Reply to "Comment on 'Fluctuation-dissipation relations in the nonequilibrium critical dynamics of Ising models' "

Peter Mayer,[1] Ludovic Berthier,[2,3] Juan P. Garrahan,[2,4] and Peter Sollich[1]
[1]*Department of Mathematics, King's College, Strand, London, WC2R 2LS, United Kingdom*
[2]*Theoretical Physics, University of Oxford, 1 Keble Road, Oxford, OX1 3NP, United Kingdom*
[3]*Laboratoire des Verres, Université Montpellier II, 34095 Montpellier, France*
[4]*School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, United Kingdom*
(Received 12 March 2004; published 2 July 2004)

We have recently shown that in nonequilibrium spin systems at criticality the limit X^∞ of the fluctuation-dissipation ratio $X(t,t_w)$ for $t \gg t_w \gg 1$ can be measured using observables such as magnetization or energy [Phys. Rev. E **68**, 016116 (2003)]. Pleimling argues in a Comment [preceding paper, Phys. Rev. **70**, 018101 (2004)] on our paper that for such observables correlation and response functions are dominated by one-time quantities dependent only on t, and are therefore not suitable for a determination of X^∞. Using standard scaling forms of correlation and response functions, as used by Pleimling, we show that our data do have a genuine two-time dependence and allow $X(t,t_w)$ and X^∞ to be measured, so that Pleimling's criticisms are easily refuted. We also compare with predictions from renormalization-group calculations, which are consistent with our numerical observation of a fluctuation-dissipation plot for the magnetization that is very close to a straight line. A key point remains that coherent observables make measurements of X^∞ easier than the traditionally used incoherent ones, producing fluctuation-dissipation plots whose slope is close to X^∞ over a much larger range.

DOI: 10.1103/PhysRevE.70.018102 PACS number(s): 05.70.Ln, 75.40.Gb, 75.40.Mg

In our recent paper [1] we analyzed out-of-equilibrium fluctuation-dissipation (FD) relations in ferromagnetic spin systems quenched to criticality. One measures a response at time t to a perturbation at an earlier time t_w, the waiting time, and compares with the corresponding two-time correlation. The FD ratio (FDR), $X(t,t_w)$, then captures how much the response deviates from what would be expected in equilibrium. In many situations, T/X can be thought of as an effective temperature $T_{\rm eff}$ governing the out-of-equilibrium dynamics [2]. In the context of critical dynamics the role of the long-time limit value X^∞ of $X(t,t_w)$ for $t \gg t_w \gg 1$ as a universal amplitude ratio has been emphasized, see e.g. [3].

Exact results in [1] for the $d=1$ case with $T_c=0$, showed that X^∞ is identical for all spin observables, whether one considers incoherent (short-range) observables or coherent (long-range) ones such as the total magnetization. For the coherent case, the limiting FD plot at long times is in fact a straight line, from which X^∞ can be determined trivially. Similar results were found for the case of bond observables, where the incoherent observable corresponds to an indicator for a local domain wall while the coherent observable is the total energy. X^∞ was again found to be identical for these observables. The advantage of using coherent observables is much more dramatic here: for the incoherent case the window in the FD plot where the slope is close to X^∞ shrinks to zero with increasing times, while for the coherent observable one finds again a straight line FD plot of slope X^∞. Numerical simulations in $d=2$ strongly suggested that these results carry over to higher dimensions. In particular, FD plots for both the magnetization and the energy were numerically indistinguishable from straight lines. We also found the resulting values for X^∞ to be equal within numerical error, suggesting that there may be a well-defined effective temperature $T_{\rm eff}$ for a broad range of observables.

In the preceding Comment [4], Pleimling argues that magnetization and energy are unsuitable for measuring X^∞ because their correlation and response functions are dominated by one-time contributions depending only on the measurement time t. We show in this Reply that Pleimling's remarks trivially apply in the regime $t \gg t_w$, but say nothing about the regime where t and t_w are of the same order. It is in this regime that our numerical data were taken, and so they do carry nontrivial two-time information. Pleimling also argues that our results are not supported by renormalization group (RG) calculations [5]. We show explicitly that the RG results are in agreement, predicting a limiting FD plot for the magnetization which is very close to a straight line.

