta \left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \left[ C_{ji}(t, s) - \langle \sigma_j(t) \tanh\left(\beta \sum_{k \neq i} J_{ik} \sigma_k(s)\right) \rangle \right]. \quad (22)$$

The hyperbolic tangent is the equilibrium value of the spin  $\sigma_i$  in the Weiss field created by all other spins at time  $s$ . Using the notation  $\sigma_i^{\text{Weiss}}(s) = \tanh\left(\beta \sum_{k \neq i} J_{ik} \sigma_k(s)\right)$ , the fluctuation-dissipation relation is rewritten far-from-equilibrium as

$$R_{ji}(t, s) = \beta \left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \langle \sigma_j(t) [\sigma_i(s) - \sigma_i^{\text{Weiss}}(s)] \rangle \quad (23)$$

This relation generalises equation (1). The response function  $R(t, s)$  turns out to be related to time-derivatives of the correlation function of the spin at time  $t$  with the fluctuations of the spin at time  $s$  around the equilibrium average  $\sigma_i^{\text{Weiss}}(s)$  in its Weiss field. In this sense, this relation is still a fluctuation-dissipation relation but valid far-from-equilibrium. It is very general since no assumption has been made on the dimension of the space or on the set of exchange couplings  $J_{ij}$  during the calculation. Moreover, it applies for any initial conditions  $\wp(\{\sigma\}, 0)$ . The appearance of the prefactor  $1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}$  is not related to the Ising-Glauber model but comes from the Markovian property of the dynamics. Generalised response functions are easily calculated in the same manner. One has for example for the second-order term:

$$\begin{aligned}
R_{kji}^{(2)}(t, s, r) &= \left( \frac{\delta^2 \langle \sigma_k(t) \rangle}{\delta h_j(s) \delta h_i(r)} \right)_{h \rightarrow 0} \quad (t > s > r) \\
&= \beta \left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \langle \sigma_k(t) \delta \sigma_j(s) \delta \sigma_i(r) \rangle. \quad (24)
\end{aligned}$$

where  $\delta \sigma_j(s) = \sigma_j(s) - \sigma_j^{\text{Weiss}}(s)$ . The calculation of higher-order derivatives of the transition rate may be necessary as for example for the non-linear term

$$\begin{aligned}
R_{kii}^{(2)}(t, s, s) &= \left( \frac{\delta^2 \langle \sigma_k(t) \rangle}{\delta h_i^2(s)} \right)_{h \rightarrow 0} \quad (t > s) \\
&= -2\beta^2 \left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \langle \sigma_k(t) \sigma_i^{\text{Weiss}}(s) \delta \sigma_i(s) \rangle. \quad (25)
\end{aligned}$$

These relations are moreover easily extended to other models and other dynamics. For the Glauber dynamics defined as a local equilibration of a degree of freedom in its Weiss field, the relations (23) to (26) hold for the  $\mathcal{O}(n)$  or the  $q$ -state Potts for example where  $\sigma_i(s)$  has to be replaced by the local order parameter at time  $s$  on the site  $i$  and  $\sigma_i^{\text{Weiss}}(s)$  by its average value in the Weiss field.

### 3.2 Equilibrium limit and violation ratio

We will show in this section that the usual expression of the FDT (1) is recovered in the equilibrium limit. At equilibrium, any two-time function is invariant under a time-translation. As a consequence, the two derivatives  $\frac{\partial}{\partial s}$  and  $\frac{\partial}{\partial t}$  in the relation (23) cancel each other in the equilibrium limit. Using the master equation (7) of

the conditional probability, the time-derivative of the correlation function is written as

$$\begin{aligned}
\frac{\partial}{\partial s} C_{ji}^{\text{eq}}(t-s) &= -\frac{\partial}{\partial t} C_{ji}^{\text{eq}}(t-s) \\
&= -\sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \sigma'_i \frac{\partial \wp(\{\sigma\}, t | \{\sigma'\}, s)}{\partial t} \wp_{\text{eq}}(\{\sigma'\}) \\
&= \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \sigma'_i \frac{\partial \wp(\{\sigma\}, t | \{\sigma'\}, s)}{\partial s} \wp_{\text{eq}}(\{\sigma'\}) \\
&= C_{ji}^{\text{eq}}(t-s) - \sum_{\{\sigma\}, \{\sigma'\}, \{\sigma''\}} \sigma_j \sigma'_i \wp(\{\sigma\}, t | \{\sigma''\}, s) W(\{\sigma'\} \rightarrow \{\sigma''\}) \wp_{\text{eq}}(\{\sigma'\}).
\end{aligned} \tag{26}$$

