Interface fluctuations, bulk fluctuations and dimensionality in the off-equilibrium response of coarsening systems

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Abstract

The relationship between statics and dynamics proposed by Franz, Mezard, Parisi and Peliti (FMPP) for slowly relaxing systems [Phys.Rev.Lett. **81**, 1758 (1998)] is investigated in the framework of non disordered coarsening systems. Separating the bulk from interface response we find that for statics to be retrievable from dynamics the interface contribution must be asymptotically negligible. How fast this happens depends on dimensionality. There exists a critical dimensionality above which the interface response vanishes like the interface density and below which it vanishes more slowly. At $d = 1$ the interface response does not vanish leading to the violation of the FMPP scheme. This behavior is explained in terms of the competition between curvature driven and field driven interface motion.

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Recently Franz, Mezard, Parisi and Peliti (FMPP) have proposed [1,2] a connection between static and dynamic properties of slowly relaxing systems. This is of fundamental importance for disordered systems such as spin glasses, since the low temperature equilibrium properties are hard to compute and still object of controversy after many years of intensive study. The existence of a bridge between statics and dynamics then offers a useful alternative tool for the investigation of the equilibrium state.

Here we are interested in the analysis of this connection for non disordered coarsening systems, such as a ferromagnet quenched below the critical point. In this case the structure of the equilibrium state is simple and well known. Therefore, these systems are particularly suitable for a detailed understanding of the method. Nonetheless, existing results are quite puzzling. For the nearest neighbors Ising model numerical results in space dimension $d \geq 2$ [3] fit into the FMPP scheme, while recent exact analytical results in the $d = 1$ case [4] show a qualitatively different behavior excluding any connection between the relaxation properties and the structure of the equilibrium state. In this paper we investigate the problem through a careful analysis of the linear response function as the space dimensionality is changed. This allows to put together the rich and interesting picture of what goes on in the off equilibrium response of a coarsening system and to uncover the mechanism whereby the FMPP scheme is or is not verified.

Let us first outline the problem. We consider a phase ordering system with a scalar order parameter quenched at the time $t = 0$ from high temperature to a final temperature T below the critical point. The time evolution takes place by formation and coarsening of domains of the opposite equilibrium phases [5]. The characteristic feature of the process is the coexistence of fast and slow dynamics. Within domains local equilibrium is reached rapidly while the coarsening process is slow. In the case of non conserved order parameter, as it will be considered here, the typical domain size grows like $L(t) \sim t^{1/2}$. This phenomenology suggests the split of the order parameter into the sum of two independent components [6]

$$\phi(\vec{x}, t) = \psi(\vec{x}, t) + \sigma(\vec{x}, t) \tag{1}$$

where $\psi(\vec{x},t)$ describes equilibrium thermal fluctuations within domains, the ordering component $\sigma(\vec{x},t)$ takes values $\pm m_T$ in the bulk of domains with the change of sign occurring at the interfaces and m_T is the equilibrium spontaneous magnetization. The split (1) accounts well for the observed behavior [7] of the autocorrelation function $C(t,t') = \langle \phi(\vec{x},t)\phi(\vec{x},t')\rangle$ where $t \geq t' \geq 0$. This quantity can be written as the sum of two terms

$$C(t,t') = C_{st}(t-t') + C_{ag}\left(\frac{t}{t'}\right) \tag{2}$$

representing, respectively, the stationary dynamics of thermal fluctuations $\psi(\vec{x},t)$ and the slow out of equilibrium dynamics of $\sigma(\vec{x},t)$ obeying an aging form. At equal times $C_{st}(t-t'=0) = m_0^2 - m_T^2$, where m_0 is the $T=0$ spontaneous magnetization, and $C_{ag}(1) = m_T^2$. Furthermore, due to the wide separation of time scales, in the range of time over which C_{st} decays to zero the aging contribution remains practically constant $C_{ag}(t/t') \simeq m_T^2$.

