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A far-from-equilibrium fluctuation–dissipation relation for an Ising–Glauber-like model

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Abstract

We derive an exact expression of the response function to an infinitesimal magnetic field for an Ising–Glauber-like 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 complicated correlation function and so the expression is a generalization of the equilibrium fluctuation–dissipation theorem in the special case of this model. Correspondence with the Ising–Glauber model is discussed. A discrete-time version of the relation is implemented in Monte Carlo simulations and then used to study the ageing 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 fluctuation–dissipation ratio.

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1. Introduction

Knowledge about out-of-equilibrium processes is far from being as advanced as for systems at thermodynamical 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 $R^{\mathrm{eq}}(t-s)$ 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 $C^{\mathrm{eq}}(t-s)$:

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

In the Ising case, the response function reads $R_{ji}(t,s) = \delta\langle\sigma_j(t)\rangle/\delta h_i(s)$ 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 generalized by adding a multiplicative factor $X(t,s)$ which moreover depends on time only through the correlation function:

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

The quantity $\beta^{\rm eff}(t,s) = \beta X(C(t,s))$ is interpreted as an effective inverse 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 equation (2) to be valid for any times t and s, one can relate the integrated response function to the fluctuation–dissipation (FD) ratio:

$$\chi(t,s) = \int_0^s R(t,u)\,\mathrm{d}u \sim \beta\int_{C(t,0)}^{C(t,s)} X(C)\,\mathrm{d}C. \tag{3}$$

The FD 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] and so on. 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 FD 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 generalization of the equilibrium FDT has recently become an increasingly popular issue. Let us mention two of them: an approximate generalization 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 generalization of the FDT for trap models [13].

In the present work, we study the dynamics of an Ising–Glauber-like model. In section 2, we describe the model and its dynamics which are studied analytically in section 3. The response function to an infinitesimal magnetic field is exactly calculated far-from-equilibrium. It turns out that the response function is no longer related to a time-derivative of the spin–spin correlation function but to time-derivatives of a more complicated correlation function. The equilibrium limit is shown to have the usual form. In section 4, 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 nonlinear effects due to the use of a finite magnetic field, (iii) the FD ratio can be computed without resorting to the Cugliandolo conjecture (2) and (iv) we can calculate the response function $R(t,s)$ and the FD 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 at and below the critical temperature T_c. In both cases, the expected scaling behaviour of the response function in the ageing regime is well reproduced by the numerical data. The value of the exponent a, still controversial, is estimated and the FD ratio is computed. Our estimate of X_∞ 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 FD ratio depends on time not only through the correlation function.

2. Our Ising–Glauber-like model

2.1. Useful relations on Markov processes

We consider a classical Ising model whose degrees of freedom are N scalar variables $\sigma_i = \pm 1$ located at the nodes of a d-dimensional lattice. Let us denote by $\wp(\{\sigma\}, t)$ the probability to observe the system in the state $\{\sigma\}$ at time t. We first define a discrete-time Markov chain by the master equation

$$\wp(\{\sigma\}, t+\Delta t) = (1-\Delta t)\wp(\{\sigma\}, t) + \Delta t \sum_{\{\sigma'\}} W(\{\sigma'\} \to \{\sigma\}, t)\wp(\{\sigma'\}, t) \tag{4}$$

where $W(\{\sigma\} \to \{\sigma'\}, t)$ is the transition rate per unit time from the state $\{\sigma\}$ to the state $\{\sigma'\}$ at time t. The condition $\sum_{\{\sigma'\}} W(\{\sigma\} \to \{\sigma'\}, t) = 1$ ensures the normalization of the probability $\wp(\{\sigma\}, t)$ at any time t. The system is not forced to make a transition at each time step, i.e. the transition rate may have non-zero diagonal elements $W(\{\sigma\} \to \{\sigma\}, t)$. In the continuous-time limit $\Delta t \to 0$, the master equation (4) goes to

$$\left(1 + \frac{\partial}{\partial t}\right)\wp(\{\sigma\}, t) = \sum_{\{\sigma'\}} W(\{\sigma'\} \to \{\sigma\}, t)\wp(\{\sigma'\}, t). \tag{5}$$

It is easily shown that the conditional probability, $\wp(\{\sigma\}, t|\{\sigma'\}, s)$ with $s < t$, defined by the Bayes relation

$$\wp(\{\sigma\}, t) = \sum_{\{\sigma'\}} \wp(\{\sigma\}, t|\{\sigma'\}, s)\wp(\{\sigma'\}, s) \tag{6}$$

also satisfies the same master equation (4)

$$\begin{aligned}\wp(\{\sigma\}, t+\Delta t|\{\sigma'\}, s) &= (1-\Delta t)\wp(\{\sigma\}, t|\{\sigma'\}, s) \\ &\quad + \Delta t \sum_{\{\sigma''\}} W(\{\sigma''\} \to \{\sigma\}, t)\wp(\{\sigma''\}, t|\{\sigma'\}, s)\end{aligned} \tag{7}$$

or in the continuous-time limit $\Delta t \to 0$

$$\left(1 + \frac{\partial}{\partial t}\right)\wp(\{\sigma\}, t|\{\sigma'\}, s) = \sum_{\{\sigma''\}} W(\{\sigma''\} \to \{\sigma\}, t)\wp(\{\sigma''\}, t|\{\sigma'\}, s). \tag{8}$$

