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LETTER TO THE EDITOR

Non-universal freezing in an alternating-bond Glauber chain

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Abstract. Analytical and Monte Carlo techniques are used to study a Glauber Ising chain with spatially modulated coupling strengths, under slow cooling approaching absolute zero. The spin configuration freezes if an appropriately-defined effective time does not diverge. The relationship between energy and cooling rate is found to be non-universal with respect to the cooling programme. Rate-matching arguments are used to clarify this non-universality, to categorize freezing behaviours, and to remove ambiguities present in previous discussions.

When a thermodynamic system is cooled at a finite rate, it will depart from equilibrium when internal rates become too slow for the system to keep up with the external cooling. Depending upon the details of the system and the cooling programme, the system may then remain in the non-equilibrium state indefinitely. Such a situation occurs in the preparation of amorphous solids, spin glasses and other glassy systems. The frozen state is heavily dependent upon the cooling schedule, in particular upon the cooling rate.

The relationship between the cooling rate and the frozen values of such quantities as residual entropy and energy have been a topic of recent interest. This is related to the problem of simulating the equilibrium properties of such a system. A power law relationship of energy ε with respect to cooling time τ

$$\varepsilon \propto \tau^{-\mu} \tag{1}$$

has been conjectured by Grest *et al* [1] for non-NP-complete problems, whereas a modified logarithmic law

$$\varepsilon \propto (\log \tau)^{\alpha} \tag{2}$$

has been proposed by Huse and Fisher [2] as a more general relationship.

The validity of either relationship (1) or (2) is difficult to establish rigorously. There is a dearth of analytical results in this area, and many simulational results are only obtained over one or two decades of τ, and so may fit either law equally well. However, under slow cooling exact results have been obtained for simple kinetic Ising models without random disorder. Although such systems arguably bear little relationship to real glassy systems, they give insight into the mechanism of freezing itself. This helps

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us to understand more complex systems, just as studies of Ising systems have helped our understanding of the behaviour both near to and far from equilibrium. Kob and Schilling [3, 4] have modelled a chain of particles, coupled by anharmonic double-well forces, by a kinetic Ising chain with an energy barrier, and under a cooling programme of the form

$$\mathrm{d}T/\mathrm{d}t = \tau^{-1} f(T) \tag{3}$$

obtain a relationship of the form (1). Simulations of the chain of particles [5] only agree with the predictions of the Ising approximation for very small values of the energy barrier. Jäckle *et al* [6] have studied perhaps the simplest exactly-solvable collective system with intrinsically activated relaxational dynamics, an Ising chain with alternating values for the nearest-neighbour coupling strengths, and obtained two universality classes of cooling programme. However, one of these universality classes occurs for a cooling programme that is not of the form (3).

In this letter, we summarize and extend the analytic results of [6] for two universality classes of cooling of the form (3). We then compare these results with our Monte Carlo simulations of this system under slow cooling.

The model we consider is an Ising chain with alternating coupling constants, that is described with the following Hamiltonian

$$\mathcal{H} = -\sum_i J_i \sigma_i \sigma_{i+1} \tag{4}$$

where

$$\sigma_i = \pm 1 \tag{5}$$

and

$$J_i = \begin{cases} A & \text{for } i \text{ odd,} \\ B\ (<A) & \text{for } i \text{ even.} \end{cases} \tag{6}$$

The system is subject to Glauber single spin-flip dynamics, where the probability per unit time W_Δ for a spin-flip energy by a change Δ is

$$W_\Delta = \frac{1}{2}\left(1 - \tanh\frac{\beta\Delta}{2}\right). \tag{7}$$

We have normalized the unit of time to the bare spin-flip rate. By choosing alternating values for the coupling constants, there are no zero-energy spin-flips, so that all processes require an activation energy. This fact gives rise to a non-universal value for the dynamic critical exponent $z = 1 + A/B$ [7]. It also means that the spin configuration may not evolve at absolute zero temperature. Thus the system may freeze in a non-equilibrium state if the system is cooled to approach zero temperature asymptotically.