The sum over  $\{\sigma'\}$  can be performed when replacing the transition rate by its definition (13). One obtains

$$\begin{aligned}
&\sum_{\{\sigma'\}} \sigma'_i W(\{\sigma'\} \rightarrow \{\sigma''\}) \wp_{\text{eq}}(\{\sigma'\}) \\
&= \frac{1}{\mathcal{Z}} \sum_{\{\sigma'\}} \sigma'_i \frac{\left[ \prod_{k \neq i} \delta_{\sigma'_k, \sigma''_k} \right] e^{\beta \sum_{k \neq i} J_{ik} \sigma'_i \sigma''_k}}{\sum_{\sigma = \pm 1} e^{\beta \sum_{k \neq i} J_{ik} \sigma \sigma''_k}} e^{\beta \sum_{k, l < k} J_{kl} \sigma'_k \sigma'_l} \\
&= \wp_{\text{eq}}(\{\sigma''\}) \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma''_k \right).
\end{aligned} \tag{27}$$

Replacing in (26) and identifying with (23), one gets the expression of the equilibrium FDT (1) for the Ising-Glauber model:

$$R_{ji}^{\text{eq}}(t-s) = \beta \frac{\partial}{\partial s} C_{ji}^{\text{eq}}(t-s) = \beta \langle \sigma_j(t) [\sigma_i(s) - \sigma_i^{\text{Weiss}}(s)] \rangle_{\text{eq}}. \tag{28}$$

Taking the ratio of the far-from-equilibrium response function (23) with this quantity, one can form the violation ratio

$$X_{ji}(t, s) = \frac{\left(1 + \frac{\partial}{\partial s} + \frac{\partial}{\partial t}\right) \langle \sigma_j(t) [\sigma_i(s) - \sigma_i^{\text{Weiss}}(s)] \rangle}{\langle \sigma_j(t) [\sigma_i(s) - \sigma_i^{\text{Weiss}}(s)] \rangle}. \tag{29}$$

This quantity depends on both the times  $s$  and  $t$  and cannot be trivially rewritten as a function of the correlation function  $C(t, s)$  only. However, Cugliandolo conjecture (2) is expected to hold only asymptotically. We will now study numerically the asymptotic behaviour of this violation ratio for the homogeneous 2d-Ising model during a quench.

## 4 Monte Carlo simulation of the 2d-Ising model

The expression (23) of the response function given above will able us to study the aging displayed by the Ising-Glauber model more accurately than previous works that were based on the numerical estimate of the integrated response function. To deal properly in Monte Carlo simulations with the time-derivatives entering the expression (23), one has to work out its equivalent in discrete time. This will be done in the first part of this chapter. In the second part, simulations of the Glauber dynamics of the two-dimensional Ising model during a quench from the paramagnetic phase to the ferromagnetic one are presented. The system is



expected to display aging, interpreted [15] as the existence of growing domains corresponding to competing ferromagnetic states. Reversible processes occur in the bulk of domains while domain walls rearrangements are irreversible processes. We will distinguish quenches at the critical temperature  $T_c$  and below. In both cases, lattice sizes  $128 \times 128$ ,  $256 \times 256$  and  $362 \times 362$  were simulated and the data averaged over respectively  $N_{\text{config}} \simeq 3000$ , 10000 and 5000 initial configurations. For all data, error bars were estimated as the standard deviation around the average value.

