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Persistence and dynamics in the ANNNI chain

Parongama Sen and Subinay Dasgupta

Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700 009, India

E-mail: parongama@vsnl.net and subinay@vsnl.net

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Abstract

We investigate both the local and global persistence behaviour in the ANNNI (axial next-nearest-neighbour Ising) model. We find that when the ratio κ of the second neighbour interaction to the first neighbour interaction is less than 1, $P(t)$, the probability of a spin to remain in its original state up to time t shows a stretched exponential decay. For $\kappa > 1$, $P(t)$ has an algebraic decay but the exponent is different from that of the nearest-neighbour Ising model. The global persistence behaviour shows similar features. We also conduct some deeper investigations in the dynamics of the ANNNI model and conclude that it has a different dynamical behaviour compared to the nearest-neighbour Ising model.

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1. Introduction

The tendency of a spin in an Ising system to remain in its original state following a quench to zero temperature has been extensively studied over the last few years and is well established as an example of the phenomenon called persistence in dynamical systems [1]. Quantitatively, persistence is measured by the probability $P(t)$ that a spin does not flip up to time t. $P(t)$ shows a power-law behaviour, i.e., $P(t) \sim t^{-\theta}$, where θ is a new exponent not related to any other static or dynamic exponent. This phenomenon has been observed and studied quite extensively in Ising models with nearest-neighbour interaction in different dimensions [1–3].

Apart from such 'local' persistence, one can also study the 'global' persistence [4] behaviour by measuring the probability $P_G(t)$ that the order parameter does not change its sign till time t. At the critical temperature, the probability that the individual spins will not be flipped till time t has an exponential decay, while the global persistence shows an algebraic decay: $P_G(t) \sim t^{-\theta_G}$. The critical temperature of the Ising model in one dimension being zero, the global persistence becomes a quantity of interest together with the local persistence

at zero temperature. Exact values of the exponents for the nearest-neighbour Ising chain are known to be $\theta = 0.375$ [2] and $\theta_G = 0.25$ [4].

In this paper, our objective is to investigate the effect of frustration on (local and global) persistence, by computer simulation of an ANNNI (axial next-nearest-neighbour Ising) chain [5] at zero temperature. This model has the Hamiltonian

$$H = -\sum_{i=1}^{L}(S_i S_{i+1} - \kappa S_i S_{i+2}), \tag{1}$$

where S_i is the spin (± 1) at the ith site and κ (>0) is the parameter which represents the amount of frustration. We choose this particular model for our study because it is perhaps the simplest classical model with tunable frustration and because this model as such shows very interesting static and dynamic behaviour [5–8]. As regards static behaviour, the ground state is ferromagnetic for $\kappa < 0.5$, antiphase ($++--$ type) for $\kappa > 0.5$ and highly degenerate for $\kappa = 0.5$. On the other hand, zero-temperature dynamics using a single spin-flip does not lead to the ground state for $0 < \kappa < 1$ but does lead to the ground state for $\kappa > 1$ [7].

Our main observation is that for $0 < \kappa < 1$ there is no persistence (i.e., no algebraic decay of $P(t)$) while for $\kappa > 1$ there *is* persistence albeit with a persistence exponent different from that of the unfrustrated nearest-neighbour Ising model (i.e., $\kappa = 0$). We also claim, using some novel approaches, that as regards domain dynamics, the ANNNI model belongs to a different dynamical universality class for $\kappa > 1$.

In section 2, we describe the model and the studies on local persistence for $\kappa < 1$ and $\kappa > 1$. In section 3, the dynamics of the domains for $\kappa > 1$ is analysed in detail. The global persistence behaviour is presented in section 4. Since the behaviour at $\kappa = 1$ is unique, we have discussed it in a separate section (section 5). The results are summarized and discussed in section 6.

2. Local persistence in ANNNI chain

2.1. The model

We take an ANNNI chain of L spins in one dimension with periodic boundary condition in a random configuration (infinite temperature) and quench it to zero temperature. Thus, our updating rule is that a spin is selected randomly from the system, it is flipped (not flipped) if its energy is positive (negative), and it is flipped with probability 0.5 if its energy is zero. L is always chosen to be a multiple of 4 to ensure complete antiphase ordering. We have used $L = 8000$–$12\,000$ (unless otherwise mentioned) and averaged the results over 10^3–10^4 configurations as necessary.

