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Slow Quenching for a One-Dimensional Kinetic Ising Model: Residual Energy and Domain Growth

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A one-dimensional kinetic Ising model with Glauber dynamics subjected to a slow continuous quench to zero temperature is studied. For a rather general class of cooling schemes, described by a time-dependent temperature $T(t)$, the mean domain size $L(t)$ is calculated along with the residual energy $e_{\text{res}}(r)$ as a function of the cooling rate r. If the attempt frequency $\alpha = \alpha_0 \exp(-\varepsilon/kT)$, entering into the transition rates, is temperature dependent (i.e., the barrier ε is nonzero), the asymptotic growth of $L(t)$ is given by $L(\infty) - L(t) \sim \exp[-\varepsilon/kT(t)]$. For this case the residual energy exhibits a power-law behavior $e_{\text{res}}(r) \sim r^{\delta/2(1+\delta)}$ for r small, where $\delta = 4J/\varepsilon$ and J is the nearest neighbor coupling constant. For $\varepsilon = 0$ and for certain cooling schemes the residual energy is zero and $L(t) \sim t^{1/2}$, independent of r.

KEY WORDS: Glauber model; cooling rate dependence; domain growth; residual energy.

1. INTRODUCTION

In the last few years the study of systems subjected to an instantaneous quench has attracted a lot of activity. One of the primary interests has been the domain growth and the asymptotic behavior of the intermediate structure function $S(\mathbf{q}, t)$. The function $S(\mathbf{q}, t)$ is believed to obey a scaling law which states that the $(\mathbf{q}, t)$ dependence is given by $|\mathbf{q}| \cdot L(t)$, where $L(t) \sim t^{\phi}$ is the mean linear size of a domain. Mainly two types of models have been used: kinetic Ising models and time-dependent Ginzburg–Landau models. For details and references see the review by Gunton *et al.*[1]

The aim of this paper is to study the influence of a *continuous* quench with *finite* cooling rate. I use the one-dimensional Ising model with Glauber dynamics. At a certain time t_f, i.e., at a certain temperature

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$T_f = T(t_f)$, the system will fall out of equilibrium and will freeze into a nonequilibrium state. Thus, apart from $L(t)$, also the residual quantities, e.g., the residual energy $e_{\text{res}}(r)$ per particle, which is the energy of the frozen state with respect to the ground-state energy, becomes of particular interest.

This model exposed to a heat bath with time-dependent temperature $T(t)$ was solved by Reiss[2] and discussed by him for a rapid quench. I investigate the opposite limit of slow quenching, for which I calculate the mean domain size $L(t)$ for $t \to \infty$ and the cooling rate dependence of the residual energy $e_{\text{res}}(r)$.

The use of a one-dimensional kinetic Ising model is motivated by recent work[3,4] on a chain of particles with anharmonic and competing interactions. In ref. 3 we showed that the configuration space can be decomposed into 2^N nonoverlapping cells (N is the number of particles). These cells can be labeled uniquely by a sequence $\sigma = \{\sigma_n\}$ of Ising variables $\sigma_n = \pm 1$, $n = 1, 2, \ldots, N$. Furthermore, each cell contains exactly *one* local minimum of the potential energy, its energy being given by the Ising Hamiltonian:

$$E(\sigma) = J_0 \sum_{n \neq m} \eta^{|\eta - m|} \sigma_n \sigma_m - h \sum_n \sigma_n \tag{1}$$

where J_0, η, and h depend on the coupling constants of the interactions. J_0 is always negative and η is between $-1/3$ and $+1/3$. The crucial property of the model is that the phase space state of the particles can easily be decomposed into a configurational part, described by the Ising variables, and a vibrational one. For low kinetic energy per particles (with respect to the barriers between adjacent cells), i.e., for low temperatures, the σ_n change slowly with respect to the fast vibrational modes. Therefore, one can consider the latter as a heat bath inducing transitions between the cells, i.e., transitions from $\sigma \to \sigma'$. Consequently, the chain of particles may be regarded as a realization of a one-dimensional kinetic Ising model.

