Off-equilibrium generalization of the fluctuation dissipation theorem for Ising spins and measurement of the linear response function

Eugenio Lippiello,* Federico Corberi,† and Marco Zannetti‡

Istituto Nazionale di Fisica della Materia, Unità di Salerno and Dipartimento di Fisica "E.R. Caianiello," Università di Salerno, 84081 Baronissi (Salerno), Italy

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We derive for Ising spins an off-equilibrium generalization of the fluctuation dissipation theorem, which is formally identical to the one previously obtained for soft spins with Langevin dynamics [L.F. Cugliandolo, J. Kurchan, and G. Parisi, J. Phys. I **4**, 1641 (1994)]. The result is quite general and holds both for dynamics with conserved and nonconserved order parameters. On the basis of this fluctuation dissipation relation, we construct an efficient numerical algorithm for the computation of the linear response function without imposing the perturbing field, which is alternative to those of Chatelain [J. Phys. A **36**, 10 739 (2003)] and Ricci-Tersenghi [Phys. Rev. E **68**, 065104(R) (2003)]. As applications of the new algorithm, we present very accurate data for the linear response function of the Ising chain, with conserved and nonconserved order parameter dynamics, finding that in both cases the structure is the same with a very simple physical interpretation. We also compute the integrated response function of the two-dimensional Ising model, confirming that it obeys scaling $\chi(t,t_w) \simeq t_w^{-a} f(t/t_w)$, with $a=0.26\pm0.01$, as previously found with a different method.

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I. INTRODUCTION

In the recent big effort devoted to the understanding of systems out of equilibrium, of particular interest is the problem of the generalization of the fluctuation dissipation theorem (FDT). The autocorrelation function $C(t-t')$ of some local observable and the corresponding linear response function $R(t-t')$ in equilibrium are related by the FDT

$$R(t-t') = \frac{1}{T}\frac{\partial C(t-t')}{\partial t'}. \tag{1}$$

The question is whether an analogous relation also exists away from equilibrium, namely, whether it is still possible to connect the response function to properties of the unperturbed dynamics, possibly in the form of correlation functions.

A positive answer to this question exists when the time evolution is of the Langevin type. Consider a system with an order parameter field $\phi(\vec{x})$ evolving with the equation of motion

$$\frac{\partial \phi(\vec{x},t)}{\partial t} = B(\phi(\vec{x},t)) + \eta(\vec{x},t), \tag{2}$$

where $B(\phi(\vec{x},t))$ is the deterministic force and $\eta(\vec{x},t)$ is a white, zero-mean Gaussian noise. Then, the linear response function is simply given by the correlation function of the order parameter with the noise

$$2TR(t,t') = \langle \phi(\vec{x},t)\,\eta(\vec{x},t')\rangle, \tag{3}$$

where T is the temperature of the thermal bath and $t \geqslant t'$ by causality. It is straightforward [1] to recast the above relation in the form

$$TR(t,t') = \frac{1}{2}\frac{\partial C(t,t')}{\partial t'} - \frac{1}{2}\frac{\partial C(t,t')}{\partial t} - A(t,t'), \tag{4}$$

where

$$A(t,t') \equiv \frac{1}{2}[\langle \phi(\vec{x},t) B(\phi(\vec{x},t'))\rangle - \langle B(\phi(\vec{x},t))\,\phi(\vec{x},t')\rangle] \tag{5}$$

is the so-called asymmetry. Equation (4) [or (3)] qualifies as an extension of the FDT out of equilibrium, since in the right-hand side unperturbed correlation functions appear and, when time translation and time inversion invariance holds, reduces to the equilibrium FDT (1). In Appendix A we show that this equation holds in the same form both for conserved order parameter (COP) and nonconserved order parameter (NCOP) dynamics.

The next interesting question is whether one can do the same also in the case of discrete spin variables, where there is no stochastic differential equation and, therefore, Eq. (3) is not available. For spin variables governed by a master equation, this problem has been considered in recent papers by Chatelain [2], Ricci-Tersenghi [3], Diezemann [4], and Crisanti and Ritort [5]. However, although important for computational and analytical calculations, their results, as we shall explain below, cannot be regarded as generalizations of the FDT in the sense of Eq. (4). In Refs. [2,3], a scheme is presented where $R(t,t')$ is related to unperturbed correlation functions which, however, are not computed in the *true* dynamics of the system. Rather, as will be clarified in Sec. IV, these correlation functions are computed through an auxil-

*Email address: lippiello@sa.infn.it
†Email address: corberi@sa.infn.it
‡Email address: zannetti@na.infn.it

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iary dynamical rule, instrumental to the construction of an algorithm for the computation of $R(t,t')$. On the other hand, in Refs. [4,5], $R(t,t')$ is related to quantities that can be extracted from the dynamics of the unperturbed system, but not all of them can be put in the form of correlation functions.

Instead, we have succeeded in deriving for Ising spin systems a genuine off equilibrium generalization of the FDT, which takes exactly the same form as Eqs. (4) and (5) and which holds, as in the Langevin case, for NCOP (spin flip) and COP (spin exchange) dynamics. Furthermore, using this result we have derived an efficient numerical method for the computation of the response function, without imposing the perturbing conjugate field, which is alternative to those of Refs. [2,3].

The paper is organized as follows. In Sec. II we introduce the formalism and derive the off equilibrium FDT. In Sec. III we introduce the dynamics in discrete time in order to develop a numerical algorithm based on the fluctuation dissipation relation. Section IV is devoted to a comparative discussion of our method with those of Chatelain and Ricci-Tersenghi. In Sec. V the algorithm is applied to the investigation of the scaling properties of the response function in the one dimensional Ising model with NCOP (Sec. V A) and COP dynamics (Sec. V B). As a further application of the method we study in Sec. VI the integrated response function of the Ising model in $d=2$. In Sec. VII we make concluding remarks.

