Journal of Statistical Physics, Vol. 61, Nos. 1/2, 1990

Transient Dynamical Behavior and Phase Transitions in Magnetic Systems

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Received November 1, 1989; final May 17, 1990

It was recently suggested that transient dynamical properties were of some use to predict equilibrium critical properties of 2D and 3D models of statistical mechanics on the lattice. We investigate such dynamical properties for three related models with competitive interactions, namely the ANNNI model, the brickwork model, and the BNNNI model. In spite of known differences in their equilibrium phase diagrams, our simulations display similar transient dynamical behaviors for all three models. The reliability of this method for probing equilibrium properties seems therefore questionable even for rather simple magnetic models without any structural disorder.

KEY WORDS: Phase transitions; dynamics; ANNNI model; Monte Carlo method.

1. INTRODUCTION

Recently, a new dynamical method was proposed for probing phase diagrams in statistical mechanics.[1] It is grounded on the idea that comparing the evolution, for the same sample of the thermal noise, of two distinct initial configurations of the system may given some insight on the phase diagram. At high temperature, the system rapidly forgets its initial condition and consequently the distance between the two configurations rapidly vanishes (provided the dynamical behavior is not chaotic). On the contrary, at low temperature, the system is generally in a phase where several valleys coexist; the two configurations may then be trapped in dif-

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0022-4715/90/1000-0329$06.00/0

ferent regions so that their distance will never vanish. However, few exact results[2] have been established so far which connect these transient dynamical properties and the equilibrium phase diagram of the system, relating changes of dynamical regime to phase transitions. If such a link was established, one could then rely on less time-consuming simulations than the standard Monte Carlo methods to study the equilibrium properties.

A priori the long-time behavior is not related in a simple way to short-time properties and an appropriate validity criterion for applying the above method is lacking. However, analytical studies of a class of mean field models[3–6] have shown that this method can predict correctly the (mean-field) phase boundaries at equilibrium. Moreover, for 2D and 3D nearest-neighbor Ising models, the results derived from such simulations are also in very good agreement with the known location of the ferromagnetic–paramagnetic transition. The q-state standard Potts model is also well behaved in this respect (at least for $q = 3, 4, 5$).[7] On the other hand, the reliability of this new method for testing the equilibrium phase diagram of more complex models (3D spin glass,[3] XY model[7]) remains more questionable. One should nevertheless note that even if a reliable estimate for the 3D spin glass was not found by this method, it has been suggested that the "distance method" is suitable for giving more insight into the phase diagram properties of spin glasses and for finding evidence of an Almeida–Thouless line in finite-dimensional systems.[9]

Barber and Derrida[10] have recently studied the ANNNI (axial next nearest neighbor Ising) model. Their conclusions were that the ferromagnetic and paramagnetic phases as well as an antiphase could be identified within this approach. They also suggested that some features of the observed dynamical behavior were related to the floating phase of the ANNNI model. However, the extension of this floating phase was significantly larger than in other works.[11,12] The main goal of the present paper is to study and compare the transient dynamical behaviors of three different models, namely the ANNNI model, the brickwork model, and the BNNNI (biaxial next nearest neighbor Ising) model (see Section 2 for the precise definition of the models). These three models pertain to the same class (competing interactions, no structural disorder), but display significantly different physical properties, thus providing a good testing ground for the above method. The brickwork model is a modified version of the ANNNI model. It turns out to be exactly solvable[13,14] and one can show rigorously that no floating phase exists in this model. It was previously used to check indirectly the validity of the conventional Monte Carlo simulations of the ANNNI model. Monte Carlo simulations of the brickwork model were shown to exhibit metastability, which led to a spurious similarity with Monte Carlo simulations of the ANNNI model.[14,15] The BNNNI model is an isotropic version of the ANNNI model. The very existence of a floating phase for this model is still a subject of controversy. As will be shown in this work, all three models display fairly similar transient dynamical behaviors (see Section 3 for the description of the method and Section 4 for the results) in spite of the differences in their equilibrium phase diagrams. The strong connection between the transient dynamical behavior and the equilibrium phase diagram which was observed in simple models is no longer present. As advocated in the conclusion, as soon as the model presents nontrivial phases (due to competition or frustration, for instance) the connection between transient and equilibrium properties becomes quite loose, which impairs the confidence one can have in this dynamical approach for probing thermodynamics.

