

# Floating Phase in 2D ANNNI Model

Anjan Kumar Chandra and Subinay Dasgupta  
*Department of Physics, University of Calcutta,  
 92 Acharya Prafulla Chandra Road,  
 Calcutta 700009, India.*

(Dated: November 5, 2018)

We investigate whether the floating phase (where the correlation length is infinite and the spin-spin correlation decays algebraically with distance) exists in the temperature( $T$ ) - frustration parameter ( $\kappa$ ) phase diagram of 2D ANNNI model. To identify this phase, we look for the region where (i) finite size effect is prominent and (ii) some relevant physical quantity changes somewhat sharply and this change becomes sharper as the system size increases. For  $\kappa < 0.5$ , the low temperature phase is ferromagnetic and we study energy and magnetization. For  $\kappa > 0.5$ , the low temperature phase is antiphase and we study energy, layer magnetization, length of domain walls running along the direction of frustration, number of domain-intercepts that are of length 2 along the direction of frustration, and the number of domain walls that do not touch the upper and/or lower boundary. In agreement with some previous studies, our final conclusion is that, the floating phase exists, if at all, only along a line.

PACS numbers: 05.70.Jk, 05.10.Ln, 64.60.Fr

## I. INTRODUCTION

The two-dimensional Axial Next-Nearest Neighbor Ising (ANNNI) model (spin =  $\frac{1}{2}$ ) is a square lattice Ising model with nearest neighbor ferromagnetic interaction along both the axial directions and second neighbor anti-ferromagnetic interaction along one axial direction. The Hamiltonian is,

$$\mathcal{H} = -J \sum_{x,y} s_{x,y} [s_{x+1,y} + s_{x,y+1} - \kappa s_{x+2,y}] \quad (1)$$

where the sites  $(x,y)$  runs over a square lattice, the spins  $s_{x,y}$  are  $\pm 1$ ,  $J$  is the nearest-neighbor interaction strength and  $\kappa$  is a parameter of the model. For positive values of  $\kappa$  the second-neighbor interaction introduces a frustration. This is one of the simplest frustrated classical Ising model with a tunable frustration and has been studied over a long time ([1, 2, 3] for review). The most widely studied aspect of this model is the phase diagram in the  $T - \kappa$  phase space, where  $T$  stands for temperature. It is easy to prove analytically that [1, 2, 3] at zero temperature, the system is in a ferromagnetic state for  $\kappa < 0.5$ , and in antiphase ( $++--++--\dots$  along  $x$  direction and all like spins along  $y$  direction) for  $\kappa > 0.5$  with a “multiphase” state at  $\kappa = 0.5$ . (The multiphase state comprises of all possible configurations that have no domain of length 1 along the  $x$  direction.)

From Monte Carlo simulations and approximate analytic calculations, some early studies had proposed a phase diagram (Fig. 1) consisting of a ferromagnetic phase (for  $\kappa < 0.5$ ) and antiphase (for  $\kappa > 0.5$ ) at low temperature along with a paramagnetic phase at high temperature (for all  $\kappa$  values). The crucial point is, between the ordered and the disordered phases for  $\kappa > 0.5$ , there may be a so-called “floating” phase characterized by (i) a spin-spin correlation that decays algebraically

with distance and (ii) an incommensurate, continuously varying modulation. An approximate analytic treatment by Villain and Bak [4] predicted that (for  $\kappa > 0.5$ ) as temperature increases from zero, there is a second order Pokrovsky-Talapov type commensurate-incommensurate phase transition from antiphase to the floating phase followed by a Kosterlitz-Thouless transition from the floating to the paramagnetic phase. This leads to a phase diagram shown schematically in Fig. 1. Several computational studies (see [1, 5]) also confirmed such a phase diagram. Later, Shirahata and Nakamura [5] have measured the dynamical exponent by studying the non-equilibrium relaxation of order parameter at  $\kappa = 0.6$  and  $0.8$  and concluded that the floating phase exists, if at all, over a narrow temperature range only. The central problem in this study is that the identification of order parameter is ambiguous for  $\kappa > 0.5$ , in the sense that it is difficult to identify a physical observable that relaxes algebraically at the critical temperature. One may note that the antiphase magnetization

$$M_{\langle 2 \rangle} = \sum_{x,y} s_{x,y}^{\langle 2 \rangle} s_{x,y}$$

does not satisfy this criterion [5]. (Here,  $s_{x,y}^{\langle 2 \rangle}$  is the spin distribution for perfect antiphase distribution.) Recently, a density matrix renormalization group analysis [6] has also excluded the presence of any incommensurate phase over an extended region.

The 2D ANNNI model is related to the transverse ANNNI chain by Suzuki-Trotter transformation [7, 8, 9, 10]. This quantum Ising model has also been studied widely. Numerical and approximate analytic studies [9, 11, 12] had predicted that the floating phase exists in the transverse ANNNI chain over a region, as shown in Fig. 1. However, recently we have shown [13] that for this model, the floating phase exists over a wide re-

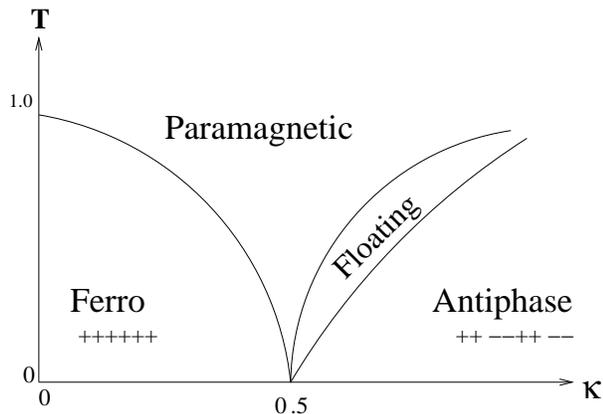


FIG. 1: Schematic phase diagram of the two-dimensional ANNNI model according to previous studies.

gion extending from  $\kappa < 0.5$  to  $\kappa > 0.5$ . There is thus a controversy about the existence of algebraically decaying phase in 2D ANNNI model.

In this article, we shall present Monte Carlo simulation of 2D ANNNI model with a view to locating the floating phase, if any. For  $\kappa < 0.5$ , one can easily identify the magnetization as the order parameter and for this case we have therefore, measured

1. internal energy
2. magnetization.

