Generic features of the fluctuation dissipation relation in coarsening systems

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The integrated response function in phase-ordering systems with scalar, vector, conserved, and nonconserved order parameter is studied at various space dimensionalities. Assuming scaling of the aging contribution $\chi_{ag}(t,t_w)=t_w^{-a_\chi}\hat{\chi}(t/t_w)$ we obtain, by numerical simulations and analytical arguments, the phenomenological formula describing the dimensionality dependence of a_χ in all cases considered. The primary result is that a_χ vanishes continuously as d approaches the lower critical dimensionality d_L. This implies that (i) the existence of a nontrivial fluctuation dissipation relation and (ii) the failure of the connection between statics and dynamics are generic features of phase ordering at d_L.

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After the groundbreaking work of Cugliandolo and Kurchan [1] on mean-field spin glasses, the study of the out-of-equilibrium linear response function has been gaining an increasingly important role in the understanding of slow relaxation phenomena. The key concept is that of the fluctuation dissipation relation (FDR) [2]. In terms of the response function $\chi(t,t_w)$ integrated over the time interval (t_w,t), an FDR arises if $\chi(t,t_w)$ depends on time only through the autocorrelation function $C(t,t_w)$. If this happens, there remains defined a function $\chi=S(C)$ which generalizes the fluctuation dissipation theorem into the out-of-equilibrium regime.

The existence of an FDR is important for several reasons [2]. Here, we focus on a specific aspect: to what extent the FDR shape is revealing of the mechanism of relaxation and of the structure of the equilibrium state. In particular, we aim at dispelling the common belief that relaxation by coarsening and a simple equilibrium state do *necessarily* imply a flat or trivial FDR, i.e., $S(C)=1-q_{EA}$ when C falls below the Edwards-Anderson order parameter q_{EA}.

To appreciate the relevance of the problem, notice that, by reversing the argument, a nonflat FDR would rule out coarsening. This is a statement of far-reaching consequences. For instance, an argument of this type plays a role in the discrimination between the mean field and the droplet picture of the low-temperature phase of finite dimensional spin glasses [3]. In that case, the final conclusion may well be right, but for the argument to be sound, the behavior of the response function, when relaxation proceeds by coarsening, needs to be thoroughly understood.

As a contribution in this direction, we have undertaken a large program of systematic investigation of the FDR in the phase ordering systems [4], the workbench for the study of all aspects of relaxation driven by coarsening. We have considered pure ferromagnetic systems quenched from above to below the critical point. We have covered the whole spectrum of systems with nonconserved (NCOP), conserved (COP), scalar $(N=1)$, and vector $(N>1)$ order parameter at different space dimensionalities d, where N is the number of components of the order parameter. The manifold of the systems considered is displayed in Table I. Some of these (marked by a dot) have been studied before. With the new entries, the picture becomes rich enough to promote to *generic* the behavior previously observed in the case of the Ising model [5–8] and in the large-N model [9]. Namely, that FDR is flat for $d>d_L$ and nonflat for $d=d_L$ [10], where d_L is the lower critical dimensionality. The implication is that a flat FDR is not a necessary condition for coarsening.

To explain, let us recall [2] that one can write $\chi(t,t_w)=\chi_{st}(t-t_w)+\chi_{ag}(t,t_w)$. The first is the stationary contribution due to the fast degrees of freedom which rapidly equilibrate with the bath, while the second is the aging contribution coming from the slow out-of-equilibrium degrees of freedom. One can also show, in general, that a flat FDR is obtained if $\chi_{ag}(t,t_w)$ vanishes asymptotically [2,6]. Now, in phase ordering for large t_w, one expects the scaling behavior

$$\chi_{ag}(t,t_w)=t_w^{-a_\chi}\hat{\chi}(t/t_w), \tag{1}$$

from which it follows that the FDR is or is not flat according to $a_\chi>0$ or $a_\chi=0$. Therefore, investigating the FDR shape requires the investigation of a_χ.

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TABLE I. The manifold of systems considered. Entries with dots correspond to systems studied in Refs. [5–8].