We begin by reviewing the construction of the FD plots from which we determine $X(t,t_w)$, since Pleimling argues that the introduction of some one-time quantities render our plots unsuitable. Consider a connected two-time correlation function $C(t,t_w)=\langle A(t)B(t_w)\rangle - \langle A(t)\rangle\langle B(t_w)\rangle$, with A, B two observables, and the conjugate response $R(t,t_w) = T\delta\langle A(t)\rangle / \delta h_B(t_w)|_{h_B=0}$. Here h_B is the field thermodynamically conjugated to B and a factor of T has been included in the response. The nonequilibrium FDR $X(t,t_w)$ is defined via

$$R(t,t_w) = X(t,t_w)\frac{\partial}{\partial t_w}C(t,t_w). \tag{1}$$

This relation can be cast in terms of the step response $\chi(t,t_w)=\int_{t_w}^{t} dt' R(t,t')$, i.e., the response to a field h_B switched on at t_w and kept constant since:

$$\frac{\partial}{\partial t_w}\chi(t,t_w) = -R(t,t_w)$$
$$= -X(t,t_w)\frac{\partial}{\partial t_w}C(t,t_w)$$
$$= X(t,t_w)\frac{\partial}{\partial t_w}[C(t,t) - C(t,t_w)]. \qquad (2)$$

Two things are important to note. First, the correlation $C(t,t_w)$ is a connected one, see the definition above. Second, it is physically sensible to compare the integrated response $\chi(t,t_w)=\int_{t_w}^{t} dt' R(t,t')$ to the integral $\int_{t_w}^{t} dt'(\partial/\partial t')C(t,t') = C(t,t)-C(t,t_w) \equiv \Delta C(t,t_w)$, rather than just to $C(t,t_w)$. These observations are irrelevant in the usual situation of incoherent spin observables, for which one-time correlations are constant, but are important in our case where they do change in time (a situation sometimes referred to as physical aging). This point is discussed in detail in Refs. [1,6–8].

From (2) it follows that a parametric plot of $\chi(t,t_w)$ versus $\Delta C(t,t_w)$ has slope $X(t,t_w)$. This is obvious if t_w is varied along the curve while t is held fixed. However, if a series of such plots converges to a limit plot for $t\to\infty$, then this limit plot and its slope X can clearly be obtained by varying either t_w or t, as long as both times are large. For shorter times or if no limit plot exists, plots where t is varied and t_w is fixed will not in general have a slope related to X, whether one plots $\chi(t,t_w)$ versus $C(t,t_w)$ or versus $\Delta C(t,t_w)$. However, in the simple case where $X(t,t_w)$ is constant, one has from (2) that $\chi(t,t_w)=X\Delta C(t,t_w)$, so that a $(\Delta C,\chi)$-plot does have the correct slope. A (C,χ)-plot does not, on the other hand, since $(\partial\chi/\partial t)(t,t_w)=X(d/dt)C(t,t)-X(\partial C/\partial t)(t,t_w) \neq -X(\partial C/\partial t)(t,t_w)$. This lends further support to our choice of plotting χ versus ΔC rather than C [9].

For systems where $C(t,t)$ does not converge for $t\to\infty$ it is convenient to consider normalized functions $\tilde{\chi}(t,t_w) = \chi(t,t_w)/C(t,t)$ and $\tilde{C}(t,t_w)=C(t,t_w)/C(t,t)$ [1,6,8]. According to (2) these are also linked by

$$\frac{\partial}{\partial t_w}\tilde{\chi}(t,t_w) = X(t,t_w)\frac{\partial}{\partial t_w}[1-\tilde{C}(t,t_w)]. \qquad (3)$$

Again, X is the slope of a plot of $\tilde{\chi}$ versus $1-\tilde{C}$. If a limit plot is approached for large times, either t or t_w can be varied to obtain this plot. Explicitly, if for large times X depends on t and t_w only through $\tilde{C}(t,t_w)$, the shape of the limit plot follows by integration of (3) as

$$\tilde{\chi}(t,t_w) = \int_{\tilde{C}(t,t_w)}^{1} d\tilde{C}X(\tilde{C}). \qquad (4)$$

In equilibrium $X(t,t_w)\equiv 1$ and one recovers the standard FDT relation $\tilde{\chi}(t,t_w)=1-\tilde{C}(t,t_w)$.