For  $\kappa > 0.5$ , the ordered phase is “antiphase” and it is difficult to identify the order parameter unambiguously. In this case, we have measured

1. internal energy,
2. layer magnetization (magnetization perpendicular to the direction of frustration)
3. length of domain walls running along the direction of frustration
4. number of domain-intercepts that are of length 2 over a straight line along the direction of frustration
5. number of dislocations measured as the number of domain walls that do not touch the upper and/or lower boundary.

We shall discuss later (Sec. III) the significance of these quantities in the context of our work.

From the measurement of a suitable physical quantity  $Q(t)$  at a time  $t$ , the critical point (or, for that matter, the critical region) could be identified from the general principle that at the critical point the quantity  $Q(t) - Q(\infty)$  is expected to vanish algebraically as a function of time  $t$ . While this characteristic is handy for the case  $Q(\infty) = 0$ , it is not usable when  $Q(\infty) \neq 0$ , as very large time simulation is required to measure the quantity  $Q(\infty)$  itself. In such cases, we have utilized two essential

features of critical phenomena : (i) For a finite lattice, the correlation time will diverge as [14]

$$\tau \sim L^z.$$

Hence, the quantity  $Q(t)$  will depend strongly on the system size only at the critical temperature  $T_c$  even at finite values of  $t$ . (ii) the equilibrium value  $Q(\infty)$  will undergo a sudden change, which is detectable even for small size and becomes more and more drastic as the system size increases.

As mentioned above, the results from non-equilibrium relaxation study [5] and the density matrix renormalization group analysis [6] contradicts the previous studies [5, 9, 15] as regards the extent of the floating phase. This paper confirms the conclusion of the former two studies by Monte Carlo simulation. One should note that all these studies agree at sufficiently low temperatures. We measure some observables that play a crucial role in the underlying physics and that have not been analyzed till now.

In Sections II and III we shall present the simulation studies for  $\kappa < 0.5$  and  $\kappa > 0.5$  respectively. All the simulation studies were performed with sequential Metropolis algorithm using periodic boundary conditions in X and Y directions and the results were averaged over 10 to 50 realizations. In Section IV we shall study the correspondence between the 2D ANNNI model and the transverse ANNNI chain and in Section V present conclusions. Our final conclusion is that the divergent correlation time exists only along a line. The phase diagram obtained is presented in Fig. 2. Everywhere in this communication temperature is measured in unit of  $T_c^{(0)} = 0.44069$ , the critical temperature for nearest-neighbor interaction ( $\kappa = 0$ ). This diagram is in qualitative agreement with that obtained by Shirahata and Nakamura [5] and Derian, Gendiar and Nishino [6]. The small difference between our results and those obtained by these authors seems to be due to the small ( $\sim 1000 \times 1000$ ) size of our simulation, compared to that of Shirahata and Nakamura ( $\sim 6399 \times 6400$ ).

## II. SIMULATION STUDIES FOR $\kappa < 0.5$

### A. Energy

Before we consider the measurements on the 2D ANNNI model itself, let us break off for a discussion on critical behavior of energy relaxation in general. Internal energy  $E$  is always unambiguously defined, in contrast to the order parameter, which for some phase transitions (like our system for  $\kappa > 0.5$ ) may not be easy to identify and measure. However, since  $E(\infty) \neq 0$ , it is difficult to study the time variation of the quantity  $E(t) - E(\infty)$ , as mentioned above. The relaxation of energy has also been studied elsewhere [16, 17].

We shall now consider the case of  $\kappa = 0$  (only nearest-neighbor interaction), and obtain the exponent, following

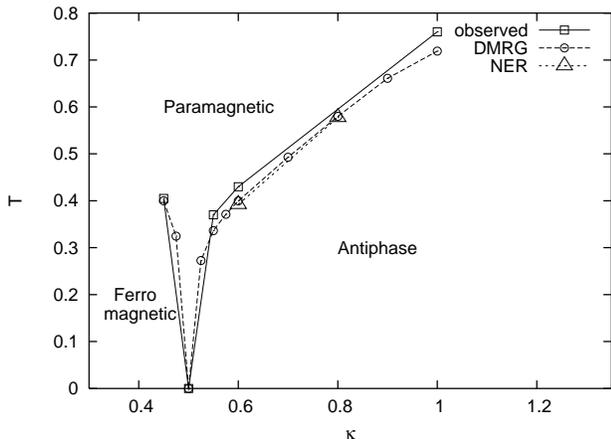


FIG. 2: The phase diagram of the two-dimensional ANNNI model as obtained from the present study, from non-linear relaxation (NER) [5] and density matrix renormalization group (DMRG) [6]. The temperature is measured in units of  $T_c^{(0)} = 0.44069$  as mentioned in the text.

standard scaling arguments [16, 18, 19]. Starting from the standard diffusion equation for the (non-conserved) order parameter  $\psi$

$$\frac{\partial \psi}{\partial t} = -\Gamma \frac{\partial F}{\partial \psi}$$

one obtains

$$\frac{\partial F}{\partial t} = -\frac{1}{\Gamma} \left( \frac{\partial \psi}{\partial t} \right)^2,$$

where  $F$  is the appropriate free energy and  $\Gamma$  is a parameter of the model. The identity  $E = \partial(\beta F)/\partial \beta$ , where  $E$  is the total internal energy then gives,

$$\frac{\partial E}{\partial t} = -\frac{1}{\Gamma} \left( 1 + \beta \frac{\partial}{\partial \beta} \right) \left( \frac{\partial \psi}{\partial t} \right)^2. \quad (2)$$

