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Analytic study of domain growth in the Ising model with quenched impurities

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We analytically study the one-dimensional kinetic Ising model with Glauber dynamics in the presence of quenched impurities. We derive the evolution equations for the expectation value of spin and the equal-time pair correlation function. The scaling form of the structure factor is given by $G_k(t) = (1-\rho)t^{1/2}g((1-\rho^2)k^2t,\rho^2t)$ with the impurity concentration ρ, and its scaling function is calculated at zero temperature. We also obtain the average pinned domain size at long time for quenches to $T=0$ in one dimension, and find that it scales inversely with impurity concentration for the small ρ. [S1063-651X(97)50205-4]

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Recently, the effects of impurities or vacancies on domain growth have attracted more and more attention [1–6]. In real materials the presence of impurities or vacancies is quite important since they play a significant role in determining the properties of the material. There are two kinds of impurities [2]: quenched impurities, which are immobile and have the form of macroscopic second-phase particles, and diffusing impurities, which take the form of individual atoms and show behavior similar to diffusing vacancies. Numbers of theoretical works, especially computer simulations, have been carried out to study the mechanism of quenched [1,2] and diffusing [2–6] impurities.

Most of the simulations are based on the kinetic Ising model, where a system is quenched from an initial high temperature to a final temperature less than T_c. This nonequilibrium process exhibits many important dynamic scaling behaviors which have been of great interest [7,8]. For the domain growth without impurities, the equal-time pair correlation function $G(r,t)$ and its Fourier transformation, the equal-time structure factor $G_k(t)$ have the scaling forms $G(r,t)=f(r/L)$ and $G_k(t)=L^d g(kL)$, respectively, where d is the spatial dimensionality and $L(t)$ is the correlation length characterizing the domain structure and scales as $L(t)\sim t^n$. It is well known [7,8] that the growth exponent n is 1/2 for the nonconserved order parameters and 1/3 for the conserved order parameters. Moreover, the scaling functions have been obtained exactly [9,10] for the one-dimensional Ising model with Glauber dynamics [11]. However, the presence of impurities has been shown to affect these scaling properties [1–4]. In the simulations of a two-dimensional nonconserved Ising model with quenched and random impurities carried out by Grest and Srolovitz [1], the average domain size $L(t)$ was observed to increase as $t^{1/2}$ at early times, and then become pinned at a constant which scales as the inverse square root of the impurity concentration ρ for quenches to $T=0$, or become a logarithmic growth for quenches to a final $T>0$. The scaling behaviors of domain growth for the simulations of mixed spin flip and impurities diffusing dynamics are similar, that is, $L(t)$ was found to crossover from the $t^{1/2}$ growth law to a saturate value [2] or an effectively logarithmic growth behavior [3]. While the growth law for the impurity mechanism has been studied in considerable detail, the scaling forms of the correlation function and structure factor have received less attention.

In this paper we analytically study the one-dimensional Ising model with Glauber spin-flip dynamics at zero temperature in the presence of quenched impurities, and exactly calculate the scaling forms of the equal-time structure factor and correlation function, as well as the average domain size in the pinned state. The Hamiltonian for this Ising model is written as

$$\mathcal{H}=-J\sum_{i=1}^{N} n_i n_{i+1}\sigma_i\sigma_{i+1}, \tag{1}$$

where $\sigma_i=\pm 1$ is the normal spin variable, $n_i=0,1$ is the site occupation variable, and $n_i=0$ represents the impurity on the lattice. Thus, $S_i=n_i\sigma_i$ is defined as $+1$ for the up spin, -1 for the down spin, and 0 for the impurity.

In this kinetic model the impurities are randomly placed on the lattice with concentration ρ and become immobile. The up or down spin is flipped with Glauber probability $W=[1-\tanh(\beta\Delta\mathcal{H}/2)]/2$, where $\Delta\mathcal{H}$ is the change of the total energy associated with the spin flip, and $\beta=1/k_BT$. Therefore, using Eq. (1) and the identity $\tanh[\beta J(S_1+S_2)]=x(S_1+S_2)+y(S_1^2S_2+S_1S_2^2)$, where $S_i=\pm 1,0$, $x=\tanh\beta J$, and $y=(1/2)\tanh 2\beta J-\tanh\beta J$, we obtain the transition probability for this one-dimensional nonconserved Ising model

$$W(n_i,\sigma_i)=\tfrac{1}{2}\{1-n_i\sigma_i[x(n_{i-1}\sigma_{i-1}+n_{i+1}\sigma_{i+1}) +yn_{i-1}n_{i+1}(\sigma_{i-1}+\sigma_{i+1})]\}. \tag{2}$$

The master equation for the spin configuration probability $p(n_1,\sigma_1,\ldots,n_N,\sigma_N,t)$ is

$$\frac{dp(n_1,\sigma_1,\ldots,n_N,\sigma_N,t)}{dt}=-\sum_i W(n_i,\sigma_i)p(n_1,\sigma_1,\ldots,n_i,\sigma_i,\ldots,n_N,\sigma_N,t) +\sum_i W(n_i,-\sigma_i)p(n_1,\sigma_1,\ldots,n_i,-\sigma_i,\ldots,n_N,\sigma_N,t). \tag{3}$$