Moreover, one can work out a master equation for the time s. It reads

$$\begin{aligned}\wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta t) &= (1+\Delta t)\wp(\{\sigma\}, t|\{\sigma'\}, s) \\ &\quad - \Delta t \sum_{\{\sigma''\}} W(\{\sigma'\} \to \{\sigma''\}, s)\wp(\{\sigma\}, t|\{\sigma''\}, s)\end{aligned} \tag{9}$$

and in the continuous-time limit $\Delta t \to 0$

$$\left(1 - \frac{\partial}{\partial s}\right)\wp(\{\sigma\}, t|\{\sigma'\}, s) = \sum_{\{\sigma''\}} W(\{\sigma'\} \to \{\sigma''\}, s)\wp(\{\sigma\}, t|\{\sigma''\}, s). \tag{10}$$

This last equation might be obtained simply 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 of $t - s$ only. 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 (8) then reads

$$\frac{\partial}{\partial t}\hat{\wp}(t, s) = (\hat{W} - \mathbb{1})\hat{\wp}(t, s) \tag{11}$$

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

$$\begin{aligned}\wp(\{\sigma\}, t|\{\sigma'\}, s) &= \sum_{\{\sigma''\}}\langle\{\sigma\}|\exp\left(\int_s^t (\hat{W} - \mathbb{1})\,\mathrm{d}t'\right)|\{\sigma''\}\rangle\wp(\{\sigma''\}, s|\{\sigma'\}, s) \\ &= \langle\{\sigma\}|\exp((\hat{W} - \mathbb{1})(t - s))|\{\sigma'\}\rangle\end{aligned} \tag{12}$$

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

2.2. *The model and its dynamics*

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

$$\wp_{\mathrm{eq}}(\{\sigma\}) = \frac{1}{\mathcal{Z}}\exp(-\beta\mathcal{H}(\{\sigma\})) = \frac{1}{\mathcal{Z}}\exp\left(\beta\sum_{k,l<k} J_{kl}\sigma_k\sigma_l\right) \tag{13}$$

where ferromagnetic couplings correspond to $J_{kl} > 0$. The condition of stationarity $\frac{\partial}{\partial t}\wp_{\mathrm{eq}}(\{\sigma\}) = 0$ leads according to the master equation (5) to a constraint on the transition rates

$$\sum_{\{\sigma'\}}[\wp_{\mathrm{eq}}(\{\sigma'\})W(\{\sigma'\} \to \{\sigma\}, t) - \wp_{\mathrm{eq}}(\{\sigma\})W(\{\sigma\} \to \{\sigma'\}, t)] = 0. \tag{14}$$

The equation (14) is satisfied when the detailed balance holds

$$\wp_{\mathrm{eq}}(\{\sigma'\})W(\{\sigma'\} \to \{\sigma\}, t) = \wp_{\mathrm{eq}}(\{\sigma\})W(\{\sigma\} \to \{\sigma'\}, t). \tag{15}$$

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

$$W(\{\sigma\} \to \{\sigma'\}, t) = \frac{1}{N}\sum_{k=1}^{N} W_k(\{\sigma\} \to \{\sigma'\}) \tag{16}$$

where the transition rate for a single spin-flip is

$$W_k(\{\sigma\} \to \{\sigma'\}) = \left[\prod_{l\neq k}\delta_{\sigma_l,\sigma'_l}\right]\frac{\exp\left(\beta\sum_{l\neq k}J_{kl}\sigma'_k\sigma'_l\right)}{\sum_{\sigma=\pm 1}\exp\left(\beta\sum_{l\neq k}J_{kl}\sigma\sigma'_l\right)}. \tag{17}$$

In this last expression, only the single-spin flip $\sigma_k \to \sigma'_k$ is allowed. The product of Kronecker deltas ensures that all other spins are unmodified during the transition. After the transition, the spin σ_k takes the new value σ'_k, chosen according to the equilibrium probability distribution $\wp_{\mathrm{eq}}(\{\sigma\})$. In the case of the Ising chain, the transition rates (16) are equivalent to Glauber's ones [14]. We will use a slightly different dynamics consisting of a sequential update of spins. Let us choose a sequence of lattice sites $\{\kappa(t) \in \{1, \ldots, N\}, \forall t = n\Delta t, n \in \mathbb{N}\}$ and let us define the transition rates in discrete time as

$$W(\{\sigma\} \to \{\sigma'\}, t) = W_{\kappa(t)}(\{\sigma\} \to \{\sigma'\}). \tag{18}$$