2. THE MODELS

In this section we recall the definition of the three models we study in the following (see also Fig. 1). We consider $N \times N$ Ising spins $S_{i,j}$ ($i = 1,..., N$; $j = 1,..., N$) ($S_{i,j} = \pm 1$) on a square lattice. The usual ANNNI model is then described by the Hamiltonian

$$H = -J_1 \sum_{i,j} (S_{ij} S_{i+1,j} + S_{i,j} S_{i,j+1}) - J_2 \sum_{i,j} S_{i,j} S_{i+2,j}$$

J_1 is a ferromagnetic coupling, J_2 an antiferromagnetic coupling, and the positive parameter $\kappa = -J_2/J_1$ quantifies the competition between the two interactions. A complete report on the properties of this model can be found in Selke's review.[16] Let us recall the main features of the phase diagram. For $0 < \kappa < 0.5$ the low-temperature phase is ferromagnetic and the high-temperature phase is paramagnetic. For $\kappa > 0.5$ the low-temperature phase is an antiphase, whereas at high temperature the system is in a disordered phase; these two phases are separated by a floating phase. Moreover, a disorder line splits the disordered phase.

A modified version of the ANNNI model is the so-called brickwork ANNNI model. It is governed by the following Hamiltonian (N is assumed even):

$$\begin{aligned} H = &-J_1 \sum_{i=1}^{N-1} \sum_{j=1}^{N/2} S_{i,2j-1} S_{i+1,2j} - J_1 \sum_{i=1}^{N} \sum_{j=1}^{N/2-1} S_{i,2j} S_{i,2j+1} \\ &- J_2 \sum_{i=1}^{N} \sum_{j=1}^{N/2-1} S_{i,2j} S_{2,2j+2} - J_3 \sum_{i=1}^{N} \sum_{j=1}^{N/2} S_{i,2j-1} S_{i,2j} \end{aligned}$$

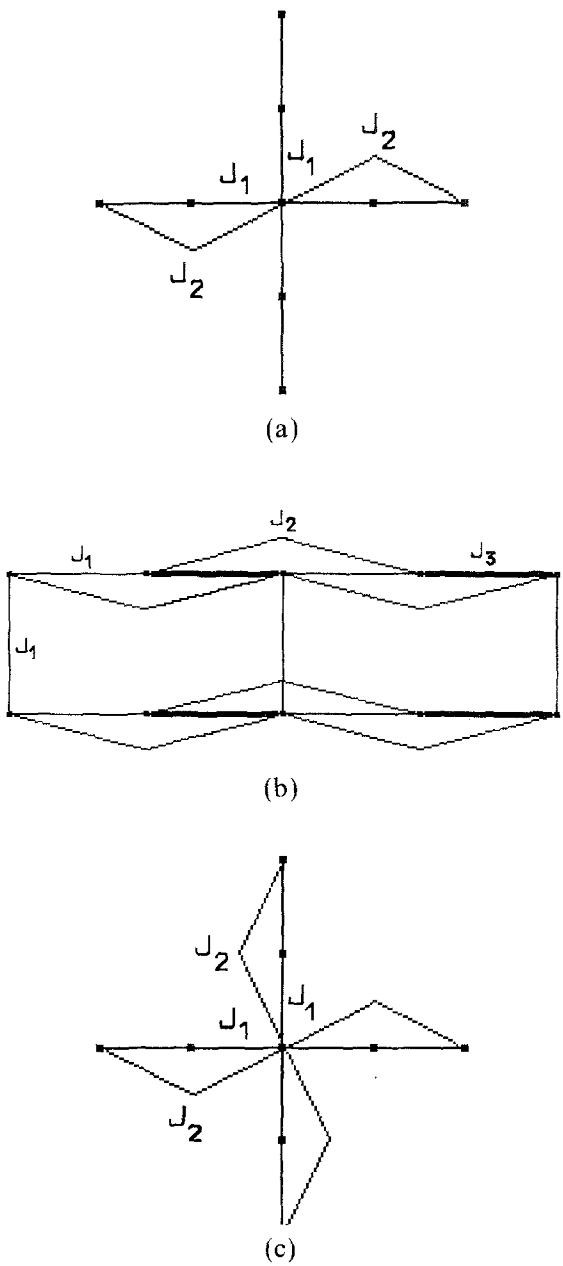


Fig. 1. Definitions of the three models; the different kinds of couplings (between nearest neighbors or next nearest neighbors) are indicated. (a) ANNNI model, (b) Brickwork model, (c) BNNNI model.