II. FLUCTUATION DISSIPATION RELATION FOR ISING SPINS

We consider a system of Ising spins $s_i=\pm 1$ executing a Markovian stochastic process. The problem is to compute the linear response $R_{i,j}(t,t')$ on the spin at the site i and at the time t, due to an impulse of external field at an earlier time t' and at the site j. Let

$$h_j(t) = h\delta_{i,j}\theta(t-t')\theta(t'+\Delta t - t) \tag{6}$$

be the magnetic field on the jth site acting during the time interval $[t',t'+\Delta t]$, where θ is the Heavyside step function. The response function then is given by [2,5]

$$R_{i,j}(t,t') = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\left.\frac{\partial\langle s_i(t)\rangle}{\partial h_j(t')}\right|_{h=0}, \tag{7}$$

where

$$\left.\frac{\partial\langle s_i(t)\rangle}{\partial h_j(t')}\right|_{h=0} = \sum_{[s],[s'],[s'']} s_i p([s],t|[s'],t'+\Delta t) \times \left|\frac{\partial p^h([s'],t'+\Delta t|[s''],t')}{\partial h_j}\right|_{h=0} p([s''],t') \tag{8}$$

and $[s]$ are spin configurations.

Let us concentrate on the factor containing the conditional probability in the presence of the external field $p^h([s'],t'+\Delta t|[s''],t')$. In general, the conditional probability for Δt sufficiently small is given by

$$p([s],t+\Delta t|[s'],t) = \delta_{[s],[s']} + w([s']\to[s])\Delta t + O(\Delta t^2), \tag{9}$$

where we have used the boundary condition $p([s],t|[s'],t) = \delta_{[s],[s']}$. Normalization of the probability implies

$$\sum_{[s']} w([s]\to[s']) = 0. \tag{10}$$

Furthermore, the transition rates must verify detailed balance

$$w([s]\to[s'])\exp(-\mathcal{H}[s]/T) = w([s']\to[s])\exp(-\mathcal{H}[s']/T), \tag{11}$$

where $\mathcal{H}[s]$ is the Hamiltonian of the system. In the following we separate explicitly the diagonal from the off-diagonal contributions in $w([s]\to[s'])$

$$w([s]\to[s']) = -\delta_{[s],[s']}\sum_{[s'']\neq[s]} w([s]\to[s'']) + (1-\delta_{[s],[s']})w([s]\to[s']), \tag{12}$$

where we have used Eq. (10).

Introducing the perturbing field as an extra term $\Delta\mathcal{H}[s] = -s_j h_j$ in the Hamiltonian, to linear order in h the most general form of the perturbed transition rates $w^h([s]\to[s'])$ compatible with the detailed balance condition is (see Appendix B)

$$w^h([s]\to[s']) = w^0([s]\to[s'])\left\{1 - \frac{1}{2T}h_j(s_j - s_j') + M([s],[s'])\right\}, \tag{13}$$

where $M([s],[s'])$ is an arbitrary function of order h/T symmetric with respect to the exchange $[s]\leftrightarrow[s']$ and $w^0([s]\to[s'])$ are unspecified unperturbed transition rates, which satisfy detailed balance. Note that, since Eq. (11) reduces to an identity for $[s]\neq[s']$, Eq. (13) does not hold for the diagonal contribution $w^h([s]\to[s])$ which, in turn, can be obtained by the normalization condition $\Sigma_{[s']}w^h([s]\to[s'])=0$. In the following, for simplicity, we will take $M([s],[s'])=0$ and the role of a different choice for $M([s],[s'])$ will be discussed in Sec. IV.

Using Eqs. (9), (12), and (13) we obtain

$$T\left.\frac{\partial p^h([s],t+\Delta t|[s'],t)}{\partial h_j}\right|_{h=0} = \Delta t\,\delta_{[s],[s']}\frac{1}{2}\sum_{[s'']\neq[s]} w^0([s]\to[s''])(s_j - s_j'') + \Delta t(1-\delta_{[s],[s']})\frac{1}{2}w^0([s]\to[s'])(s_j' - s_j) \tag{14}$$

and inserting this result in Eq. (8), the response function can be written as the sum of two contributions [6,7]

$$TR_{i,j}(t,t') = \lim_{\Delta t\to 0}[TD_{i,j}(t,t',\Delta t) + T\overline{D}_{i,j}(t,t',\Delta t)], \quad (15)$$

where the first term comes from the diagonal part of Eq. (14)

$$TD_{i,j}(t,t',\Delta t) = \frac{1}{2}\sum_{[s],[s']} s_i p([s],t|[s'],t'+\Delta t) \times \sum_{[s'']\neq[s']} w^0([s']\to[s''])(s'_j - s''_j)p([s'],t'), \quad (16)$$

whereas $\overline{D}_{i,j}$ takes all the off-diagonal contributions

$$T\overline{D}_{i,j}(t,t',\Delta t) = \frac{1}{2}\sum_{[s],[s'],[s'']\neq[s']} s_i p([s],t|[s'],t'+\Delta t)(s'_j - s''_j) \times w^0([s'']\to[s'])p([s''],t'). \quad (17)$$

Using the time translational invariance of the conditional probability $p([s],t|[s'],t'+\Delta t)=p([s],t-\Delta t|[s'],t')$, one can write $D_{i,j}(t,t',\Delta t)$ in the form of a correlation function

$$TD_{i,j}(t,t',\Delta t) = -\frac{1}{2}\langle s_i(t-\Delta t)B_j(t')\rangle, \quad (18)$$

where

$$B_j = -\sum_{[s'']}(s_j - s''_j)w^0([s]\to[s'']). \quad (19)$$

Using Eqs. (9) and (12) the off-diagonal contribution can be written as

$$T\overline{D}_{i,j}(t,t',\Delta t) = \frac{1}{2}\frac{\Delta C_{i,j}(t,t')}{\Delta t}, \quad (20)$$

where

$$\Delta C_{i,j}(t,t') = \langle s_i(t)[s_j(t'+\Delta t) - s_j(t')]\rangle = \sum_{[s],[s'],[s'']} s_i(s'_j - s''_j)p([s],t|[s'],t'+\Delta t) \times p([s'],t'+\Delta t|[s''],t')p([s''],t'). \quad (21)$$

