Dynamical frustration in ANNNI model and annealing

Parongama Sen and Pratap Kumar Das
Department of Physics, University of Calcutta, 92 Acharya Prafulla Chandra Road, Kolkata 700009, India.

Zero temperature quench in the Axial Next Nearest Neighbour Ising (ANNNI) model fails to bring it to its ground state for a certain range of values of the frustration parameter $\kappa$, the ratio of the next nearest neighbour antiferromagnetic interaction strength to the nearest neighbour one. We apply several annealing methods, both classical and quantum, and observe that the behaviour of the residual energy and the order parameter depends on the value of $\kappa$ strongly. Classical or thermal annealing is found to be adequate for small values of $\kappa$. However, neither classical nor quantum annealing is effective at values of $\kappa$ close to the fully frustrated point $\kappa = 0.5$, where the residual energy shows a very slow algebraic decay with the number of MCS.

Keywords: frustration, zero temperature quenching, domain dynamics, small world network, freezing, Suzuki Trotter mapping

I. INTRODUCTION

Simulated annealing is usually applied to systems with frustration, like spin glasses and optimisation problems, where the energy landscape is complex with many spurious minima. There are certain other systems, however, which have very simple energy landscape picture and ground states, but still the system fails to reach its ground state during a energy-lowering dynamical process. This situation corresponds to “dynamical frustration”. We have specifically considered the case of the axial next nearest neighbour (ANNNI) chain, where such a situation is encountered. In section II, we elaborate the notion of dynamic frustration with examples and in section III, the dynamics in ANNNI model is discussed in detail. The results of application of the classical and quantum annealing are discussed in sections IV and V. Summary and some concluding comments are given in the last section.

II. DYNAMIC FRUSTRATION IN ISING MODELS

Quenching dynamics in magnetic systems has been a topic of intense research over the last few decades. In quenching dynamics, the system has a disordered initial configuration corresponding to a high temperature. As the temperature is suddenly decreased quite a few interesting phenomena take place like domain growth [1,2], persistence [3–6] etc.

The Ising model maybe regarded as the simplest model describing magnetic properties of many real systems and it shows a rich dynamical behaviour with respect to the above phenomena. The dynamics of Ising models has been extensively studied in lattices of different dimensions as well as on graphs and networks.

In dynamical studies, the system is allowed to evolve from the initial configuration following a certain prescription and the commonly used dynamical rule at zero temperature is the Glauber dynamics, i.e., a spin is chosen randomly and flipped if it makes the energy lesser, not flipped if energy increases and flipped with probability $1/2$ if there is no energy change.

The zero temperature deterministic dynamics in Ising models can be visualised as the motion of interfaces and the domains grow in size as the interfaces annihilate on approaching each other (Fig. 1). In one dimension, a zero temperature quench of the Ising model ultimately leads to the equilibrium configuration, i.e., all spins point up (or down).

In two or higher dimensions, however, the system does not always reach equilibrium [7–12]. Such a situation corresponds to dynamical frustration when the system gets frozen in a metastable state which does not correspond to the ground state. For example, in the two dimensional lattice (Fig. 2), the dynamics stops at a higher energy when the domain walls are straight and appear without any corner. The system thus acquires a “striped phase”, where the number of stripes is an even number. In dimensions higher than two, there maybe other kind of frozen states in which the system gets locked.

This kind of freezing or blocking is also encountered in ferromagnetic Ising models on random graphs and small world networks where there are finite number of random long range bonds. In the random graph, any two spins are connected with a finite probability while in the small world network, random long range connections occur in addition to nearest neighbour links. In these cases, the...
domain walls may get pinned resulting in a frozen state [13–17]. Recently, freezing has been observed on scale-free networks also, where, although the system is locked in an excited state, the dynamics continues indefinitely [18].