Basically, this model is related to the standard ANNNI model by suppressing every second vertical coupling and strengthening every second horizontal coupling, as shown in Fig. 1. The partition function can be calculated exactly using a standard dimer method. The phase diagram has been proposed by Beale *et al.*[12] (see Fig. 8 in that reference) for $J_3 = 2J_1$. It exhibits just order–disorder transitions without any intermediate floating phase, in contrast with the standard ANNNI model.

The third model we investigate is the BNNNI model. It can be deduced from the ANNNI model by adding a next nearest neighbor interaction on the second direction, thus restoring the isotropy of the model. The equilibrium phase diagram of this model is still a matter of controversy. The first Monte Carlo simulations made by Hornreich *et al.*[17] and Selke and Fisher[18] seemed to indicate the existence of an incommensurate phase for $\kappa > 0.5$. However, more recent simulations[19] suggest that, instead of a two-transition scenario, only one (first-order) transition leads from the ordered (chessboard) phase to the disordered phase. More recently the problem of the very existence of a floating phase was reconsidered by Oitmaa and Velgakis[20] (using series expansions), Velgakis and Oitmaa[19] (via Monte Carlo simulations), and Oitmaa *et al.*[22] (by finite-size study). The conclusions of these works rather supported the existence of a floating phase, although it was impossible to decide unambiguously.[4]

3. THE SIMULATIONS

We now describe the method used for the simulations and define the quantities we measured. We consider $N = L^2$ spins. In order to ensure an efficient vectorization of the code, the lattice was chosen as follows. Duplicating the N spins leads to a rectangular lattice of size $L \times 2L$ with the L-periodic horizontal conditions: $S_{i,j} = S_{i,j+L}$. Moreover, we impose periodic boundary conditions on this new lattice. It is then allowed to update at the same time all the spins located on the diagonal defined by $i = j + k$ for given k ($k = 1, \ldots, L$), as these spins do not interact directly. In the following, a time step of the simulation will therefore correspond to the sequential update of the L different diagonals.

As in Barber and Derrida,[10] the dynamical evolution of the system is based on a heat bath algorithm. To update the spin $S_{i,j}$ at time $t + dt$ ($dt = 1/L$), one first computes the local field $h_{i,j}(t)$ at time t. One then chooses $S_{i,j}(t + dt)$ to be ± 1 with probability $1/2 \pm \tanh[h_{i,j}(t)/T]$. To

[4] In the problem of the 3-state chiral Potts model, a study based on Monte Carlo simulations and partial analytical results also supported the idea of a floating phase, even in the case of *isotropic interaction.*[23]

compare the relative evolution of two different initial configurations $\{S_{i,j}(0)\}$ and $\{S'_{i,j}(0)\}$ for the same sample of the thermal noise, we update the two corresponding configurations at time t $\{S_{i,j}(t)\}$ and $\{S'_{i,j}(t)\}$ according to

$$S_{i,j}(t+dt) = \text{sign}[1/2 + 1/2 \tanh h_{i,j}(t)/T - z_{i,j}(t)]$$
$$S'_{i,j}(t+dt) = \text{sign}[1/2 + 1/2 \tanh h'_{i,j}(t)/T - z_{i,j}(t)]$$

where $z_{i,j}(t)$ is a random number (the same in both equations) uniformly distributed between zero and one.

Several quantities can be used to characterize such a relative evolution. The first one is a Hamming distance $D(t)$ between the two configurations at time t:

$$D(t) = 1/4N \sum [S_{i,t}(t) - S'_{i,j}(t)]^2$$

Here the sum is extended over the whole lattice and $D(t)$ ranges between 0 and 1. The survival probability $P(t)$ is computed to be the fraction (averaged over noise) of initial conditions for which the two configurations are still different at time t.

We also examined the behavior of other quantities, such as the probability $P_t(\varepsilon)$ that at time t the two configurations are at a distance smaller than ε.

The initial configurations considered in this work will be two types: a first group of simulations will be done with two different configurations chosen among the ground states of the model. The results thus obtained will be compared with simulations starting from configurations chosen at random under the constraints $S'_{i,j}(0) = -S_{i,j}(0)$.