Therefore, putting together Eqs. (18) and (20) and taking the limit $\Delta t\to 0$ we obtain

$$TR_{i,j}(t,t') = \frac{1}{2}\frac{\partial C_{i,j}(t,t')}{\partial t'} - \frac{1}{2}\langle s_i(t)B_j(t')\rangle. \quad (22)$$

In order to bring this into the form of Eqs. (4) and (5), we notice that from Eqs. (9) and (12) follows

$$\frac{d\langle s_j(t)\rangle}{dt} = \sum_{[s]} s_j\frac{dp([s],t)}{dt} = -\sum_{[s]}\sum_{[s'']\neq[s]} s_j w^0([s]\to[s''])p([s],t) + \sum_{[s],[s']\neq[s]} s_j w^0([s']\to[s])p([s'],t). \quad (23)$$

Hence, after the change of variables $[s]\to[s''],[s']\to[s]$ in the second sum, one obtains

$$\frac{d\langle s_j(t)\rangle}{dt} = -\sum_{[s]}\sum_{[s'']\neq[s]}(s_j - s''_j)w^0([s]\to[s''])p([s],t) = \langle B_j(t)\rangle. \quad (24)$$

In a similar way, it is straightforward to derive

$$\frac{\partial C_{i,j}(t,t')}{\partial t} - \langle B_i(t)s_j(t')\rangle = 0 \quad (25)$$

and subtracting this from Eq. (22) we finally find

$$TR_{i,j}(t,t') = \frac{1}{2}\frac{\partial C_{i,j}(t,t')}{\partial t'} - \frac{1}{2}\frac{\partial C_{i,j}(t,t')}{\partial t} - A_{i,j}(t,t'), \quad (26)$$

where $A_{i,j}(t,t')$ is given by

$$A_{i,j}(t,t') = \frac{1}{2}[\langle s_i(t)B_j(t')\rangle - \langle B_i(t)s_j(t')\rangle]. \quad (27)$$

Equations (26) and (27) are the main result of this paper. They are identical to Eqs. (4) and (5) for Langevin dynamics, since the observable B entering in the asymmetries (5) and (27) plays the same role in the two cases. In fact, Eq. (24) is the analog of

$$\frac{\partial\langle\phi(\vec{x},t)\rangle}{\partial t} = \langle B(\phi(\vec{x},t))\rangle \quad (28)$$

obtained from Eq. (2) after averaging over the noise.

In summary, Eq. (26) is a relation between the response function and correlation functions of the unperturbed kinetics, which generalizes the FDT. Furthermore, Eq. (26) applies to a wide class of systems. In addition to being obeyed by soft and hard spins, it holds both for COP and NCOP dynamics. Moreover, as is clear by its derivation, Eq. (26) does not require any particular assumption on the Hamiltonian nor on the form of the unperturbed transition rates.

III. DYNAMICS IN DISCRETE TIME: THE NUMERICAL ALGORITHM

We now discuss the numerical implementation of the fluctuation dissipation relation derived above, as a method to compute the response function without imposing the external magnetic field (6). Let us recall that Eq. (22) was obtained letting $\Delta t\to 0$

$$TR_{i,j}(t,t') = \frac{1}{2}\lim_{\Delta t\to 0}\left[\frac{\Delta C_{i,j}(t,t')}{\Delta t} - \langle s_i(t-\Delta t)B_j(t')\rangle\right]. \quad (29)$$

In the simulations of an N-spin system, time is discretized by the elementary spin updates. Measuring time in Monte Carlo steps, the smallest available time $\epsilon=1/N$ is the one associated to a single update. Then, in discrete time, Eq. (29) reads

$$TR_{i,j}(t,t') = \frac{1}{2}\frac{C_{i,j}(t,t'+\epsilon) - C_{i,j}(t,t')}{\epsilon} - \frac{1}{2}\langle s_i(t-\epsilon)B_j(t')\rangle \tag{30}$$

and we use this for the numerical calculation of the response function. For completeness we also give the expression for the integrated response function

$$\chi_{i,j}(t,[\bar{t},t_w]) = \int_{t_w}^{\bar{t}} R_{i,j}(t,t')dt', \tag{31}$$

which correspond to the application of a constant field between the times t_w and $\bar{t}$. From Eq. (30) we have

$$T\chi_{i,j}(t,[\bar{t},t_w]) = T\epsilon\sum_{t'=t_w}^{\bar{t}} R_{i,j}(t,t') = \frac{1}{2}[C_{i,j}(t,\bar{t}) - C_{i,j}(t,t_w)] - \frac{\epsilon}{2}\sum_{t'=t_w}^{\bar{t}} \langle s_i(t-\epsilon)B_j(t')\rangle, \tag{32}$$

where $t-\epsilon \geqslant \bar{t} > t_w \geqslant 0$ and $\Sigma_{t'=t_w}^{\bar{t}}$ stands for the sum over the discrete times in the interval $[t_w,\bar{t}]$.

