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Dynamics of random interfaces in an order-disorder transition

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A computer-simulation study of the dynamic structure factor has been carried out for the two-dimensional Ising antiferromagnet at several temperatures below T_c. The scaling function for the structure factor depends weakly on temperature. The corresponding second moment as well as a characteristic domain size exhibits an Allen-Cahn time dependence, but with temperature-dependent prefactors which disagree with their theory in two dimensions. Additional theoretical work seems necessary to understand the temperature dependence of the scaling function and the domain size.

Recently considerable attention has been given to problems involving the motion of random interfaces, which arise in a wide range of physical phenomena. One particular example involves the development of order in a system quenched below its order-disorder transition temperature. The average domain size in such a case is thought to satisfy a $t^{1/2}$ growth law, where t is the time, as has been predicted by many authors,[1-6] most notably Allen and Cahn.[1] The Allen-Cahn theory predicts that the normal component of the interface velocity is proportional to the curvature of the interface, with the proportionality constant being an Arrhenius-type kinetic coefficient. In recent computer-simulation "controlled-growth" studies (in which an initial domain of a specified shape is allowed to evolve in a background of the opposite phase) the Allen-Cahn law has been verified at low temperatures, but is found to break down at higher temperatures for a two-dimensional order-disorder model.[7] This breakdown is manifest via a temperature-dependent prefactor of the $t^{1/2}$ law which is not present in the Allen-Cahn theory and which the authors of the controlled-growth study attribute to important roughening effects omitted from this theory. It should be pointed out, however, that these controlled-growth studies are extremely simple approximations to the real behavior of a quenched system, in which one has a larger number of interacting domains, which have in general rather irregular shapes. Thus although studying the rate of collapse of isolated domains is useful, it is not as realistic as studies of the cluster-distribution function and structure factor of quenched systems.

In this regard the theoretical study[8] by Ohta, Jasnow, and Kawasaki (OJK) is useful in that they have obtained an explicit scaling function for the dynamical structure factor $S(k,t)$ starting with the Allen-Cahn equation of motion (which omits noise). Their scaling function was shown to be in reasonable agreement with Monte Carlo studies for both the two-[4] and three-[3]dimensional models at the one temperature studied in each case. (Their scaling function is closely related to one obtained in an earlier theory by Kawasaki, Yalabik, and Gunton.[5]) However, since the noise term omitted in the Allen-Cahn equation appears to become more important at higher temperatures,[7,9,10] one would expect the OJK scaling theory to become less accurate at higher temperatures. The interface becomes increasingly diffuse as well, rather than sharp as assumed in the OJK theory, as the temperature increases. This should also affect the behavior of $S(k,t)$.

In this paper we study the temperature dependence of the dynamical structure factor for several temperatures below T_c for the two-dimensional kinetic Ising antiferromagnet. We find a temperature dependence for the (time-dependent) second moment of the structure factor and for a characteristic domain size, which suggests that the Allen-Cahn theory is incorrect in two dimensions, as predicted in the earlier controlled-growth studies.[7] As noted above, our current studies go beyond the controlled-growth studies of the Allen-Cahn equation in that we do not restrict ourselves to a subset of domain configurations.[7,9] We also find small temperature-dependent deviations from the OJK scaling function, as one would expect. However, we must add one word of caution about the previous[3,4] and present computer studies of this model. Namely, one encounters significant fluctuations (finite-size effects) in the Monte Carlo data for $S(k,t)$ which make it extremely difficult to draw definitive conclusions from the data. In particular we have encountered finite-size "slab" effects such as discussed in Refs. 3 and 4. We have done our best to minimize fluctuations by making many independent runs, as discussed below. Nevertheless, perhaps the major conclusion of this work is that one is going to study much larger systems before the temperature dependence of this dynamical model is well understood.