In ref. 4 we calculated the residual energy $e_{\text{res}}(r)$ for this chain by numerical integration of the Newtonian equations of motion including a damping term. For finite damping constant r (corresponding to a cooling rate) the initially equilibrated configuration relaxed to one of the local minima. The data for $e_{\text{res}}(r)$ could be fitted by a *power law*

$$e_{\text{res}}(r) \sim r^{\mu}$$

with $\mu = \mu_1(\eta)$ for $0.02 < r < 0.8$ and $\mu = \mu_2(\eta) > \mu_1(\eta)$ for $0.004 < r < 0.02$. We interpreted this power-law behavior as the freezing of *independent* two-level systems with energy Δ and barrier B, for which it was shown that[5]

$$e_{\text{res}} \sim r^{\Delta/B}$$

for $r \to 0$. The one-dimensional model exhibits a hierarchy of Δ/B values. Although the exponent μ_1 coincided approximately with one of these Δ/B values, μ_2 did not. However, further numerical investigations have shown that the independent two-level system approach is not quite correct. This demands an improved description, which I believe to be a kinetic Ising model subjected to a continuous quench.

2. THE MODEL

Because the coupling constants in ref. 4 were chosen such that $h=0$ and $0<\eta<0.15$, the Hamiltonian (1) is well approximated by the nearest neighbor Ising model

$$H = -J\sum_n \sigma_n \sigma_{n+1} \tag{2}$$

with $J = -2J_0\eta > 0$. To describe the kinetics, I use the Glauber dynamics. This is justified by the numerical simulation showing that the relaxation occurs through a sequence of *single spin flips*. Thus, I use for the transition probability for the jth spin[6]

$$w_j(\sigma) = \frac{\alpha}{2}\left[1 - \frac{\gamma}{2}\sigma_j(\sigma_{j-1} + \sigma_{j+1})\right] \tag{3a}$$

where

$$\gamma(T) = \tanh\frac{2J}{kT} \tag{3b}$$

$$\alpha(T) = \alpha_0 \exp\left(-\frac{\varepsilon}{kT}\right) \tag{3c}$$

α_0 is a constant setting the time scale and $\varepsilon > 0$ is related to the barrier heights. Because for the present model the barriers depend on σ_{j-1} and σ_{j+1}, a more realistic Ansatz for α would be

$$\alpha(T) = \alpha_1(T)[1 + \alpha_2(T)(\sigma_{j-1}\cdot\sigma_{j+1})] \tag{4}$$

Nevertheless, I will use α from (3c). Since for η small the barriers do not depend too strongly on σ_{j-1} and σ_{j+1}, this should not be a bad approximation. It furthermore makes it possible to solve the equation of motion for the spin correlation function exactly even with a time-dependent temperature.

My goal now is to calculate the mean domain size $L(t)$ for $t \to \infty$ and the residual energy $e_{\text{res}}(r)$. For the one-dimensional Ising model these two quantities follow immediately from the spin correlation function $\langle \sigma_j \sigma_{j+1} \rangle(t)$, which is related to the density of domain walls $\rho_w(t)$ by

$$\rho_w(t) = \tfrac{1}{2}[1 - \langle \sigma_j \sigma_{j+1} \rangle(t)] \tag{5a}$$

Then

$$L(t) = 1/\rho_w(t) \tag{5b}$$

and

$$e_{\text{res}} = 2J\rho_w(t = \infty) \tag{5c}$$

$L(t)$ is measured in units of the lattice constant. Using the transition rate (3), one finds that the correlation functions $C_n(t) = \langle \sigma_j \sigma_{j+n} \rangle(t)$ satisfy the differential equation[6]

$$\dot{C}_n = -2\alpha C_n + \alpha\gamma(C_{n-1} + C_{n+1}), \qquad n \neq 0 \tag{6}$$

with

$$C_0(t) \equiv 1$$

and where translational invariance is assumed.