4. RESULTS

4.1. The ANNNI Model

We considered three different values of κ, namely $\kappa = 0.1$, 0.2, 0.8, and a lattice of size $L = 32$. The averaging was performed over 100 samples of the thermal noise. The dynamical evolution starting from ground-state initial conditions (ferromagnetic states for $\kappa < 0.5$ and antiphase for $\kappa > 0.5$) was stopped after $t_0 = 500$ steps and we focused on the temperature dependence of $P(t_0)$ and $D(t_0)$ (results are displayed on Figs. 2a–2c).

For $\kappa = 0.1$, $P(t_0)$ displays a sharp drop for $T \approx 2.1$, which is also the temperature at which $D(t_0)$ begin to decrease rapidly. Three different regimes can be seen in the behavior of $D(t_0)$. For $0 < T < 1.8$, $D(t_0)$ remains

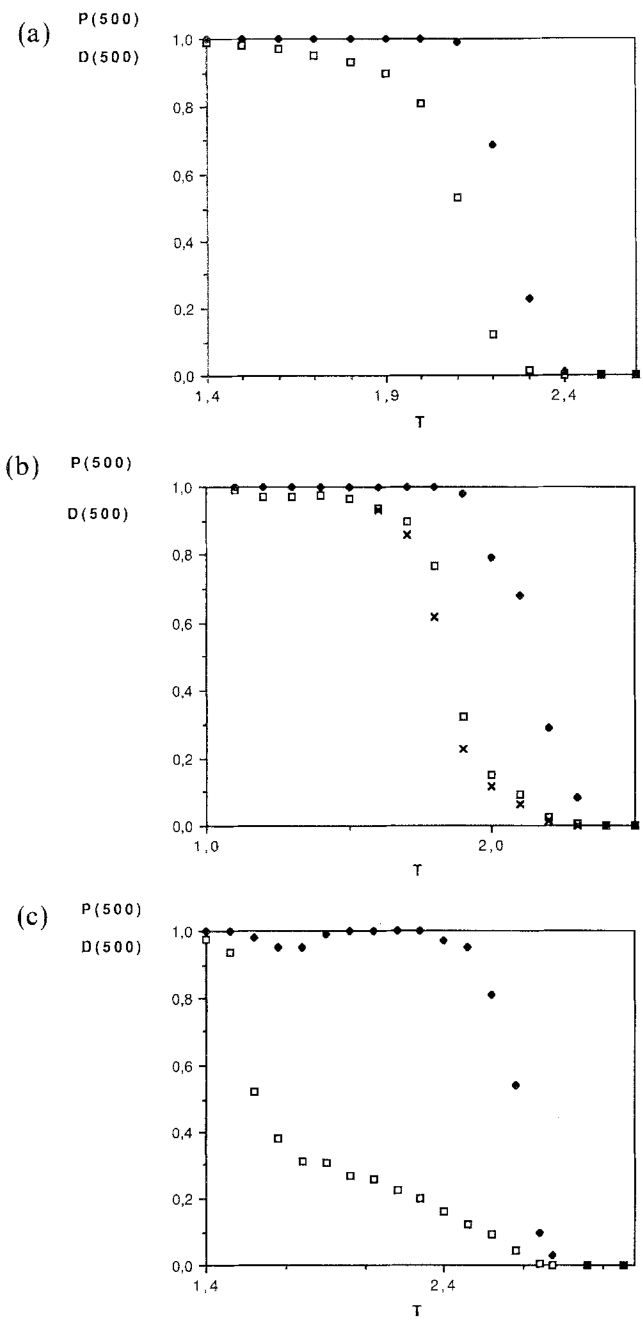


Fig. 2. The ANNNI model: Temperature dependence of the Hamming distance $D(t_0 = 500)$ (open squares) and of the survival probability $P(t_0 = 500)$ (black diamonds) for ground-state initial conditions and different values of κ (simulations were performed for $L = 32$ with averaging over 100 samples). (a) $\kappa = 0.1$, (b) $\kappa = 0.2$ [the Hamming distance (crosses) for $L = 128$ is also displayed], (c) $\kappa = 0.8$.

close to unity, $D(t_0)$ then decreases rapidly in the range $1.8 < T < 2.3$, and for $T > 2.3$, $D(t_0)$ vanishes. This behavior is very slightly affected when increasing the size of the system, averaging over a larger set of samples, and choosing a larger time t_0. The transition temperature $T \approx 2.2$ [observed for both $P(t_0)$ and $D(t_0)$] is in good agreement with the temperature of the ferromagnetic/paramagnetic transition as reported by Final and de Fontaine.[24]

For $\kappa = 0.8$, the situation seems rather different. Indeed, in this case an additional regime where $D(t_0)$ decreases slowly and roughly linearly is observed in a large range of temperatures $(1.7 < T < 3)$. It should be noticed that the drop in $P(t_0)$ does not coincide with the onset of this regime; indeed, $P(t_0)$ remains close to unity in much of this intermediate domain.