From now on we describe the system in terms of the density of kinks on the weak bonds $K = \frac{1}{2}(1 - \langle\sigma_i\sigma_{i+1}\rangle)$ (i even), which is proportional to the energy of the system at low temperatures (when there are vanishingly few kinks on the strong bonds). The quantity K is also a measure of the inverse average domain size. The system is translationally invariant over even multiples of the lattice constant, and so the correlation functions are functions not only of the separation of the spins but also of whether the spins are even or odd. The equations of motion of the four different spin-spin correlation functions are coupled linear differential equations, whose coefficients are functions of time when temperature is varied. Elimination between these equations

yields a tractable form only in the limit of slow cooling and low temperatures. In this limit, the equation of motion of the even–even correlation function $g(x, t) \equiv \langle \sigma_i \sigma_{i+x} \rangle$ is

$$\frac{\partial g}{\partial t} = \omega \left(\frac{\partial^2}{\partial x^2} - \frac{1}{\xi^2} \right) g \tag{8}$$

where $\xi = \exp(2\beta B)$ is the equilibrium correlation length and $\omega = \exp[-2\beta(A-B)]$ is the Arrhenius factor associated with spin-flips at domain walls. Both are time dependent (through the time dependence of temperature) during a cooling procedure. We make a change of variable to the *effective time* $u \equiv \int_0^t \omega \, dt$, and use an integrating factor $\exp \int_0^u \xi^{-2} \, du$, to transform (8) into a standard diffusion equation. The correlation function will therefore not relax to its zero temperature value if the final effective time $u(t=\infty)$ is *finite*. This will always be the case if the zero temperature is reached in finite time, but not necessarily if we choose cooling programmes that approach absolute zero asymptotically in accordance with the third law of thermodynamics.

The equation may be exactly solved by standard techniques. If the initial cooling rate is much slower than the initial equilibration rate then the final solution is found to be independent of the initial conditions. For two classes of cooling programme, both consistent with (3), asymptotic analysis in the limit of slow cooling yields:

(i) For a cooling programme of the form

$$\omega = \omega(0) \exp(-t/\tau) \tag{9}$$

the asymptotic frozen kink density varies like

$$K \propto \tau^{-1/z}. \tag{10}$$

(ii) For a different cooling programme, of the form

$$\omega = \omega(0)/(1 + t/\tau)^d \tag{11}$$

the form obtained for the dependence of the frozen kink density upon the cooling parameters τ and d is:

$$K = \tau^{-1/\alpha} \left(\frac{d-1}{\pi} \right)^{1/2} \left(\frac{z-2}{d\xi_0^2 \alpha} \right)^{((1/2)-(1/\alpha))} \int_0^\infty (1 - \exp(-s^{-((1/2)-(1/\alpha))})) \, ds. \tag{12}$$

where $\xi_0 = \omega^{-1/(x-2)}(0)$ is the initial value of the correlation length, and α is defined by

$$\alpha = z - \frac{z-2}{d}. \tag{13}$$

Changing τ but keeping d constant yields $K \propto \tau^{-1/\alpha}$. (In [6], the particular choice $d \propto 1/\log \tau$ was made, leading to ω not being simply a function of t/τ. This cooling programme is not of the form (3), and yields a threshold behaviour $K \propto (\tau_c - \tau)^{1/2}$.)

The freezing exponent is dependent upon the non-universal dynamic critical exponent z, as would be expected. Perhaps more surprisingly, however, the freezing exponent is also non-universal with respect to the details of the cooling programme, even for systems within the same universality class for critical dynamics. This occurs in spite of the fact that we have constrained ourselves to cooling programmes of type (3) (i.e. with a well defined characteristic cooling time), which approach absolute zero only asymptotically. Whilst other dynamical phenomena (e.g. domain growth, critical dynamics) display less universality than static phenomena, it is still the case that the characteristic exponents for such phenomena are a property of a given system. By

constrast, a given system possess freezing exponents which depend continuously upon the type of cooling to which it is submitted.

To confirm this unexpected result of the analysis, we performed Monte Carlo simulations of the model system under continuous cooling. A chain of size 1024 spins was used, which was sufficiently large for finite size effects to be unimportant for the cooling programmes used, where the largest domain size was ~30 units. The choice $A/B=3$ was made, yielding $z=4$. The lattice was split into two sublattices, to exploit the vector processing capability of the machine used (Stardent 1500). The system was prepared in a state corresponding to thermal equilibrium at temperature $T=2B/k_B$, and then the temperature was changed in discrete steps, with a constant number of sweeps at each temperature. Different values for the parameter τ were obtained both by rescaling all flip probabilities by the ratio τ/τ_0, where τ_0 is the slowest cooling time, or by altering the number of Monte Carlo sweeps per temperature step. Between 16 and 60 independent runs were performed for each set of values of the cooling parameters. The results for the two classes of cooling programme were as follows.

• For the cooling of type (i), 10 values of τ in the range 3×10^2–10^6 were simulated. The kink density as a function of temperature during cooling programmes corresponding to five typical values of τ is shown in figure 1. The final value of the kink density on a log-log scale is plotted against τ in figure 2. A straight-line fit yields the gradient 0.254 ± 0.02, compared with the theoretical value $1/z=0.25$.