## 4.1 Discrete response function

During a Monte Carlo simulation, the time is a discrete variable and the dynamics is governed by the master equation

$$\wp(\{\sigma\}, t+1) = \sum_{\{\sigma'\}} \wp(\{\sigma'\}, t) W(\{\sigma'\} \rightarrow \{\sigma\}). \quad (30)$$

Replacing the continuous-time master equation (4) by (30), the response function can be calculated in an analogous manner than in the continuous case. The magnetisation at time  $t$  can be expanded as

$$\langle \sigma_j(t) \rangle = \sum_{\{\sigma\}, \{\sigma'\}, \{\sigma''\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s+1) W_h(\{\sigma''\} \rightarrow \{\sigma'\}) \wp(\{\sigma''\}, s). \quad (31)$$

Using the derivative with respect to the magnetic field (17) of the transition rate, the integrated response function between the times  $s$  and  $s+1$  is shown to be

$$\chi_{ji}(t, s) = \beta \sum_{\{\sigma\}, \{\sigma'\}} \sigma_j \wp(\{\sigma\}, t | \{\sigma'\}, s+1) \left[ \sigma'_i - \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma'_k \right) \right] \wp(\{\sigma'\}, s+1) \quad (32)$$

In discrete time, the integrated response function between the times  $s$  and  $s+1$  is identical to the response function at time  $s$  so the far-from-equilibrium fluctuation-dissipation relation (22) reads in discrete time:

$$\begin{aligned} R_{ji}(t, s) &= \beta \left[ \langle \sigma_j(t) \sigma_i(s+1) \rangle - \langle \sigma_j(t) \tanh \left( \beta \sum_{k \neq i} J_{ik} \sigma_k(s+1) \right) \rangle \right] \\ &= \beta \left[ \langle \sigma_j(t) \sigma_i(s+1) \rangle - \langle \sigma_j(t) \sigma_i^{\text{Weiss}}(s) \rangle \right]. \end{aligned} \quad (33)$$

The term  $\sigma_k(s+1)$  could be equally replaced by  $\sigma_k(s)$  in this expression since the only single-spin flip contributing to the response function between times  $s$  and  $s+1$  is the one involving the spin  $\sigma_i$  so all other spins are not changed. The equilibrium limit is worked out analogously than in equations (26) to (28) and is shown to be for a time-discrete dynamics

$$R_{ji}^{\text{eq}}(t, s) = \beta \left[ \langle \sigma_j(t) \sigma_i(s+1) \rangle_{\text{eq}} - \langle \sigma_j(t) \sigma_i(s) \rangle_{\text{eq}} \right]. \quad (34)$$

The violation ratio is then readily written as

$$X_{ji}(t, s) = \frac{\langle \sigma_j(t) \sigma_i(s+1) \rangle - \langle \sigma_j(t) \sigma_i^{\text{Weiss}}(s) \rangle}{\langle \sigma_j(t) \sigma_i(s+1) \rangle - \langle \sigma_j(t) \sigma_i(s) \rangle}. \quad (35)$$

The relations (33) and (35) are easily implemented in a Monte Carlo simulation.

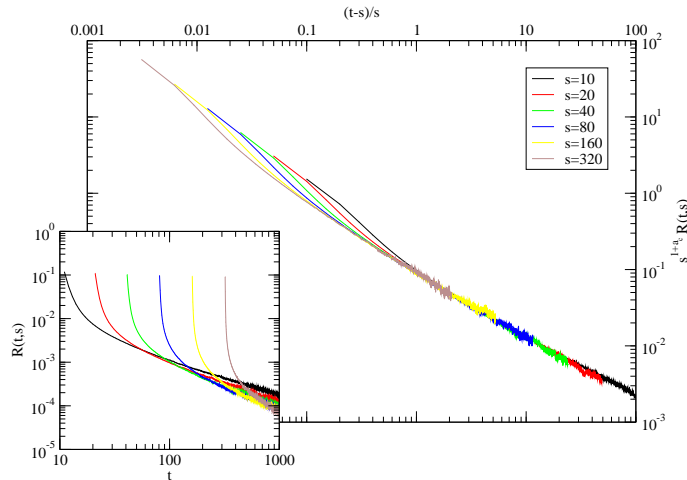


Figure 1: Response function of the 2D-Ising model during a quench at the critical temperature (inset) and collapse of the scaling function for different values of  $s$ . The data were obtained with a lattice of size  $362 \times 362$  and averaged over 5000 initial configurations. Each curve is surrounded by a clouds of dots corresponding to the lower and upper bounds of the error bars. The value  $a_c = 0.115$  was used [17].