In [1], we showed FD plots for the total magnetization $M=\sum_i s_i$ (i.e., $A=B=M$ above) and energy $E=-\sum_{(ij)}s_i s_j$ for a $d=2$ system of Ising spins s_i quenched to its critical temperature. These were produced by varying t at several fixed t_w, and without normalization. While *a priori* the slope of the plot does then not necessarily correspond to X, the numerical data for $\chi(t,t_w)$ versus $C(t,t)-C(t,t_w)$ fall on a straight line. Normalization only shrinks both axes of the plot in a t-dependent manner. The normalized plots will thus have the same slope, as shown explicitly in Fig. 1. The data clearly point towards the existence of a limit plot for large times which must be very close to a straight line. The asymptotic FDR X^∞, which is obtained for $t \gg t_w \gg 1$, i.e., $\tilde{C}\to 0$, is the slope at the end point of the limit plot (see the sketch in Fig. 2). Our data do not reach this end point, but RG calculations (see below) show that the slope should remain constant on approaching it. X^∞ can therefore be determined from the slope in the central part of the plot (i.e., the regime $t \gtrsim t_w \gg 1$).

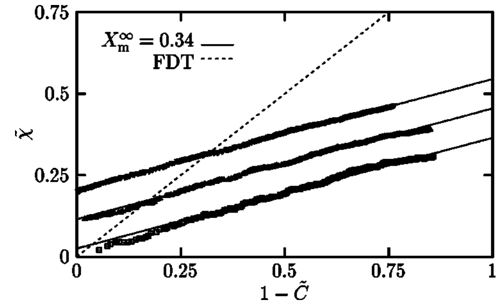

FIG. 1. Normalized FD plot for magnetization in the $d=2$ Ising model at T_c for times $t_w=46$, 193, and 720 (bottom to top). Curves have been vertically shifted by 0, 0.1, and 0.2 for clarity. The convergence for large t_w to an almost straight line of slope $X^\infty \approx 0.34$ is evident.

We now summarize the scaling relations used by Pleimling, taking as he did the case of the total magnetization as an example. For large times, one expects the two-time autocorrelation of M to scale as

$$C(t,t_w) = t_w^{a+1} f_C(t/t_w), \qquad (5)$$

with a expressed in terms of standard critical exponents as $a+1=(2-\eta)/z=(d-2\beta/\nu)/z$. The scaling function f_C decays as $f_C(r)\sim r^{\theta'}$ for large $r=t/t_w$ with $\theta'\approx 0.19$ for the $d=2$ Ising model; in the limit $r\to 1$, $f_C(r)$ has to tend to a

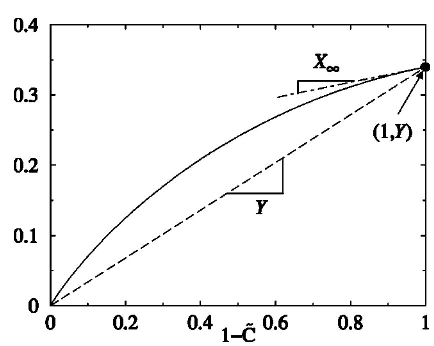

FIG. 2. Sketch of a limiting normalized FD plot (solid line). The asymptotic FDR X^∞ is the slope of the tangent at the top right end point of the plot (dotted-dashed). This end point is at $(1-\tilde{C},\tilde{\chi}) = (1,Y)$, where Y is the axis-ratio of the plot or, alternatively, the slope of the dashed line connecting the end point to the origin.