The scaling relation for the order parameter may be written as [19],

$$\psi(t, \epsilon, L, \psi_0) = b^{-\beta/\nu} \psi(b^{-z}t, b^{1/\nu}\epsilon, b^{-1}L) \quad (3)$$

where  $\epsilon = (1 - T)$  ( $T$  being the temperature measured in units of  $T_c^{(0)}$ ),  $L$  is the linear dimension of the system,  $b$  is the scaling factor, and  $\psi_0$  is the initial value of the order parameter. Also,  $\beta$  and  $\nu$  are the static critical exponents, and  $z$  is the dynamic critical exponent. Choosing  $b = t^{1/z}$  and suppressing the unimportant arguments  $L$  ( $\rightarrow \infty$ ) and  $\psi_0$ , we obtain,

$$\psi(t, \epsilon) = t^{-\beta/\nu z} \left[ \psi(1, 0) + t^{1/\nu z} \epsilon \psi'(1, 0) \right] \quad (4)$$

where  $\psi'$  is the derivative of  $\psi$  with respect to  $\epsilon$ . Substituting this form in Eq. (2), we have, for large time,

$$\Delta E \sim t^{-\sigma} \quad (5)$$

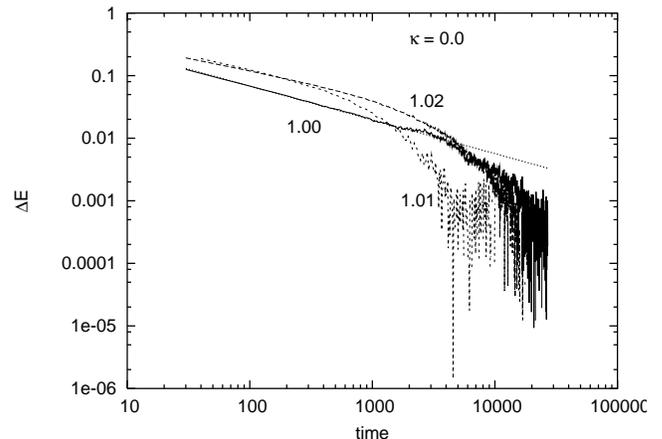


FIG. 3: Energy relaxation for a  $1000 \times 1000$  lattice for only nearest neighbor interaction i.e.  $\kappa = 0$ , starting from an ordered (all up) configuration. The straight line is a guide to the eye and fits to  $0.82t^{-0.54}$ .

where  $\Delta E$  is the energy difference  $E(t) - E(\infty)$  and  $\sigma = 1 - (1 - 2\beta)/\nu z = 0.66$ . Our simulations confirm this value of sigma (Fig. 3).

In the case of ANNNI model ( $\kappa$  non-zero but  $< 0.5$ ) we study the energy relaxation starting from ferromagnetic state. Our results for  $\kappa = 0.45$  is as follows. The  $E(t)$  vs  $t$  curve for an  $L \times L$  lattice is the same for  $L = 700, 1000$  and  $1200$  at a temperature  $T = 0.40$  (in units of  $T_c^{(0)}$ ). This happens also for  $T = 0.41$  but not for  $T = 0.404$ , where the relaxation behavior depends on  $L$  to the largest extent (Fig. 4). At  $L = 700$ , we could evaluate  $E(\infty)$  and found that  $E(t) - E(\infty)$  vs  $t$  plot shows an algebraic decay around  $T = 0.40$  but the algebraic region is most extended for  $T = 0.404$  (Fig. 5). It is hence concluded that at  $\kappa = 0.45$ , the critical point is  $T_c = 0.404 \pm 0.002$ . We could not however evaluate  $E(\infty)$  for  $L = 1000$  or  $1200$  as they involve too much computational time. Moreover, even at  $T = 0.404$ , there is some anomaly in the sense that the decay of  $E(t)$  at  $L = 1200$  is *faster* (rather than slower) than that for  $L = 700$  and  $1000$  (Fig. 4). A simulation over a longer time scale might resolve the anomaly.

It is interesting to note that at  $\kappa = 0.45$ ,  $T = 0.404$ , the exponent  $\sigma$  has a value  $0.15 \pm 0.05$ . Although it is a computationally intensive job to determine  $\sigma$  accurately, we attempted to study the apparent variation of  $\sigma$  with  $\kappa$  and found that it does not change much till  $\kappa = 0.4$  and afterwards decrease markedly.

## B. Magnetization

For  $\kappa < 0.5$ , the order parameter is magnetisation  $M$ , whose equilibrium value is zero at the critical point. Hence, an easy method of locating the critical point is to investigate where the magnetisation relaxes algebraically. It is well-known (Eq.(4)) that at  $T_c$  the magnetisation de-

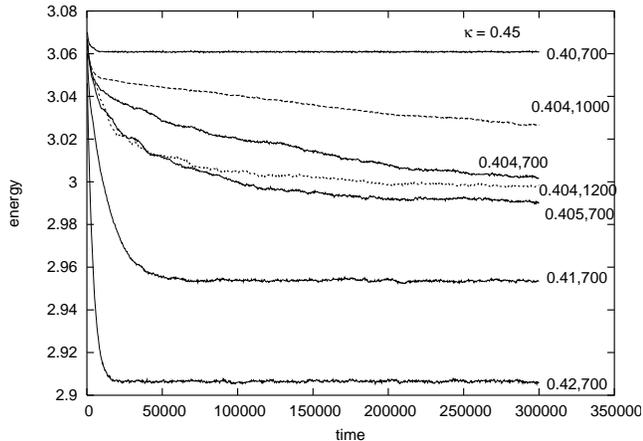


FIG. 4: Energy relaxation for  $\kappa = 0.45$  at temperature  $T$  for  $L \times L$  square lattice. The numbers at the right margin indicate  $T$  and  $L$  values. It is important to note that for  $T = 0.40, 0.405, 0.41$  and  $0.42$ , the curves for  $L = 1000$  and  $1200$  coincide with that of  $L = 700$ .

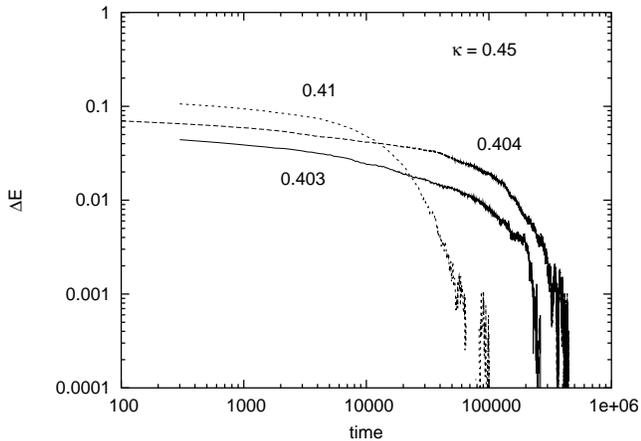


FIG. 5: Energy relaxation for  $\kappa = 0.45$  for  $700 \times 700$  lattice. The numbers indicate temperature. Note that the linear (algebraic) region is most prominent for  $T = 0.404$ . The algebraic region fits to  $0.17t^{-0.15}$ . We could not furnish the curve for  $T = 0.405$  as the system takes too long time to equilibrate.

ays as

$$M \sim t^{-\sigma'} \quad (6)$$

where  $\sigma' = \beta/\nu z$ . For  $\kappa = 0$ , the value of  $\sigma'$  is  $0.05734$ .