## 4.2 Quench at the critical temperature

During a quench at the critical temperature  $T_c$ , the asymptotic decay of the correlation function has been conjectured to be [16, 17]

$$C(t, s) \underset{t, s \gg 1}{\sim} s^{-a_c} \mathcal{C}_c(t/s) \quad (36)$$

where  $a_c = \frac{2\beta}{\nu z_c}$  and  $\mathcal{C}_c(x)$  is a scaling function that asymptotically behaves as  $\mathcal{C}_c(x) \underset{x \gg 1}{\sim} x^{-\lambda_c/z_c}$ .  $\lambda_c$  is the critical autocorrelation exponent [18] and  $z_c$  the dynamical exponent. Similarly, the asymptotic behaviour of the response function is

$$R(t, s) \underset{t, s \gg 1}{\sim} s^{-1-a_c} \mathcal{R}_c(t/s) \quad (37)$$

where the scaling function  $\mathcal{R}_c(x)$  behaves asymptotically as  $\mathcal{R}_c(x) \underset{x \gg 1}{\sim} x^{-\lambda_c/z_c}$  too.

By integrating over  $s$ , one obtains a relation similar to (37) for the integrated response function that has been checked by large-scale Monte Carlo simulations [19]. However, the relation (37) is asymptotic so is not expected to hold for the response function  $R(t, s)$  with small values of  $s$  that are the main contribution to the integrated response function. As a consequence, it is difficult to test the asymptotic behaviour of the response function in this way. Our approach permits us to avoid these problems and to test directly the relation (37).

The numerical data are plotted in figure 1. For the largest lattice size ( $L = 362$ ) and the smallest value of  $s$  ( $s = 10$ ), errors bars are at most 6 % of the value of the response function while for the largest ( $s = 320$ ), they increase up to 12 %. Indeed, in the last case, the response function is of order of  $1/N_{\text{config}}$  and so can not be sampled accurately. Nevertheless, a fairly good collapse of the data is observed indicating that  $\mathcal{R}_c(t/s) = s^{1+a_c} R(t, s)$  is indeed a scaling function (actually we have used  $(t-s)/s$  instead of  $t/s$  but this has no consequence on the asymptotic behaviour).

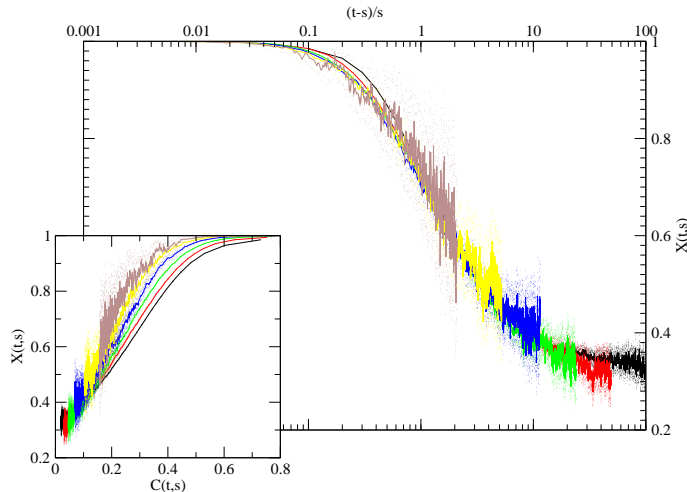


Figure 2: Violation ratio  $X(t, s)$  versus  $t$  for different values  $s$  for the Ising-Glauber model quenched at the critical temperature  $T_c$ . The data were obtained for a lattice  $362 \times 362$  and averaged over 5000 initial configurations. Each curve is surrounded by a clouds of dots corresponding to the lower and upper bounds of the error bars.

We computed the violation ratio  $X(t, s)$  using the estimator previously derived and whose expression is given by equation (35). The error bars are quite large. The numerical data are plotted in figure 2 for the largest lattice size ( $L = 362$ ). In contradistinction to Cugliandolo conjecture (2), the inset of figure 2 shows that the violation ratio does not depend on time only through the correlation function. However, it seems that it may be the case in the limit  $C(t, s) \rightarrow 0$ . On the other hand, it seems that the violation ratio depends on time only through  $t/s$  and reach a plateau for large enough values of  $t$  that we may estimate roughly to be  $X_\infty \simeq 0.33(2)$ . The same value is obtained for  $L = 256$  and  $L = 362$  excluding any possibility of finite-size effects. The limit  $X_\infty$  has been conjectured to be universal [17] but incompatible values have been numerically measured by different groups:  $X_\infty = 0.26(1)$  [20] and  $X_\infty = 0.340(5)$  [21]. Our estimate is fully compatible with the last one. The estimate  $X_\infty = 0.26(1)$  has probably been measured for a too-short time  $t$ , far from the region where Cugliandolo conjecture (2) and thus equation (3) hold. This puts stress upon the danger of using equation (3) to compute the violation ratio.