On the basis of very similar results and of a comparison with the mean-field phase diagram of Finel and de Fontaine,[24] Barber and Derrida[10] suggested that this intermediate regime was a signature of the floating phase of the ANNNI model. Indeed, the temperature of the sharp drop of $D(t_0)$ is very close to the critical boundary separating the antiphase and the floating phase for $\kappa = 0.8$. As already noted by Barber and Derrida, this intermediate regime seems to end at a temperature which exceeds by about 20% the value proposed by Finel and de Fontaine for the transition to the completely disordered phase. In addition, the sharp drop of $P(t_0)$ at $T \approx 2.5$ (a value close to the temperature proposed by Finel and de Fontaine for the floating/paramagnetic transition) is located in the midst of the intermediate region. Thus, the determination of the extent of the floating phase is not deprived of ambiguity and it is even possible that the linear decrease of $D(t_0)$ is not uniquely related to the existence of the floating phase.

The situation for $\kappa = 0.2$ is even less clear (see Fig. 2b). The behavior seems qualitatively similar to what we observed for $\kappa = 0.8$, except for the much smaller extension (T ranging from 2 to 2.4) of the intermediate region where $D(t_0)$ slowly decreases.[5] Note that this intermediate regime can also be found in the results of Barber and Derrida.[10] These authors argued that this was due to some finite-size effect in the critical region. However, increasing the size of the lattice up to $L = 128$, we found that the intermediate regime was persisting and almost no change was visible in its domain and its slope (Fig. 2b) (note that in our simulation $L = 128$ means 128×128 spins; hence the lattice is larger than the one with the corresponding L in ref. 10, which would have 128×64 spins).

[5] The existence of such an intermediate region cannot be ruled out for $\kappa = 0.1$, but its size would be very small and the conditions of the present simulations cannot lead to a definitive conclusion.

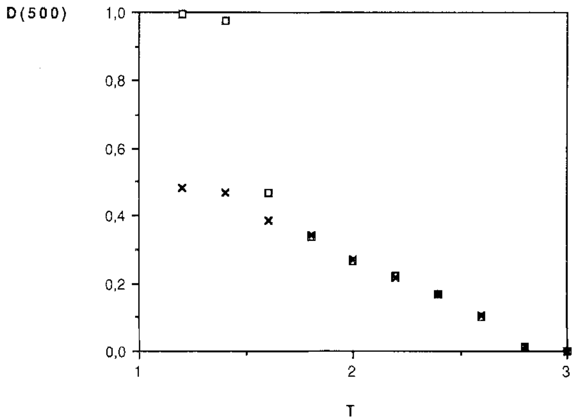


Fig. 3. The ANNNI model: Comparison of $D(500)$ for ground-state (open squares) and random (crosses) initial conditions for $\kappa = 0.8$ and $L = 64$. Other parameters are as in Fig. 2.

For obtaining additional information on the location (and nature) of the first transition we compared the behaviors of $D(t_0)$ for the two sets of initial conditions defined in Section 2. Indeed, in a stable or metastable low-temperature phase one should expect drastic differences between starting from random states and zero-temperature equilibrium states; on the other hand, at high temperature these equilibrium states no longer play any specific role. Hence, both types of initial conditions should then lead to the same behavior. The results we obtain (see Fig. 3) confirm that the first characteristic temperature [where $D(t_0)$ starts to decrease] is indeed related to the disappearance of the low-temperature phase.

4.2. The Brickwork Model

We studied the brickwork model for $J_3 = 2J_1$. The known exact results for this choice of parameters are given in ref. 10 (see Fig. 8 in that paper). Our simulations display the following features. For $\kappa = -J_2/J_1 = 0.1$ and $\kappa = 0.2$ no intermediate regime exists. For instance, for $\kappa = 0.2$ (Fig. 4a) the characteristic temperature where $P(t_0)$ and $D(t_0)$ drop off is $T \approx 1.8$. This is in a pretty good agreement with the exact value for the ferromagnetic/paramagnetic transition.