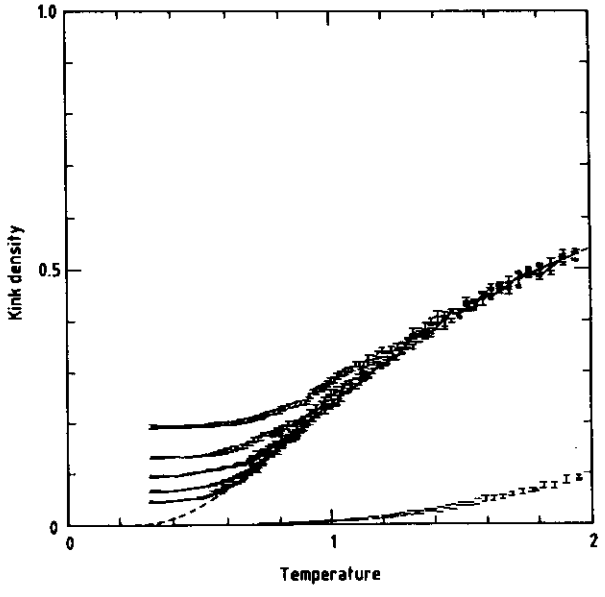

Figure 1. Kink density as a function of temperature during five cooling procedures of type (i) (see text). The lower line represents the density of kinks on strong (A) bonds. The dotted curve is the equilibrium value of the kink density.

• For the cooling of type (ii), six values of τ were simulated for $d=2$, 3, 4, 5. Figure 3 shows the kink density as a function of temperature for six different values of τ at $d=4$. Figure 4 is a log-log plot of the final kink density against τ for four different values of d. The gradients of the straight line fits are shown in table 1.

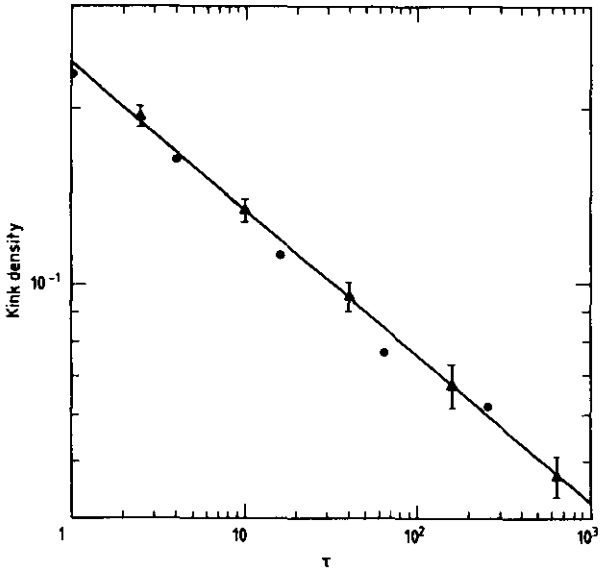

Figure 2. Frozen kink density for ten values of τ for cooling programmes of type (i), on a log–log scale (see text). The triangles (with error bars) are averaged over 32 independent runs, the circles over 16 runs. The line is a fit to the data, with gradient -0.254 ± 0.02.

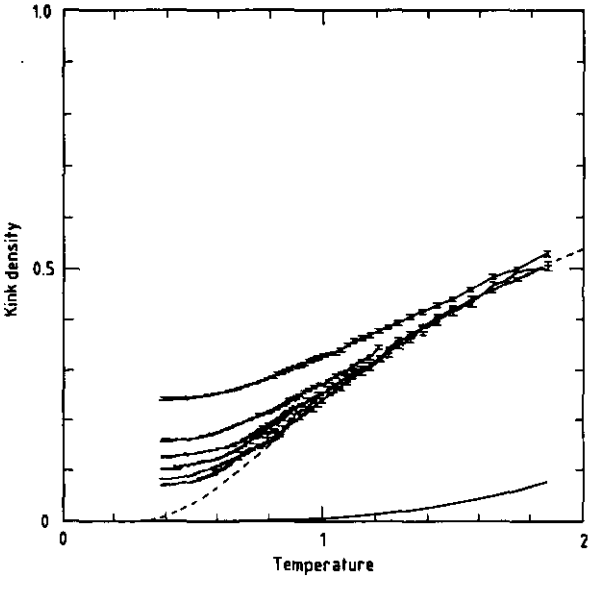

Figure 3. Kink density as a function of temperature for cooling procedures of type (ii) (see text), for six values of τ, with $d = 4$. The lower curve is the density of kinks on strong bonds. The dotted curve is the equilibrium value of the kink density.