Case I: $\kappa < 1$

For local persistence, in the entire range $0 < \kappa < 1$ the decay of $P(t)$ is not algebraic (figure 1), but rather a stretched exponential,

$$P(t) \sim \exp(-\alpha t^{\beta}) \tag{2}$$

with $\alpha = 1.06$ and $\beta = 0.45$. The exponent β as well as the coefficient α is found to be independent of κ. There is no special behaviour at $\kappa = 0.5$, the multiphase point for the ground state.

The dynamical processes occurring in the system are as follows. In the first few dynamical steps (the precise number depends on the system size) domains of size 1 are removed and one is left with domains of size $\geqslant 2$. No domain wall is annihilated or created henceforth but

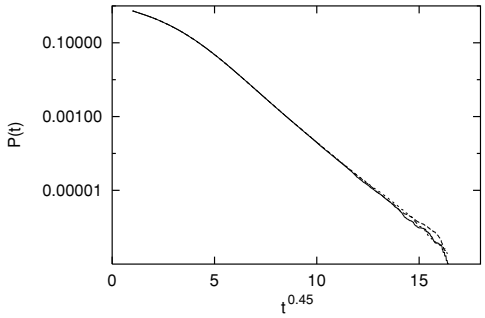

Figure 1. The variations of $P(t)$ for $\kappa < 1$ are shown for $\kappa = 0.2, 0.4, 0.6$ against $t^{0.45}$. The curves fit fairly well to a linear form in the log–linear plot indicating that $P(t)$ fits to a stretched exponential form $P(t) \sim \exp(-1.06t^{0.45})$. The local persistence seems to be independent of κ. Here the simulations have been done for $L = 12\,000$.

the dynamics continues indefinitely as all domains of size >2 are unstable. As a result, the system attains a non-equilibrium steady state but the equilibrium state is never reached and in a finite time all the spins in the system are flipped. This justifies the faster than power-law decay of $P(t)$ in the system. To illustrate our argument further, we observe from simulation studies that after the first few iterations (typically ten iterations for a system of $L = 16\,000$ spins) the number of domain walls per spin (say M/L) attains a constant value of 0.2795. This constant value of M/L is quite close to the most probable value of M/L which can be theoretically estimated easily. Under the constraint that each domain is of size $\geqslant 2$, the number of configurations in a system of L spins and M domains is

$$N(L, M) = \binom{L - M}{M}, \tag{3}$$

and the maximum value of this quantity is for

$$\frac{M}{L} = \frac{(\sqrt{5} - 1)}{2\sqrt{5}} = 0.2764. \tag{4}$$

Case II: $\kappa > 1$

For local persistence, in the range $\kappa > 1$, the behaviour of $P(t)$ agrees well with an algebraic decay

$$P(t) \sim t^{-\theta'} \tag{5}$$

at large t (figure 2). However, θ' shows a weak dependence on the time interval over which it is calculated, indicating that there is a correction to the scaling. We have calculated the slopes in the log–log plot over different intervals of time and found that θ' increases slowly with time initially but at large times ($t > 10\,000$) attains convergence to $\theta' = 0.69 \pm 0.01$. This value is considerably different from that of the ferrromagnetic Ising model. The value of θ' remains the same for all κ except at the point $1/\kappa = 0$, where the system breaks up into two independent sublattices with nearest-neighbour antiferromagnetic interactions, and θ' becomes equal to θ. The dynamics here is such that the patches of antiphase state (e.g., $+ \; + \; - \; -$) grow in size gradually and the equilibrium (lowest-energy) configuration of antiphase is reached eventually. Similar dynamics also prevails in the ferromagnetic state ($\kappa = 0$), as the regions of up (or down) spins grow in size and ultimately fill up the entire system. However, one must note that inspite of the similarity in *dynamics*, the *persistence exponents* are indeed different. In the next section we investigate the domain dynamics for $\kappa > 1$ in greater detail.

