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On the relaxation processes of the one-dimensional kinetic Ising model

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Abstract. We study various relaxation phenomena of the general single-spin-flip one-dimensional kinetic Ising model with transition rates $w_i(\sigma_i) = \frac{1}{2}\alpha(1 + \delta\sigma_{i-1}\sigma_{i+1})[1 - \frac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})]$. We show that the long-time behaviour can be described by an exponential decay (except at some special parameter values) contrary to previous numerical results. Furthermore we prove that the exponent z characterizing the disappearance of the excitation gap is not restricted. The case of $\delta = 1$ is investigated in detail.

1. Introduction

Kinetic Ising models are the simplest ones exhibiting non-trivial dynamical behaviour. They describe an Ising system in contact with a heat bath. Therefore, the time evolution of the model is stochastic and not generated by a Hamiltonian. One possible choice for the dynamics, proposed by Glauber (1963), is a model in which transitions between configurations occur due to the flipping of single spins. Glauber solved this model exactly for the one-dimensional homogeneous chain with nearest-neighbour interactions. He could give a closed expression for the time dependence of various observables and found that the relaxation is exponential, at least for long times. This is the only case so far where the whole spectrum of the time evolution operator has been worked out explicitly (Felderhof 1971). (There exists another solution (Deker and Haake 1979, Kimball 1979) from which, for example, the dynamical exponent can be extracted, but we do not know the whole spectrum in that model.)

Because of the relative simplicity of the model it seems straightforward to use numerical methods to study the dynamics as was done, for example, by Skinner (1983), Pandit *et al* (1981), Bauer *et al* (1988) (see also references therein). Some of these authors find that the relaxation of, for example, the autocorrelation function is not exponential—suprisingly enough, not even for the exactly known case. Therefore the question arises naturally as to whether one can show that, similarly to Glauber's solution, the long-time behaviour is recovered by the exponential decay or whether there are special values of the parameters appearing in the transition rates where a different type of relaxation occurs. On the other hand the kinetic Ising model gives a good description of the dynamics of some polymer melts (see, e.g., Skinner 1983) and even of glassy-like models (Kob and Schilling 1990) where one finds, in experiments and numerical simulations, a stretched exponential behaviour on the intermediate time scale and it would be useful to have predictions for longer times as well.

Both the magnetization and correlation function calculated within the Glauber model (Glauber 1963) show non-trivial critical slowing down at $T_c = 0$. The scaling theory describes the dependence of the relaxation time τ on the divergent correlation length ξ as $\tau \sim \xi^{\tilde{z}}$, where $\tilde{z}$ is the dynamical critical exponent. In the following we use another variable z instead of $\tilde{z}$, which characterizes the disappearance of the excitation gap and which will be called the gap exponent. The meaning of this distinction is that the disappearance of the gap has its origin not necessarily in the collective dynamics, as was first emphasized by Achiam and Southern (1992) in a somewhat different context. The value of z at different choices of the transition rates is not known exactly. Using approximate renormalization group treatment Achiam (1978, 1980) obtained $z = 2$ for all possible transition rates. Cordery *et al* (1981) gave physical reasons for arguing that $2 \leqslant z \leqslant 4$ and $z > 2$ can be reached only in the limit $\delta \to 1$, $T \to 0$ (δ is the parameter characterizing the different rates). From a variational calculation Haake and Thol (HT) (1980) obtained lower and upper bounds for z: $z = n + 2$ for $0 \leqslant n \leqslant 2$ and $4 \leqslant z \leqslant n + 2$ for $n \geqslant 2$. (n characterizes the correlation of the two mentioned limiting process—see also equation (12).) Numerical diagonalization of the time evolution operator (Pandit *et al* 1981) identified the upper bound of HT as the exact value. To resolve this contradiction we give a better lower bound for z and point out the differences between the various definitions of z. We show that using the definition of HT, one finds $z \geqslant (n + 1)$ for $\delta = -1$ as well, which has its origin in the existence of a conserved quantity at $\delta = \pm 1$ and is not connected with the special properties of the $T_c = 0$ critical point. The somewhat exotic $\delta = 1$ case will be treated in detail.