For $\kappa = 0.8$ (Fig. 4b), $D(t_0)$ displays an intermediate regime quite similar to the intermediate regime of the ANNNI model. At first sight this comes as a surprise in view of the absence in the brickwork model of a floating phase and even of any phase transitions other than of the ferromagnetic/paramagnetic type. This numerically observed behavior seems not to depend on the size of the lattice. We checked that in simulations of sizes up to $L = 128$ (see Fig. 4b), this intermediate regime occurs in almost the same range of temperature (T between 1.7 and 2.3). We also checked that increasing the duration of the simulation up to $t = 10{,}000$ time steps caused no significant changes in this intermediate regime. Moreover, the disappearance of the low-temperature ordered phase at $T \approx 1.7$ is confirmed by the comparison of the curves obtained for ground-state and random initial conditions (see Fig. 5).

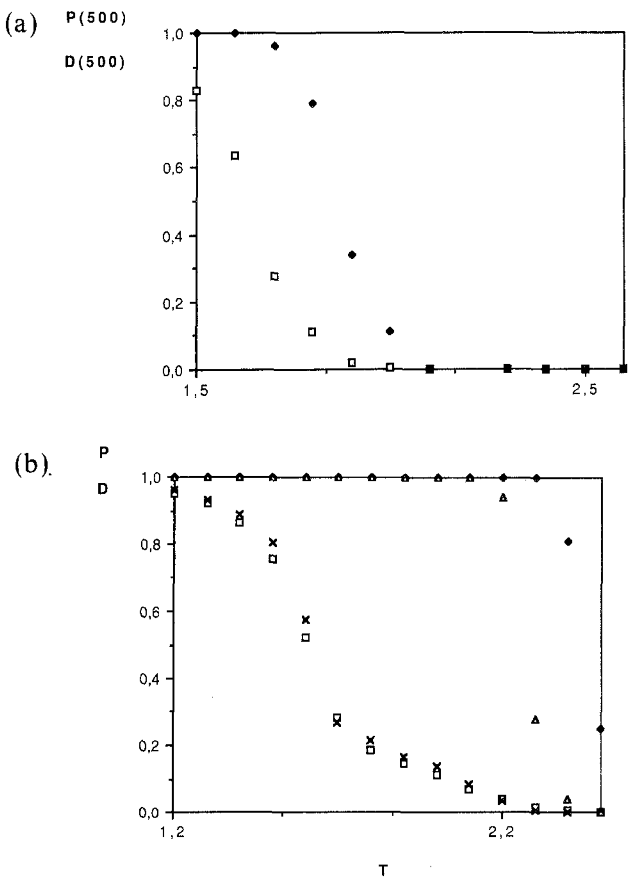


Fig. 4. The brickwork model: Temperature dependence of the Hamming distance $D(t_0 = 500)$ (open squares) and of the survival probability $P(t_0 = 500)$ (black diamonds) for ground-state initial conditions and different values of κ (simulations were performed for $L = 64$ with averaging over 100 samples). (a) $\kappa = 0.2$, (b) $\kappa = 0.8$. The Hamming distance (crosses) and the survival probability (open triangles) at time $t_0 = 250$ for $L = 128$ are also displayed.

