Coarsening in 3D nonconserved Ising model at zero temperature: Anomaly in structure and slow relaxation of order-parameter autocorrelation

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Abstract – Via Monte Carlo simulations we study pattern and aging during coarsening in a nonconserved nearest-neighbor Ising model, following quenches from infinite to zero temperature, in space dimension $d = 3$. The decay of the order-parameter autocorrelation function appears to obey a power-law behavior, as a function of the ratio between the observation and waiting times, in the large ratio limit. However, the exponent of the power law, estimated accurately via a state-of-the-art method, violates a well-known lower bound. This surprising fact has been discussed in connection with a quantitative picture of the structural anomaly that the 3D Ising model exhibits during coarsening at zero temperature. These results are compared with those for quenches to a temperature above that of the roughening transition.

Introduction. – Kinetics of phase transitions [1,2], following quenches of homogeneous systems to the state points inside the coexistence regions, remains an active area of research [3–28]. A particular interest has been in the case [1,2] when the temperature ($T$) of a magnetic system, prepared at the paramagnetic region, is suddenly lowered to a value that falls in the ferromagnetic region of the phase diagram. Following such a quench, the system evolves towards the new equilibrium via formation and growth of domains, rich in atomic magnets aligned in a particular direction. For such an evolution, in addition to the understanding of the time ($t$)-dependence of the average domain size ($\ell$) [1,2,18–22,29], there has been a significant interest in obtaining quantitative information on pattern formation [12–17], persistence [23–27] and aging [3–11,28].

Ising model [1,2] has been instrumental in the understanding of the above aspects of kinetics of phase transitions. Via computer simulations of this model, a number of theoretical expectations have been confirmed [2]. Some of these we describe below in the context of the nonconserved order parameter.

The (interfacial) curvature driven growth in this case is expected to provide [2,29]

$$\ell \sim t^\alpha; \quad \alpha = 1/2,$$

referred to as the Cahn-Allen growth law. The two-point equal-time correlation function [2], that quantifies the pattern, in this case was obtained by Ohta, Jasnow and Kawasaki (OJK) [12]. This has the form

$$C(r, t) = \frac{2}{\pi} \sin^{-1} \gamma,$$

with

$$\gamma = \exp(-r^2/8Dt),$$

where $D$ is a diffusion constant and $r$ is the scalar distance between two space points $\vec{r}_1$ and $\vec{r}_2$.

Note that $C(r, t)$ is a special case of a more general two-point two-time (space and time-dependent) order-parameter ($\psi$) correlation function [4]

$$C_{\text{gen}}(\vec{r}_1, \vec{r}_2, t, t_w) = \langle \psi(\vec{r}_1, t)\psi(\vec{r}_2, t_w) \rangle - \langle \psi(\vec{r}_1, t) \rangle \langle \psi(\vec{r}_2, t_w) \rangle,$$

for $t = t_w$, when the pattern is isotropic. On the other hand, when $\vec{r}_1 = \vec{r}_2$, $C_{\text{gen}}$ is referred to as the two-time
autocorrelation function [3,4]. This we will denote by \( C_{ag}(t, t_w) \), where \( t \) and \( t_w \) (\( \leq t \)) are usually referred to as the observation and waiting times, respectively. There exists a prediction of power-law decay for \( C_{ag} \) as [3,4]

\[
C_{ag} \sim \left( \frac{t}{t_w} \right)^{-\lambda},
\]

where \( t_w \) is the average domain size at time \( t_w \). For the aging exponent \( \lambda \), Fisher and Huse (FH) [3] predicted a lower bound

\[
\lambda \geq \frac{d}{2},
\]

where \( d \) is the space dimension.