Since the impurities initially placed at random are quenched and immobile, the impurity configuration $\{n_1,n_2,\ldots,n_N\}$ is fixed. Therefore, we can obtain the evolution equations for the expectation value of spin $\langle S_i\rangle$ and the equal-time pair correlation function $G_{ij}(t)=\langle S_i(t)S_j(t)\rangle$ for $i\neq j$ by first fixing the impurity configuration and following the derivation process of Glauber's paper [11], and then averaging over the impurity distribution. The equations of motion we derive are

$$\frac{d\langle S_i\rangle}{dt}=-\langle S_i\rangle+\langle n_i[x(S_{i-1}+S_{i+1}) +y(n_{i-1}S_{i+1}+n_{i+1}S_{i-1})]\rangle, \tag{4}$$

and

$$\frac{dG_{ij}(t)}{dt}=-2\langle S_iS_j\rangle+\langle n_i[x(S_{i-1}+S_{i+1})+y(n_{i-1}S_{i+1} +n_{i+1}S_{i-1})]S_j\rangle+\langle S_in_j[x(S_{j-1}+S_{j+1}) +y(n_{j-1}S_{j+1}+n_{j+1}S_{j-1})]\rangle. \tag{5}$$

Moreover, as the configuration and distribution of quenched impurities remain unchangeable during the kinetic process, for the site occupation variable n_i we have

$$\frac{d\langle n_i\rangle}{dt}=0,$$

$$\frac{d\langle n_in_j\rangle}{dt}=0,$$

$$\cdots\cdots$$

$$\frac{d\left\langle \prod_{i=1}^{N} n_i\right\rangle}{dt}=0. \tag{6}$$

According to the initial random distribution of impurities on the lattice with concentration ρ, Eq. (6) gives $\langle n_i\rangle=1-\rho=\text{const}$, $\langle n_in_j\rangle=(1-\rho)^2$ with $i\neq j$, ... Therefore, due to the random distribution and independent correlation between the immobile impurities as shown above, we assume that n_i and $S_j=n_j\sigma_j$ are uncorrelated for $i\neq j$, that is, $\langle n_iS_j\rangle=\langle n_i\rangle\langle S_j\rangle=(1-\rho)\langle S_j\rangle$, and similarly $\langle n_in_jS_k\rangle=(1-\rho)^2\langle S_k\rangle$, $\langle n_iS_jS_k\rangle=(1-\rho)\langle S_jS_k\rangle$, $\langle n_in_jS_kS_l\rangle=(1-\rho)^2\langle S_kS_l\rangle$, for $i\neq j\neq k\neq l$, etc. Thus, Eqs. (4) and (5) are written as

$$\frac{d\langle S_i(t)\rangle}{dt}=-\langle S_i(t)\rangle+\tfrac{1}{2}\gamma'[\langle S_{i-1}(t)\rangle+\langle S_{i+1}(t)\rangle], \tag{7}$$

and

$$\frac{dG_{ij}(t)}{dt}=-2G_{ij}(t)+\tfrac{1}{2}\gamma'[G_{ij-1}(t)+G_{ij+1}(t)+G_{i-1j}(t) +G_{i+1j}(t)], \tag{8}$$

where

$$\gamma'=(1-\rho)^2\gamma+2\rho(1-\rho)\tanh\beta J, \tag{9}$$

with $\gamma=\tanh 2\beta J$. For $i=j$, we have

$$G_{ii}(t)=\langle S_i^2\rangle=1-\rho. \tag{10}$$

It is noted that Eqs. (7) and (8) are similar to the equations derived by Glauber [11] for the pure one-dimensional Ising model without impurities except for the expression of γ'. If $\rho=0$, that is, there is no impurity, we have $\gamma'=\gamma$ from Eq. (9) and Eqs. (7) and (8) recover the results of Glauber [11]. The exact solutions to these two equations have been given by Glauber, and the scaling function of the equal-time correlation function has been exactly calculated by Bray [9] and by Amar and Family [10] for the pure one-dimensional Glauber model at zero temperature. In the following, we derive the scaling forms of the structure factor and the pair correlation function for the model with quenched impurities.