![FIG. 2. Striped phase in two dimensional Ising model under zero temperature quenching dynamics - the domain walls are straight and no spin flips can occur.](image)

In the above examples of freezing in Ising models on finite dimensional lattices, graphs and networks, a few things are to be noted
(a) The ground state is simple in all the cases
(b) There is no frustration arising out of the interactions in the system.
In addition, power law scalings with time (e.g., domain size \( \sim t^{1/\beta} \)) exist for the finite dimensional lattices [19] but in the case of networks or random graphs, one has an exponential relaxation behaviour consistent with the mean field nature of these systems [20–23].

III. DYNAMICS IN ANNNI CHAIN

We will now discuss the dynamics in the axial next nearest neighbour Ising (ANNNI) model [24] in which there is frustration but no randomness or disorder. The ANNNI model in one dimension is described by the Hamiltonian

\[
H = -J_1 \Sigma S_i S_{i+1} + J_2 \Sigma S_i S_{i+2}.
\]

The ground state of this model is well-known: it is ferromagnetic for \( \kappa = J_2/J_1 < 0.5 \); antiphase for \( \kappa = J_2/J_1 > 0.5 \) and highly frustrated for \( J_2/J_1 = 0.5 \). All configurations having domains of size \( \geq 2 \) are ground states at the point \( \kappa = 0.5 \), which we call the fully frustrated point.

The dynamics of the ANNNI chain has quite a few interesting behaviour [25,26]. When zero temperature quenching dynamics dynamics is considered, \( \kappa = 1.0 \) emerges as a dynamical transition point. For \( \kappa < 1 \), there is no conventional domain coarsening or persistence behaviour. Here, all domains of size 1 immediately vanish but domains of size two are stable such that two domain walls cannot approach each other and annihilate (Fig. 3).

![FIG. 3. Dynamics in ANNNI chain for \( \kappa < 1 \): All domains of size 1 are unstable and they immediately vanish (a). The system is left with domains of size \( \geq 2 \). A domain of size two, as shown in (b), is energetically stable as the spins within the domain satisfy the antiferromagnetic ordering with their second neighbours and energy contribution from first neighbours is zero. As a result, two domain walls have to maintain a minimum distance and cannot approach each other and annihilate.](image)

As the domain walls continue moving in the system, the number of spin flips at any time becomes a constant in time. This constant is independent of the value of \( \kappa \). That is expected as this quantity is proportional to the number of domain walls. The average number of domain walls remaining in the system (per spin) turns out to be close to 0.28 [26].

![FIG. 4. Constant residual energy of the ANNNI model with zero temperature dynamics for \( \kappa < 1 \).](image)

Unlike in the Ising model in \( d = 2 \), here the domain walls are not pinned but can move around keeping their number fixed. The energy of the system is constant as spin flips occur with zero energy cost. The system thus wanders in a subspace of iso-energy metastable states forever. As a result, the model also does not show a power-law decay in the persistence probability. Interestingly, there is no special effect of the \( \kappa = 0.5 \) point (which dictates the static behaviour) on the dynamics.
with domain sizes $\geq 2$ are nothing but the degenerate ground states of the $\kappa = 0.5$ point. The residual energy decreases as $\kappa = 0.5$ is approached from both sides.

For the sake of completeness, it should be mentioned that the ANNNI model shows conventional relaxation behaviour for $\kappa > 1$ although with a dynamic exponent different from that of the nearest neighbour Ising model.

Since the conventional dynamics does not bring the system to the ground state, one has to employ some other method to do this. Simulated annealing for the Ising model on random graphs has been attempted to "melt" the system with success [13]. For small world networks, freezing can be got rid off by letting more number of edges in the system also [27]. We discuss in the next two section the result of applying different annealing schedules to the ANNNI model for various values of $\kappa < 1$.

IV. CLASSICAL ANNEALING (CA)

We have adopted two different schemes for applying classical or thermal annealing.

Scheme A

This is the conventional scheme where one starts with a finite temperature $T = T_0$ and slowly reduces it according to a linear schedule, such that, at the $t$-th iteration step,

$$T = T_0(1 - t/\tau),$$

where $\tau$ is the total number of Monte Carlo steps (MCS). The final temperature (at $t = \tau$) is zero for any starting value of $T$.

Since for all non-zero temperature, the ANNNI model is in a paramagnetic state, one may start with a random initial configuration corresponding to $T_0$.