2. The time evolution operator

Consider a linear chain of Ising spins $\sigma_n = \pm 1$ ($n = 1, 2, \ldots, N$) with nearest-neighbour interactions. The energy of the spin system can be written as $E(\{\sigma_n\}) = -J \sum_n \sigma_n \sigma_{n+1}$, where J denotes the coupling constant. For simplicity we assume periodic boundary conditions. The master equation then reads

$$\frac{\partial P(\sigma_1, \sigma_2, \ldots, \sigma_n; t)}{\partial t} = -\sum_i w_i(\sigma_i) P(\sigma_1, \sigma_2, \ldots, \sigma_i, \ldots, \sigma_N; t) + \sum_i w_i(-\sigma_i) P(\sigma_1, \sigma_2, \ldots, -\sigma_i, \ldots, \sigma_N; t). \tag{1}$$

The transition probability $w_i(\sigma_i)$ is given by

$$w_i(\sigma_i) = \tfrac{1}{2}\alpha(1 + \delta\sigma_{i-1}\sigma_{i+1})[1 - \tfrac{1}{2}\gamma\sigma_i(\sigma_{i-1} + \sigma_{i+1})] \tag{2}$$

where $\gamma = \tanh(2J/k_B T)$; $-1 \leqslant \delta \leqslant 1$ is a further parameter, which may but need not depend on the temperature (the Glauber model is recovered by $\delta = 0$); $\alpha/2$ characterizes the time scale of the spin flips and we use $\alpha = 2$. This transition probability is the most general one for the one-spin-flip dynamics satisfying the detailed balance condition (Glauber 1963). The interpretation of the parameter δ is simple: $\delta < 0$ prefers (compared with the $\delta = 0$ case) spin flips, which does not alter the energy whereas $\delta > 0$ prefers energy changing flips. In other words one could say that $\delta < 0$ decreases the probability of domain wall creation and only allows their movement, while $\delta > 0$ means 'defect' creation and annihilation.

The time evolution of a classical stochastic model can be described by a quantum model of the same spatial dimension (Kogut 1979). The time evolution (or master) operator of this kinetic model can be expressed as (see also Siggia 1977, Kimball 1979, Peschel and Emery 1981):

$$\hat{H} = \sum_n \Big\{ 1 - \gamma(1+\delta)\sigma_n^z\sigma_{n+1}^z + \delta\sigma_n^z\sigma_{n+1}^z - \tfrac{1}{2}\sigma_n^x\left(1-\delta+(1+\delta)\sqrt{1-\gamma^2}\right) + \tfrac{1}{2}\sigma_n^x\sigma_{n-1}^z\sigma_{n+1}^z\left(1-\delta-(1+\delta)\sqrt{1-\gamma^2}\right)\Big\} \tag{3}$$

or performing a duality transformation

$$H_\delta = N - \gamma(1+\delta)\sum_n \tau_n^z + \delta\sum_n \tau_n^z\tau_{n+1}^z - \tfrac{1}{2}\left(1-\delta+(1+\delta)\sqrt{1-\gamma^2}\right) \times \sum_n \tau_n^x\tau_{n+1}^x - \tfrac{1}{2}\left(1-\delta-(1+\delta)\sqrt{1-\gamma^2}\right)\sum_n \tau_n^y\tau_{n+1}^y. \tag{4}$$

Here we introduced new variables $\tau_n^z = \sigma_n^z\sigma_{n+1}^z$, $\tau_{n-1}^x\tau_n^x = \sigma_n^x$ (σ and τ denote the Pauli matrices). The factor N in equations (3) and (4) makes the time evolution operator positive definite i.e. it leads to relaxation (Haken 1978). The Hamiltonian H_δ at special parameter values becomes simpler: (i) $\delta = 0$ the z–z coupling disappears and H_δ can be easily diagonalized by introducing lattice fermions; (ii) $H_{\delta=-1}$ is an isotropic ferromagnetic Heisenberg Hamiltonian, which does not depend on the temperature; (iii) only at the $\delta = \pm 1$ values does the Hamiltonian become rotational invariant (around the z axis), which may lead to a vanishing excitation gap (see later sections for details).