Monte Carlo (MC) simulations [30] of the Ising model have been performed [2,17] in various space dimensions, for quenches to various values of \( T \). In \( d = 2 \), the above predictions were found to be valid, irrespective of the temperature of the quench. The status is similar with respect to simulations in \( d = 3 \) also, but only at reasonably high temperatures. From the limited number of available works, it appears that the coarsening of the 3D Ising model at \( T = 0 \) is special [18-22,27, 30-32]. E.g., Olejarz et al. [20,21] recently reported an extremely slow relaxation in this case, due to the presence of a large number of metastable states involving blinker spins. These authors also pointed out unusual structural features. Following these and other [18,19] works, we have undertaken a comprehensive study of aging phenomena, via the calculations of \( C_{ag}(t, t_w) \), alongside obtaining a quantitative picture of the structural anomaly.

We have obtained the scaling property of \( C_{ag}(t, t_w) \) and quantified its functional form via analysis of results from extensive MC simulations of very large systems. We observe scaling with respect to [3] \( x = t/t_w \) and power-law decay of the corresponding function in the \( x \to \infty \) limit. The correction to this power law, in the small-\( x \) region, resembles that of the high-temperature quench [8]. The exponent of the power law has been estimated, via the calculation and convergence of an appropriate instantaneous exponent [31] (in the \( x \to \infty \) limit). The value, thus extracted, violates the FH lower bound [3]. We have discussed this striking fact in connection with the structural property [5]. Preliminary results on this issue were reported in ref. [17]. However, in this earlier work violation of the FH bound was not observed.

**Methods.** – We implement the nonconserved dynamics [2] in the MC simulations of the Ising model by using spin-flips [2,30,32] as the trial moves. We have randomly chosen a spin and changed its sign. The energies before and after a trial were calculated from the Ising Hamiltonian [1–3] \((ij)\) in the summation represents nearest neighbors

\[
H = -J \sum_{\langle ij \rangle} S_i S_j, \quad S_i = \pm 1, \quad J > 0.
\]

Following this, the moves were accepted in accordance with the standard Metropolis algorithm [3], based on the difference in energies between the original and the perturbed configurations. One MC step (MCS), the time unit used in our simulations, consists of \( N \) trial moves, where \( N \) is the total number of spins in the system. We have considered periodic boxes of simple cubic type such that \( N = L^3 \), where \( L \) is the linear dimension of a cubic box, in units of the lattice constant.

We present results from two different temperatures, viz., \( T = 0 \) and 0.6\( T_c \), where \( T_c \) the critical temperature, is approximately equal to 4.51\( J/k_B \), \( k_B \) being the Boltzmann constant. In the following we set \( k_B = 1 \), the interaction strength \( J \) and the lattice constant to unity. For both the temperatures, we start with random initial configurations, which mimic the infinite temperature scenario. Note that \( T = 0.6T_c \) lies above the roughening transition temperature [16,19,33], \( T_R \) (\( \geq 0.57T_c \)). All quantitative results are presented after averaging over a minimum of 20 independent initial configurations, with \( L = 512 \) (except one case where we have used \( L = 300 \), to gain an insight into the finite-size effects). Note that the spin variable \( S_i \) is same as the order parameter \( \psi \), that is used in the definition of the correlation function.

For the calculation of \( C(r, \ell) \) and \( \ell \) at 0.6\( T_c \), thermal noise was eliminated via the application of a majority spin rule [34]. In this method, for a chosen lattice site we determine the direction of the spins sitting in its neighborhood (including the site itself) and assign that alignment to the central spin. In addition to calculating \( \ell \) from the scaling property (see discussion in results part) of \( C(r, \ell) \) as

\[
C(\ell, t) = a, \quad (8)
\]

\( a \) being a pre-assigned number that, in this work, will be fixed at 0.5, we have also obtained it from the first moment of the domain-size distribution function [34], \( P(\ell_d, t) \), as

\[
\ell = \int \ell_d P(\ell_d, t) d\ell_d. \quad (9)
\]

Here \( \ell_d \) is the distance between two consecutive domain boundaries along any Cartesian direction. In the exercise related to the scaling property of \( C(r, \ell) \) we will use \( \ell \) obtained from eq. (8). On the other hand, for quantifying the aging property via \( C_{ag}(t, t_w) \) we will use \( \ell \) calculated from eq. (9). Note that there exist other methods as well, for the calculation of \( \ell \). All these methods provide results proportional to each other.