We have calculated the residual energy and the order parameter as functions of $\tau$; the former is expected to approach zero and the latter should increase towards unity with larger values of $\tau$.

In Fig. 5, we show the behaviour of $E_r$ against $\tau$ for different $\kappa$ values. These simulations have been done for a system of 100 spins keeping $T_0 = 10$. The number of configurations $n$ over which averaging has been done decreases with $\tau$: starting with $n = 1000$ for smaller values of $\tau$, it is decreased to $n = 100$ for very large $\tau$ values. While for $\kappa = 0.2$, we find a stretched exponential decay, the nature of the curves changes to a power law decay for higher values of $\kappa$. Close to 0.5 it has a very slow decay. Corresponding to a power law fit $E_r \sim \tau^{-\alpha}$, $\alpha$ is very small here, e.g., for $\kappa = 0.4$, $\alpha = 0.08 \pm 0.01$, and for $\kappa = 0.6$, $\alpha = 0.03 \pm 0.01$. The slowing down of the decay pattern of $E_r$ seems to depend on the closeness to $\kappa = 0.5$ as well as on the nature of the ground state. For the various values of $\kappa$ for which the annealing scheme has been employed, the slowest decay is observed at $\kappa = 0.6$, when the system is close to $\kappa = 0.5$ and the ground state is also antiphase. The power law remains valid for $\kappa > 0.5$ with an increasing value of $\alpha$.

We have also checked the efficiency of this scheme for different values of $T_0$. Note that the decrease in $T$ is made with a slope equal to $T_0/\tau$ (eq. 2), so we compare the results for different $T_0$'s by plotting $E_r$ against $\tau/T_0$. For $\kappa = 0.4$ or 0.6, $E_r$ is independent of $T_0$ (as long as $T_0$ is not very small compared to 1) while for $\kappa = 0.2$, lowering $T_0$ makes the decay faster at large $\tau$. However, when $T_0$ is made smaller than unity the decay does not become faster any more. This plot (Fig. 6) also shows that for $\kappa$ close to 0.5, the power law behaviour is actually valid over a large range of $\tau$ which is not so apparent from Fig. 5.

FIG. 5. Residual Energy vs. MCS $\tau$ in the ANNNI model for different values of $\kappa < 1.0$. The decay is slow close to $\kappa = 0.5$. $T_0 = 10$ here.

FIG. 6. The residual energy vs the number of MCS ($\tau$) for different starting values of $T_0$. The scaled data shows a good collapse for $T_0 \geq 1$ for $\kappa = 0.4, 0.6$. For $\kappa = 0.2$, the decay is fastest for $T_0 = 1$ (filled circles). The data for $\kappa = 0.6$ and 0.2 have been shifted for clarity.
Thus $E_r$ depends strongly on $\kappa$: not only does the functional form change from a stretched exponential to power law, there is also a non-universal exponent $\alpha$ which depends on the value of $\kappa$. The role of $\kappa = 0.5$ is felt clearly as the annealing is least effective close to this point.

While estimating the order parameter (OP), it should be noted that for $\kappa < 0.5$, the order parameter is just the magnetisation while for $\kappa > 0.5$, it is the average of the four sublattice magnetisations defined as

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

(3) as in [26]. In Fig. 7, we plot the behaviour of the OP with $\kappa$ for different values of $\kappa$. The behaviour of the order parameter is also $\kappa$ dependent. The variations with $\tau$ are not smooth: the reason is that decreasing energy is not necessarily equivalent to increasing the order parameter. However it seems to have a rough power law increase for all values of $\kappa$ (Fig. 7). As expected, the growth of the order parameter is slowest at $\kappa = 0.6$.

Thus we find that this annealing schedule is not very effective near $\kappa = 0.5$ but works well for small values of $\kappa$. It is not possible to detect whether there is a value of $\kappa$ for which the behaviour of the residual energy changes from stretched exponential to power law from the present numerical study.