In comparison to Glauber dynamics, only the spin-flip involving the spin $\sigma_{\kappa(t)}$ is possible at time t. In the continuous-time limit $\Delta t \to 0$, the two dynamics are equivalent up to a rescaling of time $t \to t/N$ (found for example in the definition of a Monte Carlo step). Indeed, when iterating the master equation (4) N times, one obtains

$$\begin{aligned}\wp(\{\sigma\}, t+N\Delta t) &= (1-N\Delta t)\wp(\{\sigma\}, t)\\ &\quad + \Delta t \sum_{\{\sigma'\}} \wp(\{\sigma'\}, t) \sum_{n=0}^{N-1} W_{\kappa(t+n\Delta t)}(\{\sigma'\} \to \{\sigma\}) + \mathrm{O}(\Delta t^2).\end{aligned} \tag{19}$$

and the Glauber dynamics is recovered if $\{\kappa(t+n\Delta t)\}_{n=0,\ldots,N-1}$ is any circular permutation of the set of lattice sites $\{1, \ldots, N\}$. The equivalence of the two dynamics may not hold in the thermodynamic limit $N \to +\infty$. Despite the fact that the time-dependence of the transition rates (18) breaks the time-translation invariance of the conditional probabilities, the effective transition rate in equation (19) is time-independent and thus the time-translation invariance is restored in the continuous-time limit if $\{\kappa(t)\}$ is periodic of period $N\Delta t$. Again, this may no longer be true in the thermodynamic limit. In the following, we will assume that $\{\kappa(t)\}$ satisfies the two above discussed conditions, i.e. being periodic of period $N\Delta t$ and that any N consecutive values are a circular permutation of $\{1, \ldots, N\}$.

3. Fluctuation–dissipation relation

3.1. Far-from-equilibrium fluctuation–dissipation relation

A magnetic field h_i is coupled to the spin σ_i between the times s and $s + \Delta t$. During this interval of time, the transition rates are changed to

$$W^h_{k=\kappa(s)}(\{\sigma\} \to \{\sigma'\}) = \left[\prod_{l\neq k} \delta_{\sigma_l,\sigma'_l}\right] \frac{\exp\left(\beta\left[\sum_{l\neq k} J_{kl}\sigma'_k\sigma'_l + h_i\sigma'_k\delta_{k,i}\right]\right)}{\sum_{\sigma=\pm1} \exp\left(\beta\left[\sum_{l\neq k} J_{kl}\sigma\sigma'_l + h_i\sigma\delta_{k,i}\right]\right)} \tag{20}$$

in order to take into account the additional Zeeman term $\beta h_i\sigma_i$ in the Hamiltonian of the equilibrium probability distribution (13). The transition rates are all identical to the case $h_i = 0$ apart from the single-spin flip W^h_i involving the spin σ_i.

Using the Bayes relation and the discrete-time master equation (4), the average of the spin σ_j at time $t > s$ can be expanded in the following form:

$$\begin{aligned}\langle\sigma_j(t)\rangle &= \sum_{\{\sigma\}} \sigma_j \wp(\{\sigma\}, t)\\ &= \sum_{\{\sigma\},\{\sigma'\}} \sigma_j \wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta t)\wp(\{\sigma'\}, s+\Delta t)\\ &= \sum_{\{\sigma\},\{\sigma'\}} \sigma_j \wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta t)\Bigg[(1-\Delta t)\wp(\{\sigma'\}, s)\\ &\quad + \Delta t \sum_{\{\sigma''\}} W^h_{\kappa(s)}(\{\sigma''\} \to \{\sigma'\})\wp(\{\sigma''\}, s)\Bigg].\end{aligned} \tag{21}$$

W^h_i being the only quantity depending on the magnetic field in equation (21), only the second term remains when $\kappa(s) = i$ after taking derivatives with respect to the magnetic field . The derivative then leads to

$$\left[\frac{\partial\langle\sigma_j(t)\rangle}{\partial h_i}\right]_{h_i\to 0} = \Delta t\,\delta_{\kappa(s),i}\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_j\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)$$
$$\times\left[\frac{\partial W_i^h}{\partial h_i}(\{\sigma''\}\to\{\sigma'\})\right]_{h_i\to 0}\wp(\{\sigma''\},s) \qquad (22)$$

This quantity is the magnetization on site j at time t when an infinitesimal magnetic field is applied to the site i between s and $s+\Delta t$, i.e. an integrated response function that we will denote $\chi_{ji}(t,[s;s+\Delta t])$. The derivative of the transition rate W_i^h defined by equation (20) is easily taken and reads

$$\left[\frac{\partial W_i^h}{\partial h_i}(\{\sigma''\}\to\{\sigma'\})\right]_{h_i\to 0} = \beta W_i(\{\sigma''\}\to\{\sigma'\})\left[\sigma_i' - \tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\right]. \qquad (23)$$

It turns out to involve the transition rate of the zero-field dynamics (17). Due to this property, the integrated response function can be expressed in terms of thermodynamic averages of the zero-field dynamics. Inserting (23) into (22), the integrated response function is rewritten as

$$\chi_{ji}(t,[s;s+\Delta t]) = \beta\Delta t\,\delta_{\kappa(s),i}\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_j\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)$$
$$\times\left[\sigma_i' - \tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\right]W_i(\{\sigma''\}\to\{\sigma'\})\wp(\{\sigma''\},s) \qquad (24)$$

The summation over $\{\sigma''\}$ can be performed by using the discrete-time master equation (4). One obtains

$$\chi_{ji}(t,[s;s+\Delta t]) = \beta\delta_{\kappa(s),i}\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)\left[\sigma_i' - \tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\right]$$
$$\times\left[\wp(\{\sigma'\},s+\Delta t) - (1-\Delta t)\wp(\{\sigma'\},s)\right] \qquad (25)$$