The ground state of H_δ, which is equivalent to the equilibrium state of the original Ising model and which has, therefore, the eigenvalue $\lambda_0 = 0$, can be constructed in a simple way:

$$|\phi_0\rangle = \otimes_i |g_i\rangle \qquad |g_i\rangle = |\uparrow\rangle_i + g|\downarrow\rangle_i/\sqrt{1+g^2} \tag{5}$$

where $\otimes$ denotes the direct product and $g = ((1-\gamma)/(1+\gamma))^{1/4}$ does not depend on δ. This feature is the consequence of the δ-independence of the detailed balance condition and consequently of the equilibrium state.

Now we should realize that the following identities hold

$$H_\delta = (1+\delta)H_{\delta=0} - \delta H_{\delta=-1} = (1-\delta)H_{\delta=0} + \delta H_{\delta=1}. \tag{6}$$

Since H_δ, $H_{\delta=0}$ and $H_{\delta=\pm1}$ have a common ground state one can conclude that the excitation gap Δ satisfies the following inequalities (see also HT (1980))

$$(1-|\delta|)\Delta_{\delta=0} \leqslant \Delta_\delta \leqslant (1+|\delta|)\Delta_{\delta=0} \tag{7}$$

for all δ, γ values, where $\Delta_{\delta=0} = 1-\gamma$ is known from the exact solution (Felderhof 1971). Here it is important to note that the lower and upper bounds can also be reached, since $H_{\delta=\pm1}$ have gapless continuous spectra. This disappearance of the gap can be easily demonstrated using a spin-wave excitation-like variational wavefunction constructed as follows

$$|\phi_k\rangle = \sum_k \mathrm{e}^{\mathrm{i}kl}|\psi_l\rangle \tag{8}$$

$$|\psi_l\rangle = |g_1\rangle \otimes |g_2\rangle \otimes \ldots \otimes |g_{l-1}\rangle \otimes |-1/g_l\rangle \otimes |g_{l+1}\rangle \otimes \ldots \otimes |g_N\rangle. \tag{9}$$

This state is orthogonal to the ground state since

$$\langle g|-1/g\rangle = \frac{\langle\uparrow| + g\langle\downarrow|}{\sqrt{1+g^2}} \frac{|\uparrow\rangle - 1/g|\downarrow\rangle}{\sqrt{1+1/g^2}} = 0. \tag{10}$$

$|\phi_k\rangle$ is not an eigenstate, but because of its orthogonality to the ground state we get an upper bound of the excitation gap

$$\Delta \leqslant \Delta_k = \langle\phi_k|H_\delta|\phi_k\rangle = 4 - 2\gamma(1+\delta)\frac{1-g^2}{1+g^2} + \frac{2\cos k}{(1+g^2)^2}\left[4g^2\delta - (1-\delta)(1+g^4) + 2(1+\delta)\sqrt{1-\gamma^2}g^2\right]. \tag{11}$$

This is a complicated k-dependent expression, but one can easily conclude that: (i) Δ_k becomes zero only at $\delta = \pm 1$; and (ii) the zero value can be reached at $k = 0$ for $\delta = -1$ and at $k = \pi$ for $\delta = 1$. Unfortunately this simple spin-wave-like excitation fails to reproduce the known gap value at $\delta = 0$.

The reason why the ground state can be explicitly constructed is that the time evolution operator of the kinetic model involves special correlations among the coupling constants and the magnetic field. Similar simplification of the ground state for Heisenberg models were realized earlier, for example, by Kurmann *et al* (1982) and were explained by the existence of the so called disordered lines (Ruján 1982, and references therein). In these models the ground state is simple but the excitations are not known at all.

Concluding this section we can realize from equation (7) that the gap of the time evolution operator is always finite for $\delta \neq \pm 1$, indicating exponential time decay of the original model, at least for long times.

3. The gap exponent

As already mentioned in the introduction there is some controversy concerning the value of the dynamic critical exponent $\tilde{z}$ if the limits $T \to 0$ and $\delta \to 1$ are performed simultanously. We shall see in this section that the limiting processes $T \to 0$ and $\delta \to -1$ show similar peculiarities and that the whole controversy has its origin in the definition of $\tilde{z}$ and therefore we shall use z in the following, which is well defined.