**Scheme B**

In this scheme, we first let the system evolve from a random configuration (corresponding to a high temperature) using the zero temperature dynamics and then, after a few steps, apply scheme A. The difference here is, we let the system reach one of the metastable states under zero temperature dynamics, heat it to a finite temperature $T_0$ which is then gradually decreased.

In the ANNNI chain, for the first 100 iterations, the temperature is kept zero such that when re-heated, the system is in one of the metastable iso-energy states. We find that this scheme accelerates the decay of the residual energy remarkably for small values of $\kappa$ (e.g., $\kappa = 0.2$) at large $\tau$. However, for higher values, e.g., $\kappa = 0.3, 0.4, 0.6$, for which scheme A gave a power law decay of $E_r$, the results are identical to that of scheme A. Thus near the $\kappa = 0.5$ point, this scheme is also seen to fail to bring the system to its static ground state.

This scheme is highly appropriate for cases where the system has a fractional probability to end up in a metastable or frozen state not corresponding to the ground state. Here it is not possible to predict whether a random initial configuration will reach the ground state under zero temperature dynamics or not. A good example is the two dimensional Ising model as it reaches a frozen state in about 30% cases. It is useless to apply scheme A here because 70% of the cases do not require any annealing at all. Therefore in order to see whether CA is useful, it should be better to apply scheme A to an initial configuration of frozen state which can be assumed to have evolved from a perfectly random initial state with zero temperature Glauber dynamics. Thus effectively it has undergone a period of cooling at zero temperature and when scheme A is now applied to it, it is equivalent to scheme B.

We have performed some simulation on a square lattice of size $L = 40$, where the number of stripes $s$ is equal to 2 or 4. In each case, we find that the behaviour of both the residual energy and the magnetisation is exponential which means that the scheme works very well in this case. In Fig. 8, we show the variation of the residual energy and magnetisation for $s = 2$. The exponential relaxation is easily understood, as the thermal perturbation breaks the structure of the domain walls and the system is then again free to evolve dynamically. The results are identical for $s = 2$ and 4 at large $\tau$. It may be mentioned

![Figure 7](image-url)

**FIG. 7.** Order parameter vs. MCS $\tau$ in the ANNNI model for different values of $\kappa < 1.0$. The growth is slow close to $\kappa = 0.5$.

![Figure 8](image-url)

**FIG. 8.** Order parameter (magnetisation) and residual energy versus MC time $\tau$ in the 2-$d$ Ising model under scheme B. The value of $T_0$ is 1 here. The dashed line has slope equal to $3.33 \times 10^{-5}$ in the log-linear plot.
here that for a value of the stripe number $s$ comparable to $L$, the situation is very similar to the ANNNI model (as stripe sizes have to be $\geq 2$) and then the exponential behaviour may no longer be present. However, the probability of a large value of $s$ is small and so, we have not considered values of $s > 4$.

V. QUANTUM ANNEALING (QA)

Although the classical annealing methods work quite well for the ANNNI model for small $\kappa$, we find that close to the $\kappa = 0.5$ point, it leads to very slow relaxation. In several situations, quantum annealing is far more efficient in decreasing the energy of the system [28, 29] and we therefore apply this method in the ANNNI model. Here instead of thermal fluctuation, quantum fluctuation is considered to induce tunnelling to enable the system reach the ground state for $\kappa < 1$.

The Hamiltonian for the quantum ANNNI chain is:

$$H = -J_1 \Sigma S_i S_{i+1} + J_2 \Sigma S_i S_{i+2} - \Gamma \Sigma S_i$$

(4)

This can be mapped to a 2-dimensional classical model [30, 31] using the Suzuki-Trotter formula:

$$H = -J_1 \Sigma S_{\alpha,i} S_{\alpha,i+1} + J_2 \Sigma S_{\alpha,i} S_{\alpha,i+2} - J_p \Sigma S_{\alpha,i} S_{\alpha+1,i}$$

(5)

where

$$J_p = -PT/2\ln(\tanh(\Gamma/PT))$$

and $\alpha$ denotes the $\alpha{}th$ row in the Trotter direction. Subsequently, one can use a linear schedule for the transverse field as in [29] and find out the results for $E_r$ and the order parameter. However, it is not possible to make $\Gamma$ equal to zero in the last step as that would make $J_p$ infinite.