3. CONTINUOUS QUENCH

The cooling process will be described by a time-dependent temperature $T(t)$ of the heat bath determined by

$$dT/dt = -rf(T) \tag{7}$$

r is the cooling rate and $f(T)$ is positive and decreases to zero monotonically with $T \to 0$ such that $T(t) \to 0$ for $t \to \infty$.[2] For example, $f(T) = T$ describes exponential cooling. In order to calculate $\langle \sigma_j \sigma_{j+1} \rangle(t)$, one has to solve Eq. (6) with *time-dependent* coefficients $\alpha(t) = \alpha(T(t))$ and $\gamma(t) = \gamma(T(t))$. This was done in ref. 2 by introducing a new dimensionless time scale τ

$$\tau(t) = \int_0^t dt' \, \alpha(t') \, \gamma(t') \tag{8}$$

[2] To guarantee that $T = 0$ is not reached in a finite time, f has to approach zero at least linearly in T. This restriction is only for convenience and does not restrict the results.

The solution of Eq. (6) for $n=1$ is then given by [here $\gamma(\tau)$ denotes $\gamma(t(\tau))$]

$$C_1(\tau)=\frac{2}{\pi}\eta_0\int_0^\pi d\Theta\,\frac{\sin^2\Theta\exp(2\tau\cos\Theta)}{1-2\eta_0\cos\Theta+\eta_0^2}\exp\left[-2\int_0^\tau d\tau'\,\frac{1}{\gamma(\tau')}\right]$$
$$+\int_0^\tau d\tau'\,\frac{I_1(2\tau')}{\tau'}\exp\left[-2\int_0^{\tau'}d\tau''\,\frac{1}{\gamma(\tau-\tau'')}\right] \tag{9}$$

I_1 is the modified Bessel function and $\eta_0=C_1(0)=\tanh J/kT_0$ is the equilibrium correlation function for $T_0=T(0)$. Because the system is cooled to zero temperature, the final state depends sensitively on whether $\tau_m\equiv\tau(\infty)$ is finite or not. At least for $f(T)$ decreasing algebraically with $T\to 0$ it follows from (3b), (3c), and (7) that $\tau_m<\infty$ if $\varepsilon>0$. For $\varepsilon=0$, as is usually the case in Monte Carlo dynamics, it is $\tau(t)\sim t$, leading to $\tau_m=\infty$. In the following I will determine $C_1(\tau)$ for $\tau\to\tau_m$, i.e., $t\to\infty$ and $r\ll 1$. The r will be measured in units of α_0.

4. DOMAIN SIZE AND RESIDUAL ENERGY

4.1. For $\epsilon>0$

First of all we need $\tau(t)$ for large t. Substituting (3b) and (3c) into (8) and using $x=\varepsilon/kT(t)$ as an integration variable, one finds with (7) that (here and in the following I omit the technical details because the calculations, while straightforward, are laborious)

$$\tau(t)\cong\tau_m-\frac{1}{r}\,g(T(t))\,e^{-\varepsilon/kT(t)}[1-e^{-\delta\varepsilon/kT(t)}] \tag{10a}$$

where

$$\tau_m=\frac{1}{r}\int_{\varepsilon/kT_0}^\infty dx\;g(x)e^{-x}\tanh\frac{\delta}{2}x \tag{10b}$$

$$g(x)\equiv\varepsilon/[kx^2f(\varepsilon/kx)]>0 \tag{10c}$$

and

$$\delta=4J/\varepsilon \tag{10d}$$

Note that $\tau_m\sim r^{-1}$, i.e., on the τ scale the system has more "time" to find its ground state if r gets smaller, demonstrating that τ and not t is the relevant quantity to describe the quenching.

$C_1(\tau)$ is the sum of two terms, $\bar{C}_1$ and $\bar{\bar{C}}_1$. The term $\bar{C}_1$ contains the influence of the initial condition. Noticing that only small Θ contribute to

the integral in $\bar{C}_1(t)$, one finds, using (10a) (quantities independent of t and r will be denoted by a_0, a_1, etc., and chosen such that $a_i > 0$),

$$\bar{C}_1(t) \cong \bar{C}_1(t=\infty)\left[1+\frac{2}{r}\, g(T(t)) e^{-(1+\delta)\varepsilon/kT(t)}\right] \tag{11a}$$

with

$$\bar{C}_1(t=\infty) \cong a_1 r^{3/2} e^{-2a_0/r} \tag{11b}$$

The second term $\bar{\bar{C}}_1(t)$ becomes

$$\bar{\bar{C}}_1(t) \cong \bar{\bar{C}}_1(t=\infty) - 2(a_2 r^{\delta-1} + a_3 r^{(\delta-2)/2(1+\delta)})\, g(T(t)) e^{-\varepsilon/kT(t)}$$