	NCOP		COP	
d	$N=1$	$N>1$	$N=1$	$N>1$
1	•		•	
2	•	$N=10$	$N=1$	$N=4$
3	•	$N=2$, $N=5$	$N=1$	$N=5$
4	•	$N=6$	$N=1$	

Let us see the situation with this exponent. In the Ising model [5–8] and in the large-N model [9], we have found that a_χ depends on dimensionality according to

$$a_\chi = \begin{cases} \delta\left(\dfrac{d-d_L}{d_U-d_L}\right) & \text{for } d < d_U, \\ \delta \quad \text{with log corrections} & \text{for } d = d_U, \\ \delta & \text{for } d > d_U, \end{cases} \tag{2}$$

where δ enters the time dependence of the density of defects and d_L, d_U are the two special dimensionalities (with $d_L < d_U$) where $a_\chi = 0$ and above which $a_\chi = \delta$, respectively. The density of defects goes like $\rho(t) \sim L(t)^{-n} \sim t^{-\delta}$, where $L(t) \sim t^{1/z}$ is the typical defect distance, z is the dynamic exponent, and $n=1$ or $n=2$ for scalar or vector order parameter [4]. Hence, $\delta = n/z$. Here, we present strong evidence supporting Eq. (2) as the generic pattern of behavior.

We have computed $\chi(t,t_w)$ for systems quenched from infinite to zero final temperature. In all cases we have used the time-dependent Ginzburg-Landau equation [4], except for NCOP with $N>1$ and $d>2$ where the Bray-Humayun [11] algorithm has been used [12]. After computing $\chi_{st}(t-t_w)$ from equilibrium simulations, we have obtained $\chi_{ag}(t,t_w) = \chi(t,t_w) - \chi_{st}(t-t_w)$. To get a_χ, one ought to extract the t_w dependence of $\chi_{ag}(t,t_w)$ for fixed $x = t/t_w$ [8]. However, this is computationally very demanding and would make it impossible to get the vast overview we are aiming for. So, we have measured a_χ from the large-t behavior for a fixed t_w, assuming $\chi_{ag}(t,t_w) \sim t^{-a_\chi}$. This holds if $\hat{\chi}(x) \sim x^{-a_\chi}$ for $x \gg 1$, which has been verified in the NCOP scalar case [6,8], and it is an exact result in the soluble models [5,9]. The assumption is that it holds in general. The choice of t_w is inessential provided it is larger than some microscopic time necessary for scaling to set in [8].

The time dependence of $\chi_{ag}(t,t_w)$ is depicted in Figs. 1–3. We have extracted a_χ from the asymptotic power-law decay and we have collected all results, old and new, in Fig. 4. At d_L we have used the parametric plot $\chi_{ag}(C)$ (insets of Figs. 1–3), showing more effectively the absence of asymptotic decay, due to $a_\chi = 0$. In Fig. 4, we have also displayed the values of a_χ predicted by Eq. (2). The comparison with the computed values is quite good. For convenience, we have collected in Table II the values of all the parameters entering Eq. (2). Figure 4 is the main result in the paper.

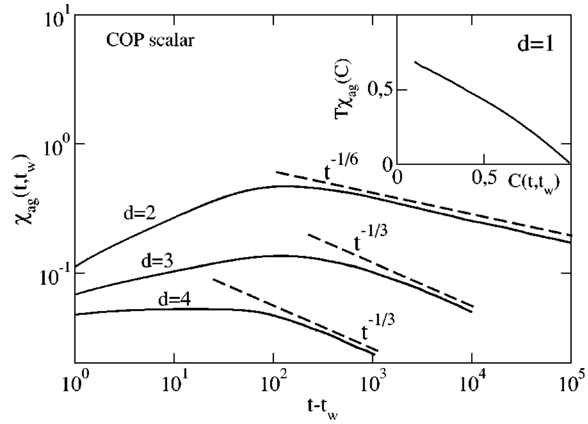

FIG. 1. $\chi_{ag}(t,t_w)$ against $t-t_w$ for $N=1$ with COP. Lattice sizes, realizations, and t_w: 512^2, 41, and 30 for $d=2$; 128^3, 39, and 40 for $d=3$; 60^4, 6, and 31 for $d=4$. The dashed lines are the slopes from Eq. (2). In the inset: parametric plot for $d=1$ from Ref. [7]

Let us now comment on the results. From Fig. 4 it is evident that the pattern of behavior predicted by Eq. (2) is obeyed with good accuracy in the scalar cases, with $d_L=1$ and $d_U=3$. In the vector cases, given the great numerical effort needed, values of N were chosen according to the criterion of the best numerical efficiency, together with the requirement to simulate both systems with $(N<d)$ and without $(N>d)$ stable topological defects. The overall behavior of the data in Fig. 4 shows that Eq. (2) represents the dimensionality dependence of a_χ well also in the vector case with $d_L=2$ and $d_U=4$. Finally, the insets in Fig. 1–3 (together with the analogous figures for the $d=1$ Ising model in Refs. [5,7] and in the large-N model [9]) show quite clearly that $a_\chi=0$ and a nonflat FDR are common features in phase ordering kinetics at d_L.