**Results.** – In fig. 1(a) we show two snapshots, taken during the evolution of the 3D Ising model, following a quench from infinite temperature to \( T = 0 \). Growth in the system is clearly visible. To check for the structural self-similarity in the growth, in fig. 1(b) we have shown \( C(r, \ell) \) vs. \( r/\ell \) plots. A nice collapse of data from various different times (\( \geq 1000 \)) implies the scaling form [2]

\[
C(r, t) = \tilde{C}(r/\ell(t)), \quad (10)
\]
Coarsening in 3D nonconserved Ising model at zero temperature: etc.

Fig. 1: (Colour online) (a) Snapshots during the evolution of the 3D nonconserved Ising model. Pictures from two different times are shown. The locations of the “up” spins are marked. The linear dimension of the system is $L = 64$. (b) Plots of two-point equal-time correlation function vs. $r/\ell$. Data from five different times are included. The box size corresponds to $L = 512$. All results are from $T = 0$.

where $\tilde{C}(y)$ is independent of time, a requirement for the self-similarity. While this qualitative feature is the same as that exhibited [2,17] by the model in $d = 2$ or for quenches to much higher values of $T$ in $d = 3$, we will later see that $\tilde{C}$ in the present case differs from that for the above cases. This difference may have an important consequence in the aging property. Unless otherwise mentioned, all results below are for quenches to $T = 0$.

Next we focus our attention to the aging property. In fig. 2 we present plots of $C_{\text{ag}}(t, t_w)$ vs. $t - t_w$, from three different values of $t_w$. As expected, no time translation invariance is observed [11] and the decay becomes slower with the increase of $t_w$, implying aging in the system. However, the autocorrelation function for different $t_w$ values exhibits data collapse when plotted vs. $\ell/\ell_w$ [3]. This is demonstrated in fig. 3. The solid line in this figure represents a power law with exponent $\lambda = 1.67$. This value was predicted by Liu and Mazenko (LM) [4], via a calculation that uses a Gaussian auxiliary field ansatz [2,4]. LM constructed a dynamical equation for $C_{\text{gen}}(\vec{r}_1, \vec{r}_2, t, t_w)$ as [4]

$$\frac{\partial C_{\text{gen}}(\vec{R}, t, t_w)}{\partial t} = \nabla^2 C_{\text{gen}}(\vec{R}, t, t_w) + \frac{K}{t} C_{\text{gen}}(\vec{R}, t, t_w),$$

(11)

where $\vec{R} = \vec{r}_1 - \vec{r}_2$ and the constant $K$ depends upon $d$. An (approximate) solution of this equation, in the asymptotic limit, for $\vec{R} = 0$, provides a power law for $C_{\text{ag}}(t, t_w)$:

$$C_{\text{ag}}(t, t_w) \sim \ell^{-\lambda}; \quad \lambda = d - 2K.$$  

(12)

In $d = 3$ [4] one obtains $\lambda \simeq 1.67$. The LM line in fig. 3, however, is in significant disagreement with the simulation data, even for a very large value of $\ell$. Note that the presented data sets cover an overall length scale lying between 50 and 250. As observed in previous studies in different dimension or at other temperatures, here also the scaling function exhibits continuous bending [8,10]. (The sharp bending towards the end, however, is related to the finite-size effects. This fact is
demonstrated in the inset by presenting data from different system sizes. Such bending occurs at fixed fraction (\( \approx 0.4 \)) of the system sizes, marked by the arrows.) Even though a fair agreement of the simulation data with the LM prediction is not yet observed, a trend for arriving at a better agreement with the latter or at least with a power-law behavior may be appreciated with the increase of \( x \). The continuous bending perhaps implies [8] the presence of correction(s) for smaller \( x \). In such a situation, if indeed a power-law behavior is expected in the \( x \rightarrow \infty \) limit, for the estimation of the exponent it is instructive to calculate the instantaneous exponent as [8,31]

\[
\lambda_i = -\frac{d\ln C_{ag}(t, t_w)}{d\ln x}.
\]