From this result one obtains in leading order in $\exp[-\varepsilon/kT(t)]$ {note that $\exp[-\varepsilon/kT(t)] \ll 1$ for $rt \gg 1$} with the use of Eq. (5)

$$L(\infty) - L(t) \cong (a_2 r^{\delta-1} + a_3 r^{(\delta-2)/2(1+\delta)})\, g(T(t)) e^{-\varepsilon/kT(t)} \tag{12}$$

where the t dependence of $L(t)$ is completely determined by that of the bath temperature $T(t)$.

To calculate $C_1(t=\infty)$ and thus e_{res} it remains to estimate $\bar{\bar{C}}(t=\infty)$. Substituting $\tau = \tau_m$ into the second term of Eq. (9), it follows for $r \ll 1$ that

$$\bar{\bar{C}}_1(t=\infty) \cong 1 - a_4 R^{\delta} - \frac{4^{1/\delta}}{\sqrt{\pi}}\, \Gamma\left(\frac{2\delta+1}{2\delta+2}\right) R^{\delta/2(1+\delta)} \tag{13a}$$

where

$$R(r) = r\frac{k}{\varepsilon}\left(\frac{\ln r}{1+\delta}\right)^2 f\left(-\frac{\varepsilon(1+\delta)}{k \ln r}\right) \tag{13b}$$

Since $\bar{C}_1(t=\infty)$ can be neglected with respect to $\bar{\bar{C}}_1(t=\infty)$, one finds in leading order in r, omitting the logarithmic corrections, the *power law behavior*

$$e_{\text{res}} \sim r^{\delta/2(1+\delta)} \tag{14}$$

for $r \ll 1$. Thus, the types of cooling does not influence the exponent, but only the logarithmic corrections [cf. (13b)], which is similar to behavior found for the two-level system.[5] The power law (14) can also easily be obtained by more physical arguments: The *relaxation rate spectrum* for the Glauber model for fixed temperature is well known. Apart from the zero eigenvalue, the spectrum is given by[7]

$$\lambda(q, T) = \alpha(T)[1 - \gamma(T) \cos q] \tag{15}$$

where q lies in the first Brillouin zone. It is reasonable to assume that the system falls out of equilibrium at that temperature T_f for which the cooling rate equals the lowest relaxation rate. For the kinetic Ising model this yields the criterion

$$r = \min_q \lambda(q, T_f) \tag{16a}$$

and with the use of (15) one gets

$$r = \alpha(T_f)[1 - \gamma(T_f)] \tag{16b}$$

If $r \ll 1$, the temperature T_f will be much smaller than ε/k and J/k. Thus, using $J/kT_f \gg 1$, one finds for $\gamma(T_f)$ in leading order $\gamma(T_f) \cong 1 - 2e^{-4J/kT_f}$ [cf. Eq. (3b)]. With this result and (3c) one obtains from (16b) that

$$r \cong 2e^{-(\varepsilon + 4J)/kT_f}$$

which can be solved for e^{-2J/kT_f}, yielding

$$e^{-2J/kT_f} \cong (r/2)^{\delta/(1+\delta)2} \tag{17a}$$

At T_f the equilibrium correlation function η_f takes the value

$$\eta_f = \eta_f(T_f) = \tanh J/kT_f \cong 1 - 2e^{-2J/kT_f} \tag{17b}$$

Substituting (17a) into (17b), one gets

$$e_{\text{res}}(r) \sim r^{\delta/2(1+\delta)}$$

in agreement with (14).