At this stage Eq. (2) is a phenomenological formula. Apart from the exact solution of the large-N model [9], there is no derivation of Eq. (2). Here, we propose an argument for the dependence of a_χ on d in the scalar case. It is based on two simple physical ingredients: (a) the aging response is

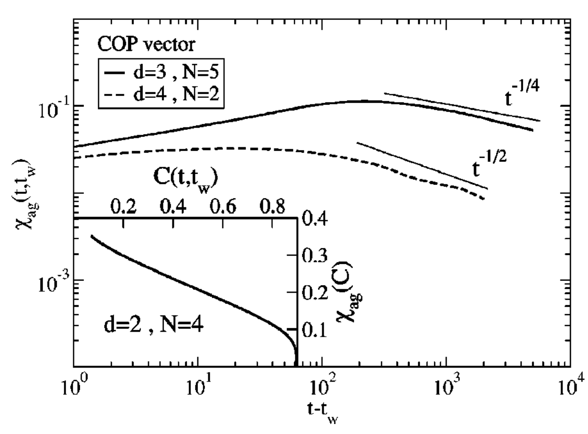

FIG. 2. $\chi_{ag}(t,t_w)$ against $t-t_w$ with COP. Lattice sizes, realizations, and t_w: 96^3, 89, and 35 for $d=3$ and $N=5$; 50^4, 82, and 35 for $d=4$ and $N=2$. The dashed lines are the slopes from Eq. (2). In the inset: parametric plot for $d=2, N=4$. Lattice size, realizations, and t_w: 512^2, 232, 500.

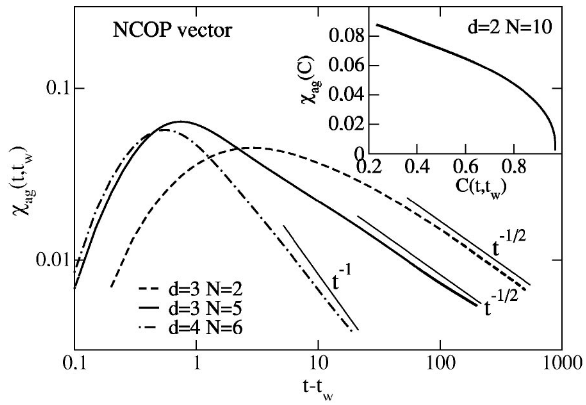

FIG. 3. $\chi_{ag}(t,t_w)$ against $t-t_w$ with NCOP. Lattice sizes, realizations, and t_w: 180^3, 1445, and 2 for $d=3$ and $N=2$; 140^3, 1486, and 0.3 for $d=3$ and $N=5$; 40^4, 486, and 0.3 for $d=4$ and $N=6$. In the inset: parametric plot for $d=2$ and $N=10$. Lattice size, realizations, and t_w: 1024^2, 22, and 20.

given by the density of defects $\rho(t)$ times the response of a single defect [6] $\chi_{ag}(t,t_w)=\rho(t)\chi^s_{ag}(t,t_w)$, and (b) each defect responds to the perturbation by optimizing its position with respect to the external field in a quasiequilibrium way. In $d=1$ this occurs via a displacement of the defect [6]. In higher dimensions, since defects are spatially extended, the response is produced by a deformation of the defect shape.