The static correlation length ξ of the $d = 1$ Ising model is given by $\xi^{-1} = \log\coth(J/k_{\mathrm{B}}T)$ and $\xi \to \infty$ as $T \to 0$. Instead of ξ and T we always use γ in the following and we utilize the relation $\xi \sim (1-\gamma)^{1/2}$ as $\gamma \to 1$. The simultaneous limits $\delta \to \pm 1$ and $\gamma \to 1$ will be characterized by the exponent n, which is defined through

$$1 - |\delta| = (1-\gamma)^{n/2}. \tag{12}$$

For the sake of completeness we first treat the $|\delta| \neq 1$ case. We saw in the previous section that there exist δ-dependent lower and upper bounds for the gap: $(1-|\delta|)\Delta_{\delta=0} \leqslant \Delta \leqslant (1+|\delta|)\Delta_{\delta=0}$. Since we keep $(1-|\delta|)$ finite and $\Delta_{\delta=0} \sim (1-\gamma)$ we can immediately conclude that $z = 2$ for these cases. This result was also found by all the previously cited authors.

Let us now pay attention to the different definitions of z: Haake and Thol (1980), Pandit *et al* (1981) and Bauer *et al* (1988) define z from the gap of the master operator, whereas Cordery *et al* (1981) investigate only equilibrium quantities and their values correspond to $\tilde{z}$ whereas the other authors calculate z. We argue in the following that we have to make a strict distinction between these definitions, as they are not directly comparable. We show that the physical picture used by Cordery *et al* (1981) is applicable for the non-equilibrium situation as well and leads to the same value for z as the one conjectured from the behaviour of the gap of the master operator.

First we take a closer look at the gap. From equation (11) we get for $k = 0$ and for $k = \pi$

$$\Delta_{k=0} = 4\sqrt{1-\gamma^2}(1+\delta) \qquad \Delta_{k=\pi} = 4(1-\delta). \tag{13}$$

From these upper bounds for Δ one can derive a lower bound for z. Using equation (12) one arrives at $n \leqslant z \leqslant (n+2)$ as $\delta \to 1$ and $(n+1) \leqslant z \leqslant (n+2)$ as $\delta \to -1$ for *all* n values. Consequently we can give a better lower bound for z than the formerly known values (and we can discuss the $\delta \to \pm 1$ cases in the same way), which means that z can reach any positive value. The numerical results of Pandit *et al* (1981) suggest that the upper bound coincides with the exact value.

On the other hand equation (13) shows that the gap disappears at $\delta = \pm 1$ independently of the temperature, which is a simple consequence of the existence of conserved quantities. For $\delta = -1$ the energy stays constant while the corresponding observable for $\delta = 1$, which is a bit more tricky, will be explicitly constructed in the next section.

Now we proceed to show how one can find the time scale leading to the exponent $z = (n+2)$. Let us first treat the $\delta = -1$ case. In the equilibrium state the relaxation of, for example, the autocorrelation function can be derived using the physical picture of Cordery *et al* (1981). The typical cluster size is proportional to the correlation length ξ and the cluster decays through the diffusive motion of the domain wall, since the flipping of a spin inside a homogeneous cluster costs too much energy (it takes much more time). The time scale of the decay of the cluster is, therefore, determined by the number of diffusive steps needed to cross the length ξ, i.e. $\tau \sim \xi^2$. It means that $z = 2$.

Another question is how the equlibrium configuration can be reached from a given initial state. The probability of the following transition $\uparrow\uparrow\uparrow \to \uparrow\downarrow\uparrow$ (creation of domain walls) is proportional to $(1+\delta)(1-\gamma) \sim \xi^{n+2}$. The other rates are much larger in the $\gamma \to 1$ limit and they generate the equilibrium distribution of the walls (at a given number) on a relatively short time scale. Consequently, starting from, for example, a homogeneous initial configuration the time scale of the domain wall creation is proportional to ξ^{n+2}, which results in $z = n + 2$. It is clear that this long time corresponds to the small gap found earlier and is strongly related to the conserved quantity.