The response function $R_{ji}(t,s)$ being defined as the response of the magnetization to a magnetic pulse $h_i(t) = h_i\delta(t-s)$, it may be obtained by taking the continuous-time limit $\Delta t\to 0$ of equation (25). In this limit, spin-flip may still occur on the same sequence of sites but at times closer and closer. The function $\kappa(t)$ will be defined for all real positive values of t meaning that a spin-flip may occur at any time. In this limit expression (25) will go towards the integrated response for a magnetic field applied during an infinitesimal timestep, i.e. the response function. Using a Taylor-expansion of $\wp(\{\sigma'\},s)$ in the vicinity of $s+\Delta t$, equation (25) can be rewritten to lowest order in Δt as

$$\chi_{ji}(t,[s;s+\Delta t]) = \beta\Delta t\,\delta_{\kappa(s),i}\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)\left[\sigma_i' - \tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\right]$$
$$\times\left[\wp(\{\sigma'\},s+\Delta t) + \frac{\partial\wp}{\partial s}(\{\sigma'\},s+\Delta t)\right]. \qquad (26)$$

In the continuous-time limit $\Delta t\to 0$, the dynamic no longer depends on the sequence of sites on which spin-flips may occur. As a consequence, a derivative $\frac{\partial\wp}{\partial s}(\{\sigma'\},s)$ involves a transition rate W_i that can be reinterpreted according to the master equations as a derivative with respect to time t if $t-s$ is a multiple of $N\Delta t$ or equivalently if $\kappa(t)=i$.

$$\frac{\partial\wp}{\partial s}(\{\sigma\},t|\{\sigma'\},s)=-\frac{\partial\wp}{\partial t}(\{\sigma\},t|\{\sigma'\},s). \tag{27}$$

The term involving the time-derivative in equation (26) can thus be rewritten in the continuous-time limit as

$$\begin{aligned}\wp(\{\sigma\},t|\{\sigma'\},s)\frac{\partial\wp}{\partial s}(\{\sigma'\},s) &= \frac{\partial}{\partial s}[\wp(\{\sigma\},t|\{\sigma'\},s)\wp(\{\sigma'\},s)]\\ &\quad \underbrace{-\frac{\partial\wp}{\partial s}(\{\sigma\},t|\{\sigma'\},s)}_{=+\frac{\partial\wp}{\partial t}(\{\sigma\},t|\{\sigma'\},s)}\wp(\{\sigma'\},s).\end{aligned} \tag{28}$$

Moreover, the integrated response function $\chi_{ji}(t,[s;s+\Delta t])$ goes to the response function $R_{ji}(t,s)$ in the continuous-time limit:

$$\chi_{ji}(t,[s;s+\Delta t])=\int_s^{s+\Delta t}R_{ji}(t,u)\,\mathrm{d}u=R_{ji}(t,s)\Delta t+\mathrm{O}(\Delta t^2). \tag{29}$$

Combining equations (26), (28) and (29), the response function reads in the continuous-time limit

$$R_{ji}(t,s)=\beta\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\left\langle\sigma_j(t)\left[\sigma_i(s)-\sigma_i^{\mathrm{Weiss}}(s)\right]\right\rangle\delta_{\kappa(s),i} \tag{30}$$

where $\sigma_i^{\mathrm{Weiss}}(s)=\tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k(s)\right)$ is the equilibrium value of the spin σ_{i} in the Weiss field created by all other spins at time s. Relation (30) generalizes equation (1). The response function $R_{ji}(t,s)$ turns out to be related to time-derivatives of the correlation function of spin σ_j at time t with the fluctuations of spin σ_i at time s around the equilibrium average $\sigma_i^{\mathrm{Weiss}}(s)$ of this spin in its Weiss field. In this sense, this relation is still a fluctuation–dissipation relation but valid far-from-equilibrium. No assumption has been made on the dimension of the space or on the set of exchange couplings J_{kl} 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 equilibrium probability distribution of the model but comes from the Markovian properties of the dynamics. Generalized response functions are easily calculated along the same lines as equation (30). The second-order term for example reads

$$\begin{aligned}R^{(2)}_{kji}(t,s,r) &= \left(\frac{\delta^2\langle\sigma_k(t)\rangle}{\delta h_j(s)\delta h_i(r)}\right)_{h\to 0}\qquad (t>s>r)\\ &= \beta\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\left(1+\frac{\partial}{\partial r}+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\langle\sigma_k(t)\delta\sigma_j(s)\delta\sigma_i(r)\rangle\delta_{\kappa(r),j}\delta_{\kappa(s),i}\end{aligned} \tag{31}$$

where $\delta\sigma_j(s)=\sigma_j(s)-\sigma_j^{\mathrm{Weiss}}(s)$. Calculation of nonlinear terms requires higher-order derivatives of the transition rate such as for example

$$\begin{aligned}R^{(2)}_{jii}(t,s,s) &= \left(\frac{\delta^2\langle\sigma_j(t)\rangle}{\delta h_i^2(s)}\right)_{h\to 0}\qquad (t>s)\\ &= -2\beta^2\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\left\langle\sigma_j(t)\sigma_i^{\mathrm{Weiss}}(s)\delta\sigma_i(s)\right\rangle\delta_{\kappa(s),i}.\end{aligned} \tag{32}$$

These relations are moreover easily extended to other models. The relations (30) to (32) hold for the 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 $\sigma_i^{\mathrm{Weiss}}(s)$ by its average value in the Weiss field.