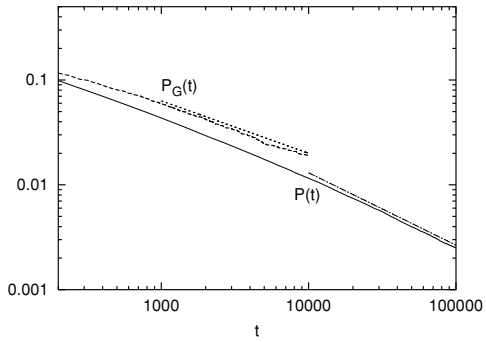

Figure 2. The variations of $P(t)$ and $P_G(t)$ are shown for $\kappa = 2.0$. Both have a power-law decay, the best fit straight lines in the log–log plot for large t show that $P(t)$ has an exponent $\sim$0.69 while $P_G(t)$ has an exponent $\sim$0.50 (see the text for the details in calculating the exponent θ'). The curves are the same for all $\kappa > 1$. Here the simulated system sizes are $L = 10\,000$ and $L = 8000$ for $P(t)$ and $P_G(t)$ respectively.

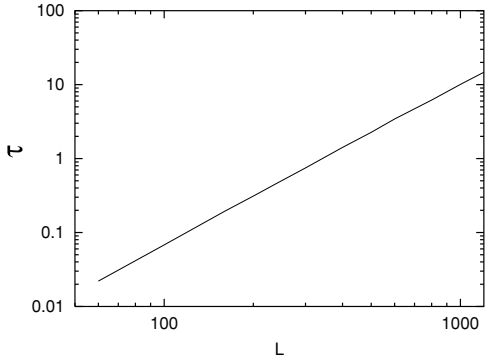

Figure 3. Lifetime τ (scaled down by 10^5) is shown against the system size L. τ increases as $L^{2.15}$. The value of $\kappa = 2.5$ here.

3. Domain dynamics for $\kappa > 1$

In some earlier studies [6, 7], it has been concluded that the ANNNI model belongs to a different dynamical universality class compared to the nearest-neighbour Ising model. However, precise values of exponents for other dynamical processes, e.g., dynamical exponent, are not available for the ANNNI model. In the nearest-neighbour ferromagnetic Ising case, the dynamical exponent $z = 2$. Here we have attempted to estimate the value of z', the dynamic exponent for the ANNNI chain.

To estimate z' directly, we have calculated the lifetimes τ defined as the time up to which the dynamics continues in the ANNNI model as a function of the system size L (figure 3). In the nearest-neighbour Ising model, this time varies as L^z, while for the ANNNI model we find

$$\tau \sim L^{z'},$$

with $z' \simeq 2.15$.

The dynamics in the nearest-neighbour Ising model can be viewed as a random walk of the domain walls which separate regions of up-spins and down-spins. The domain walls annihilate each other when they meet and their number M reduces with time as $t^{-1/z}$ with the value of z equal to 2 as mentioned above. On the other hand, in the ANNNI model, the domain

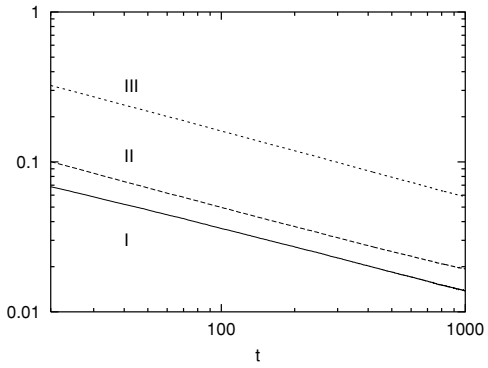

Figure 4. The time decay of M' (number of domains of length other than 2; curve maked I), of 'defect' sites D (II) and of excitation energy ΔE (III) are shown against time t ($\kappa = 2.5$). All the simulations have been done for systems with $L = 1000$ spins.

dynamics is different and the domain walls have a different role in the antiphase state. In order to compare the dynamics in these two systems, it is therefore useful to regard the domain walls in the non-frustrated ($\kappa = 0$) Ising model as 'defects' and compare its dynamics with that of an analogous quantity in the ANNNI model. We have adopted a number of ways to estimate the defects in the ANNNI model (for $\kappa > 1$) as a function of time to get an estimate of the domain decay exponent. In the following we briefly describe these methods.

First we note that the excitation energy $\Delta E(t)$ (deviation from the ground-state energy) of any state in the nearest-neighbour ferromagnetic Ising model is identical to the number of domains (apart from some multiplicative constant), and as the system relaxes to its equilibrium ground state, ΔE also shows a decay $\Delta E \sim t^{-1/2}$. In the ANNNI model also, we study the relaxation of energy by computing ΔE which shows the behaviour (figure 4) $\Delta E \sim t^{-1/z'}$ with $z' \simeq 2.40$. We claim that z' is the dynamic exponent in the ANNNI model.