We have calculated \( \lambda_i \) for the scaling functions at \( T = 0 \) and \( T = 0.6T_c \). These are plotted vs. \( 1/x \) in fig. 4(a). In both the cases linear convergence to the \( x \rightarrow \infty \) limit is visible [8]. Such an extrapolation for the \( T = 0.6T_c \) data indeed leads to a number that is consistent with the LM [4] value 1.67. Here note that in a later work [27], a modified value of \( \lambda \), about 6% smaller than 1.67, was mentioned. On the other hand, for \( T = 0 \) the convergence appears to be to a smaller value. Due to oscillations in data in the large-\( x \) regime, an accurate extrapolation to \( x = \infty \) is difficult in this case. Putting more emphasis on the smaller-\( x \) region, we obtain a central value \( \lambda = 1.10 \). The large-\( x \) data symmetrically oscillate around the extrapolating straight line, from which we quote the error bar \( \pm 0.12 \). The above-quoted value of \( \lambda \) is smaller than the LM [4] one. It also violates the FH (lower) bound. We mention here that the linear trend exhibited by the data sets in fig. 4(a) imply an exponential correction factor such that [8]

\[
C_{ag}(t, t_w) = Ae^{-B x^{-\lambda}},
\]

where \( A \) and \( B \) are constants. This expression can be obtained by using \( \lambda_i = \lambda + \frac{B}{x} \) in the definition of eq. (13). Thus, while \( B \) is the slope of a \( \lambda_i \) vs. \( 1/x \) plot, \( A \) can be used as an adjustable parameter related to the normalization of \( C_{ag}(t, t_w) \). From the exercises in fig. 4(a), we obtain \( B = 0.45 \) and 1.11, respectively, for \( T = 0 \) and \( 0.6T_c \).

To confirm the authenticity of the above analysis and that of eq. (14), in fig. 4(b) we have shown a comparison where the continuous lines correspond to eq. (14). In the latter equation we have used the values of \( B \) and \( \lambda \) that have been obtained from the exercises in fig. 4(a). Notice that the continuous lines, particularly for \( T = 0.6T_c \), do not converge to unity at \( x = 1 \). This is because, at high temperature the autocorrelations exhibit jump at time scales related to the equilibration of domain magnetization. Data before that should be discarded to obtain information on the global relaxation. Here, the value of \( A \) was adjusted to a lower value, since, instead of discarding the small-\( x \) data, the overall plot was normalized in such a way that \( C_{ag} \) is unity at \( x = 1 \). In any case, the agreement between the simulation data and eq. (14) is extremely good, at both the temperatures. This validates our conclusion on the values of \( \lambda \), and thus, the violation of the FH bound for \( T = 0 \). In this figure the larger range of data for \( T = 0.6T_c \) than that for \( T = 0 \) is because of the fact that a smaller value of \( t_w \) than \( \ell_w \), is considered at the nonzero temperature.