Exact expressions of the autocorrelation and response functions have been obtained for the 1D Ising–Glauber model [2] in the thermodynamic limit. It turns out in this case that the response function does not satisfy equation (30). As noted after equation (19), the dynamics is equivalent to Glauber's one in the continuous-time limit $\Delta t \to 0$ except perhaps in the thermodynamic limit $N \to +\infty$. The discrepancy of the response function with equation (30) in the case of the Ising chain shows that the equivalence of the two dynamics breaks in the thermodynamic limit and that equations (30) to (32) hold only for finite systems.

3.2. Equilibrium limit

We will show in this section that the usual expression of the FDT (1) is recovered in the equilibrium limit. At equilibrium, the probability distribution $\wp_{\rm eq}(\{\sigma\})$ does not depend on time. As a consequence, the integrated response function can be written according to equation (26) as

$$\chi_{ji}^{\rm eq}(t,[s;s+\Delta t]) = \beta\Delta t\delta_{\kappa(s),i}\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t) \times\left[\sigma_i' - \tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\right]\wp_{\rm eq}(\{\sigma'\}). \quad (33)$$

The hyperbolic tangent can be expressed in terms of the transition ratio of the zero-field dynamics (17)

$$\begin{aligned}\tanh\left(\beta\sum_{k\neq i}J_{ik}\sigma_k'\right)\wp_{\rm eq}(\{\sigma'\}) &= \sum_{\{\sigma''\}}\sigma_i''\frac{\left[\prod_{k\neq i}\delta_{\sigma_k'',\sigma_k'}\right]\exp\left(\beta\sum_{k\neq i}J_{ik}\sigma_i'\sigma_k'\right)}{\sum_{\sigma=\pm1}\exp\left(\beta\sum_{k\neq i}J_{ik}\sigma\sigma_k'\right)}\frac{\exp\left(\beta\sum_{k,l<k}J_{kl}\sigma_k''\sigma_l''\right)}{\mathcal{Z}} \\ &= \sum_{\{\sigma''\}}\sigma_i''W_i(\{\sigma''\}\to\{\sigma'\})\wp_{\rm eq}(\{\sigma''\}). \end{aligned} \quad (34)$$

Inserting in equation (33), the integrated response function reads

$$\chi_{ji}^{\rm eq}(t,[s;s+\Delta t]) = \beta\Delta t\delta_{\kappa(s),i}\left[\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\,\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)\sigma_i'\wp_{\rm eq}(\{\sigma'\}) - \sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_j\,\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t)\sigma_i''W_i(\{\sigma''\}\to\{\sigma'\})\wp_{\rm eq}(\{\sigma''\})\right]. \quad (35)$$

The first term can be expressed as a thermodynamic average while in the second, one needs to first get rid of the transition rate. The Kronecker delta constrains the only possible spin-flip to involve site i at time s. As a consequence, $W_i(\{\sigma''\}\to\{\sigma'\})$ can be replaced by $W_{\kappa(s)}(\{\sigma''\}\to\{\sigma'\})$ and the master equation (9) can be applied to equation (35). Moreover, one can show that

$$\wp(\{\sigma\},t|\{\sigma''\},s) = (1-\Delta t)\wp(\{\sigma\},t|\{\sigma''\},s+\Delta t) + \Delta t\sum_{\{\sigma'\}}W(\{\sigma''\}\to\{\sigma'\},s)\wp(\{\sigma\},t|\{\sigma'\},s+\Delta t) + {\rm O}(\Delta t^2). \quad (36)$$

This relation is obtained by first putting alone $\wp(\{\sigma\}, t|\{\sigma''\}, s)$ in the left-hand side of the master equation (9) and then by iterating the relation to make $\wp(\{\sigma\}, t|\{\sigma''\}, s)$ disappear in the right-hand side. Equation (36) is then used to eliminate the transition rate from equation (35):

$$\chi_{ji}^{\mathrm{eq}}(t, [s; s+\Delta t]) = \beta\delta_{\kappa(s),i}\left[\Delta t\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta t)\sigma_i'\wp_{\mathrm{eq}}(\{\sigma'\})\right.$$
$$-\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\}, t|\{\sigma'\}, s)\sigma_i'\wp_{\mathrm{eq}}(\{\sigma'\})$$
$$\left.+(1-\Delta t)\sum_{\{\sigma\},\{\sigma'\}}\sigma_j\wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta t)\sigma_i'\wp_{\mathrm{eq}}(\{\sigma'\})\right]. \quad (37)$$