4.2. For $\epsilon = 0$

The main effect of $\varepsilon = 0$ is that $\tau(t) \cong t$. In this section we consider only such cooling schemes for which $T = 0$ is reached only in an infinite time implying $\tau_m = \infty$. Taking this into account, it follows from Eq. (9) that

$$C_1(t = \infty) = 1$$

i.e., the residual energy is zero for all cooling rates r. Again as for $\varepsilon > 0$ the asymptotic behavior of $L(t)$ stems from $\bar{\bar{C}}_1(t)$. The asymptotic behavior of $\bar{\bar{C}}_1(t)$ is easily deduced from (9), leading to

$$L(t) \cong (\pi t)^{1/2}$$

independent of r. This result coincides with that obtained for a *sudden* quench to $T = 0$, where the $t^{1/2}$ behavior is found in general, i.e., also in higher dimension, provided the order parameter is nonconserved.[1]

5. DISCUSSION AND CONCLUSION

I have studied the one-dimensional kinetic Ising model with Glauber dynamics subjected to a *slow* quench. If the attempt frequency α is temperature dependent, i.e., the barrier ε is nonzero, the asymptotic domain growth is proportional to $\exp[-\varepsilon/kT(t)]$. Thus, the time dependence of $L(t)$ is governed by that of the temperature.

A more interesting result with respect to our recent work[4] is the power law behavior for the residual energy. The exponent $\delta/[2(1+\delta)]$ is *not* universal, but depends on the ratio $\delta = 4J/\varepsilon$. Qualitatively, this coincides with the behavior of the two-level system, only the functional dependence of the exponent on δ being different. To understand this difference, consider the system at low temperatures before it falls out of equilibrium. In this case the most relevant spin configurations possess large ferromagnetic domains of up and down spins separated by walls. There are two processes leading to an energy relaxation:

(i) *Within* a domain a spin may still flip between up and down, forming a two-level system. The freezing of these give a residual energy proportional to r^{δ}.[5] Such a contribution actually occurs in the present result [see the second term in (13a)].

(ii) The walls can *diffuse* and may become neighboring after a certain time, i.e., the configuration looks like

$$\cdots + + + + - + + + \cdots$$

Now, the central down spin may relax. This mechanism determines the cooling rate dependence of the residual energy in leading order, as is obvious from (13a). It is the diffusion process altering the exponent. This becomes still more obvious if one considers the case $J \gg \varepsilon$, i.e., $\delta \gg 1$. Using this and τ as a new variable, Eq. (6) reduces approximately to a *pure* diffusion equation for $C_1(\tau)$. Within the "time" $\tau_m \sim r^{-1}$ [cf. (10b)] only regions of length smaller than $\tau_m^{1/2}$ can approach local equilibrium. This implies that the mean domain size at τ_m, i.e., at $t = \infty$, is given by

$$L(\infty) \sim \tau_m^{1/2} \sim r^{-1/2}$$

and therefore

$$e_{\text{res}} \sim r^{1/2}$$

in agreement with (14) for $\delta \gg 1$.

Further, I emphasize that the power law behavior is easily obtained from the physical criterion that the cooling rate r equals the *lowest*

relaxation rate at T_f. Although it is well known[8] that the one-dimensional kinetic Ising model shows nonuniversal behavior for the dynamical critical exponent, one still expects a power law behavior for $e_{\text{res}}(r)$ if the dynamics is changed.

To make a reasonable comparison with the numerical results for $e_{\text{res}}(r)$, one has to investigate the chain of particles for r values down to about 10^{-4} and for different η. This work is in progress. For $\eta = 0.135$ (yielding $4J = 0.028$) and $3.3 \times 10^{-4} \leqslant r \leqslant 2 \times 10^{-2}$ we have already found a power law behavior with exponent equal to 0.282 ± 0.03. For the chain model one must distinguish between two relevant barriers B_i $(i = 1, 2)$: $B_1 \cong 0.0126$ for the $(+-+ \to +++)$ transition and $B_2 \cong 0.0244$ for the $(+--\to ++-)$ transition. Using for ε the values of B_1 and B_2, one finds for the exponent in (14) the value 0.345 and 0.256, respectively. The numerical value is just in between. The analytical result could still be improved using Eq. (4) as dynamics, thus taking the σ dependence of the barriers into account.

Finally, we mention that for vanishing barriers and a certain class of continuous quenches to zero-temperature we have found zero residual energy and a $t^{1/2}$ behavior for the domain growth, which is also found for instantaneous quenches, i.e., a finite cooling rate does not influence the growth law.

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