We have studied the dynamical evolution of a quenched nearest-neighbor Ising antiferromagnet (at zero magnetic field) by standard Monte Carlo methods employing Kawasaki spin-exchange dynamics.[3,4] The system of $N = 60\times 60$ sites was quenched from an initially disordered state at an "infinite" temperature $T = 4000T_c$ ($J/k_BT = 0.000\,11$) to several different low temperatures below T_c ($0.1T_c$, $0.15T_c$, $0.2T_c$, $0.25T_c$, $0.3T_c$, $0.4T_c$, $0.5T_c$, $0.6T_c$, $0.7T_c$). The time evolution was followed up

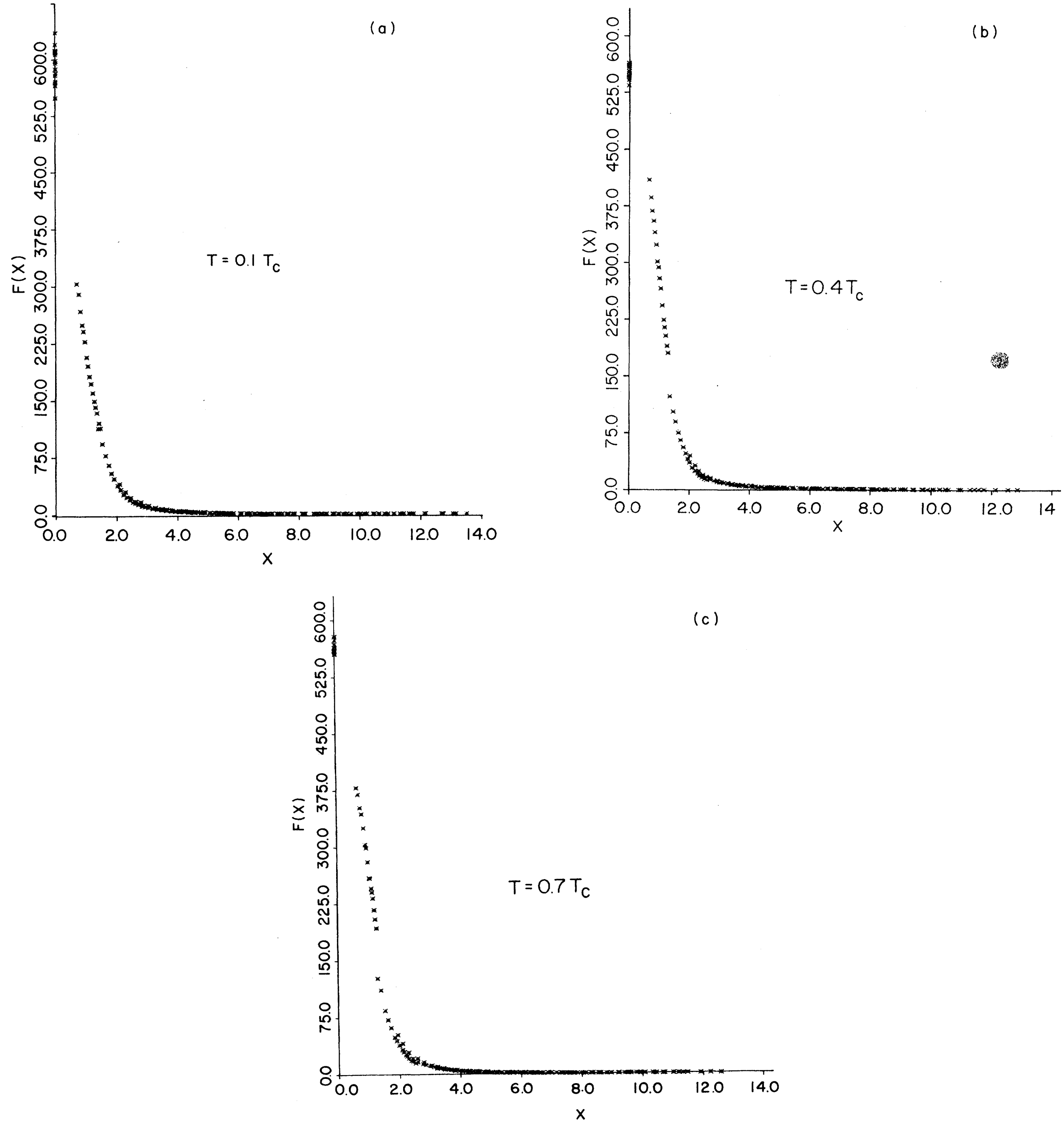

FIG. 1. Scaled (unnormalized) structure factor on a regular scale at temperature $0.1T_c$, $0.4T_c$, and $0.7T_c$.