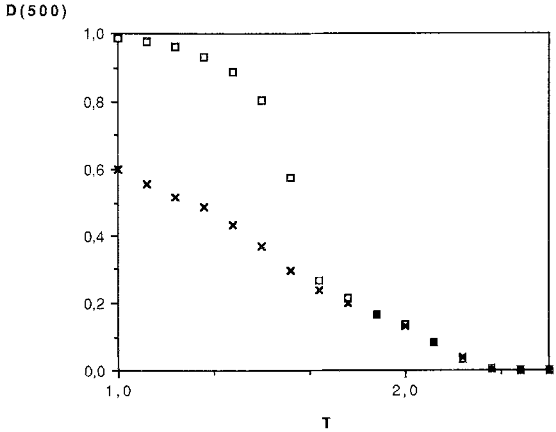


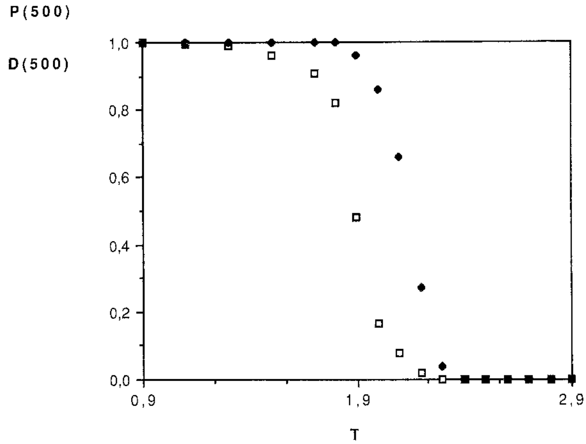
Fig. 5. The brickwork model: Comparison of $D(500)$ for ground-state (open squares) and random (crosses) initial conditions for $\kappa = 0.8$. Other parameters are as in Fig. 4.

We therefore suggest that such an intermediate dynamical regime indeed exists in the brickwork model and is no artifact of our simulations. It would be tempting to identify this intermediate regime not with a floating phase, but with the $q = 1/4$ modulated region of the equilibrium phase diagram. However, it seems to extend well above the $q = 1/4$ regime proposed by Beale *et al.*[12] Nevertheless, it is possible that such a "phase" affects the transient dynamics beyond its equilibrium range. In such a case, a new dynamical criterion to characterize a floating phase and to distinguish it from a modulated regime would be required. Indeed, if this hypothesis was true, this would entail that the dynamical quantities we used are equally sensitive to true thermodynamic phase transitions as well as nonsingular changes in the system properties (such as in the oscillations of spatial correlations).

4.3. The BNNNI Model

The very existence of a floating phase for the BNNNI model, even for $\kappa > 0.5$, is still controversal, as conventional Monte Carlo simulations and such techniques as high-temperature expansions or transfer matrix methods give ambiguous results. On the other hand, an intermediate regime clearly stands out in our simulations even for $\kappa = 0.2$.

We first discuss the simulations with $L = 32$ and ground states of the "checkerboard" type as initial conditions. For $\kappa = 0.1$, $P(t_0)$ and $D(t_0)$ both present a sharp decrease near $T \approx 1.8$ (see Fig. 6a). This last value agrees



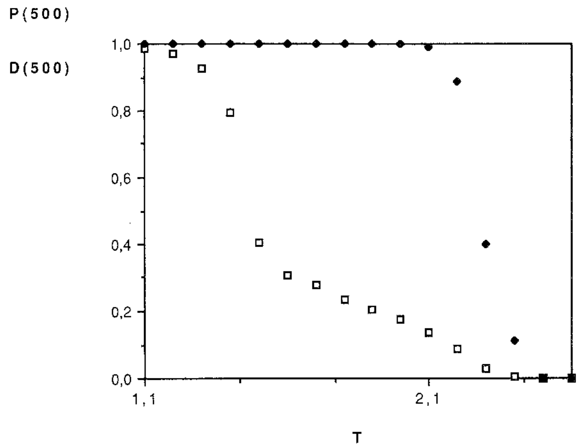


Fig. 6. The BNNNI model: Temperature dependence of the Hamming distance $D(t_0=500)$ (open squares) and of the survival probability $P(t_0=500)$ (black diamonds) for ground-state initial conditions and different values of κ (simulations were performed for $L=32$ with averaging over 100 samples). (a) $\kappa=0.1$, (b) $\kappa=0.2$.

well with the critical temperature proposed by Oitmaa and Velgakis[20] from series expansions: $T_c=1.8$. A narrow intermediate regime might exists, but we could not reach any definitive conclusion.

The situation is clearly different for $\kappa=0.2$, as the behavior of $D(t_0)$ displays a wide intermediate regime, as shown on Fig. 6b. The first drop of this quantity occurs for $T=1.4$ [on the other hand, the brutal decrease of $P(t_0)$ occurs in the midst of this intermediate region at $T=2.1$]. Comparing these results with those obtained for random initial conditions