constant to have consistency with the scaling of the equal-time correlation $C(t,t)\sim t^{(d-2\beta/\nu)/z}=t^{a+1}$. A similar scaling relation holds for the response, $R(t,t_w)=t_w^a f_R(t/t_w)$. As a result, $X(t,t_w)$ becomes for large times a function of r [3]; this is confirmed by explicit RG calculations [5]. The normalized two-time correlation

$$\tilde{C}(t,t_w) = \frac{C(t,t_w)}{C(t,t)} = (t_w/t)^{a+1}\frac{f_C(t/t_w)}{f_C(1)}, \tag{6}$$

likewise only depends on $r=t/t_w$. Eliminating r, X can be expressed for large times as a function of $\tilde{C}$. As discussed above, it follows that a plot of $\tilde{\chi}$ versus $1-\tilde{C}$ must approach a limiting shape for large times; this is consistent with our numerical data in Fig. 1. Explicitly, if $\tilde{C}(r)$ and $X(r)$ are known then the limit plot is from (4)

$$\tilde{\chi}(\tilde{C}) = \int_1^{r(\tilde{C})} \mathrm{d}r\left(-\frac{\mathrm{d}\tilde{C}}{\mathrm{d}r}\right)X(r), \tag{7}$$

where $r(\tilde{C})$ is the inverse function of $\tilde{C}(r)$ and the minus arises because $\tilde{C}(r)$ is a decreasing function.

Pleimling deduces from (5) that, in the limit $t\to\infty$ at fixed t_w, $C(t,t)-C(t,t_w)\approx C(t,t)$ because $C(t,t_w)\ll C(t,t)$. This is correct, but not surprising. As stated above, one generically expects that $\tilde{C}(t,t_w)=C(t,t_w)/C(t,t)\to 0$ for $t\gg t_w$. On the other hand, from (6) one sees that $C(t,t_w)$ remains comparable to $C(t,t)$ as long as t and t_w are of the same order. The "rapid" approach of $C(t,t)-C(t,t_w)$ to $C(t,t)$ which Pleimling asserts thus actually occurs only for $t-t_w$ of order t_w, in agreement with the data in his Figs. 1 and 2. For the step response $\chi(t,t_w)$, Pleimling shows similarly that this becomes independent of t_w for $t\to\infty$ and grows with the same power law as $C(t,t)$, so that the ratio $\tilde{\chi}(t,t_w)=\chi(t,t_w)/C(t,t)$ approaches a constant which we shall call Y [10]. Summarizing, for $t\to\infty$ at fixed t_w, one has $\tilde{C}\to 0$ and $\tilde{\chi}\to Y$. Referring to Fig. 2, Pleimling's statements thus fix a single point on the limiting normalized FD plot, namely its "end point" on the right. Geometrically, Y is the axis ratio of the FD plot. It is important to stress that Pleimling's reasoning says nothing about the rest of the limiting FD plot, which corresponds to the time regime where t and t_w are of the same order: his limit $t\to\infty$ at fixed t_w always implies the assumption $t\gg t_w$. It is also clear from Fig. 2 that the axis ratio Y and the asymptotic slope X^∞ of the FD plot are not in general related.

Pleimling's criticism would apply if we had contrived only to collect data in the regime $t\gg t_w$. Such data would, in a normalized FD plot, fall very close to the plot's end point at $(1-\tilde{C},\tilde{\chi})=(1,Y)$. In an unnormalized plot, the t-dependent stretching of the plot by $C(t,t)$ would then indeed mean that the data trivially fall on a straight line. This line would be t_w-independent and have slope Y rather than X^∞. To check for such trivial behavior, it is sufficient to normalize the data as explained above. We re-emphasize that, as Fig. 1 shows, our data are not in the regime where such trivial behavior is expected, covering a wide range of values of $1-\tilde{C}$ and remaining well away from the end point of the plot. Our observation of a close-to-straight line FD plot is therefore not explained by scaling arguments, and remains highly nontrivial. This is transparent from Pleimling's own data [4]: one sees that his FD plots in Fig. 3 actually show data for which the t_w-dependence of $C(t,t)-C(t,t_w)$ (his Fig. 1) and $\chi(t,t_w)$ (his Fig. 2) is still significant. For example, for $t_w=46$ and $t=2t_w$, $\chi(t,t_w)$ is still significantly (around 30%) below $\chi(t,0)$ but the corresponding point in the FD plot is already on the t_w-independent straight line.