### 4.3 Quench below the critical temperature

The same analysis can be done below  $T_c$ . In this regime, The correlation function decays as [16, 17]

$$C(t, s) \underset{t, s \gg 1}{\sim} M_{\text{eq}}^2 \mathcal{C}(t/s) \quad (38)$$

where  $M_{\text{eq}}$  is the equilibrium magnetisation and  $\mathcal{C}(x)$  a scaling function that asymptotically behaves as  $\mathcal{C}(x) \underset{x \gg 1}{\sim} x^{-\lambda/z}$ . The autocorrelation exponent  $\lambda$  and the dynamical exponent  $z$  are expected to take different values than at  $T_c$ . The response function is expected to scale as [16, 17]

$$R(t, s) \underset{t, s \gg 1}{\sim} s^{-1-a} \mathcal{R}(t/s) \quad (39)$$

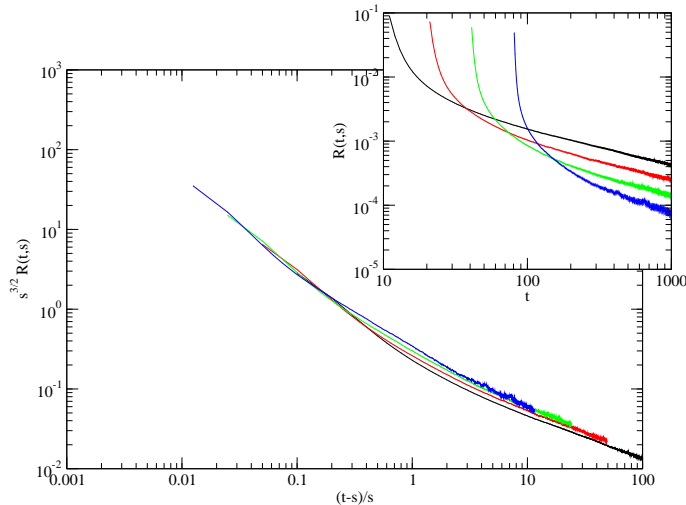


Figure 3: Response function of the 2D-Ising model during a quench at the temperatures  $T = J/0.6 \simeq \frac{3}{4}T_c$  (inset) and collapse of the scaling function for different values of  $s$ . The data were obtained for a lattice  $256 \times 256$  and averaged over 10000 initial configurations. Each curve is surrounded by a clouds of dots corresponding to the lower and upper bounds of the error bars.

where  $\mathcal{R}(x) \underset{x \gg 1}{\sim} x^{-\lambda/z}$ . A controversy exists concerning the value of  $a$  that has been estimated to be either  $1/4$  [22] or  $1/2$  [23, 24]. Our numerical data are presented in the figure 3. We studied lattice sizes only up to  $L = 256$  but calculations were made for two temperatures:  $J/0.6 \simeq \frac{3}{4}T_c$  and  $J/0.9 \simeq T_c/2$ . The error bars are much smaller than in the critical case for small values of  $s$ . The relative error is at most 2.6 % for  $s = 10$  at  $\frac{3}{4}T_c$  but increase faster with  $s$ : the relative error increases up to 11 % for  $s = 80$ . As a consequence, the study was limited to the values of  $s$  ranging from  $s = 10$  to  $s = 80$ . The response function displays the expected scaling behaviour (39) with  $a = 1/2$ . However, the collapse is not perfect, especially for the smallest values of  $s$  but a very small variation of  $a$  does not improve it. The response function has probably strong corrections as already noted by Henkel *et al.* [19, 25]. The value  $a = 1/4$  in particular improve the collapse for the small values of  $s$ . This observation is compatible with the claim of a cross-over from  $a = 1/4$  to  $a = 1/2$  [23] for large values of  $s$ .