to 200 Monte Carlo steps/spin (MCS/spin) omitting the first 40 MCS/spin from the analysis. We have studied the evolution of the circularly averaged Fourier transform of the staggered structure factor

$$S(\vec{k},t)=N^{-1}\left|\sum_{m,n}(-1)^{m+n}e^{i\vec{k}\cdot\vec{r}}\sigma(\vec{r})\right|^2, \quad (1)$$

where $\sigma(\vec{r})=\pm 1$ is the spin at site $\vec{r}=m\hat{i}+n\hat{j}$ and the wave number $|\vec{k}|=2\pi j/\sqrt{N}$ with $j=0,1,\ldots,10$. Owing to the large fluctuations in the Monte Carlo data for the structure factor, we have analyzed our data using 41 independent runs. We have used the standard deviation as an estimate for the error bars of the structure-factor data, even though there may be large systematic errors (such as finite-size effects) which are difficult to determine. The standard deviation is approximately less than 10% for the structure factor.

Our data for the structure factor is most conveniently shown in the scaling form[3,4]

$$F(x)=k_2(t)S(k,t) \quad (2)$$

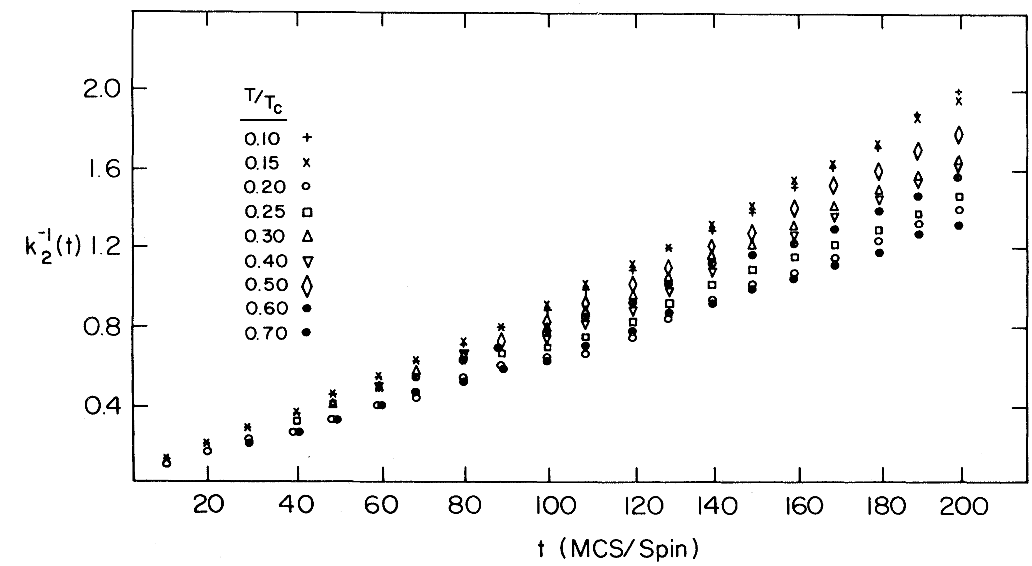

FIG. 2. Inverse second moment as a function of Monte Carlo time at different temperatures. Reasonably linear time dependence for all temperatures is evident. Time is measured in units of $\tau=\tau_0\exp(\epsilon/k_B T)$, where ϵ is an activation energy. Estimated error bars $\pm 12\%$.

in Fig. 1, where the second moment of the structure factor is

$$k_2(t)=\sum_{0\le k\le k_c} k^2 S(k,t) \Big/ \sum_{0\le k\le k_c} S(k,t),\quad k_c=\pi/3 \tag{3}$$