At  $\kappa = 0.45$  the magnetization is found to relax algebraically only around  $T = 0.405 \pm 0.002$ , which therefore is the critical temperature (Fig. 6). That the critical temperature at  $\kappa = 0.45$  lies between  $0.40$  and  $0.41$  is also verified by the fact that there is a sudden change in the equilibrium value of magnetization as temperature increases from  $0.40$  to  $0.41$ , and that this change becomes more and more sudden as the lattice size increases (Fig. 7).

The exponent for magnetization decay turns out to be  $\sigma' = 0.02 \pm 0.005$  at  $\kappa = 0.45, T = 0.404$ . As for the case

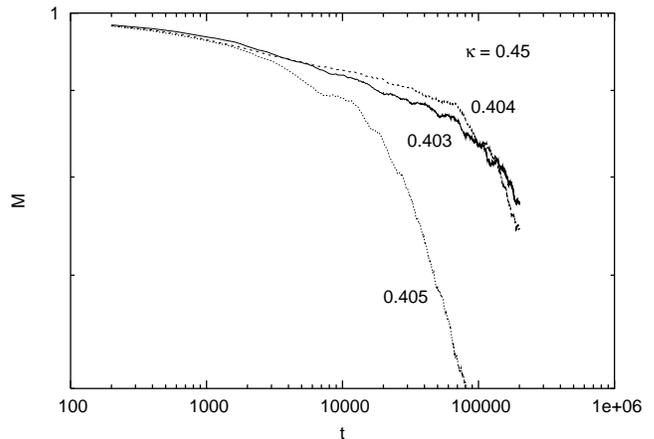


FIG. 6: Relaxation of magnetization at  $\kappa = 0.45$  at for  $1000 \times 1000$  lattice. The linear (algebraic) region is most prominent for  $T = 0.404$  and fits to  $1.08t^{-0.017}$ .

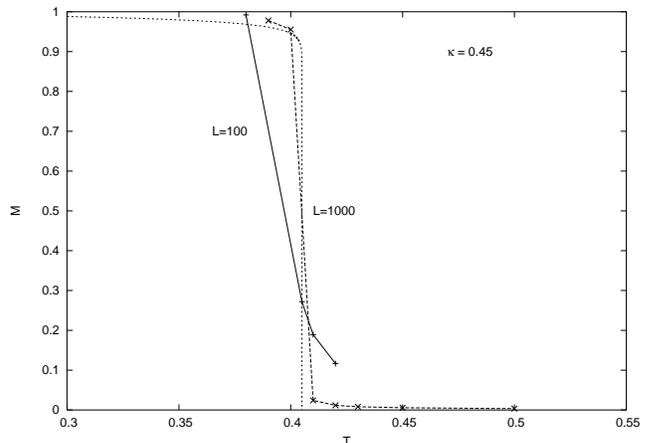


FIG. 7: Equilibrium value of magnetization at  $\kappa = 0.45$  as a function of temperature.

of energy relaxation, it is a computationally intensive job to determine  $\sigma'$  accurately. Approximate measurements indicate that just like  $\sigma$ , the exponent  $\sigma'$  also remains more or less the same up to  $\kappa = 0.4$  and starts decreasing markedly at higher  $\kappa$ . Further investigations on the apparent variation of  $\sigma$  and  $\sigma'$  is in progress.

### III. SIMULATION STUDIES FOR $\kappa > 0.5$

In this case, it is difficult to identify the order parameter, as mentioned above. It can be easily proved [1, 2, 3] that, at low temperature the system is in a perfectly ordered state with like spins along the Y axis and  $++ -$  pattern repeated along the X direction. The domain walls thus run exactly parallel to the Y axis. Moving along the X (Y) axis, one finds domains of length 2 ( $L$ ), for an  $L \times L$  system. As one increases the temperature, after some temperature  $T_c$  (called the lower critical

temperature), domains of length larger than 2 appear along the X direction. The domain walls now run not always parallel to the Y axis. They start from the lower boundary and terminate at the upper, but they often take small steps parallel to the X axis. Along the Y axis the domains are now sometimes less than  $L$  in length. Villain and Bak [4] pointed out that the number of domains that do not touch *both* boundaries is crucial and represents some sort of “dislocation”. This number is almost zero immediately above  $T_c$  but suddenly increases at some temperature  $T_2$ . While  $T_c$  marks a second order commensurate-incommensurate (Pokrovsky-Talapov type) transition,  $T_2$  marks a Kosterlitz-Thouless type transition. For  $T > T_2$  domains of small size appear in X and Y direction and the system is in a paramagnetic state. For  $T_c < T < T_2$ , Villain and Bak claimed that, the wavelength of modulation changes continuously with temperature and the correlation length is infinity, leading to a spin-spin correlation that decays algebraically with distance.

To study the two transitions, one at  $T = T_c$  and the other at  $T = T_2$ , we measure several quantities always starting the simulation with antiphase as the initial configuration.

(1) Internal energy is studied in the same way as done for  $\kappa < 0.5$ .

(2) Layer magnetization is defined (following [5]) as the magnetization of a chain along the Y axis averaged over all such chains :

$$m_l = \frac{1}{L} \sum_{x=1}^L |m_x| \quad (7)$$

where,

$$m_x = \frac{1}{L} \sum_{y=1}^L s_{x,y}$$

Obviously, this quantity should be 1 for  $T < T_c$  and zero above  $T_2$ . Hence, the size dependence of the relaxation of  $m_l$  and the algebraic nature of relaxation of  $m_l$  would indicate a diverging correlation length. Shirahata and Nakamura [5] have studied this quantity to identify the upper transition temperature  $T_2$  at  $\kappa = 0.60$  and  $0.80$ .

(3) The sum of length of the segments of domain walls that are parallel to the X axis, divided by the system size gives a quantity (say,  $d_x$ ) which is strictly zero in the perfect antiphase, but increases suddenly to some non-zero value at  $T_c$ . Its measurement leads to an estimate of  $T_c$ .