Combining the relations (38) and (39), the violation ratio  $X(t, s) = R(t, s)/\beta \frac{\partial}{\partial s} C(t, s)$  is predicted to vanish as  $s^{-a}$  below  $T_c$ . Our numerical estimates for  $T = J/0.6 \simeq \frac{3}{4}T_c$  are plotted in figure 4. The statistical errors decrease with the temperature so much less fluctuations than at  $T_c$  are observed. As expected, the violation ratio is equal to 1 for small values of  $t - s$ , signal that the main contribution to the response function is due to equilibrium processes. On the other hand, it vanishes in the limit  $t \sim s \gg 1$  as  $s^{-1/2}$ . As shown in figure 4, the data for  $s^{1/2}X(t, s)$  collapse for large values of  $t/s$ . Moreover, the figure 4 shows unambiguously that the violation ratio does not depend on time only through the correlation function. This makes the relation (3) invalid. The study of the violation of the equilibrium FDT by the usual method relying on the equation (3) would have led to erroneous values of the violation ratio.

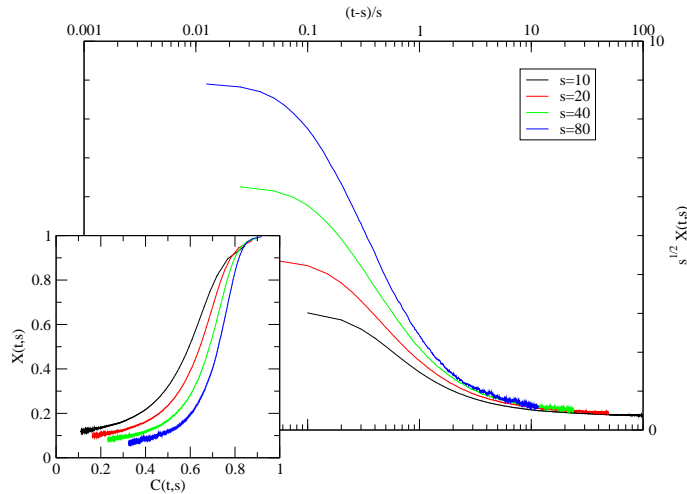


Figure 4: Violation ratio  $X(t, s)$  versus  $t$  for different values  $s$  for the Ising-Glauber model quenched at the temperature  $J/0.6k_B \simeq \frac{3}{4}T_c$ . The data were obtained for a lattice  $256 \times 256$  and averaged over 10000 initial configurations. Each curve is surrounded by a clouds of dots corresponding to the lower and upper bounds of the error bars.

## 5 Conclusion

Using a formalism similar to Kubo's one in the quantum case, we derive an exact expression of the response function of the Ising-Glauber model far-from-equilibrium (equation (23)). The response function turns out to be related to time-derivatives of a correlation function involving the fluctuations of the spin excited by the magnetic field around the equilibrium average in its Weiss field. In this sense, the expression is a generalisation of the equilibrium fluctuation-dissipation. Our expression is quite general: no assumption has been made during its derivation on the dimension of the space, the set of exchange couplings or the initial conditions. Moreover, it can be easily extended to other classical models and generalised and non-linear response functions can be obtained analogously. The calculation has been made possible because the dynamics consists in the equilibration of a given spin in its Weiss field, i.e. the transition rates do not depend on the state of the spin before the transition. It would be instructive to know whether an expression similar to (23) would be still obtained in a more general case. The role played by detailed balance is also of interest. We give also the expression of the response function in the case of a discrete-time dynamics that can be implemented in Monte Carlo simulations. Our approach gives thus access to the response function and the violation ratio directly. In particular, the violation ratio can be obtained without assuming true the Cugliandolo conjecture (2). We then study numerically the homogeneous two-dimensional Ising-Glauber model quenched from the paramagnetic phase to the ferromagnetic one. Both the response function and the violation ratio display the expected scaling behaviour both at  $T_c$  and below  $T_c$ . The values of the exponent  $a$  and of the limiting value of the violation ratio  $X_\infty$  are confirmed. The Cugliandolo conjecture (2) does not hold for this model apart perhaps at  $T_c$  in the limit of vanishing correlation functions. This would explain discrepancies of previous estimates of  $X_\infty$  relying on Cugliandolo conjecture. The above-presented numerical procedure may be extended to many different systems and would provided a unambiguous test of Cugliandolo conjecture. We are currently studying the dynamics of spin-glasses in this framework.

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