The two terms of order Δt cancel and there remains only

$$\chi_{ji}^{\mathrm{eq}}(t, [s; s+\Delta t]) = \beta\delta_{\kappa(s),i}\langle\sigma_j(t)[\sigma_i(s+\Delta t) - \sigma_i(s)]\rangle_{\mathrm{eq}} \quad (38)$$

and in the continuous-time limit, one obtains equilibrium fluctuation–dissipation:

$$R_{ji}^{\mathrm{eq}}(t, s) = \beta\delta_{\kappa(s),\mathrm{i}}\frac{\partial}{\partial s}\langle\sigma_j(t)\sigma_i(s)\rangle_{\mathrm{eq}} = \beta\delta_{\kappa(s),\mathrm{i}}\big\langle\sigma_j(t)\big[\sigma_i(s) - \sigma_i^{\mathrm{Weiss}}(s)\big]\big\rangle_{\mathrm{eq}} \quad (39)$$

where the last member is simply equation (30) at equilibrium. One recovers the usual equilibrium fluctuation–dissipation relation up to a Kronecker delta due the fact that the response function is non-zero only for times at which a spin-flip involving the spin connected to the magnetic field occurs. However, the sequence of spin-flips being assumed to be periodic with a period $N\Delta t$, in the limit $\Delta t \to 0$ the Kronecker delta may become useless. Unexpectedly, equation (39) holds in the thermodynamic limit in the case of the 1D Ising–Glauber model.

4. Monte Carlo simulations of the 2D Ising model

The discrete-time analogue of expression (30) of the response function enables us to study the ageing displayed by the Ising–Glauber model more accurately than in previous works that were based on the numerical estimate of the integrated response function. In the first part of this section, the algorithm is given. 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 ageing, associated with the existence of growing domains corresponding to competing ferromagnetic states [15]. Reversible processes occur in the bulk of domains while domain wall rearrangements are irreversible. We will distinguish between quenches at the critical temperature T_c and below. In both cases, lattice sizes 128×128, 256×256 and 362×362 were simulated and the data averaged over 3000, 10 000 and 5000 initial configurations respectively. 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, time is a discrete variable and the time step is set to $\Delta t = 1$. Monte Carlo simulations indeed implement the Markov process defined by the master equation (4) with the choice $\Delta t = 1$. The Markov chain is simulated by averaging over multiple spin histories. Changing or not the sequence of spin-flips leads in the large-time limit to the same dynamics up to a time-renormalization corresponding to the definition of a Monte Carlo step (MCS) as shown in section 2.2. The response function can only be defined for continuous time processes since the magnetic field needs to be applied during an infinitesimal time step. However, the integrated response function during one spin-flip $\sigma_i \to \sigma_i'$ is the best estimator for the response function $R_{ij}(t,s)$ that we can define. Inserting $\Delta t = 1$ into equation (25), the estimator of the response function is simply

$$\chi_{ji}(t,[s;s+1]) = \beta\delta_{\kappa(s),i}\big\langle\sigma_j(t)\big[\sigma_i(s+1) - \sigma_i^{\rm Weiss}(s+1)\big]\big\rangle \tag{40}$$

where $\sigma_i^{\rm Weiss}(s) = \tanh\big(\beta\sum_{k\neq i}J_{ik}\sigma_k'(s)\big)$. In the following, we will be interested only in response functions of the form $R_{ii}(t,s)$. In order to reduce statistical fluctuations, we have then estimated the response function $R(t,s)$ as an average over all spin-flips during one MCS:

$$R(t,s) = \frac{1}{N}\sum_{n=0}^{N-1}\chi_{\kappa(s+n)\kappa(s+n)}(t,[s+n;s+n+1]). \tag{41}$$

The calculation of this quantity is quite simple. Let the simulation evolve until time s. For each of the N next spin-flips $\sigma_i \to \sigma_i'$, store the quantity $\sigma_i' - \sigma_i^{\rm Weiss}$. Note that σ_i' may be equal to σ_i, meaning that the system has not changed during this time step. However, in strict application of equation (40), one has nevertheless to store $\sigma_i - \sigma_i^{\rm Weiss}$. After N spin-flips, let the system evolve again until time t. Calculate the response function for each site i by multiplying the quantity $\sigma_i' - \sigma_i^{\rm Weiss}$ stored by the new value of the spin σ_i and add all these one-site response functions. Repeat the simulation as many times as necessary and average the results. The integrated response function can be easily calculated by numerical integration of the response function.

The time-derivative of the correlation function $\frac{\partial}{\partial s}C_{ji}(t,s)$ at time s can be estimated by $\langle\sigma_j(t)[\sigma_i(s+1) - \sigma_i(s)]\rangle$. Again, this quantity is averaged over all spin-flips during one MCS. The FD ratio (2) can be estimated as

$$X(t,s) = \frac{R(t,s)}{\beta\frac{\partial}{\partial s}C(t,s)} = \frac{\sum_{n=0}^{N-1}\big\langle\sigma_{\kappa(s+n)}(t)\big[\sigma_{\kappa(s+n)}(s+1) - \sigma_{\kappa(s+n)}^{\rm Weiss}(s+1)\big]\big\rangle}{\beta\sum_{n=0}^{N-1}\big\langle\sigma_{\kappa(s+n)}(t)\big[\sigma_{\kappa(s+n)}(s+1) - \sigma_{\kappa(s+n)}(s)\big]\big\rangle}. \tag{42}$$

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]

$$C(t,s) \underset{t,s\gg 1}{\sim} s^{-a_c}\,\mathcal{C}_c(t/s) \tag{43}$$

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

$$R(t,s) \underset{t,s\gg 1}{\sim} s^{-1-a_c}\,\mathcal{R}_c(t/s) \tag{44}$$

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 (44) for the integrated response function that has been checked by large-scale Monte Carlo simulations [19]. However, relation (44) 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 (44).