We develop the argument for a 2D system, the extension to arbitrary d being straightforward. A defect is a sharp interface separating two domains of opposite magnetization. In order to analyse $\chi^s_{ag}(t,t_w)$ we consider configurations with a single defect as depicted in Fig. 5. The corresponding integrated response function reads [6] $\chi^s_{ag}(t,t_w)=1/(h^2\mathcal{L}^{d-1})\int dx\, dy\overline{\langle S(x,y)\rangle h(x,y)}$, where $S(x,y)$ is the order parameter field which saturates to ± 1 in the bulk of domains. $h(x,y)$ is the external random field with expectations $\overline{h(x,y)}=0$, $\overline{h(x,y)h(x',y')}=h^2\delta(x-x')\delta(y-y')$, and $\mathcal{L}$ is the linear system size. The overbar and angular brackets denote averages over the random field and thermal histories, respectively. With an interface of shape $z_w(y)$ at time t_w (Fig. 5), we can write $\chi^s_{ag}(t,t_w)=-1/(h^2\mathcal{L}^{d-1})\overline{\int_{\{z\}}E_hP_h(\{z(y)\},t)}$, where $P_h(\{z(y)\},t)$ is the probability that an interface profile $\{z(y)\}$ occurs at time t and $E_h=-\int_0^{\mathcal{L}}dy\int_{z_w(y)}^{z(y)}dx\, h(x,y)\mathrm{sign}[z(y)-z_w(y)]$ is the magnetic energy. We now introduce assumption (b) making the ansatz for the correction to the unperturbed probability $P_0(\{z(y)\},t)$ in the form of a Boltzmann factor $P_h(\{z(y)\},t)=P_0(\{z(y)\},t)\exp(-\beta E_h)\simeq P_0(\{z(y)\},t)[1-\beta E_h]$. Then, $\chi^s_{ag}(t,t_w)=-1/(h^2\mathcal{L}^{d-1})\overline{\int_{\{z\}}E_h(1-\beta E_h)P_0(\{z(y)\},t)}$. Taking into account that the linear term in E_h vanishes by symmetry, and neglecting $z_w(y)$ with respect to $z(y)$ for $t\gg t_w$, we eventually find $\beta^{-1}\chi^s_{ag}(t,t_w)=\mathcal{L}^{1-d}\int_{\{z\}}\int_0^{\mathcal{L}} dy|z(y)|P_0(\{z(y)\},t)$. This defines a length which scales as the roughness of the interface [13] given by $W(t)=[\mathcal{L}^{1-d}\int_{\{z\}}\int dy\, z(y)^2P_0(\{z(y)\},t)]^{1/2}$. The behavior of $W(t)$ in the coarsening process can be inferred from an argument due to Villain [14]. In the case $d\leqslant 3$, when interfaces are rough [15], for NCOP one has $W(t)\sim t^{(3-d)/4}$, while for COP $W(t)\sim t^{(3-d)/6}$, with logarithmic corrections in both cases for $d=3$. For $d>3$ interfaces are flat and $W(t)\simeq$ const. Finally, multiplying χ^s_{ag} by $\rho(t)\sim L(t)^{-1}$ Eq. (2) is recovered [16] and d_U is identified with the roughening dimensionality $d_R=3$.

In summary, we have investigated the scaling properties of the response function over a large variety of systems designed to bring forward the generic features when relaxation is driven by coarsening. The primary result is that the exponent a_χ depends on dimensionality, and that it vanishes smoothly as $d\to d_L$. This implies that a nontrivial FDR is not exceptional; rather, it is the rule for coarsening systems at d_L. Another important consequence is that the failure of the connection between statics and dynamics at d_L [6] is also a generic feature of coarsening. The connection between the FDR and the overlap probability function is derived [17]

TABLE II. Parameters entering Eq. (2).

	$N=1$		$N>1$	
	NCOP	COP	NCOP	COP
z	2	3	2	4
δ	1/2	1/3	1	1/2
d_L	1		2	
d_U	3		4	

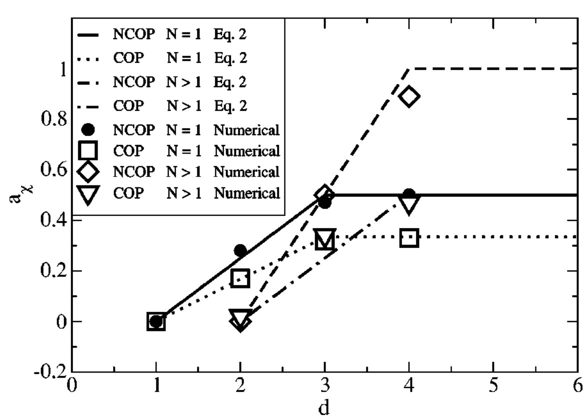

FIG. 4. Exponent a_χ from Eq. (2) and from best fit of numerical data.

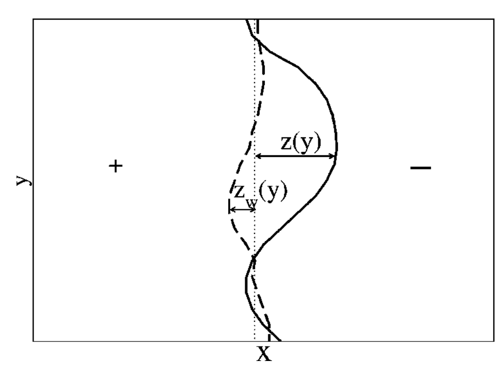

FIG. 5. Configurations with a single interface at time t_w (dashed line) and at time t (continuous line).

under the assumptions of stochastic stability and that $\chi(t,t_w)$ goes to the equilibrium value as $t\to\infty$. The latter assumption does not hold at d_L due to the existence of a nonflat FDR (insets of Fig. 1–3), which makes the limiting value of $\chi(t,t_w)$ rise above the equilibrium value. Obviously, the important and, as of yet, unanswered question is why all this happens at d_L. The scaling behavior of the response function reported in this paper adds to the many already existing challenges posed by a theory of phase ordering kinetics.

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