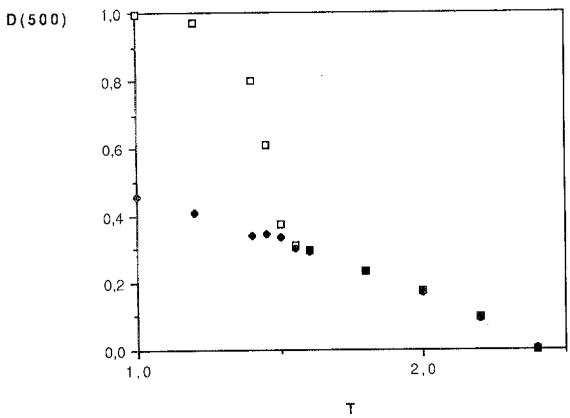


Fig. 7. The BNNNI model: Comparison of $D(500)$ for ground-state (open squares) and random (crosses) initial conditions for $\kappa = 0.2$. Other parameters are as in Fig. 6.

(see Fig. 7) and recalling that the numerical value proposed by Oitmaa *et al.*[22] for the critical temperature is $T_c(0.2) = 1.41$, one would be tempted to identify the onset of the intermediate regime with the equilibrium phase transition. However, the meaning of the intermediate regime is still quite obscure, as an intermediate floating phase seems very improbable for $\kappa = 0.2$ in the light of previous results.[20-22]

5. CONCLUSION

In this work we compared the ANNNI model, the brickwork model, and the BNNNI model with respect to some of their transient dynamical properties. The analysis has been carried out on the basis of the comparison of the temporal evolution of two initial conditions submitted to the same thermal noise. We saw that the Hamming distance $D(t_0)$ between the two configurations measured at some fixed time t_0 depends on the temperature and that at the ferromagnetic/paramagnetic transition of the three models $D(t_0)$ displays a sharp drop. However, in contrast with the suggestion of Barber and Derrida,[10] the identification of the floating phase in the ANNNI model on the basis of $D(t_0)$ remains far from unambiguous. Indeed, all three models display very similar intermediate regimes, while it is well known that no floating phase exists for the brickwork model and the existence of a floating phase is far from being established for the BNNNI model.

One could think of the survival probability $P(t_0)$ or the distribution function $P_{t_0}(\varepsilon)$ (defined in Section 3) as giving other helpful criteria for the localization of the phase transitions. Indeed, in all the models we studied $P(t_0)$ displays a sharp drop when the temperature is increased. Except in the case of the 2D Ising model, this occurs at a significantly higher temperature than the drop of $D(t_0)$. For the ANNNI model this could be related to the occurrence of the floating phase and the sharp drop of the survival probability might indicate the transition to the high-temperature disordered phase. However, the brickwork model displays the very same behavior, although no floating phase is present. Therefore no reliable identification of such a behavior with some true thermodynamic phase seems possible. In addition, we cannot identify unambiguously the observed behavior with the $q = 1/4$ regime (at equilibrium) of the correlation function, since the brickwork model displays strong metastability and freezing effects[(15)] and transient quantities such as $P(t_0)$ are, by their very definition, sensitive to such nonequilibrium phenomena. The consideration of $P_{t_0}(\varepsilon)$ did not yield significant new information in this respect.[6]

In view of these results, we conclude that there is a low efficiency of this method for predicting phase diagrams. One basic and obvious problem is that no characteristic time *a priori* exists for distinguishing between "spurious" transient behavior and an "equilibrium-like" dynamical regime. Therefore the only *a priori* possible definition for the observation time t_0 should be the unique characteristic time of the problem, namely the equilibrium time. Of course the same problem for choosing the observation time range appears if one considers the temporal dependence of dynamical quantities rather than their behavior at fixed time. Moreover, there is in general no clear correspondence (if any) between an observed dynamical regime and equilibrium phases (apart from the critical slowing down which characterizes *transitions* between phases).

However, limiting the scope of these ideas can give grounds for more optimism. For mean-field models (at least with no structural disorder) the equilibrium phase transition corresponds also to a change in the transient behavior. In addition, it seems that in all the models studied up to now such a change always accompanied the transition from the low-temperature phase.

[6] One can also define[(7)] a response function as the derivative of $D(t_0)$ with respect to an external magnetic field. In the case of the Ising model this quantity displays near the critical temperature a sharp peak reminiscent of the susceptibility divergence at T_c. This feature is also found in the ANNNI model at the transition from the low-temperature phase. However, this does not provide a new characterization of the intermediate regime.

ACKNOWLEDGMENTS

One of the authors (D.H.) acknowledges fruitful discussions with Drs. O. Golinelli and A. Neumann.

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