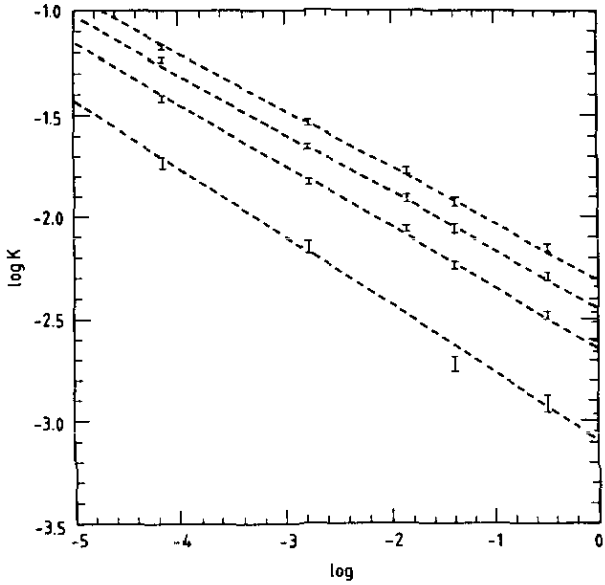

Figure 4. log (frozen kink density) as a function of log τ, for cooling programmes of type (ii), for six values of τ at each of four values of d (see text). The straight lines are each fits to the data for a particular value of d; for the gradients, see table 1.

Table 1. Gradients g_0 of a plot of log τ against log K, for cooling programmes of type (ii), divided by the theoretical values g_α.

d	g_0/g_α
2	0.95 ± 0.06
3	0.97 ± 0.02
4	1.04 ± 0.02
5	0.99 ± 0.02

To test the d-dependence of the final kink density, figure 5 is a plot of K_r against $(d=1)^{1/2}$, where

$$K_r = K \frac{\tau^{1/\alpha}(d\xi_0^2\alpha/(z-2))^{((1/2)-(1/\alpha))}}{\int_0^\infty (1-\exp(+s^{+((1/2)-(1/\alpha))}))\,\mathrm{d}s}. \tag{14}$$

At each value of d, the different points correspond to different values of τ, which are coincident due to the removal of the τ dependence in K_r. The straight line is the theoretical fit of a straight line through the origin, predicted by (12).

The exponent for the cooling class (i) is easily explained by arguments based on movement of domain walls [8]. Single spin-flips at domain walls occur at a rate proportional to ω, and after a number of the order of ξ^2 of such flips a given domain wall reaches and annihilates with another domain wall. The equilibration time of this system is therefore $\xi^2/\omega = \xi^z$ [7], so that we expect the system to fall out from equilibrium when the cooling time satisfies $\tau \approx \xi^z$, reproducing (10).

In order to explain the results (13), however, we need to be much more precise in our definition of the cooling rate. The system falls out of equilibrium in response to

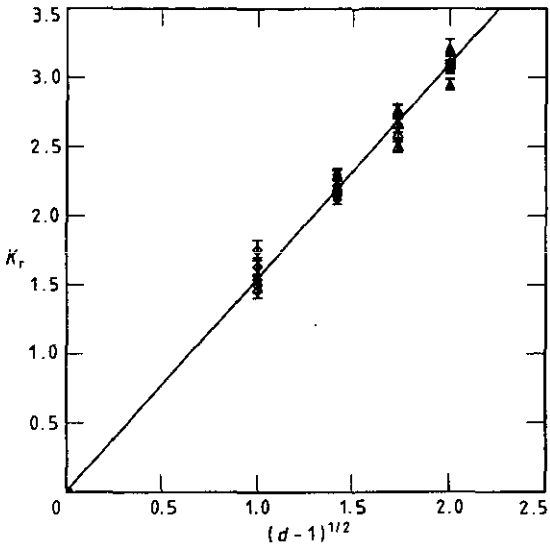

Figure 5. Frozen kink densities from the logarithmic cooling programmes, plotted in the form K_r against $(d-1)^{1/2}$ (see text). The straight line is a least squares fit, constrained to pass through the origin. Open diamonds: $d=2$; filled diamonds: $d=3$; open triangles: $d=4$; filled triangles: $d=5$.