Secondly, a direct measure of the defects defined to be simply the spins that do not belong to $++--$ type states has also been done (e.g., in the distribution $++--+++--$, the seventh spin is a defect, while in $++--++++$ the seventh and eighth spins are defects). Our simulation shows that the number of such defects, D, *also* decreases as $t^{-1/z'}$ for all $\kappa > 1$ with $z' \simeq 2.30$.

A third way to estimate z' is to count the number of domains which are not of length 2, i.e., domains which do not satisfy the antiphase configuration. As mentioned earlier, in [7], the dynamics of domains of different lengths were studied from which it was concluded that the ANNNI chain belongs to a new universality class. Here we count all domains of size other than two. We find a power-law variation of this quantity (say M') again with exponent $1/z'$ where $z' \simeq 2.30$. All the above results are shown in figure 4.

From all the above estimates, we conclude that the dynamic exponent is $z' = 2.3 \pm 0.1$ for the ANNNI model in one dimension.

It is possible, in principle, to calculate the value of z' also from the relation

$$P(t \to \infty, L) \sim L^{-z'\theta'}, \tag{6}$$

when the dynamics has stopped altogether [9]. However, such an estimate would require simulations up to $L^{z'}$ number of Monte Carlo steps for a system of size L. We could get these data only for systems with $L \leqslant 1000$ which is insufficient to give a good scaling of $P(t \to \infty, L)$ with L.

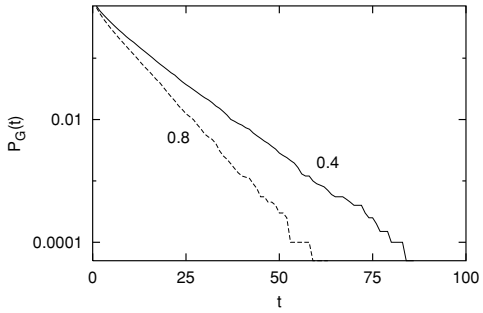

Figure 5. The variations of $P_G(t)$ for $\kappa < 1$ are shown. The labels indicate the values of κ. The exponential decay is accompanied by different exponents for $0 < \kappa < 0.5$ and $0.5 < \kappa < 1.0$. The system size is $L = 12\,000$ here.

4. Global persistence

We shall now present our results on *global* persistence. In this context one needs to be careful in defining the order parameter for different values of κ. For $\kappa < 0.5$, the global persistence may be calculated in terms of the magnetization as for the ferromagnetic nearest-neighbour Ising model and the global persistence shows an exponential decay:

$$P_G(t) \sim \exp(-0.10t). \tag{7}$$

In the entire range $0.5 < \kappa < \infty$, one needs to define the antiphase order parameter. It is not easy to put forward such a definition in a straightforward manner. One may be tempted to define the sublattice magnetization

$$S_1 + S_2 - S_3 - S_4 + S_5 + S_6 - S_7 - S_8 + \cdots$$

as the order parameter but such a definition does not work because the antiphase has a four-fold degeneracy. We propose instead to consider the magnetizations over four sublattices:

$$m_\alpha = \sum_{j=0}^{L/4-1} S_{\alpha+4j}; \qquad \alpha = 1, 2, 3, 4 \tag{8}$$

as the order parameter. The global persistence function $P_G(t)$ is evaluated for each sublattice and an average over the four sublattices is taken. We have verified that for $\kappa = 0$, with this definition of order parameter one gets a power-law decay of $P_G(t)$ with the known exponent 0.25.

For $0.5 < \kappa < 1$, $P_G(t)$ again has an exponential decay

$$P_G(t) \sim \exp(-0.16t) \tag{9}$$

which is faster than that observed in the region $0 < \kappa < 0.5$ (equation (7)). The results for global persistence for $\kappa < 1$ are shown in figure 5.

For $\kappa > 1$ there is algebraic decay of the global persistence (figure 2)

$$P_G(t) \sim t^{-\theta'_G}, \tag{10}$$

with $\theta'_G \simeq 0.5$, which is different from the exponent for the nearest-neighbour Ising model in one dimension. It should be noted that for $\kappa = 0$ the global persistence behaviour could be analysed exactly [4] because the dynamics is essentially that of some independent random walkers which annihilate each other. There is no such simplification here, as the jth spin in the αth sublattice, namely $S_{\alpha+4j}$, is independent of the neighbouring spins in the same sublattice, but depends on the jth spin in the other sublattices.