Suppose, next, that at the time $t_w > 0$ a small random field with expectations $\overline{h(\vec{x})} = 0$, $\overline{h(\vec{x})h(\vec{y})} = h_0^2\delta(\vec{x}-\vec{y})$ is switched on. Given the structure (1), the perturbation affects only the ordering component $\sigma(\vec{x},t)$, leaving thermal fluctuations unaltered, exactly as it happens in the equilibrium ordered phase under the action of an external field. Therefore, each unperturbed configuration is mapped into a new one $\phi(\vec{x},t) \rightarrow \phi_h(\vec{x},t) = \psi(\vec{x},t) + \sigma_h(\vec{x},t)$ with a modified ordering component. In general, the perturbation will modify both the bulk and the interface behavior of $\sigma(\vec{x},t)$. Accordingly, to linear order we may write

$$\begin{aligned}\sigma_h(\vec{x},t) = \sigma(\vec{x},t) &+ \int d\vec{x}'\chi_B(\vec{x}-\vec{x}',t,t_w)h(\vec{x}') \\ &+ \int d\vec{x}'\chi_I(\vec{x}-\vec{x}',t,t_w)h(\vec{x}')\end{aligned} \tag{3}$$

where the bulk response function χ_B, accounting for the change in the magnetization within domains, must be related to thermal fluctuations via the equilibrium fluctuation dissipation theorem (FDT)

$$\begin{aligned}&T\chi_B(\vec{x}-\vec{x}',t,t_w) = \\ &\quad C_{st}(\vec{x}-\vec{x}',t-t_w=0) - C_{st}(\vec{x}-\vec{x}',t-t_w).\end{aligned} \tag{4}$$

At this point one can already get a glimpse on what conditions must be realized for statics and dynamics to be connected. Since the bulk response function χ_B probes the equilibrium fluctuations and that is where the information on the equilibrium state is stored, for the FMPP scheme to work the interface contribution χ_I must disappear. Current belief is that indeed this is what happens [2,3,8] assuming that χ_I goes like the interface density $\rho_I(t) \sim L^{-1}(t) \sim t^{-1/2}$. However, to a closer scrutiny things are not so straightforward and the interface contribution turns out to have more structure than hitherto believed. In particular, there is an unexpected dependence on dimensionality which, in the end, accounts for the discrepancies in the Ising model mentioned above. Before entering the calculation of χ_I, it is useful to complete the outline of the problem illustrating a few points.

i) *FMPP scheme.* Averaging over the external field and the noise the on site total response function is given by

$$\chi(t,t_w) = \frac{1}{h_0^2 V} \int d\vec{x}\overline{\langle \phi_h(\vec{x},t)\rangle h(\vec{x})} = \chi_B(t,t_w) + \chi_I(t,t_w). \tag{5}$$

In the FMPP scheme one assumes that this quantity obeys the out of equilibrium generalization of the FDT proposed by Cugliandolo and Kurchan [9], namely that for large times $\chi(t,t_w)$ depends on the time arguments through the autocorrelation function $\chi(C(t,t_w))$. Furthermore, one assumes that $\lim_{t\to\infty} \chi(t,t_w) = \chi_{eq}$, where χ_{eq} is the equilibrium response function. With these two hypothesis, the connection between statics and dynamics is derived in the form

$$D(q) = \tilde{P}(q) \tag{6}$$

where $D(q) = -T_F \left[\frac{d^2\chi(C)}{dC^2}\right]_{C=q}$ is the dynamical quantity, while $\tilde{P}(q) = \lim_{h\to 0} P_h(q)$ is the static one. $P_h(q)$ is the overlap distribution in the perturbed Gibbs state. We recall that for a ferromagnetic system in the unperturbed Gibbs state below T_C the overlap distribution is given by [10]

$$P(q) = \frac{1}{2}\delta(q - m_T^2) + \frac{1}{2}\delta(q + m_T^2). \tag{7}$$

ii) *Validity of the FMPP scheme.* If in (5) we take into account only the bulk contribution χ_B, neglecting χ_I, then the FMPP scheme is verified. In fact, using (2) and recalling that $C_{ag}(t/t') \simeq m_T^2$ in the range of times where $C_{st}(t-t')$ decays to zero, from (4) follows

$$T\chi(C) = \begin{cases} C(t,t) - C(t,t_w) & \text{for } m_T^2 < C < m_0^2 \\ m_0^2 - m_T^2 & \text{for } C \leq m_T^2. \end{cases} \tag{8}$$