Here we recall a recent observation of structural differences [20,21] of \( T = 0 \) coarsening dynamics of a 3D nonconserved Ising model with other situations. For that matter, in fig. 5(a) we show a comparison of \( C(r, t) \) at \( T = 0 \) with that at \( 0.6T_c \). There exists a significant difference between the two cases [17]. The one at \( 0.6T_c \) is in nice agreement with the OJK function, described by eqs. (2) and (3) (see the continuous line).
In the case of usual nonconserved Ising dynamics, $\beta = 0$. Thus, YRD bound coincides with the FH bound. A question now arises on the value of $\beta$ at $T = 0$. Recall that there exists a difference in $C(r, t)$ starting from an intermediate length scale. This is consistent with the previous report, that observed a sponge-like structure [20,21]. In fact, we also find holes inside the domains of “up” and “down” spins. See the comparison between the two-dimensional cuts of the snapshots (see fig. 5(b)), obtained from the evolutions following quenches to $T = 0$ and $0.6T_c$. Essentially, the domains of the two types of spins are interpenetrating in an unusual manner at $T = 0$ and creating a porous structure. In that case, we expect a different form of the $P(\ell_d, t)$ at $T = 0$, from that at $T = 0.6T_c$. This is shown in fig. 6(a). Even though the large $\ell_d$ behavior is exponential for both the temperatures (see the log-linear choice of the plots), indeed the smaller $\ell_d$ behavior is quite different in the two cases. This is due to the presence of the porosity at $T = 0$, which is expected to enhance the values of the distribution at small $\ell_d$. This feature is consistent with the above-mentioned difference in $C(r, t)$. Such difference in $C(r, t)$ is expected to provide a disagreement between $S(k, t)$, in the intermediate to small-$k$ range, at the two temperatures.

To understand the difference between the decay of $C_{\text{ag}}(t, \ell_w)$ at the two chosen temperatures, we ask the question if the above-mentioned structural mismatch is responsible for that. Here we note, Yeung, Rao and Desai (YRD) [5] mentioned that the FH bound should be valid only for nonconserved order-parameter dynamics. The latter type of dynamics, of course, is being studied in this paper. The above conclusion of YRD was drawn [5] by considering the known structural differences between conserved and nonconserved cases. Since, by now, we know that there exists a difference between $T = 0$ and higher-temperature structures even within the nonconserved framework [17,20,21], further concrete discussion and results with respect to this is worth presenting.

YRD obtained a modified lower bound [5]

$$\lambda \geq \frac{d + \beta}{2},$$  \hspace{1cm} (15)

where $\beta$ is the exponent for the small wave number ($k$) power-law behavior of the structure factor (Fourier transform of $C(r, t)$) [15]:

$$S(k, t) \sim k^{\beta}.$$  \hspace{1cm} (16)

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In fig. 6(b) we present log-log plots of $S(k, t)$ vs. $k$, for the two chosen temperatures. Times were chosen in such a way that $\ell_w$ values are approximately the same for the two temperatures. The small-$k$ behavior is certainly not consistent with $\beta = 0$. However, for $T = 0.6T_c$, the value of $\beta$ is very close to zero ($\simeq -0.2$). (Note here that in $d = 2$ and at high $T$ in $d = 3$, various authors [5,15,17] confirmed that $\beta \approx 0$.) For the validity of the YRD bound at $T = 0$ one requires $\beta \approx -0.8$. The small-$k$ behavior of $S(k, t)$ at $T = 0$ is reasonably consistent with this number—we see the solid line in fig. 6(b). We should mention here that for finite $L$ it is not possible to access values of $k$ very close to 0. If that becomes possible, by considering large $L$, one “may” observe a behavior consistent with $\beta = 0$, even for $T = 0$, though such a convergence may occur at smaller values of $k$ than that for the higher-temperature case. This can be appreciated from the inset of fig. 6(b) where we presented the instantaneous exponent

$$\beta_i = \frac{d \ln S(k)}{d \ln k},$$  \hspace{1cm} (17)

as a function of $k$. Here we have included data in the range that lie above $\ell = \ell_w$. This raises the question, what upper value of $k$ should be considered to be small? For an answer, we provide a brief discussion on how the YRD bound was obtained.
The derivation [5] of the YRD bound required an integration over $k$, involving the structure factors at $t$ and $t_w$, viz.,