IV. COMPARISON WITH DIFFERENT ALGORITHMS

Expressions for the response function in a discretized time dynamics have been derived previously by Chatelain [2] and Ricci-Tersenghi [3]. Restricting to transition rates of the heat-bath form and to the case of single flip dynamics they have obtained

$$T\chi_{i,j}(t,[\bar{t},t_w]) = \sum_{I(\bar{t},t_w)}\sum_{\tau=t_w}^{\bar{t}} \delta_{j,I(\tau)}\langle s_i(t)[s_j(\tau) - s_j^W(\tau)]\rangle_{I(\bar{t},t_w)}, \tag{33}$$

where $I(\tau)$ is the index of the site updated at the discrete time τ, $I(\bar{t},t_w)$ is a specific sequence of $I(\tau)$'s between the times t_w, and $\bar{t}$, $s_j^W(\tau)=\tanh[\beta h_j^W(\tau)]$ and $h_j^W(\tau)$ is the local field due to the spins interacting with s_j.

It is important to stress the differences between Eqs. (33) and (32). Although in the right-hand-side (RHS) of Eq. (33) there appears an unperturbed correlation function, this is computed in the *ad hoc* kinetic rule introduced for the purpose of evaluating the response function. In Eq. (32), instead, the average in the RHS is computed in the true unperturbed dynamics of the system. This important difference arises because of the presence of the delta function $\delta_{j,I(\tau)}$ in Eq. (33), which constrains to update at the time τ only the spin at the site j, where the external field is applied. Then, in the averaging procedure, only the subset of dynamical trajectories with $I(\tau)=j$ are considered, while all the others get zero statistical weight, which is not what happens in the true unperturbed dynamics. Equation (33), therefore, although useful for the computation of the response function, is operatively restricted to a numerical protocol with a sequential updating satisfying the constraint imposed by the delta function $\delta_{j,I(\tau)}$. The correlations functions appearing in this equation cannot be extracted numerically from the behavior of the original unperturbed system, and cannot be accessed in an experiment.

Another difference between Eq. (33) and Eq. (32) concerns the choice of $M([s],[s'])$. Our results are obtained with $M([s],[s'])=0$. Instead, Eq. (33) corresponds to $M([s],[s'])\neq 0$. In fact, Eq. (33) assumes heat bath transition rates $w([s]\to[s'])=\{\exp[-\mathcal{H}[s']/T]\}/\{\exp[-\mathcal{H}[s]/T]+\exp[-\mathcal{H}[s']/T]\}$; expanding this expression to first order in powers of h/T, and comparing with Eq. (13), one has

$$M([s],[s']) = \frac{h_j}{2T}(s_j' - s_j)\frac{e^{\mathcal{H}[s']/T} - e^{\mathcal{H}[s]/T}}{e^{\mathcal{H}[s']/T} + e^{\mathcal{H}[s]/T}}. \tag{34}$$

Retaining $M([s],[s'])$ in Eq. (13) and following the same steps as for $M([s],[s'])=0$, one finds the extra term

$$\Delta R(t,t') = \frac{T}{h_j}\sum_{[s],[s'],[s'']} s_i p([s],t|[s'],t') \times M([s'],[s''])[w^0([s''] \to [s'])\times p([s''],t') - w^0([s'] \to [s''])p([s'],t')] \tag{35}$$

in addition to the quantities already present on the RHS of Eq. (26). This term cannot be related to correlation functions. It is generally believed that the large-scale–long-time properties of the dynamics (perturbed or not) do not depend too much, within a given universality class, on the form of the transition rates. Then one expects the corrections $\Delta R(t,t')$ introduced by different choices of $M([s],[s'])$ to be negligible. Indeed, as will be shown in Secs. V and VI, numerical results obtained for the Ising model in $d=1,2$ with the two algorithms are not sensitive to the choice of $M([s],[s'])$.

V. RESPONSE FUNCTION OF THE ISING CHAIN

As an application of the numerical method, we compute the autoresponse function $R(t,t')=R_{i,i}(t,t')$ in the $d=1$ Ising model, with and without conservation of the order parameter. We consider the system prepared in the infinite temperature equilibrium state and quenched to the finite temperature $T>0$ at the time $t=0$. Since the critical temperature vanishes for $d=1$, the final correlation length $\xi_{\rm eq}$ is finite and equilibrium is reached in a finite time $\tau_{\rm eq}\sim\xi_{\rm eq}^z$, where z is the dynamic exponent. For deep quenches $\tau_{\rm eq}$ is large and, after a characteristic time $t_{\rm sc}$, a well defined nonequilibrium scaling regime sets in for $t_{\rm sc}<t<\tau_{\rm eq}$, characterized by the growth of the domains with a typical size $L(t)\sim t^{1/z}$. We study the scaling properties of the response function $R(t,t')$ when both t and t' belong to the scaling regime.

A. Nonconserved dynamics

The linear response function in the model with single spin flip dynamics has been computed analytically [8–10]. This case, therefore, is useful as a test for the accuracy of the

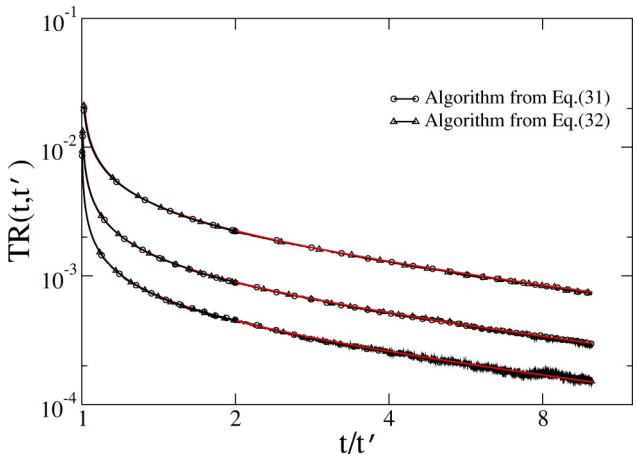

FIG. 1. $R(t,t')$ in the $d=1$ Ising model with NCOP, $T=0.3J$, and $J=1$. The number of spins is $N=10^4$, $t'=100$, 250, 500, (MCS) from top to bottom. Data from different algorithms correspond to different symbols. Continuous curves are the plots of Eq. (36).

algorithm. In the aging regime $t' \leqslant t \leqslant \tau_{\rm eq}$ the autoresponse function $R(t,t')$ is given by [9]

$$TR(t,t') = e^{-(t-t')} I_0(t-t') e^{-2t'} [I_0(2t') + I_1(2t')], \quad (36)$$

where $I_n(x)$ are the modified Bessel functions.