For $\delta = 1$ the situation is more complicated. Here one needs a two-step process to find the shortest time scale in equilibrium (Cordery *et al* 1981), since the defect motion is strongly depressed: $\uparrow\uparrow\downarrow\downarrow\downarrow\rightarrow\uparrow\uparrow\downarrow\uparrow\downarrow\rightarrow\uparrow\uparrow\uparrow\uparrow\downarrow$. The probability of the first process is proportional to $(1-\gamma)$ and that of the second to 1. Therefore the two-step movement happens on a time scale $\sim \xi^2$. The length of the cluster is $\sim \xi$ and it should be crossed by a diffusive particle, therefore we arrive at $\tau \sim \xi^4$ in equilibrium. A similar two-step process works in the non-equilibrium case as well: $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\rightarrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\rightarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow$. The transition rate for the first process is proportional to $(1-\delta)$ and for the second one to 1. It means that the typical time to annihilate two defects is $\tau \sim \xi^n$. On the other hand the wall movement is a much faster process and can, at this level, be treated as diffusion. Consequently it takes $\sim \xi^2$ steps to create a domain of length ξ, i.e. $\tau \sim \xi^{n+2}$. This leads immediately to the previously conjectured result of $z = (n+2)$.

Concluding this section we gave a new upper bound for the gap of the master operator and showed that it can be arbitrarily small. Furthermore we argued applying a physically motivated cluster picture that the generation of the equilibrium cluster configuration leads to $z = (n+2)$, in agreement with numerical data (Pandit *et al* 1981). Therefore it is important to define different relaxation times for equilibrium and for non-equilibrium quantities in the $d = 1$ kinetic Ising model. These arguments show that we can get arbitrary large z values because of the existence of a metastable state (which is, for example, a periodic arrangement of two-up and two-down clusters for $\delta = 1$) and the long time scale corresponds to the escape from this metastable 'valley'.

4. The $\delta = 1$ case

In this section we construct the conserved quantity coupled to $\delta = 1$ and comment on the special properties of other observables at this parameter value as well.

Since the steady creation and annihilation of domain walls is a more complicated process than the motion of defects, a mapping onto the $\delta = -1$ case will be performed first. Introducing new spin variables $s_{4i+j} = (-1)^{[i/2]}\sigma_{4i+j}$, where $[\cdot]$ denotes the integer part. The description of the dynamic process in terms of these new variables is equivalent to the original model. The new transition probabilities are given through

$$w_i(s_i) = (1 - \delta s_{i-1}s_{i+1})[1 - \tfrac{1}{2}\gamma(-1)^i s_i(s_{i-1} - s_{i+1})] \tag{14}$$

where we have utilized $s_i s_{i+1} = (-1)^i \sigma_i \sigma_{i+1}$. In this way one can define lattice gas variables: $n_i = [1 + (-1)^i \sigma_i \sigma_{i+1}]/2$. $n_i = 1$ corresponds to a defect in the Ising model with the spins s_i, but its meaning in terms of the σ_is is more complicated, since it depends explicitly on the site, i.e. the translational invariance is lost. One further difference compared with the original $\delta = -1$ model is the temperature dependence of the hopping rates. If p_i denotes the transition probability of the particle to the correct neighbouring place, then they are given through $p_i = [1/2 + (-1)^i\gamma/2]$ and $p_i + q_i = 1$ defines the transition probability to the other side. Since the number of the lattice gas particles is conserved, one can study the different values separately. For the probability $P(l,t)$ that the site l at time t is occupied the following equation holds

$$\dot{P}(l,t) = -P(l,t) + p_l P(l+1,t) + q_l P(l-1,t) \tag{15}$$

which leads to the well known diffusive motion with temperature-dependent diffusion constant. For the two-, three-, etc particle distributions similar equations hold.