Eq. (6) then implies $\tilde{P}(q) = \delta(q - m_T^2)$. The presence of one δ-function instead of two as in (7) does not mean that in the limit $h \to 0$ symmetry is broken. Rather, it means that from a response due only to thermal fluctuations it is impossible to distinguish one pure state from the other and everything goes as if symmetry was broken. Numerical simulations of the Ising model for $d \geq 2$ [3] show evidence for convergence toward the structure (8) in the parametric plot of χ versus C as t_w becomes large (Fig. 1). This indicates that the interface term χ_I in (5) must be asymptotically negligible.

iii) *Violation of the FMPP scheme.* From the exact analytical solution of the $d = 1$ Ising model one finds a different behavior. In $d = 1$ it is important to realize that in order to make compatible the existence of a linear response regime, which requires $\frac{h_0}{T} << 1$ and therefore $T > 0$, with the existence of an equilibrium state of the form (7), one must take the limit $J \to \infty$ in the ferromagnetic coupling. This in turn implies $m_T^2 = m_0^2$. Hence, if (8) were to hold, $T\chi(t,t_w)$ would vanish. Instead, one finds [4] $T\chi(C) = (\sqrt{2}/\pi)\arctan\left[\sqrt{2}\cot(\pi C/2)\right]$ which yields $D(q) = \pi\cos(\pi q/2)\sin(\pi q/2) \,/\, \left[2 - \sin\left(\frac{\pi}{2}q\right)\right]^2$ and which is in no way related to (7), as shown in Fig. 1. Furthermore, notice that $J = \infty$ leads to the suppression of thermal fluctuations within domains. Therefore, from the above analytical form and $\chi(t,t_w) = \chi_I(t,t_w)$ follows $\lim_{t\to\infty} T\chi_I(t,t_w) = \lim_{C\to 0} T\chi(C) = 1/\sqrt{2}$. Therefore, the violation of the FMPP scheme in $d = 1$ is due to an asymptotically dominant interface contribution.

Having made clear the necessity of investigating the relative importance of the bulk and interface terms as dimensionality is varied, we now introduce a semiphenomenological model for $\chi_I(t,t_w)$. This is based on the standard methods of the late stage theory in phase ordering kinetics [5], when only interface motion is of interest. Dropping the bulk term in (3) and defining $\sigma_I(\vec{x},t) = \sigma(\vec{x},t) + \int d\vec{x}' \chi_I(\vec{x}-\vec{x}',t,t_w)h(\vec{x}')$ we resort for this quantity to the time dependent Ginzburg-Landau model without thermal noise

$$\frac{\partial \sigma_I}{\partial t} = \nabla^2 \sigma_I + m_T^2 \sigma_I - \sigma_I^3 + h(\vec{x}). \tag{9}$$

Next, in order to allow for the action of the field on the interface motion, while keeping the domain saturation fixed at the unperturbed level $\pm m_T$, we make the ansatz

$$\sigma_I(\vec{x},t) = \frac{u(\vec{x},t)}{\sqrt{1+\frac{u^2(\vec{x},t)}{m_T^2}}} \tag{10}$$

and we make an approximation of the gaussian auxiliary field (GAF) type [5,11]. The idea is that the non-linearity of the transformation (10) is enough to take care of the non-linearity in the problem and the auxiliary field $u(\vec{x},t)$ can be treated in mean field theory. Inserting (10) in (9) and linearizing the equation of motion for $u(\vec{x},t)$ we find