In order to improve the signal to noise ratio, we have extracted $R(t,t')$ from the integrated autoresponse function $\chi(t,[t'+\delta,t'])$ by choosing δ in the following way. Expanding for small δ we have

$$\frac{\chi(t,[t'+\delta,t'])}{\delta} \simeq R(t,t') + \frac{\delta}{2}\frac{\partial R(t,t')}{\partial t'}, \quad (37)$$

then, for a given level of accuracy, $R(t,t')$ can be obtained from $\chi(t,[t'+\delta,t'])/\delta$ if δ is chosen appropriately small. Notice that, assuming scaling $R(t,t')=t^{-(a+1)}f(t'/t)$, from Eq. (37) one has that, for a given value of $x=t'/t$, the second term on the RHS produces a relative correction $\Delta R(t,t')/R(t,t')=(1/2)[f'(x)/f(x)](\delta/t)$ of order δ/t. In our simulations we have chosen $\delta=1$ and, since the simulated times are $t \geqslant 100$, we have always $\delta/t \leqslant 10^{-2}$. In the following it is understood that all numerical results for $R(t,t')$ are obtained in this way.

In Fig. 1 we compare the numerical results obtained by means of the algorithm (32), for three different values of t', with the exact solution (36). We have also plotted the data obtained using the algorithm (33) of Ricci-Tersenghi [3], finding an excellent agreement between the curves generated by the different algorithms and the analytical expression (36).

The physical meaning of the exact solution can be understood by replacing Eq. (36) with the simple interpolating formula

$$TR(t,t') = A_z t'^{-1/z}(t-t'+t_0)^{1/z-1} \quad (38)$$

obtained by replacing the Bessel functions with the dominant term in the asymptotic expansion and by inserting t_0 as a regularization of $R(t,t')$ at equal times. For NCOP $z=2$. With $A_2=1/(\sqrt{2}\pi)$ and $t_0=1/(2\pi)$ the simple algebraic form (38) gives a very good approximation of the exact solution all over the time domain, from short to large time separations. Rewriting Eq. (38) as

$$TR(t,t') \sim L(t')^{-1} TR_{\rm sing}(t-t'), \quad (39)$$

where

$$TR_{\rm sing}(t-t') = A_z(t-t')^{1/z-1} \quad (40)$$

the physical meaning becomes clear, since $L(t')^{-1}$ is proportional to the density of defects $\rho(t')$ at time t', and $R_{\rm sing}(t-t')$ can be interpreted as the response associated to a single defect. In other words, Eq. (39) means that the total response is given by the contribution of a single defect times the density of defects at the time t'. As a matter of fact, Eqs. (39) and (40) are the particular realization of a general pattern for the aging part of the response function [11]

$$R(t,t') \sim L(t')^{-1} R_{\rm sing}(t-t') f(t/t'). \quad (41)$$

The presence of the scaling function $f(t/t')$ in Eq. (41) for $d>1$ can be explained as follows: in $d=1$ interfaces are pointlike and the interaction between them always produces annihilation. This is accounted for by the defect density $L(t')^{-1}$, so $f(t/t') \equiv 1$. In higher dimension, however, defects are extended objects whose interaction can produce a wealth of different situations, which are globally described by a suitable scaling function $f(t/t')$.

B. Conserved dynamics

The generality of the structure of Eqs. (39) and (40) may soon be tested by looking at the response function in the Ising chain with COP dynamics. While for NCOP the system enters the scaling regime almost immediately, since $t_{\rm sc} \simeq 1$, for COP the time $t_{\rm sc}$ for the onset of the scaling regime is of the order of the characteristic time $\tau_{\rm ev} \sim \exp(4J/T)$ for the separation (evaporation) of a spin from the boundary of a domain. The equilibration time, instead, is given by $\tau_{\rm eq} \sim \exp(10J/T)$ [12]. In order to have a large scaling regime, namely, $\tau_{\rm eq} \gg t_{\rm sc}$, it is necessary to take $T/J \ll 1$, and to choose $t_w > t_{\rm sc}$. Simulations of the system in these conditions are excessively time demanding with a conventional Monte Carlo algorithm. Therefore we have resorted to the fast algorithm of Bortz, Kalos, and Lebowitz [13], which is much more efficient at low temperatures. With a conventional algorithm a number of attempts proportional to $\tau_{\rm ev}$ is necessary on average before the evaporation of a spin from a domain occurs. Then, at low temperatures, a huge amount of attempted moves are rejected, causing a very low efficiency. The algorithm of Bortz, Kalos, and Lebowitz, instead, is rejection free: moves are always accepted and time is increased proportionally to the inverse probability associated with them. We stress that this is not an approximate kinetics, but a clever implementation of the exact dynamics.

From the unperturbed system the response function is extracted through Eq. (32), as in the case of NCOP. About the choice of δ, for COP the simulated times are $t \geqslant 10^7$ and we can have $\delta/t \leqslant 10^{-2}$, as required for the correction term in

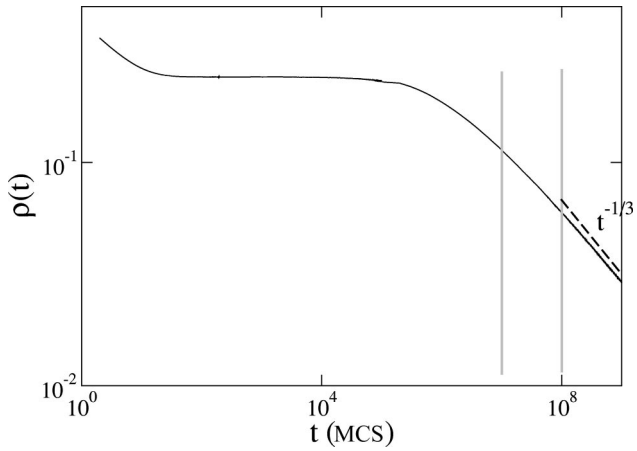

FIG. 2. $\rho(t)$ in the $d=1$ Ising model with COP, $T=0.3J$ and $J=1$. The number of spins is $N=10^4$. The range of time used in the simulations for the computation of the response function is in between the vertical lines. The dashed line represents the asymptotic law $\rho(t)\sim t^{-1/3}$.