Now we derive the time dependence of this particle for $\delta \neq 1$ and construct a quantity which always relaxes exponentially, independently of the system parameters. To this end we start from the master equation for the two spin correlation function

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\sigma_i\sigma_k\rangle = -\langle\sigma_i\sigma_k(w_k(\sigma_k) + w_i(\sigma_i))\rangle \tag{16}$$

(see, for example, the original paper from Glauber). Introducing $q_{i,k} = (-1)^i\langle\sigma_i\sigma_k\rangle(t)$ we can write

$$\begin{aligned}\dot{q}_{i,i+1} &= -2q_{i,i+1}+\delta(q_{i-1,i}+q_{i+1,i+2})+\tfrac{1}{2}\gamma(1+\delta)(q_{i,i+2}+q_{i-1,i+1})+\gamma(-1)^i(1+\delta)\\ \dot{q}_{i,i+2} &= -2q_{i,i+2} - \tfrac{1}{2}\gamma(1+\delta)(q_{i,i+1} - q_{i+1,i+2} + q_{i,i+3} - q_{i-1,i+2})\\ &\qquad + \delta(-1)^i(\langle\sigma_{i-1}\sigma_i\sigma_{i+1}\sigma_{i+2}\rangle + \langle\sigma_i\sigma_{i+1}\sigma_{i+2}\sigma_{i+3}\rangle).\end{aligned} \tag{17}$$

Summing over i we arrive at

$$\dot{Q}_1 = \sum_i \dot{q}_{i,i+1} = -2(1-\delta)Q_1 \qquad \dot{Q}_2 = \sum_i \dot{q}_{i,i+2} = -2Q_2. \tag{18}$$

It means that the time dependence of Q_2 is independent of δ and of the temperature and that $\dot{Q}_1 = 0$ for $\delta = 1$.

Concluding this section we note that for $\delta = 1$, similarly to $\delta = -1$, a conserved quantity exists, which can even be interpreted as a particle number. Furthermore we have found a special correlation function Q_2, whose time dependence is independent of the system parameters and which relaxes exponentially even for zero temeperature. This means that Q_2 should be orthogonal to all low-lying excitations, which might give some information about these states.

5. Discussion

Earlier numerical studies by Skinner (1983), Budemir and Skinner (1985) and Bauer *et al* (1988) found non-exponential decay of the correlation functions of the $d = 1$ kinetic Ising model. These studies used either small systems or were able to treat only short times (e.g. Budemir and Skinner used only times where the value of the autocorrelation function exceeded 0.1, since otherwise their method was unreliable). This means that their stretched exponential decay belongs to this time regime, although they argue that this decay could have a relevance for longer times as well.

We could show, however, that the master operator always has a finite gap for $\delta \neq \pm 1$, which yields exponential relaxation for long times, except for quantities which are orthogonal to the ground state. It is not a simple task to find the long time behaviour numerically, since, as we saw, the relaxation times increase as the limiting values of δ are approached. On the other hand, it is known (Spohn 1989) that the decay of the autocorrelation function for $\delta = -1$ is non-exponential and is asymptotically proportional to $\exp(-\sqrt{t/\tau})$. Consequently one probably sees a continuous transition from exponential to non-exponential decay at a given time scale changing δ. A similar calculation for $\delta = 1$ does not exist at the moment, but an analogy with the previous section suggests that a similar relaxation function can be found for this case as well.

It is important to note that the equilibrium state strongly depends on the dynamics and if we have $\delta = \pm 1$ then these states can have a completely different structure as in the neighbourhood of these limiting values. It makes somehow the application of the temperature-dependent Gibbs measure for $\delta = -1$ questionable (Spohn 1989) and therefore we should define these values as limits which should be performed before the long time limit.

On the other hand it is important to emphasize again the difference between the gap exponent z and the dynamic critical exponent $\tilde{z}$ (Achiam and Southern 1992). z characterizes the disappearance of the excitation gap, whereas $\tilde{z}$ appears in the scaling relations. As we have explicitly stated the disappearance of the gap is connected with the existence of a conserved quantity and has nothing to do with collective phenomena. It probably results from the singularity of the amplitude in a $\tau \sim A(T)\xi^{\tilde{z}}$-like expression†. The increase of $A(T)$ is a completely different physical phenomenon from the increase in $\tilde{z}$, although both lead to a vanishing gap.

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† I thank the referee calling my attention to this point.