and $x=k/[k_2(t)]^{1/2}$. If scaling holds, F depends only on the scaling variable x. As can be seen from Fig. 1 the scaling behavior seems to work very well in a wide temperature region, $(0.1\text{—}0.7)T_c$. It can also be seen from Fig. 1 that $F(x)$ has a weak dependence on the temperature, which is most notable in the region $x \lesssim 1.0$. Thus there appear to be small deviations from the OJK scaling.[11] At higher x values (>3.0) a least-squares analysis of the form $F(x)\sim x^{-a}$ yields an estimate of $a \simeq 2.7\pm 0.1$ over the temperature region from $0.1T_c$ to $0.7T_c$. This asymptotic large-x behavior differs from the OJK prediction[8] $a=d+1$ by about 10%, but this difference could be due to finite-size effects. The time dependence of the second moment at different temperatures is shown in Fig. 2. One would expect that the time dependence of $k_2(t)$ would be essentially the same as that of $\bar{R}^{-2}(t)$, where $\bar{R}(t)$ is the average domain size. Thus the theory would suggest that $k_2^{-1}(t)$ be linear in time to a good first approximation. As can be seen in Fig. 2 this is the case for all these temperatures. It is worth pointing out, however, that if one takes the OJK prediction for the structure function, one obtains for the second moment the relation $k_2^{-1}(t)=\bar{R}^2(t)G(k_m\bar{R}(t))$, where $k_m=\pi/a$ is an ultraviolet cutoff due to the lattice constant a. (The function G must be calculated numerically and would diverge in the absence of this cutoff.) We have plotted this function G for different values of t and have found that it displays a $t^{1/2}$ behavior. Thus strictly speaking the OJK theory predicts that $k_2^{-1}(t)$ has an additional time dependence beyond the leading linear term due to $\bar{R}^2(t)$. However, within the interval of time studied in our computer experiment, this additional time dependence is too weak to be observed. We should also note that in our calculation of the second moment $k_2(t)$ of the structure factor [Eq. (3)] we introduced an ultraviolet cutoff, $k_c=\pi/3$. In a lattice with lattice constant $a=1$, however, the correct cutoff is the edge of the Brillouin zone, $k_m=\pi$. We have analyzed the tail of the structure factor for $k>\pi/5$ and find a power-law decay given by $Ak^{-\alpha}$ with $\alpha\simeq 2.7$. To study the effect of the cutoff on $k_2(t)$ and the scaling of $S(k,t)$ we have recalculated the second moment by including the power-law tail in the sums of Eq. (3) out to k_m. We find that $k_2^{-1}(t)$ remains linear in time over the time interval we have studied. The scaling of the structure factor is also qualitatively unchanged. $k_2^{-1}(t)$ does change by a constant factor, but this factor does not affect our conclusions. We should also note that the OJK theory predicts a Porod-law type of behavior for the tail, i.e., $k^{-(d+1)}$. The use of this form rather than our empirical form $k^{-2.7}$ in the above analysis leads to the same conclusions as given above.

An alternative way to determine a length scale has been suggested recently by Sadiq and Binder.[12] In our case this corresponds to the definition

$$\bar{L}(t)=\sqrt{S(0,t)/N}\,/\psi_{eq}(T)\,, \tag{4}$$

which follows from the sum rule $S(k=0,t)=N\langle\psi^2(t)\rangle$. Here $\psi(t)$ and $\psi_{eq}(T)$ denote the time-dependent and equilibrium values of the order parameter, respectively. Although our values of $S(0,t)$ exhibit significant fluctuations from run to run, the behavior of $\bar{L}^2(T)$ as determined by (4) is quite similar to $k_2^{-1}(t)$, as can be seen in