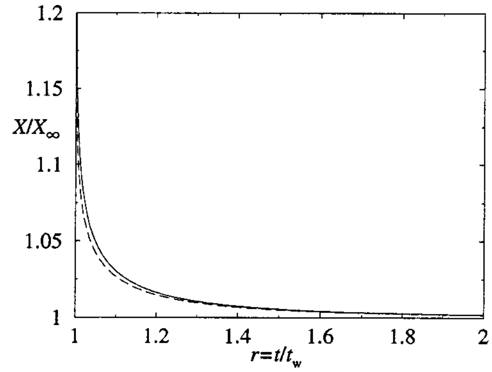

FIG. 3. RG predictions for $X(t,t_w)/X^\infty$ as a function of the time ratio $r=t/t_w$, for the two versions of the scaling functions $F=1+\epsilon^2\Delta F$ (solid line) and $F=\exp(\epsilon^2\Delta F)$ (dashed line). See text for details.

We now comment on Pleimling's statement that our numerical results are not supported by the RG calculations of [5]. These calculations give $X(t,t_w)$ as a function of the time ratio $r=t/t_w$ in the form

$$X(r) = X^\infty\frac{F_R(r)}{F_{\partial C}(r)}, \tag{8}$$

where F_R and $F_{\partial C}$ are appropriate scaling functions for $R(t,t_w)$ and $(\partial C/\partial t_w)(t,t_w)$, consistent with the definition (1). Both scaling functions are of the form $F(r)=1+\epsilon^2\Delta F(r)$, within a second-order expansion in $\epsilon=4-d$. The extrapolation to $d=2$, $\epsilon=2$ therefore has a certain arbitrariness. To $\mathcal{O}(\epsilon^2)$ in the RG calculation one could replace $F(r)$ by e.g., $\exp[\epsilon^2\Delta F(r)]$. We show both versions of the resulting RG predictions for $X(r)$ in Fig. 3. It is clear that $X(r)$ is close to X^∞ except for $r\approx 1$; where it does deviate, the RG predictions also become less reliable. The near-constancy of $X(r)$ already suggests that the FD plot will be almost straight.

To find the limiting normalized FD plot predicted by RG explicitly, we combined the RG result for the scaling function $F_{\partial C}(r)$ with the scaling exponents as quoted by Pleimling to obtain $\mathrm{d}\tilde{C}/\mathrm{d}r$ and then used (7). The result is shown in Fig. 4 and demonstrates that the RG calculations predict a limiting FD plot which is extremely close to a straight line. Quantitatively, the plot is shifted upwards from a straight line of slope X^∞ by no more than $0.01X^\infty$; its axis ratio Y therefore also lies no more than 1% above X^∞. Contrary to Pleimling's remark, our numerical data are therefore entirely consistent with RG calculations.

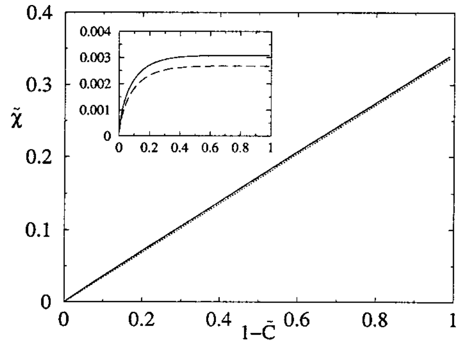

FIG. 4. RG prediction for long-time limit of the normalized FD plot for the magnetization. Two versions are shown (solid and dashed), corresponding to the two choices of scaling function from Fig. 3, but are indistinguishable by eye. Both are extremely close to a straight line of slope X^{∞} (dotted). To make the small differences visible, $\tilde{\chi}-X^{\infty}\tilde{C}$ is shown in the inset.