(4) Moving in the X-direction, one may note the lengths of domain intercepts encountered, and compute the ratio

$$f_2 = n_2/n_t$$

where  $n_2$  is the number of domains of length 2 and  $n_t$  is the total number of domains. This ratio is 1 for  $T < T_c$

and decreases for higher  $T$ . We note the region over which the relaxation of  $f_2$  depends on size or is algebraic in nature.

(5) The spin domains are identified and the fraction ( $f_d$ ) of domains that do not touch the upper and/or lower boundary is counted. (Those which miss any one boundary is counted with weightage 1 and those which miss both the boundaries are given weightage 2.) This fraction measures the number of “dislocations” that drives the Kosterlitz-Thouless phase transition at  $T_2$ . We do not study the relaxation of this quantity for computational limitations, but obtain from simulation the equilibrium value away from  $T_c$ . Such measurement should lead to an estimation of the Kosterlitz-Thouless transition temperature  $T_2$ , if any.

The study of all these quantities leads us to the conclusion that the floating phase, i.e. the region between  $T_c$  and  $T_2$  extends, if at all, over a temperature range less than 0.02. Thus, the region of diverging correlation length exists *only along a line*, up to the accuracy of this study. Our study was performed at  $\kappa = 0.55, 0.60, 1.0$ . The resulting phase diagram is presented in (Fig. 2). However, it is interesting to observe that while the width of the critical region is 0.02 for  $\kappa > 0.5$ , it is much less, about 0.001, for  $\kappa < 0.5$ .

## A. Energy

The study of energy relaxation for  $\kappa > 0.5$  follows closely the procedure for  $\kappa < 0.5$ , with the only difference that the initial configuration is now the antiphase. For  $\kappa = 0.60$ , the energy relaxation depends on size predominantly at  $T = 0.43$  and  $0.44$  (Fig. 8) and for  $L = 700$ , the energy difference  $E(t) - E(\infty)$  shows an algebraic decay over an extended region of time at  $T = 0.43$  and  $0.44$  (Fig. 9). Therefore, at  $\kappa = 0.60$  we identify  $T_c$  as  $0.44 \pm 0.01$ . The curves for  $\kappa = 0.55$  are qualitatively similar to that for  $\kappa = 0.60$ , and  $T_c$  could be identified as  $0.37 \pm 0.01$ . An alternative interpretation of the results could be that the floating phase would exist, if at all, between  $T = 0.43$  to  $0.44$  ( $0.37$  to  $0.38$ ) at  $\kappa = 0.60$  ( $0.55$ ). That the energy does not show any critical behavior over an extended range of temperature, seems to indicate that the floating phase does not exist over an extended region.

We mention that we could not perform the study of energy relaxation at  $\kappa = 1$ , since for this case a reliable data needs averaging over too many configurations.

The exponent for energy relaxation  $\sigma'$  (see Eq.(5)) is found to be  $1.7 \pm 0.1$  for  $\kappa = 0.55$  and  $0.60$ . In contrast to the findings for  $\kappa < 0.5$ , we observe no marked variation of  $\sigma'$  with  $\kappa$ .

## B. Layer Magnetization

The relaxation of layer magnetization ( $m_l$ ) is qualitatively similar for  $\kappa = 0.55, 0.60$  and  $1.00$ . At  $\kappa = 0.60$

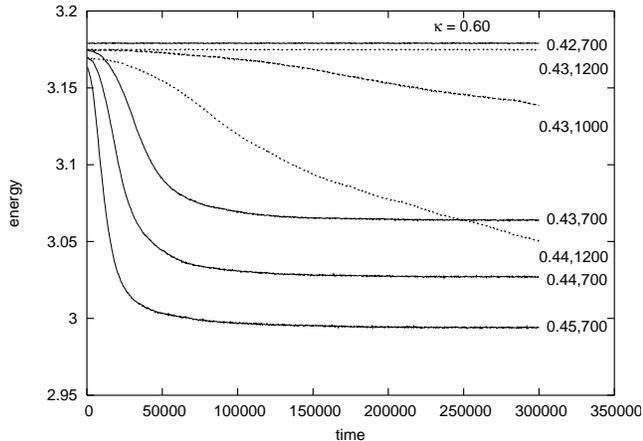


FIG. 8: Energy relaxation for  $\kappa = 0.60$  at temperature  $T$  for  $L \times L$  square lattice. The numbers at the right margin indicate  $T$  and  $L$  values. For  $T = 0.42$  and  $0.45$ , the curves for  $L = 1000$  and  $1200$  coincide with that of  $L = 700$ .

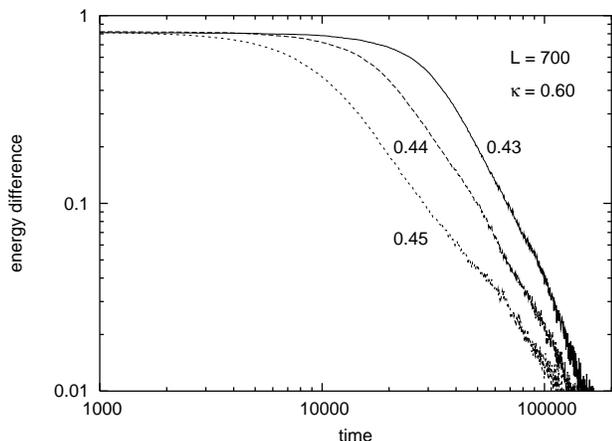


FIG. 9: Energy relaxation for  $\kappa = 0.60$  for  $700 \times 700$  lattice. The numbers indicate temperature. Note that the linear (algebraic) region is most prominent for  $T = 0.44$  and fits to  $75 \times 10^6 t^{-1.9}$ .

the relaxation shows critical slowing down and finite size effect at  $T = 0.44 \pm 0.01$  (Fig. 10), which is therefore the value of  $T_2$ . The equilibrium value of layer magnetization also shows a sharp fall (that becomes sharper as the system size increases) at this temperature, at  $\kappa = 0.60$  (Fig. 11). For  $\kappa = 0.55$  the value of  $T_2$  can be estimated in a similar manner to be  $0.37 \pm 0.01$ . We could not observe the curve for equilibrium value of layer magnetization at  $\kappa = 1$  because for this case one needs too long simulation to get the equilibrium value.