$$\frac{\partial u}{\partial t} = \nabla^2 u + m_T^2 u - \frac{3}{m_T^2}\langle (\nabla u)^2 \rangle + h(\vec{x}) \tag{11}$$

where $\langle (\nabla u)^2 \rangle$ is evaluated self-consistently. The key point is that the linear equation (11) allows $u(\vec{x},t)$ to grow unboundedly yielding via (10) $\sigma_I(\vec{x},t) \simeq m_T sign[u(\vec{x},t)]$ which enforces the saturation of domains at the required unperturbed value. Making a further mean field approximation through the replacement of (10) by $\sigma_I(\vec{x},t) = m_T \frac{u(\vec{x},t)}{\sqrt{S(t)}}$ with $S(t) = \langle u^2(\vec{x},t) \rangle$, we have $\chi_I(t,t_w) = m_T \chi_u(t,t_w)/\sqrt{S(t)}$ where χ_u is the response of the auxiliary field. Computing $\chi_u(t,t_w)$ and $S(t)$ from (11) and defining $\chi_{eff}(t,t_w)$ by $\chi_I(t,t_w) = \rho_I(t)\chi_{eff}(t,t_w)$ we find our main result

$$\chi_{eff}(t,t_w) = t^{1-\frac{d}{2}} F(t_w/t) \tag{12}$$

with $F(x) = A\int_x^1 dy y^{-\frac{d+2}{4}} (1-y+\frac{t_0}{t})^{-d/2}$. Here A is a dimensionality dependent constant and t_0 is a microscopic time related to the momentum cutoff Λ by $t_0 = \Lambda^{-2}$. The meaning of Eq. (12) can be made transparent regarding the response of the system as due to a set of interfaces each contributing through an effective response χ_{eff}. From (12) follows that this quantity obeys

$$\chi_{eff}(t, t_w) \sim (t - t_w)^{\alpha} \tag{13}$$

with $\alpha = 0$ for $d > 2$, $\alpha = 1 - d/2$ for $d < 2$ and $\chi_{eff} \sim \log(t - t_w)$ for $d = 2$ [12]. Eq. (13) applies both in the short ($t - t_w << t_w$) and in the large ($t - t_w >> t_w$) time region, with a change in the prefactor taking place about $t - t_w \simeq t_w$. The full time dependence of $\chi_{eff}(t, t_w)$ obtained by plotting out Eq. (12) for different values of d is displayed in Fig. 2a. A completely analogous behavior is obtained in the Ising model. We have computed $\chi_I(t, t_w)$ for $d = 1, 2, 3, 4$ in the Ising case by suppressing spin flips in the bulk of domains and we have plotted $\chi_{eff}(t, t_w)$ in Fig. 2b [13] . The common features of Fig. 2a and Fig. 2b may be summarized stating that in both cases χ_{eff} obeys the power law (13) and that there exists a critical dimensionality d_c such that the exponent α is zero for $d > d_c$ while it grows positive with decreasing dimensionality for $d < d_c$, reaching in both cases the final value $\alpha = 1/2$ at $d = 1$. The differences are that $d_c = 2$ in the GAF approximation, while from the Ising simulations there is a good evidence (Fig. 2b) for $d_c = 3$. One particular consequence of this, on which we comment below, is that while in the former case we have $\alpha = 0$ with logarithmic growth at $d = 2$, instead in the $d = 2$ Ising model one finds $\alpha = 1/4$ (Fig. 2b).

The interpretation of the above results goes as follows. In the perturbed system interface motion is driven not only by curvature, as in the unperturbed case [5], but also by the external field. These two mechanisms compete. For $d > d_c$ the curvature mechanism dominates. The external field then affects only the spins strictly belonging to the interface. Within a microscopic time χ_{eff} saturates (see lines for $d = 3$ in Fig. 2a and for $d = 4$ in Fig. 2b) leaving the overall response χ_I to decrease as $\rho_I(t)$. Instead, if dimensionality is low enough ($d \leq d_c$) to weaken the curvature mechanism to the point that the field driven motion may start to play a role in the response, then the single interface response χ_{eff} grows with time like t^{α} counteracting the default decrease in χ_I due to $\rho_I(t)$. This effect can be understood realizing that when interfaces are field driven the field produces a large scale optimization of domain positions with respect to field configurations [14]. $d = 1$ is the extreme case where there is no more curvature mechanism. Then, interface motion is entirely field driven yielding χ_{eff} which grows like $t^{1/2}$ and compensates exactly for $\rho_I(t)$ producing a non vanishing $\lim_{t\to\infty} \chi_I(t, t_w)$.