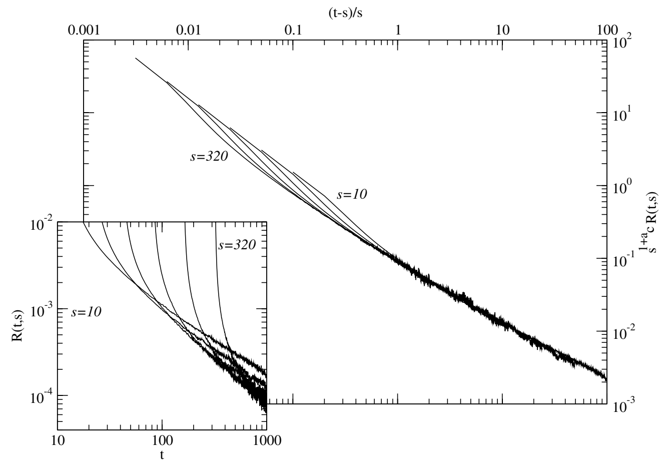

Figure 1. Response function of the 2D Ising model during a quench at the critical temperature (inset) and collapse of the scaling function for different values of s. The data were obtained with a lattice of size 362×362 and averaged over 5000 initial configurations. The value $a_c = 0.115$ was used [17].

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 the order of $1/N_{\text{config}}$ and so cannot 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).

We computed the FD ratio $X(t, s)$ using the estimator previously derived and whose expression is given by equation (42). The error bars are quite large. The numerical data are plotted in figure 2 for the largest lattice size ($L = 362$). In contradistinction to the Cugliandolo conjecture (2), the inset of figure 2 shows that the FD ratio does not depend on time only through the correlation function. However, it seems that it may be the case in the limit $C(t, s) \to 0$. On the other hand, it seems that the FD ratio depends on time only through t/s and reaches a plateau for $s = 10$ and $s = 20$ and for large enough values of t that we may estimate roughly to be $X_\infty \simeq 0.32(3)$. Compatible values are obtained for $L = 256$ and $L = 362$ excluding any possibility of finite-size effects. The limit X_∞ has been conjectured to be universal [17] but incompatible values have been given by different groups: $X_\infty = 0.26(1)$ [20] and $X_\infty = 0.340(5)$ [21] by Monte Carlo simulations and $X_\infty \simeq 0.35$ [22] for the O(1) model in dimension $d = 4 - \epsilon$. Our estimate is compatible with the last two. The estimate $X_\infty = 0.26(1)$ has probably been measured for too short a time t, far from the region where the Cugliandolo conjecture (2) and thus equation (3) hold. This stresses the danger of using equation (3) to compute the FD 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]

$$C(t, s) \underset{t,s \gg 1}{\sim} M_{\text{eq}}^2 \, \mathcal{C}(t/s) \qquad (45)$$

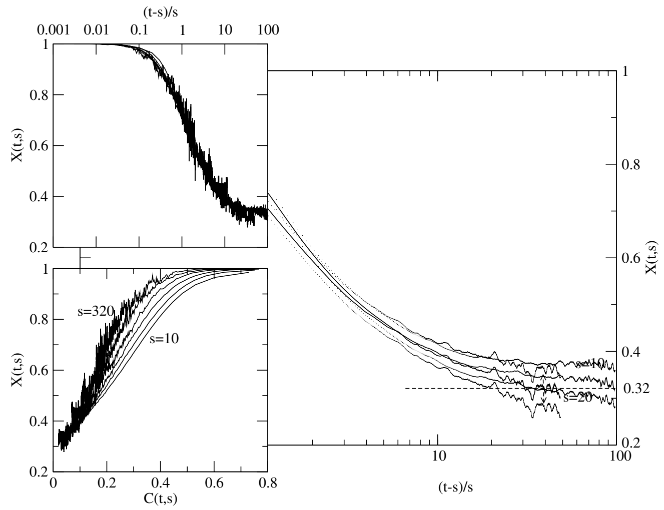

Figure 2. FD ratio $X(t, s)$ versus t for different values s for the Ising–Glauber model quenched at the critical temperature T_c. The data were obtained for a lattice 362×362 and averaged over 5000 initial configurations. In the right-hand graph, data have been averaged over every 20 successive data points in order to smooth the curves. The dashed line corresponds to the estimate of X_∞ given in the text and the arrow to its error bar.

where M_{eq} is the equilibrium magnetization 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 λ and the dynamical exponent z are expected to take values which are different from those at T_c. The response function is expected to scale as [16, 17]

$$R(t, s) \underset{t,s\gg 1}{\sim} s^{-1-a}\, \mathcal{R}(t/s) \tag{46}$$

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 [23] or 1/2 [24, 25]. Our numerical data are presented in 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 increases 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 (46) 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 significantly. The value $a = 1/4$ in particular improves the collapse for small values of s only. The response function has probably strong corrections to scaling. Note that corrections have already been taken into account for the study of the scaling behaviour of the integrated response function [19, 26].