### C. Length of domain walls parallel to the direction of frustration

Like layer magnetisation, this quantity ( $d_x$ ) shows critical slowing down and finite size effect at  $T = 0.44$  for

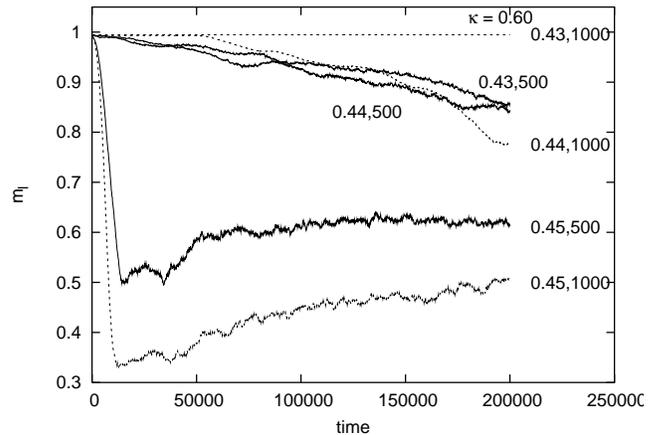


FIG. 10: Relaxation of layer magnetization for  $\kappa = 0.60$  at temperature  $T$  for  $L \times L$  square lattice. The numbers at the right margin indicate  $T$  and  $L$  values.

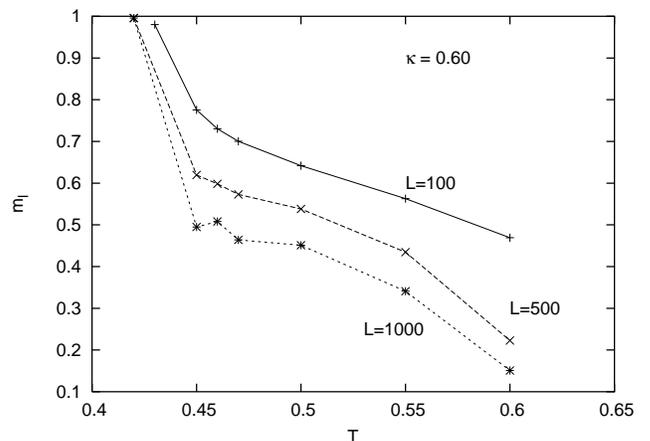


FIG. 11: Equilibrium value of layer magnetization at  $\kappa = 0.60$  as a function of temperature.

$\kappa = 0.60$  (Fig. 12). The equilibrium value of  $d_x$  shows a sharp rise at this temperature (Fig. 13), and this rise becomes sharper as the system size increases. Hence, the study of  $d_x$  indicates that  $T_c$  is  $0.44 \pm 0.01$  for  $\kappa = 0.60$ . In the same manner, the value of  $T_c$  is estimated to be  $0.37 \pm 0.01$  for  $\kappa = 0.55$  and  $0.76 \pm 0.01$  for  $\kappa = 1.00$ .

### D. Fraction of domains that have length 2

A study of this quantity ( $f_2$ ) leads to  $T_c = 0.44 \pm 0.01$  for  $\kappa = 0.60$ , since size-dependent slowing down of the relaxation of  $f_2$  is observed at this temperature (Fig. 14). Moreover, a sharp fall of the equilibrium value of  $f_2$  is observed at this temperature and this fall becomes slightly sharper as the system size increases from 100 to 1000 (Fig. 15). In a similar manner, the critical temperature for  $\kappa = 0.55$  and  $1.00$  is obtained as  $0.37 \pm 0.01$  and  $0.76 \pm 0.01$  respectively.

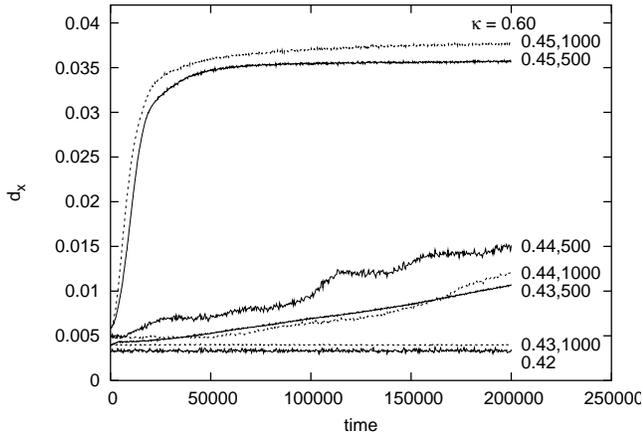


FIG. 12: Relaxation of  $d_x$  for  $\kappa = 0.60$  at temperature  $T$  for  $L \times L$  square lattice. The numbers at the right margin indicate  $T$  and  $L$  values. For  $T=0.42$ , the curves for  $L=500$  and 1000 coincide.

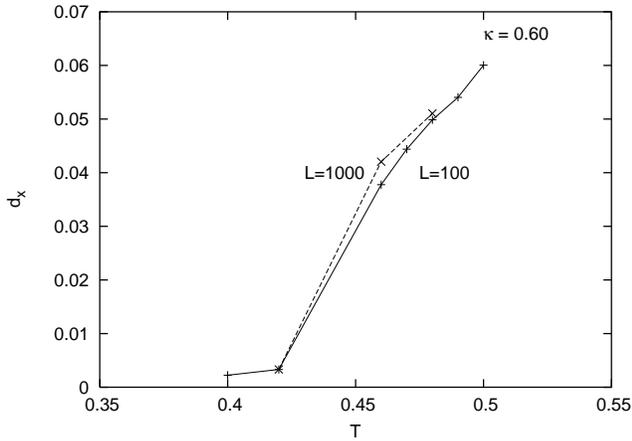


FIG. 13: Equilibrium value of  $d_x$  at  $\kappa = 0.60$  as a function of temperature.