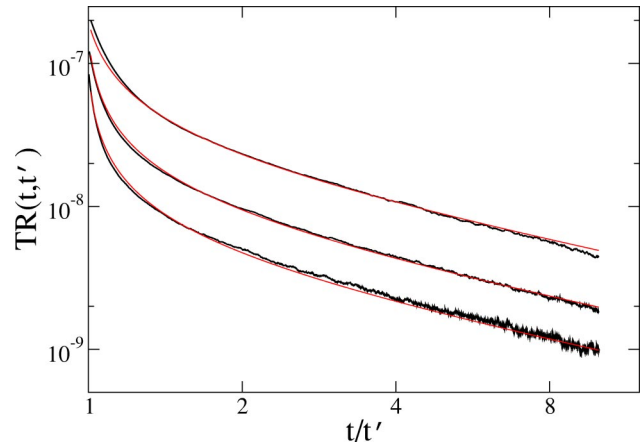

FIG. 3. $R(t,t')$ in the $d=1$ Ising model with COP, $T=0.3J$ and $J=1$. The number of spins is $N=10^4$, $t'=10^7$, 2.5×10^7, 5×10^7 (MCS) from top to bottom. Continuous curves are the plots of Eqs. (39) and (40). Fitting parameters are $A_3=0.24$, $t_0=5\times10^5$.

Eq. (37) to be negligible, with $\delta=10^5$. We have performed simulations with $T=0.3J$, corresponding to $t_{sc}\simeq6\times10^5$ and $\tau_{eq}\simeq3\times10^{14}$. In these conditions the scaling regime is very large. Actually, after a very narrow initial regime, where single spins diffuse until they are adsorbed on an interface, no evaporations occur and the system is frozen up to times of order τ_{ev}. In this time regime the density of defects $\rho(t)$ stays constant, as shown in Fig. 2. Then, for $t\gtrsim\tau_{ev}$, the evaporation-condensation mechanism takes place and the systems gradually enters the scaling regime. The range of times explored for the computation of the response function is shown in Fig. 2. This has been chosen as a compromise between the necessity to go to the largest accessible times, in order to work well inside the scaling regime, and to speed up the simulation to have a good statistics. For COP, the observation of the asymptotic behavior $\rho(t)\sim t^{1/z}$, with $z=3$, requires very large time [14]. In the range of times explored for the computation of $R(t,t')$ the effective exponent $z_{eff}=-[d\ln\rho(t)/d\ln t]^{-1}$ has reached the value $z_{eff}=3.44$.

We have plotted in Fig. 3 the numerical data for $R(t,t')$ together with the curves obtained from the analytical form (38), where we have substituted for z the above value of z_{eff} and we have used A_3 and t_0 as fitting parameters. The comparison is good and suggests that the physical interpretation, behind the form (39) and (40) of the response function, applies also to the $d=1$ Ising model with spin exchange dynamics [15]. We expect the more general form (41) to hold in higher dimension with COP.

VI. RESPONSE FUNCTION OF THE $D=2$ ISING MODEL

As a further application of the numerical method, we compute the zero field cooled (ZFC) magnetization $\chi(t,t_w)=\chi(t,[t,t_w])$ in the $d=2$ Ising model with NCOP, quenched from the infinite temperature equilibrium state to a temperature below T_c. This quantity has already been measured both by applying the perturbation [11,16–18] or by means of the algorithm of Ricci-Tersenghi [3]. In Fig. 4 we compare results obtained with our method and with that of Ricci-Tersenghi, for several values of t_w in the scaling regime. The agreement between the two algorithms is excellent also in this case. The equivalence of the two algorithms both in $d=1$ and in $d=2$ suggests, recalling the discussion at the end of Sec. IV, that different choices of $M([s],[s'])$ do not produce significant differences.

Let us comment on the behavior of $\chi(t,t_w)$. As it is well known, in the late stage of phase-ordering the interior of the growing domains is equilibrated, while interfaces are out of equilibrium. Then, a distinction can be made between bulk and interface fluctuations. Accordingly, for the ZFC one has [21–23]

$$\chi(t,t_w)=\chi_{st}(t,t_w)+\chi_{ag}(t,t_w). \tag{42}$$

Here $\chi_{st}(t,t_w)$ is the contribution from the bulk of domains, which behaves as the equilibrium response $\chi_{eq}(t,t_w)$ in the

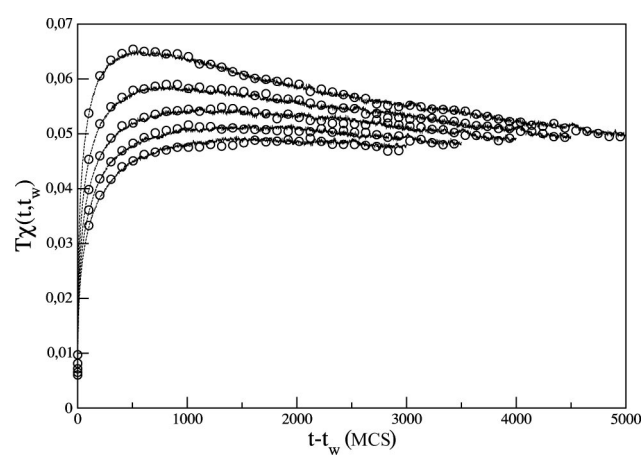

FIG. 4. $\chi(t,t_w)$ in the $d=2$ Ising model with NCOP, $T=J=1$. The number of spins is $N=1600^2$, $t_w=1\times10^3$, $t_w=1.5\times10^3$, $t_w=2\times10^3$, $t_w=2.5\times10^3$, $t_w=3\times10^3$, from top to bottom. Circles represent data obtained with the algorithm of Eq. (32), continuous lines are the results with the Ricci-Tersenghi method (33).