In summary, we have investigated the relationship between the out of equilibrium response function and the structure of the equilibrium state for coarsening systems. For the FMPP scheme to hold, the out of equilibrium response must be dominated by equilibrium fluctuations in the bulk of domains. This we have made precise by separating the bulk from interface response and by analyzing the behavior of the interface contribution $\chi_I(t, t_w)$. On the basis of a GAF model we have found that there exists a critical dimensionality $d_c = 2$ such that for $d > d_c$ $\chi_I(t, t_w)$ behaves like the interface density $\rho_I(t)$, while for $d < d_c$ it vanishes slower than $\rho_I(t)$ and does not vanish anymore at $d = 1$, yielding the violation of the FMPP scheme. We have explained this behavior identifying d_c as the dimensionality below which the external field competes effectively with the curvature in driving interface motion. The overall picture is confirmed by numerical results for the Ising model, apart from the upward shift from $d_c = 2$ to $d_c = 3$ in the critical dimensionality. This means that in the Ising case the field driven mechanism competes with the curvature even more efficiently than in the GAF approximation. In particular, the field driven mechanism is clearly observable in the $d = 2$ Ising model where $\alpha = 1/4$ makes the interface response much less preasymptotic than what was estimated on the basis of the interface density argument. Finally, the counterpart of the statement that a persistent interface contribution leads to the violation of the FMPP scheme, is that even if $\chi_I(t, t_w)$ vanishes asymptotically, due to the field driven interface motion it may vanish so slowly to hide the realization of the FMPP scheme.

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[12] A logarithmic correction in the response function for $d = 2$ was first derived in Ref. [8].

[13] For $d = 1$ the data closely reproduce $\chi_{eff}(t, t_w)$ computed analytically from the exact form of Ref. [4].

[14] This can be checked very accurately by computing the response function in simulations

without bulk flip and with initial configurations containing only one interface.

FIGURES

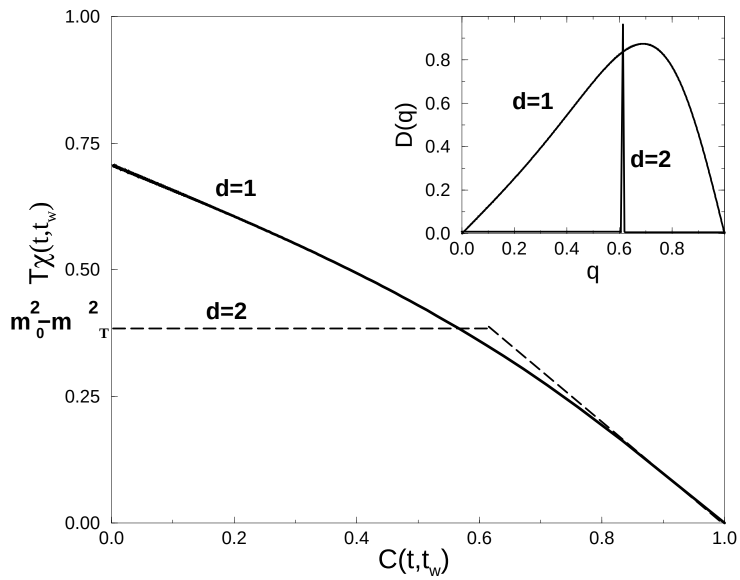

FIG. 1. $T\chi(t, t_w)$ for the Ising model. For $d = 2$ the curve shows the expected behavior on the basis of Eq. (8) for $t_w \to \infty$ with $T = 2.2, J = 1$. For $d = 1$ the curve is the plot of the analytic form of Ref. [4]. The inset shows the corresponding $D(q)$.