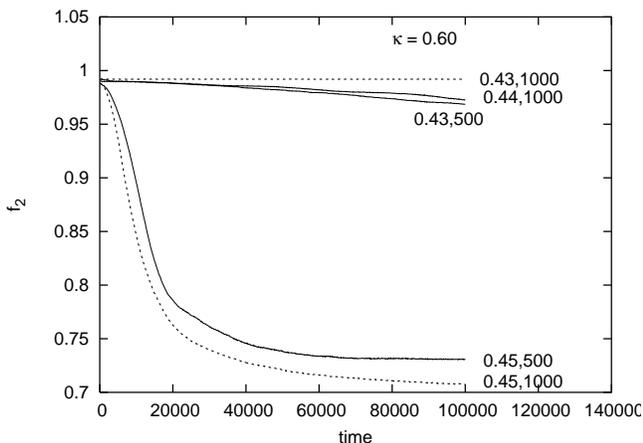


FIG. 14: Relaxation of  $f_2$  for  $\kappa = 0.60$  at temperature  $T$  for  $L \times L$  square lattice. The numbers at the right margin indicate  $T$  and  $L$  values.

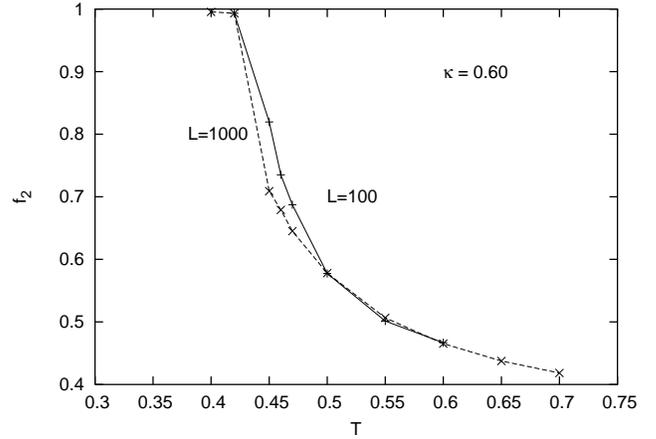


FIG. 15: Equilibrium value of  $f_2$  at  $\kappa = 0.60$  as a function of temperature.

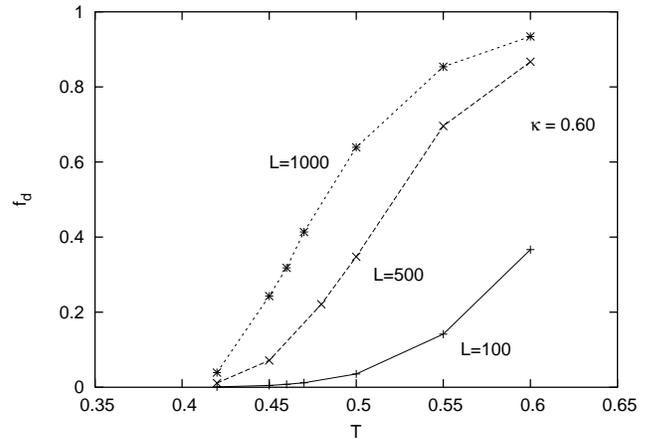


FIG. 16: Equilibrium value of  $f_d$  at  $\kappa = 0.60$  as a function of temperature.

### E. Fraction of domains that do not touch the boundary ( $f_d$ )

We could not study the relaxation of this quantity since averaging over too many realisations is necessary for a reasonably smooth curve. Rather, we could measure the equilibrium value at temperatures where the relaxation was not prohibitively slow. It is found that for  $\kappa = 0.60$ , the critical temperature lies between 0.42 and 0.45, since a sudden change is observed in the equilibrium value of  $f_d$  in this temperature range and that this change becomes more and more sudden as the lattice size increases (Fig. 16). Similar behaviour is also observed for  $\kappa = 0.55$  between temperature 0.35 and 0.40. This study could not be done for  $\kappa = 1.0$  because of computational limitation (one has to average over a good number of realisations to get reliable data). In spite of the computational difficulties for the study of  $f_d$ , it is clear that the study of this quantity excludes the possibility of critical region with width larger than 0.02 along temperature axis.

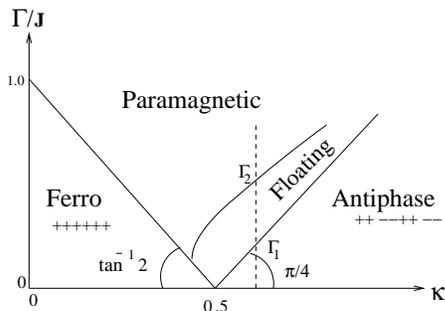


FIG. 17: Schematic phase diagram for Transverse ANNNI model (with Hamiltonian  $\mathcal{H}_q$  of Eq. (8)), after ref. [13]

#### IV. MAPPING TO QUANTUM MODEL

A quantum Ising model in  $d$  dimension is related to a classical Ising model in  $d+1$  dimension by Suzuki-Trotter transformation [7, 9, 10] and this relation is the basic idea behind quantum Monte Carlo algorithm. This transformation for the ANNNI model has been discussed in detail by Arizmendi [8] and can be summarised as follows. The quantum Ising Hamiltonian  $\mathcal{H}_q$  for the one-dimensional transverse ANNNI model with  $N$  sites is given by,

$$\mathcal{H}_q = -J' \sum_{j=1}^N (s_j^z s_{j+1}^z - \kappa s_j^z s_{j+2}^z) - \Gamma \sum_{j=1}^N s_j^x. \quad (8)$$

The ground state for this model is equivalent to a classical Ising model in two dimension with Hamiltonian

$$\mathcal{H}_{cl} = - \sum_{x=1}^N \sum_{y=1}^{mn} J_q s_{x,y} [(s_{x+1,y} - \kappa s_{x+2,y}) + p s_{x,y+1}] \quad (9)$$

in the limit ( $m \rightarrow \infty$ ) and ( $n \rightarrow \infty$ ) at a temperature  $T_q$  where

$$\frac{k_B T_q}{J_q} = \frac{m\Gamma}{J'} \quad (10)$$

( $k_B$  is the Boltzmann constant) and

$$p = \frac{m\Gamma}{2J'} \log[\coth(1/m)] \quad (11)$$

Obviously, the nearest neighbour interaction in the  $y$  direction is  $p$  times the same in the  $x$  direction and as  $m \rightarrow \infty$  this ratio  $p$  also tends to infinity.