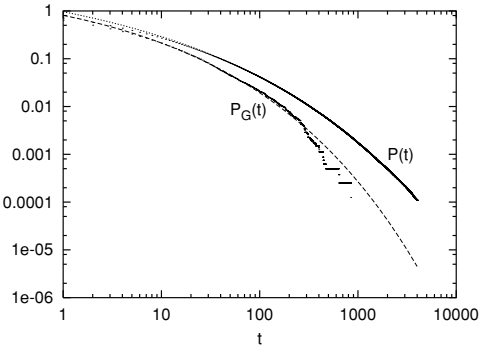

Figure 6. The variations of $P(t)$ and $P_G(t)$ for $\kappa = 1$ are shown. Both have a stretched exponential decay; the best fit curves shown in the figure are $4.39\exp(-1.69t^{0.25})$ for the global curve and $6.52\exp(-1.92t^{0.21})$ for the local curve. Data correspond to a $L = 8000$ system.

5. Dynamics at $\kappa = 1$

The point $\kappa = 1$ signifies a dynamical transition point with different dynamical behaviour on its two sides and the behaviour here is different from that for lower or higher κ values. The fraction of persistent spins $P(t)$ decays as a stretched exponential (figure 6)

$$P(t) \sim \exp(-1.92t^{0.21}) \tag{11}$$

but this decay is slower than a similar decay (equation (2)) for $0 < \kappa < 1$. As regards the behaviour of domain decay, we have found that (i) the excitation energy ΔE, (ii) the number of defects D (the sites that do not belong to the pattern $++--$), (iii) the number of domains (M') which are not of length 2, all decay as $t^{-1/z''}$ and the lifetime τ also grows with L as $L^{z''}$ with $z'' \simeq 3$.

It is interesting to note that the persistence $P(t)$ does not decay algebraically which one would expect from the fact that the dynamics does lead to the equilibrium state although at a rate much slower than that for $\kappa > 1$ [7]. This is again, we believe, a special feature related entirely to the persistence phenomena.

The dynamical transition point $\kappa = 1$ is marked by a stretched exponential decay of the global persistence also

$$P_G(t) \sim \exp(-1.69t^{0.25}), \tag{12}$$

as shown in figure 6.

6. Summary and conclusions

In summary, we have studied the persistence behaviour for the ANNNI chain for all possible values of κ, the parameter governing frustration in the model. Three regions of different behaviour of local persistence are obtained as κ is varied. The fraction of persistent sites shows a stretched exponential decay for $\kappa < 1$. At $\kappa = 1$, it is also stretched exponential with a different exponent. For $\kappa > 1$, algebraic decay of the persistence probability is observed with exponents different from that of the unfrustrated case. An estimate of the dynamical exponent z' using several approaches has been made from which we conclude $z' \simeq 2.30$. This confirms that the ANNNI model belongs to a different universality class from that of the unfrustrated nearest-neighbour Ising model for which the corresponding exponent has a

value 2. When global persistence is considered, we again observe different types of behaviour of the persistent probability in the above three regions. The behaviour of both local and global persistences is unique at $\kappa = 1$, the dynamical transition point. One should note that there is thus some abrupt change in behaviour (both of local and of global persistence) at the points $\kappa = 0, \kappa = 1$ and $1/\kappa = 0$. In other words, the behaviour changes sharply as soon as a slight amount of next-nearest-neighbour interaction is added to nearest-neighbour interaction, or a slight amount of nearest-neighbour interaction is added to next-nearest-neighbour interaction.

It should be mentioned that three regimes of persistence (namely, exponential, stretched-exponential and algebraic) have also been studied earlier, although in somewhat different contexts [10]. It should also be pointed out here that all the dynamical features obtained here are for the single spin-flip Glauber dynamics. Other types of dynamics, as considered in [6, 7] could lead to different behaviour.

Before we conclude we must also mention that for serial updating (where the sites are visited serially and updated) the results presented here remain qualitatively the same in the sense that the indices remain the same upto the accuracy of the simulation. Also, for $\kappa > 1$, one obtains the same values of the exponents even if one starts with a ferromagnetic state instead of a random state.

Acknowledgments

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