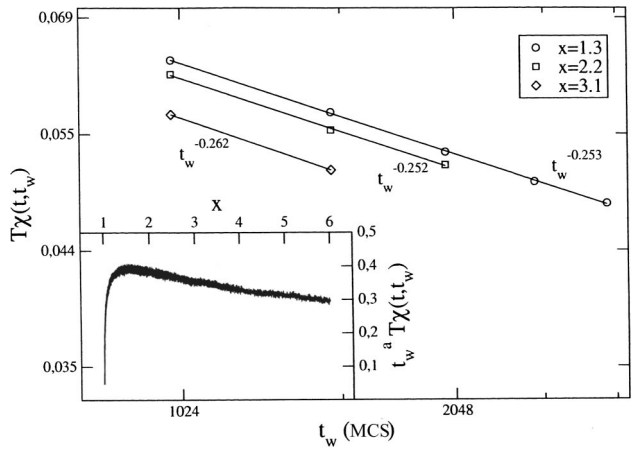

FIG. 5. The same data of Fig. 4 obtained with the algorithm of Eq. (32) plotted for fixed values of x against t_w. Straight lines are power law best fits. In the inset the data collapse for $t_w^a\chi(t,t_w)$, with $a=0.26$, is shown.

ordered state at the temperature T. This quantity, starting from zero at $t=t_w$, saturates to the value $1-M^2$, M being the equilibrium magnetization. The other term appearing in Eq. (42), namely, the additional aging contribution due to the interfaces, is much less known. It is expected to scale as

$$\chi_{\rm ag}(t,t_w) = t_w^{-a} f\left(\frac{t}{t_w}\right). \tag{43}$$

In previous studies [11,17,18], an auxiliary dynamics, which prevents flips in the bulk, was used in order to extract the aging part of the response in Eq. (42). Here, instead, we have chosen a different technique to isolate $\chi_{\rm ag}(t,t_w)$: We compute the full $\chi(t,t_w)$ in the Glauber dynamics working at a sufficiently low temperature where $\chi_{\rm st}(t,t_w)$ is negligible. In fact, by choosing $T=J$, the asymptotic value of $\chi_{\rm st}(t,t_w)$ is $1-M^2\simeq 0.0014$, much smaller than the computed values of $\chi(t,t_w)$ in the range of times considered. Then one has $\chi(t,t_w)\simeq\chi_{\rm ag}(t,t_w)$.

In addition to this difference, previous results [11,17,18] on $\chi_{\rm ag}(t,t_w)$ were obtained with the usual method where a perturbation is applied. The strength h of the perturbation must be chosen sufficiently small to work in the linear regime. However, by reducing h the signal to noise ratio lowers, and the results get worst. Then one usually runs a series of preliminary simulations in order to determine the largest value of h compatible with the requisite of working in the linear regime. While this point may be subtle, in the result presented in this paper the limit $h\to 0$ is taken analytically in the derivation of the algorithm.

We have extracted a from the data of Fig. 4 by plotting $\chi(t,t_w)$ against t_w with $x=t/t_w$ held fixed. The results are shown on a double logarithmic plot in Fig. 5. According to the scaling form (43), for different values of x the data must align on straight lines with the same slope a. This is very well compatible with the curves of Fig. 5, indicating that scaling is obeyed. Computing a as the slope of these curves we find $a=0.26\pm 0.01$. This result agrees very well with the value found in Refs. [11,17,18]. Once this exponent is known, one obtains data collapse by plotting $t_w^a\chi(t,t_w)$ against x, as shown in the inset of Fig. 5, confirming the validity of the scaling form (43).

VII. CONCLUDING REMARKS

In this paper we have derived a generalization of the FDT out of equilibrium for systems of Ising spins, which takes exactly the same form of the FDT generalization previously derived [1] for soft spins, evolving with Langevin dynamics. We have shown that this fluctuation dissipation relation, which reduces to the usual FDT when equilibrium is reached, is obeyed in complete generality both by systems with COP and NCOP. In addition to the theoretical interest, as a contribution to the understanding of the FDT in the out of equilibrium regime, our result is also promising as a convenient tool for the computation of the linear response function in numerical simulations without applying the perturbation, along the lines of Refs. [2,3]. With standard methods, the requirement to work in the linear regime, namely, with an adequately small perturbation, sometimes is very subtle and hard to be checked. This problem is avoided by this new class of algorithms. Moreover, the statistical accuracy of the results is, for comparable CPU times, much better because simulations of perturbed systems usually require additional statistical averages over realizations of the (random) perturbation. We have demonstrated the high quality of the results produced by our algorithm by computing the response function of the Ising model in $d=1$ and the integrated response function in $d=2$. In $d=2$ our results agree with those obtained with the algorithm of Ref. [3] and with previous simulations performed applying the perturbation. We confirm that $\chi(t,t_w)$ obeys a scaling form (43) with $a=0.26\pm 0.01$, in agreement with previous determinations [11,17,18] of this exponent. In $d=1$, for NCOP our results are in excellent agreement with the exact analytical solution and with the simulation made with the algorithm of Ref. [3]. In the case of COP, where no analytical solution is available, we have obtained results which substantiate the existence of the common structure (39) and (40) of the response function for COP and NCOP. These results show that the algorithm is efficient enough to give access to the direct measurement of the impulsive response function $R(t,t')$, which is too noisy to be computed with standard methods. For this reason, previous numerical studies [11,16,19,20] have been necessarily directed to the investigation of the integrated response functions, such as the thermoremanent magnetization or the zero field cooled magnetization, which are easier to compute. However, as discussed in detail in Ref. [11], it is quite a delicate task to extract the properties of $R(t,t')$ from those of the integrated response functions. Therefore, the feasibility of direct computations of $R(t,t')$ is an important development in the field, which is expected to solve a number of problems still open [11] on the scaling behavior of $R(t,t')$ for $d>1$.