the change in the equilibrium values of the system coordinates. A given coordinate falls out of equilibrium when its relaxation rate is of the order of the fractional rate of change of its equilibrium value. The relevant cooling rate is therefore specific to the property under consideration. In particular, we are interested in the domain size of the system which we identify as the inverse kink density. Then we define the cooling rate with respect to domain size as

$$r_c = \frac{d}{dt} \log \xi. \tag{15}$$

Under this definition, we see that the cooling rate for programme (i) is constant, whereas for (ii) the cooling rate becomes a function of time. We expect that the system will freeze at a point where the cooling rate is equal to the equilibration rate r_{eq}

$$r_c \propto r_{eq} = \xi^{-z} \tag{16}$$

with a constant of proportionality that is independent of τ but possibly dependent on the class of cooling programme. Using $\xi = \omega^{-1/(z-2)}$, (16) yields result (13). It is interesting to note that the d-dependent factor in (12) is not reproduced; this is to be expected, since as $d \to 1$ the system spends more and more time relaxing after departing from equilibrium, and so the approximation that the system freezes abruptly becomes less and less valid. Case (i) then corresponds to a 'natural' choice for cooling programme, since all relaxation times in the system are of Arrhenius form.

The above two choices of cooling programme yield asymptotic power law behaviour for freezing, but we might ask whether other types of relation may occur for different cooling programmes still consistant with (3). Suppose a cooling programme where the correlation length varies like $\xi = f(t/\tau)$ freezes at $t = t_F$, where the correlation length

is $\xi_F(\tau) = f(t_F/\tau)$. Then (16) produces a differential equation for (t_F/τ), which may be integrated to provide the dependence of ξ_F on τ through

$$\frac{t_F}{\tau} = \text{constant} + \int^{\tau} \xi_F^{z-1}(\tau') \frac{d\xi_F(\tau')}{d\tau'} \frac{d\tau'}{\tau'} \equiv h(\xi_F) \tag{17}$$

where h is some function specific to the choice of the functional form of ξ_F. This may be inverted to produce $h^{-1}(t_F/\tau) = \xi_F(\tau) (= \xi(t_F/\tau))$. A cooling programme that produces a prescribed freezing relation ξ_F is then given by $\xi(t/\tau) = h^{-1}(t/\tau)$. Then we make the following remarks:

- t_F/τ approaches a finite limit if ξ_F varies more slowly with τ than with $\tau^{1/z}$. A cooling programme that approaches zero temperature asymptotically must be characterized by t_F/τ diverging as τ diverges, so programmes of this type may never produce freezing relations (such as logarithmic ones) that are slower than this form. Other (faster) relationships, e.g. that arising in programme (ii), $\xi_F \sim \exp(\gamma\tau)$ etc, are possible.
- Any relationship between ξ_F and τ is possible for cooling programmes reaching absolute zero in finite time. For instance, $\xi(t/\tau) = 1/\log(1 - t/\tau)$ gives $\xi_F \sim \log(\tau)$.

In [5], Kob and Schilling chose a cooling programme of the form

$$T \propto \exp(-\gamma t)). \tag{18}$$

For γ sufficiently small, the cooling programme is equivalent to (i) in the freezing region, and so their predicted power law should hold. However, the relaxation times of their system are Arrhenius in form, and so a cooling programme of the form (9) is again a more natural choice. The choice (18) in (16) yields a transcendental equation, so there is a broad crossover region before the true asymptotic region is reached. This is supported by the fact that in some cases they were unable to obtain the predicted asymptotic behaviour, and suggests they were actually in the crossover region.

We remark that the two-level system studied by Huse and Fisher [2] is another example of a system with Arrhenius-like relaxation times. One therefore obtains a non-universal exponent if cooling schedules other than (3) are used.

If the relaxation time for a given mode is not Arrhenius-like, or the coordinates of the system are not proportional to Boltzmann factors, a cooling schedule of form (i) will not be a natural choice, and equation (16) will not yield a power law relationship. True glasses, for example, are characterized by relaxation times that obey the Vogel–Tamman–Fulcher law

$$\tau_r \sim \exp\left(\frac{A}{T - T_0}\right). \tag{19}$$

A cooling programme of the form $X \sim \exp(-t/\tau)$, where X is a Boltzmann factor, will then give a freezing relationship of the form

$$X = X_0 + \frac{(\text{constant})}{\log \tau} \tag{20}$$

where X_0 is the value of X at the initial temperature T_0.

In conclusion, we have shown for a 1D kinetic Ising model that the relationship between frozen kink density and cooling rate is non-universal with respect to the type of cooling programme used. Even for cooling programmes in the same universality class, an 'unnatural' choice can lead to a broad crossover region before the asymptotic relationship holds. For cooling programmes approaching absolute zero asymptotically,

the slowest relationship that may be obtained is a power law. For simulations that lower the temperature to absolute zero in finite time, any relationship may be obtained, and so the cooling rate needs to be specified more carefully in order to ensure that the appropriate law is observed.

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