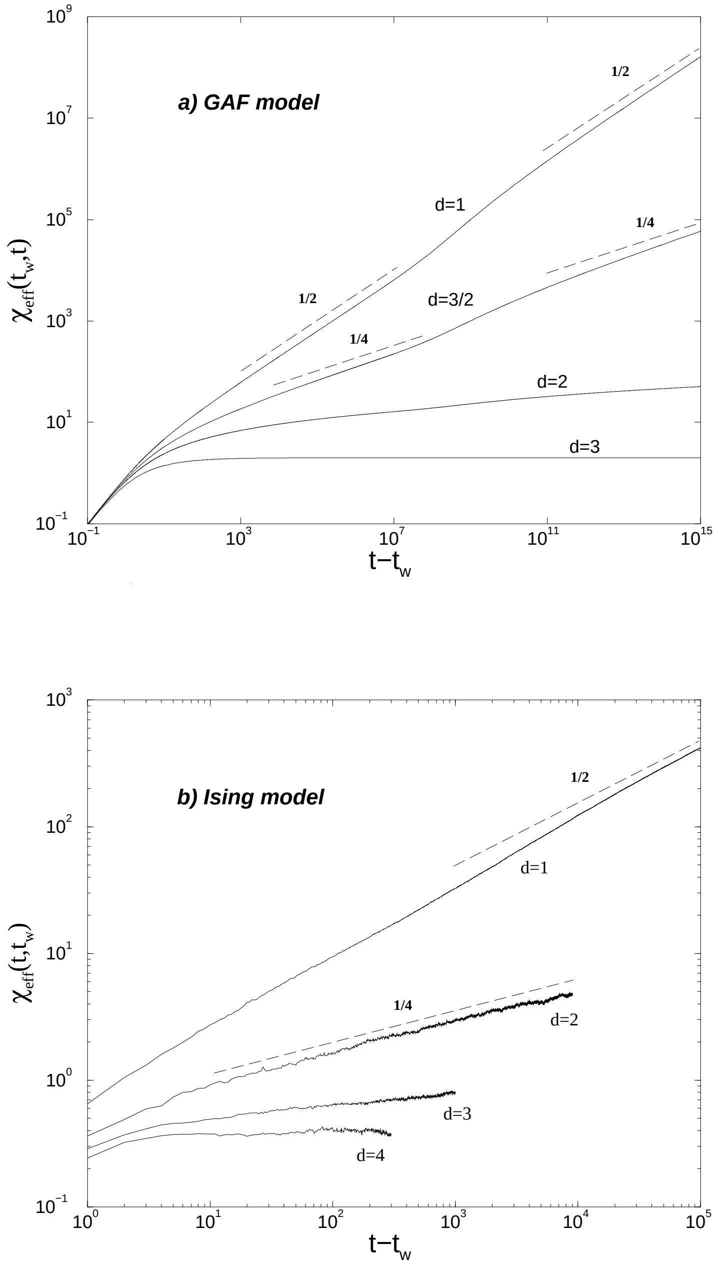

FIG. 2. $\chi_{eff}(t, t_w)$ in the semiphenomenological model with $t_w = 10^8$ (a) and in the Ising model without spin flips in the bulk (b). For $d = 1, 2, 3, 4$, the temperature, waiting time and linear system sizes L of the simulations are $T = 0.48, 2.2, 3.3, 4.4$, $t_w = 10^3, 10^3, 10^2, 10$ and $L = 10^6, 512, 128, 42$ with $J = 1$ and averages over $170, 6045, 2590, 922$ realizations. The dashed lines are power laws with the corresponding exponent α. For $d = 3$ in (b) the curve is very well fitted by $0.33+0.066 \log(t-t_w)$.