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APPENDIX A

Let us write the Langevin equation in the general form

$$\frac{\partial\phi(\vec{x},t)}{\partial t} = (i\vec{\nabla})^p[B(\phi(\vec{x},t)) + h(\vec{x},t)] + \eta(\vec{x},t), \qquad \text{(A1)}$$

where $h(\vec{x},t)$ is the external field conjugated to the order parameter, $p=0$ or $p=2$ for NCOP or COP, respectively, and the noise correlator is given by

$$\langle \eta(\vec{x},t)\eta(\vec{x}',t')\rangle = (i\vec{\nabla})^p 2T\delta(\vec{x}-\vec{x}')\delta(t-t'). \qquad \text{(A2)}$$

Fourier transforming with respect to space, these become

$$\frac{\partial\phi(\vec{k},t)}{\partial t} = k^p[\mathcal{B}([\phi],\vec{k},t) + h(\vec{k},t)] + \eta(\vec{k},t) \qquad \text{(A3)}$$

and

$$\langle \eta(\vec{k},t)\eta(\vec{k}',t')\rangle = 2Tk^p(2\pi)^d\delta(\vec{k}+\vec{k}')\delta(t-t'), \qquad \text{(A4)}$$

where $\mathcal{B}([\phi],\vec{k},t)$ is the Fourier transform of $B(\phi(\vec{x},t))$.

The linear response function is defined by

$$R(\vec{k},t,\vec{k}',t') = \left.\frac{\delta\langle\phi(\vec{k},t)\rangle_h}{\delta h(\vec{k}',t')}\right|_{h=0} \qquad \text{(A5)}$$

with $t \geqslant t'$. Notice that, since $\eta(\vec{k},t)$ and $k^p h(\vec{k},t)$ enter the equation of motion (A3) in the same way, we have

$$\left\langle \frac{\delta\phi(\vec{k},t)}{\delta\eta(\vec{k}',t')}\right\rangle = \frac{1}{k'^p}\left.\frac{\delta\langle\phi(\vec{k},t)\rangle_h}{\delta h(\vec{k}',t')}\right|_{h=0}, \qquad \text{(A6)}$$

where $\langle\cdots\rangle$ denotes averages in absence of the external field. Then, using the identity [24]

$$\langle\phi(\vec{k},t)\eta(\vec{k}',t')\rangle = 2Tk'^p\left\langle\frac{\delta\phi(\vec{k},t)}{\delta\eta(\vec{k}',t')}\right\rangle, \qquad \text{(A7)}$$

we find

$$2TR(\vec{k},t,\vec{k}',t') = \langle\phi(\vec{k},t)\eta(\vec{k}',t')\rangle \qquad \text{(A8)}$$

or in real space

$$2TR(\vec{x},t,\vec{x}',t') = \langle\phi(\vec{x},t)\eta(\vec{x}',t')\rangle \qquad \text{(A9)}$$

showing that Eq. (3) holds in the same form for NCOP and COP.

APPENDIX B

The transition rates, with and without the external field, satisfy the detailed balance condition (11). Writing $w^h([s]\to[s'])=w^0([s]\to[s'])\Delta w([s]\to[s'])$ and $\mathcal{H}^h[s]=\mathcal{H}^0[s]+\Delta\mathcal{H}[s]$, from Eq. (11) follows

$$\Delta w([s]\to[s'])\exp\left[-\frac{\Delta\mathcal{H}[s]}{T}\right] = \Delta w([s']\to[s])\exp\left[-\frac{\Delta\mathcal{H}[s']}{T}\right]. \qquad \text{(B1)}$$

Using $\Delta\mathcal{H}[s]=-s_j h_j$, Eq. (B1) is satisfied by $\Delta w([s]\to[s'])=\exp\{-[1/(2T)]h_j(s_j-s_j')\}$ up to a factor $\mathcal{M}([s],[s'])$ which satisfies $\mathcal{M}([s],[s'])=\mathcal{M}([s'],[s])$. Therefore, the most general form of the perturbed transition rates, compatible with detailed balance, is given by

$$\Delta w([s]\to[s']) = \exp\left[-\frac{1}{2T}h_j(s_j-s_j')\right]\mathcal{M}([s],[s']). \qquad \text{(B2)}$$

For $h=0$ the condition $\Delta w([s]\to[s'])=1$ implies $\mathcal{M}([s],[s'])=1$. Therefore, to linear order in the perturbation one has $\mathcal{M}([s],[s'])\simeq 1+M([s],[s'])$. Inserting this result in Eq. (B2), and expanding also the exponential term, to linear order in h/T one obtains Eq. (13).

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Tersenghi, J. Stat. Mech.: Theory Exp. **2004**, P04007 have shown that the parametric plot of $\chi(t,[t,t_w])$ versus $C(t,t_w)$ is slightly different between dynamics with COP and NCOP. Here we make a different statement. Our data support the fact that both dynamical rules produce the same form (39) and (40) of the response. This does not imply that the parametric plot $\chi(C)$ is the same. In particular, a different numerical value of the coefficient A_z and a different form of the autocorrelation function in the two cases may produce a different $\chi(C)$.

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