$$C_{ag} \sim \ell^{-\lambda} \leq \ell^{d/2} \int_0^b d\ell k^{d-1} [S(k, t_w) \hat{S}(k\ell)]^{1/2},$$  \hspace{1cm} (18)$$

where $\hat{S}$ is a time-independent scaling function and $b = \hat{T}/\ell$. $\ell$ being the domain length at time $t$. The bound in eq. (15) follows when $S(k, t_w)$ in eq. (18) is replaced by its small-$k$ behavior, as in eq. (16). Given that the growth in the considered case is slow, the value of $b$, i.e., the range of integration in $k$-space is bigger, at a given time, compared to the higher-temperature scenario, where the growth is faster. This provides more negative “effective” value of $\beta$ in this case. The dashed vertical line in fig. 6(b) corresponds to $\ell = 200$, which is essentially the limiting value that can be accessed for $L = 512$, the size of our systems, without encountering finite-size effects. Data upto this value of $\ell$ are consistent with $\beta = -0.8$. Nevertheless, the question remains, as mentioned above, with the increase of the system size a constant value of $S(k, t_w)$ may be seen for $T = 0$ and at very late time the value of $b$ may fall in that region. This will raise the value of the lower bound. In that case, do we expect a crossover in the value of $\lambda$, from the value mentioned above to the LM one? This will certainly be interesting to check. However, for that purpose, system sizes much larger than the ones considered here, because of the strong finite-size effects, must be run for an extremely long time. This exercise is not within our ability at the moment, given the limitation of computational resources available to us. Nevertheless, the system size $L = 512$, used in this work, is extremely large and contains more than 0.13 billion spins. To our knowledge, there exists only one study in the literature that considered a similar system size [19]. However, these authors ran the simulations for much shorter times, understandably due to the difficulty in handling such big systems.

Before concluding, we comment on the exponential correction factor in the decay of the autocorrelation function. The behavior of the data sets for $\beta_{\lambda}$, in the inset of fig. 6(b), appears linear as a function of $t$. This fact, when used in the definition of $\beta_i$ (eq. (17)), can produce an exponential correction factor in the small-$k$ behavior of $S(k)$. This, in turn, when used in eq. (18), may give rise to a correction in $C_{ag}(t, t_w)$ quantitatively similar to the exponential factor we obtained from numerical analysis.

**Conclusion.** – We have studied the aging property [11] during ordering in the 3D Ising model without conservation of the order parameter. Monte Carlo simulation [30] results, for quenches from infinite to zero temperature, are presented for the two-time autocorrelation function. It has been shown, like in the high-temperature case [8], that the decay of this correlation function, as a function of $x (=t/t_w)$, is a power law, with an exponential correction for small $x$. The exponent for the power law, however, is much smaller than that for the high-temperature decay [8]. While in the high-$T$ case the exponent is consistent with the theoretical prediction by Liu and Mazenko [4], that obeys a lower bound, provided by Fisher and Huse (FH) [3], for $T = 0$ this lower bound is violated. This is an extremely striking observation. Furthermore, the pattern at $T = 0$ is different from that of the high temperature. For $T = 0$, the Ohta-Jasnow-Kawasaki function [12] does not describe the two-point equal-time correlation function well. The origin of this difference has been discussed. We argue that this deviation is responsible for the violation of the FH bound. In fact our result shows that the aging exponent obeys another bound, obtained by Yeung, Rao
and Desai [5], that can account for the structural anomaly mentioned above.

In this work the results from $T = 0$ are compared with those from $0.67T_c$, that lies above the roughening transition temperature, $T_R$. In the future we will perform a more systematic study by gradually varying $T$. This will provide information on whether the surprising features that have been observed are only a zero-temperature property or there is a gradual crossover from $T = 0$ to a higher temperature. This will also reveal if $T_R$, related to the interface broadening, is responsible for the unusual structure and dynamics.

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