Considering the translationally invariant situation and averaging over the initial conditions, we can simplify Eqs. (8) and (10) as

$$\frac{dG(r,t)}{dt}=-2G(r,t)+\gamma'[G(r-1,t)+G(r+1,t)], \tag{11}$$

for $r\neq 0$, and

$$G(0,t)=1-\rho. \tag{12}$$

At zero temperature, we obtain from Eq. (9) $\gamma'=1-\rho^2$. Therefore, following the method given by Bray [9], we solve Eqs. (11) and (12) by a combination of Fourier transformation in space and Laplace transformation in time, and give the result for the equal-time structure factor $G_k(t)$ in the scaling limit provided that the initial state contains no long-range order

$$\begin{aligned}G_k(t)=&(1-\rho)2\left(\frac{t}{\pi}\right)^{1/2}\frac{(1-\rho^2)^{1/2}}{2\rho^2+(1-\rho^2)k^2}\\&\times\int_0^1 dy\; y^{-1/2}\{2\rho^2\exp(-2\rho^2 ty)+(1-\rho^2)k^2\\&\times\exp(-[2\rho^2+(1-\rho^2)k^2]t+(1-\rho^2)k^2ty)\}.\end{aligned} \tag{13}$$

Therefore, from Eq. (13) we discover that the equal-time structure factor in the presence of quenched impurities has the scaling form

$$G_k(t)=(1-\rho)t^{1/2}g((1-\rho^2)k^2t,\rho^2t), \tag{14}$$

where the scaling function $g(x,y)$ is given in Eq. (13). The pair correlation function in the scaling limit can be calculated by a Fourier transformation of the structure factor, and from Eq. (14) its scaling form is expected to be

$$G(r,t)=(1-\rho)f(r^2/(1-\rho^2)t,\rho^2t). \tag{15}$$

It is noted that for $\rho\to 0$, Eqs. (14) and (15) give the expected and well known scaling forms $G_k(t)=t^{1/2}g(k^2t)$ and $G(r,t)=f(r^2/t)$, for the one-dimensional nonconserved dynamics without impurities. Moreover, the scaling functions $g(y)$ and $f(x)$ obtained by Bray [9] are recovered from Eq. (13) as well as its corresponding Fourier transformation, respectively. For $\rho^2t\gg 1$, Eq. (13) gives $G_k(t)\to(1-\rho)2[2\rho^2(1-\rho^2)]^{1/2}/[2\rho^2+(1-\rho^2)k^2]$, which corresponds to $G(r,t)\to(1-\rho)\exp\{-[2\rho^2/(1-\rho^2)]^{1/2}r\}$.

One of the main phenomena in the two-dimensional simulations with quenched impurities [1] is the pinned domain state at long times for quenches to $T=0$. The average pinned domain size can be calculated by studying Eq. (8) with translational invariance. The solution of this equation has been given by Glauber [11] as

$$\begin{aligned}G(m,t)=\eta^m+e^{-2t}\sum_{l=1}^{\infty}&[G(l,0)-\eta^l][I_{m-l}(2\gamma't)\\&-I_{m+l}(2\gamma't)],\end{aligned} \tag{16}$$

for $m>0$, where $I_m(x)$ is the modified Bessel function of the first kind, and η is given by

$$\eta=\gamma'^{-1}[1-(1-\gamma'^2)^{1/2}]. \tag{17}$$

Thus, at $T=0$ we have $\eta=[1-\rho(2-\rho^2)^{1/2}]/(1-\rho^2)$ from Eq. (9).

It is shown from Eq. (16) that $G(m,t)$ exponentially decays to its equilibrium solution η^m. Therefore, at long times $G(1,t)$ saturates at value η, and then the average wall density [10] $n(t)=[1-G(1,t)]/2$ is written as

$$n(t)=\frac{1-\eta}{2}. \tag{18}$$

Thus, substituting Eq. (17) into Eq. (18) and using the relation $L(t)=1/n(t)$, we obtain the average pinned domain size $L(t)$ at long times for quenches to zero temperature

$$L(t)=\frac{2(1-\rho^2)}{\rho(2-\rho^2)^{1/2}-\rho^2}. \tag{19}$$

When the impurity concentration is very small, Eq. (19) gives $L(t)\sim\rho^{-1}$. This scaling result is different from that of the two-dimensional simulations where the average pinned domain size is found to scale as $\rho^{-1/2}$. This inconsistency may be attributed to the different physics of the domain wall mechanism, since the final domain size is determined by the impurity concentration at the domain edges. In two dimensions the domain growth is driven by the curvature of the domain wall, while in one-dimensional growth the domain walls perform independent random walks and their diffusion annihilation is expected to be the growth mechanism.

In summary, we have derived the evolution equations of the expectation value of spin and the equal-time correlation function for the one-dimensional kinetic Ising model with Glauber dynamics in the presence of quenched impurities. At zero temperature the scaling function of the equal-time structure factor is calculated, and the scaling forms of the structure factor and the pair correlation function are given by $G_k(t)=(1-\rho)t^{1/2}g((1-\rho^2)k^2t,\rho^2t)$ and $G(r,t)=(1-\rho)f(r^2/(1-\rho^2)t,\rho^2t)$, respectively. In fact, we can recover the well known evolution equations [11], the scaling forms of the structure factor, and the correlation function [7,8], as well as their scaling functions [9,10] for the one-dimensional Glauber model without impurities by setting $\rho = 0$ in our corresponding results. Moreover, the average pinned domain size at long times for quenches to $T = 0$ is obtained. For the small impurity concentration, it is expected to scale inversely with ρ in one dimension. It should be noted that the scaling results we have derived need to be verified by further experimental and simulation work.

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