We would first show some curious features of the results on applying this method to the ANNNI model and then try to justify the results.

The Suzuki-Trotter mapping is exact for $PT \to \infty$ but it can be a good approximation if $PT \geq 1$. One needs to find out an optimum value of $PT$ for which $E_r$ does not change with $P$. We therefore fix $PT$ and find out $E_r$ for different values of $P$ following [29]. We first fix $PT = 1$. For small $\kappa$, e.g., for $\kappa = 0.1$, the scheme indeed makes $E_r$ go down with $\tau$ quite efficiently. However, the value of $E_r$ for the same $\tau$ and different values of $P$ shows that $E_r$ actually increases with $P$. Thus results for any finite $P$ may not be reliable. Even increasing $PT$ to 2, we find that this behaviour persists. The reason for this maybe that the Suzuki-Trotter mapping works with a non-zero temperature for which the system is disordered and is always at a high energy state compared to the perfectly ordered state and therefore $E_r$ does not go to zero for large $\tau$ and $P$. These results are shown in Fig. 9.

In case of a value of $\kappa$ close to 0.5, e.g., $\kappa = 0.4$, we find that $E_r$ remains virtually a constant for all $P$ values when $PT = 1$ which apparently implies that $PT = 1$ is a good optimum value. However, $E_r$ actually remains a constant for all $\tau$ values as well showing that it does not relax at all. Thus here too the quantum annealing method will not work well. The reason is again because a non-zero temperature of the system has been used. However, the manifestation of this non-zero temperature is different for small and higher values of $\kappa$.

On hindsight, it may appear that quantum annealing is a redundant exercise in this case. However, it is interesting to find out how the redundancy makes itself known for different values of $\kappa$ in different ways.
In summary, we have shown that in systems with dynamic frustration, simulated annealing can be applied which gives results according to the nature of the system. For the ANNNI model, which has a competing interaction leading to frustration, (but well defined ground states with trivial degeneracy for $\kappa \neq 0.5$) classical annealing seems to work well for values of $\kappa$ close to $\kappa = 0$.

We have applied a different scheme of thermal annealing where the system is heated after an initial period of cooling. The results remain same in case of the ANNNI model when the frustration parameter is appreciable. But this method is useful in case of some other models where the conventional scheme is not very handy, e.g., the two dimensional Ising model. The better effectiveness of the annealing scheme for the two dimensional model in comparison to the ANNNI model may be attributed to the fact that there is no frustration in the former. The frustration present in the ANNNI model especially near $\kappa = 0.5$ makes it unresponsive to the thermal annealing while the unfrustrated two dimensional Ising model responds fast to the thermal fluctuation.

In case of the ANNNI model, it is also interesting to note that while in the dynamical studies it was shown that the $\kappa = 0.5$ point hardly has any role to play, and dynamical quantities like persistent probability, number of spins flipped at any time etc. were $\kappa$ independent, things become strongly $\kappa$ dependent under any annealing schedule with non-universal exponents governing the power law decays. The effect of $\kappa = 0.5$ is also felt as the annealing fails to make any impact close to it.

The application of a quantum annealing method with non-zero temperature also fails to "melt" the system to its ground states and its effect is differently manifested for small and large values of $\kappa$.

In fact we find that much is left to be done for a successful annealing programme near $\kappa = 0.5$, e.g., one may attempt a zero-temperature quantum annealing schedule.

Even for the classical annealing case, the change in behaviour of the residual energy as $\kappa$ is varied requires to be studied more intricately and possibly for larger system sizes. Our present study may act as a guideline for such future research work.

Lastly, we note that the variations of the residual energy does not follow a Huse-Fisher [32] type scaling in any parameter range for the ANNNI model.

Acknowledgements: We are grateful to Arnab Das and Subinay Dasgupta for very valuable discussions. P. K. Das acknowledges support from CSIR grants no. 9/28(608)/2003-EMR-I.