Combining relations (45) and (46), the FD ratio $X(t, s) = R(t, s)\big/\beta \frac{\partial}{\partial s} C(t, s)$ 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 that the data fluctuate less than at T_c. As expected, the FD ratio is equal to 1 for small values of $t - s$, signalling 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, figure 4 shows unambiguously that the FD ratio does not

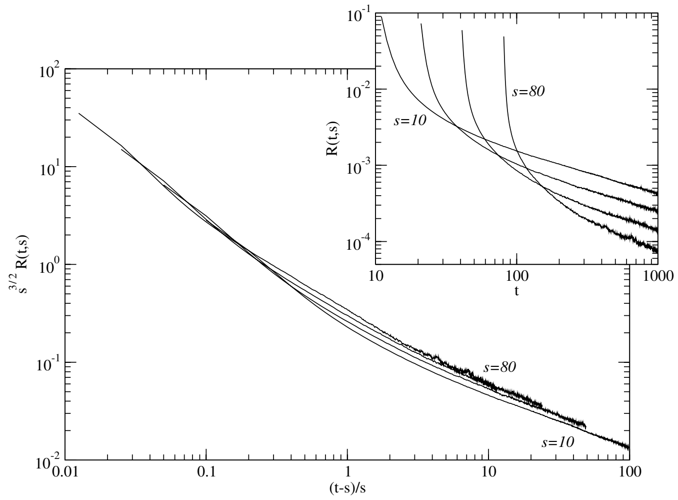

Figure 3. Response function of the 2D Ising model during a quench at the temperature $T = J/0.6 \simeq \frac{3}{4}T_c$ (inset) and collapse of the scaling function for different values of s. The data were obtained for a lattice 256×256 and averaged over 10 000 initial configurations.

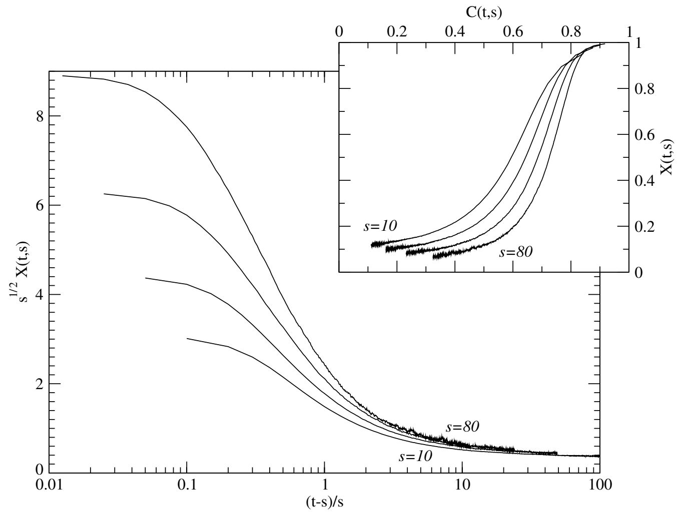

Figure 4. FD ratio $X(t,s)$ versus t for different values s for the Ising–Glauber model quenched at the temperature $J/0.6k_B \simeq \frac{3}{4}T_c$. The data were obtained for a lattice 256×256 and averaged over 10 000 initial configurations.

depend on time only through the correlation function. This makes relation (3) invalid. The study of the violation of the equilibrium FDT by the usual method relying on equation (3) would have led to erroneous values of the FD ratio.

5. Conclusion

Using a formalism similar to Kubo's one in the quantum case, we derive an exact expression of the response function of an Ising–Glauber-like model far-from-equilibrium (equation (30)).

At least for finite systems, the dynamics of our model is equivalent to the Glauber dynamics up to a time-renormalization $t \to t/N$. The derivation is possible because the dynamics consists of a sequential update of the spins and the transition rate under a magnetic field can be written as a product of the transition rate without magnetic field and of a term depending only on the final spin configuration. 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 its equilibrium average in its Weiss field. In this sense, the expression is a generalization 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. Generalized and nonlinear response functions can be obtained analogously. However, relation (30) does hold in the thermodynamic limit in the case of the 1D Ising–Glauber model because of the breaking of the equivalence of the dynamics introduced in this work with Glauber's one in the thermodynamic limit.

The calculation of the response function in discrete-time is then implemented in Monte Carlo simulations. Our approach gives access to the response function and the FD ratio directly. In particular, the FD ratio can be obtained without assuming the validity of 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 FD ratio display the expected scaling behaviour both at T_c and below T_c. The values, still controversial, of a and X_∞ are estimated to be equal to $1/2$ and 0.32(3) respectively, in agreement with some previous works. The Cugliandolo conjecture (2) does not hold for this model apart from perhaps at T_c in the limit of vanishing correlation functions. This would explain the discrepancies of previous estimates of X_∞ relying on the Cugliandolo conjecture. The above-presented numerical procedure may be extended to many different systems and would provide a unambiguous test of the Cugliandolo conjecture. We are currently studying the dynamics of frustrated systems in this framework.

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During the (long) refereing process of this paper, the method has been applied to calculate the integrate response function in Monte Carlo simulations [27].

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