As mentioned earlier, the Hamiltonian  $\mathcal{H}_q$  of Eq. (8), describing a transverse ANNNI chain, has also been studied widely and numerical and (approximate) analytic studies [9, 11, 12, 13] had predicted the existence of floating phase over a wide region extending from  $\kappa < 0.5$  to  $\kappa > 0.5$  (Fig. 17). Why then this extensive presence of floating phase does not occur in the phase diagram of Fig. 2? It seems that the explanation is the following. For the classical Hamiltonian  $\mathcal{H}_{cl}$  of Eq. (9), the

strength of nearest-neighbor interaction in the  $Y$  direction is  $p$  times stronger than that in the  $X$  direction, thus stabilizing the order in the  $Y$  direction. This raises both the upper critical temperature  $T_2$  (at which the order in the  $Y$  direction breaks down) and the lower critical temperature  $T_c$  (at which the order in the  $X$  direction breaks down). Both the temperatures are raised by almost the same amount (thus the floating phase always has negligible width) but the amount of rise depends on the value of  $p$ . Now consider the quantum Hamiltonian  $\mathcal{H}_q$ . For a given  $\kappa$  if the floating phase extends from  $\Gamma_1$  to  $\Gamma_2$  ( $\Gamma_2 > \Gamma_1$ , the difference  $\Gamma_2 - \Gamma_1$  being appreciable), then the value of  $p$  (say,  $p_2$ ) corresponding to  $\Gamma_2$  will be proportionately larger than the value of  $p$  (say,  $p_1$ ) corresponding to  $\Gamma_1$  (see Eq. (11)). Although for every value of  $p$ , one has  $T_c \approx T_2$ , the common value of  $T_c$  and  $T_2$  at  $p_2$  is appreciably larger than that at  $p_1$ . This shows that the *presence* of floating phase over a wide parameter region for the quantum model is consistent with the *absence* of the same for the classical model.

TABLE I: Conclusions regarding the critical region from the study of various observables (Sec. II and III here).  $T_0$  is the temperature (in units of  $T_c^{(0)} = 0.44069$ ) at which there is a critical region of width  $< 0.02$

$\kappa$	$T_0$
0.45	0.404
0.55	0.37
0.60	0.44
1.0	0.76

#### V. CONCLUSIONS

(1) For the 2D ANNNI model, diverging correlation length and algebraically decaying spin-spin correlation exists only along a “line”. We present in Table 1 the temperature  $T_0$  such that within the temperature range  $(T_0 - 0.01) < T < (T_0 + 0.01)$  lie both the upper critical temperature  $T_2$  and the lower critical temperature  $T_c$ . We did not conduct the study at temperature intervals smaller than 0.01 except at  $\kappa = 0.45$ .

(2) The phase diagram is topologically different for 2D ANNNI model and its Suzuki-Trotter counterpart, the 1D transverse ANNNI chain. This is in contradiction with the fact that often a quantum model and its corresponding classical counterpart show topologically similar phase diagram and have the same critical indices at the transition point. Two examples of such behavior are (i) 2D Ising model and 1D transverse Ising model with nearest neighbor interaction ( $\kappa = 0$ ) [20] and (ii) XYZ chain and eight vertex model [21].

### Acknowledgments

The work of one author (AKC) was supported by UGC fellowship. We also acknowledge the financial

support from DST-FIST for computational facility.

- 
- [1] W. Selke, Phys. Rep. **170**, 213 (1988); W. Selke, in *Phase Transitions and Critical Phenomena* edited by C. Domb and J.L. Lebowitz, Vol. 15, p. 1-72 (Academic Press 1992).
- [2] J. Yeomans, in *Solid State Physics* edited by H. Ehrenrich and D. Turnbull, Vol. 41, p. 151-200 (Academic Press 1988).
- [3] R. Liebmann, *Statistical Mechanics of Periodic Frustrated Ising Systems* (Springer-Verlag, Berlin) 1986
- [4] J. Villain and P. Bak, J. de Phys (Paris) **42**, 657 ((1981).
- [5] T. Shirahata and T. Nakamura, Phys. Rev. B **65**, 024402 (2001).
- [6] R. Derian, A. Gendiar and T. Nishino, cond-mat/0605411.
- [7] M. Suzuki, in *Quantum Monte Carlo Methods* ed. M. Suzuki, (Springer-Verlag, Berlin, Heidelberg) 1987.
- [8] C.M. Arizmendi, A.H. Rizzo, L.N. Epele and C.A. Garcia Canal, Z. Phys. B **83**, 273 (1991).
- [9] B.K. Chakrabarti, A. Dutta and P. Sen, *Quantum Ising Phases and Transitions in Transverse Ising Models* (Springer-Verlag, Berlin, Heidelberg) 1996.
- [10] B.K. Chakrabarti and A. Das, *Quantum Annealing and Related Optimization Methods* ed. B.K. Chakrabarti and A. Das (Springer-Verlag, Berlin, Heidelberg) 2005 (cond-mat/0312611).
- [11] G. Uimin and H. Rieger, Z. Phys. B **101**, 597 (1996).
- [12] A. Dutta and D. Sen, Phys. Rev. B **67**, 094435 (2003).
- [13] A.K. Chandra and S. Dasgupta, arXiv:cond-mat/0612144, Phys. Rev. E **75**, 021105 (2007).
- [14] M.E. Fisher, Phys. Rev. B **13**, 5039 (1976); K. Binder and D. W. Heermann, *Monte Carlo Simulations in Statistical Physics* (Fourth Edition) (Springer-Verlag, Berlin, Heidelberg) 2002, p.55; D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, (Springer-Verlag, Berlin, Heidelberg), 200?, Chapters 2, 4.
- [15] A. Sato and F. Matsubara, Phys. Rev. B **60**, 10316 (1999).
- [16] A.D. Rutenberg and A.J. Bray, Phys. Rev. B **51**, 5499 (1995).
- [17] S. Wansleben and D.P. Landau, Phys. Rev. B **43**, 6006 (1991).
- [18] S.K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, New York) 1976; M.E. Fisher and Z. Racz, Phys. Rev. B **13**, 5039 (1976).
- [19] H.K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B. **73**, 539 (1989); B. Zheng, Int. J. Mod. Phys. **12**, 1419 (1998); P. Sen and S. Dasgupta, J. Phys. A **35**, 2755 (2002).
- [20] D. C. Mattis, *The Theory of Magnetism*, Vol. II (Springer-Verlag, Berlin, Heidelberg) 1985, Sec. 3.6.
- [21] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic Press, London) 1982, p. 266.