As a final point, we comment on our observation in [1] that the values of X^{∞} are, to within numerical accuracy, identical for the magnetization (a spin observable) and the energy (a bond observable). While this may be surprising from the point of view of nonequilibrium critical dynamics [11], it is natural if one thinks of $T_{\rm eff}=T_c/X^{\infty}$ as an effective temperature which should govern the long-time nonequilibrium critical dynamics of all (or at least a broad range of) observables. This is supported by an analysis of the spherical model, where the values of X^{∞} for spin and bond observables do indeed coincide. We will report on a more detailed investigation of this point in a future publication.

In summary, Pleimling's criticisms of our method of measuring X^{∞} using coherent observables do not apply. His reasoning only addresses the limit $t \gg t_w$, where the normalized correlation function $\tilde{C}(t,t_w)=C(t,t_w)/C(t,t)$ is negligibly small, while our data are taken in a regime where $\tilde{C}(t,t_w)$ is of order unity. This is most easily demonstrated using a normalized FD plot of $\chi(t,t_w)/C(t,t)$ versus $1-\tilde{C}(t,t_w)$. Our observation that, for the magnetization in the $d=2$ Ising model quenched to criticality, the normalized FD plot is close to a straight line therefore remains nontrivial, and is consistent with RG predictions.

There are two key conclusions of our original study [1] which we have emphasized throughout this reply. First, FD plots for coherent observables are able to reveal nontrivial two-time dependencies in nonequilibrium dynamics, and do so unambiguously when normalized. Second, FD plots for coherent observables typically have a wide range where their slope is close to the asymptotic value X^{∞}. For measurements of X^{∞} this makes them preferable to the traditionally used incoherent observables, where this range shrinks to zero for long times.

We are grateful to P. Calabrese for discussions. We acknowledge financial support from CNRS France, EPSRC Grant Nos. 00800822, GR/R83712/01, and GR/S54074/01, E.U. Marie Curie Grant No. HPMF-CT-2002-01927, the Glasstone Fund, Nuffield Grant No. NAL/00361/G, Österreichische Akademie der Wissenschaften, and Worcester College Oxford. Some of the numerical results were obtained on Oswell at the Oxford Supercomputing Center, Oxford University.

[1] P. Mayer, L. Berthier, J. P. Garrahan, and P. Sollich, Phys. Rev. E **68**, 016116 (2003).
[2] L. F. Cugliandolo, J. Kurchan, and L. Peliti, Phys. Rev. E **55**, 3898 (1997).
[3] C. Godrèche and J. M. Luck, J. Phys. A **33**, 9141 (2000).
[4] M. Pleimling, preceding paper, Phys. Rev. E **70**, 018101 (2004).
[5] P. Calabrese and A. Gambassi, Phys. Rev. E **66**, 066101 (2002).
[6] S. Fielding and P. Sollich, Phys. Rev. Lett. **88**, 050603 (2002).
[7] A. Buhot and J. P. Garrahan, Phys. Rev. Lett. **88**, 225702 (2002).
[8] P. Sollich, S. Fielding, and P. Mayer, J. Phys.: Condens. Matter **14**, 1683 (2002).
[9] When using *normalized* FD plots, the choice of ΔC vs C is immaterial, since $\Delta C(t,t_w)/C(t,t)=1-\tilde{C}(t,t_w)$ differs from $C(t,t_w)/C(t,t)=\tilde{C}(t,t_w)$ only by a constant.
[10] The limit $t\to\infty$ here has to be understood as taken *after* the zero-field limit $h\to 0$. As Pleimling discusses, if one considers instead a fixed nonzero field then the respponse eventually becomes nonlinear, on a time scale for t which diverges for $h\to 0$. While correct, this obsevation is irrelevant for the present discussion: we have checked carefully that all our data are taken in the time window where the response is linear, as Pleimling's Fig. 2 also confirms.
[11] RG calculations of X^{∞} for the energy are in progress for the $O(n)$ model in order to clarify this point [P. Calabrese (private communication)].