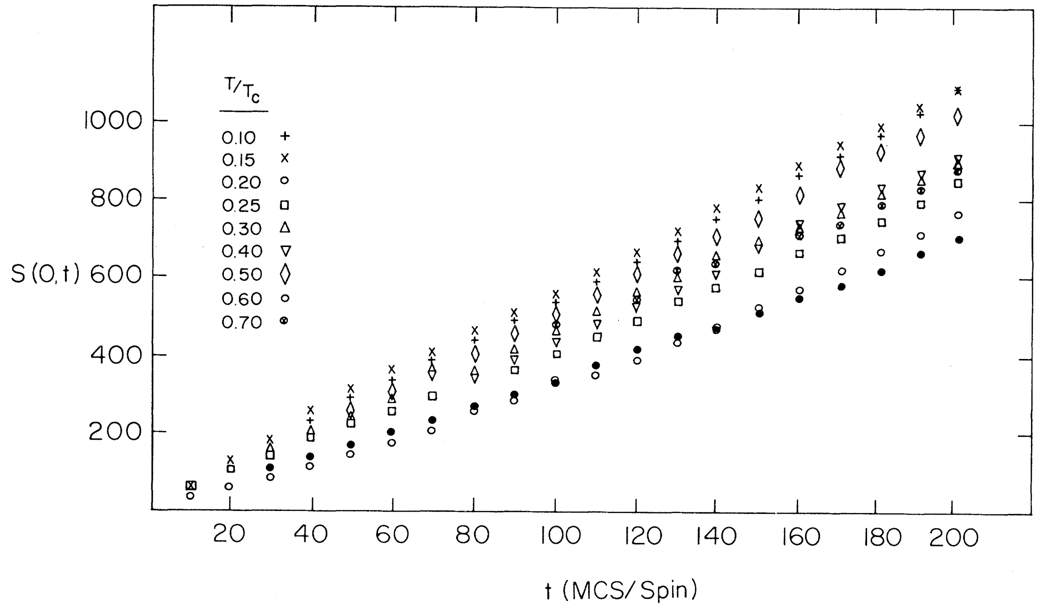

FIG. 3. An alternative length scale as a function of Monte Carlo time at different temperatures. Also here the time dependence is linear [similarly with $k_2^{-1}(t)$; see Fig. 2].

Fig. 3.

Finally we have tried to determine the temperature-dependent prefactor $A(T)$ of the second moment, which is obtained by a least-squares analysis of the form, $k_2^{-1}(t,T)=A(T)t+B(T)$ [and a similar fit for $\bar{L}^2(t)$]. The term $B(T)$ is included to describe early-time "transient effects." This form was used in the analysis of the controlled-growth experiment.[7] In particular Sahni *et al.* found a temperature region governed by an Arrhenius-type behavior $T(\lesssim 0.6T_c)$ and then a region exhibiting a different temperature behavior for $T>0.6T_c$. As can be seen in Figs. 2 or 3, our study also reveals temperature-dependent $A(T)$'s, so that in this sense our results are similar to those of Ref. 7. However, our results for $A(T)$'s do not seem to be in quantitative agreement with their work. In Fig. 4 we have plotted estimates of $A(T)$ and $A'(T)$ obtained from $k_2^{-1}(t)$ and $\bar{L}^2(t)$, respectively, which are based on our "late-time" data in the region $150\leq t\leq 200$ MCS/spin. This shows an overall tendency for the coefficient to decrease as T increases in the interval $0\leq T\leq 0.6T_c$.[13] Furthermore this dependence is the same (within the precision of our data) for $k_2^{-1}(t)$ and $\bar{L}^2(t)$. As noted above, this behavior differs from the controlled-growth results. However, our analysis is limited to a very restricted region of time. If we estimate the amplitudes $A(T)$ and $A'(T)$ in the region of time $80\leq t\leq 200$ MCS/spin, we find an overall temperature dependence which is qualitatively the same as in Fig. 4, within the precision of our data. However, in the temperature interval $(0.2$–$0.25)T_c$ there appears to be a small "dip" in the amplitudes. Therefore, at the present time we cannot give a precise form for the temperature dependence of the $A(T)$'s, since this seems to depend somewhat on the region of time which is used in the analysis. We are currently starting studies of much larger systems, in order to reduce various fluctuation effects present in this and previous studies. We hope this will allow us to make more definitive conclusions than the present study permits. In conclusion we remark that an understanding of the observed temperature dependence of the scaling function, the second moment, and $\bar{L}(t)$ requires an improvement of our current theoretical understanding, as well as improved simulation studies.

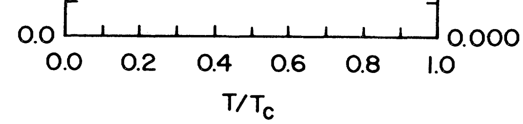

FIG. 4. Temperature-dependent prefactors $A(T)$ (circles) and $A'(T)$ (crosses) for $k_2^{-1}(t,T)$ and $\bar{L}^2(t,T)$, respectively, as obtained from the least-squares analysis of linear (in time) form $A(T)t+B(T)$. Arrows indicate the appropriate axes for $A(T)$ and $A'(T)$. An overall decreasing tendency is seen as temperature increases.

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[11]Note that OJK theory discusses a normalized structure factor $\bar{S}(k,t)$. Their predictions for the scaling function for $S(k,t)$ contains a temperature-dependent prefactor $(\Delta\psi)^2$, where $\Delta\psi$ is the discontinuity in the order parameter at the coexistence curve. We have not included this factor in our analysis since it is essentially constant in the temperature region which we have studied.

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[13]This is in qualitative agreement with the recent theory by Grant and Gunton (Ref. 10).