"2+4" Model: A Monte Carlo study

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A Monte Carlo simulation on a two-dimensional (2D) Ising-like model with competing two- and four-spin interactions was performed. We studied the magnetization (both global and by column), susceptibility, energy, specific heat, correlation functions, and structure factors of this model for small values of x, the ratio of the interaction constants, paying special attention to any evidence of modulated structures that might appear. Our results show that no modulation is present. We have found that the x dependence of the specific heat is such that all curves can be reduced to one by a simple transformation, showing some degree of scaling. The same happens with the susceptibility and the magnetization. The phase diagram for $x < 0.5$ is given.

I. INTRODUCTION

Models with competing interactions have, during the past few years, become of interest, as they are expected to display a rich variety of phases. On the other hand, there is evidence of the remarkable effects that multispin interactions have on the critical behavior of the system.[1] A few years ago Penson[2] introduced a so called "2+4" model, mixing both competing and multispin interactions. It consists of an Ising model plus a competing four-spin interaction among nearest neighbors along one direction. Using the finite-size-scaling method on the one-dimensional quantum analog, he found only one modulated phase, the so called ⟨3-1⟩ phase, and a first-order transition, for high values of the ratio of competing interactions. A year later Kolb and Penson[3] showed that this model, unlike the ANNNI (anisotropic next-nearest-neighbor Ising) model, does not exhibit an incommensurate phase either.

Different mean-field approximations of the two-dimensional (2D) classical model[4,5] also show that no modulated phase is present other than the previously mentioned, and that as the multispin interaction increases, the transition becomes first order. A similar result has been obtained using the Müller-Hartmann and Zittartz approximation and perturbative calculations.[6]

Recently, a very interesting and original application of this model was proposed by Scott[7] who considered it to be suitable to simulate the ripple phase of a lipid bilayer, below the lipid-chain melting temperature. He states, via a Monte Carlo simulation, that modulated phases are present for small ratios of the competing interaction constants.

Therefore, there are two conflicting results. In this work we perform a more exhaustive Monte Carlo simulation of the model, studying several microscopic and macroscopic quantities, obtaining the phase diagram for $x < 0.5$. After a careful search for modulated structures, we believe we can solve the discrepancy mentioned above: our results show that no modulation is present for those values of the ratio of competing interactions. Hence we conclude that modulations reported in Ref. 7 are probably due both to finite-size effects and to the relatively small number of Monte Carlo steps per site (MCS/s) used.

The article is organized as follows: in Sec. II we define the model, state the quantities studied, and give technical details on the Monte Carlo method used. In Sec. III we present an analysis of the results and we make some remarks concerning finite-size effects. The article concludes with a brief summary.

II. MODEL AND CALCULATION TECHNIQUES

A. The "2+4" model

We consider two-dimensional lattices of $N \times M$ sites (N sites in the x direction by M sites in the y direction) with full periodic boundary conditions (a torus). We set the lattice constant $a = 1$.

Along the x axis there is a pairwise interaction competing with a four-spin one while, along the y axis, there is only a pairwise ferromagnetic interaction. The corresponding Hamiltonian is

$$H = -J_x \sum_{i=1}^{M}\sum_{j=1}^{N} s_{ij}s_{ij+1} - J_y \sum_{i=1}^{M}\sum_{j=1}^{N} s_{ij}s_{i+1j} - J_4 \sum_{i=1}^{M}\sum_{j=1}^{N} s_{ij}s_{ij+1}s_{ij+2}s_{ij+3}. \quad (1)$$

We consider $J_x = J_y = J_2 > 0$ and $J_4 < 0$ with, as usual,

$$K_i = \frac{J_i}{k_B T}, \quad (2)$$

where T is the temperature and

$$x = \frac{|K_4|}{|K_2|}. \tag{3}$$

In the following we take $k_B = 1$. Moreover, we use $T = \frac{1}{K_2}$.

B. Quantities studied and calculation techniques

In all cases, we considered two lattice sizes: 80×10 and 160×20; in some cases we also studied smaller lattices (40×10). On these systems we computed the following quantities:

(i) *magnetization per site*

$$m = \langle \mu \rangle, \tag{4}$$

where

$$\mu = \frac{1}{NM} \sum_{i,j} s_{ij}; \tag{5}$$

(ii) *column magnetization per site*

$$m_j = \frac{1}{N} \langle \mu_j \rangle, \tag{6}$$

where

$$\mu_j = \frac{1}{M} \sum_{i} s_{ij}; \tag{7}$$

(iii) *specific heat per site*

$$C = \frac{1}{k_B T^2} (\langle H^2 \rangle - \langle H \rangle^2); \tag{8}$$

(iv) *susceptibility per site*

$$\chi = \frac{1}{k_B T} (\langle \mu^2 \rangle - \langle \mu \rangle^2); \tag{9}$$

(v) *correlation function (averaged over columns)*[8]

$$\Gamma(r) = \frac{1}{N} \sum_{j=1}^{N} \Gamma^j(r) \tag{10}$$

with

$$\Gamma^j(r) = \langle \mu_j \mu_{j+r} \rangle - \langle \mu_j \rangle \langle \mu_{j+r} \rangle; \tag{11}$$

(vi) *structure factor*[9]

$$S(k) = \sum_{r=1}^{\frac{N}{2}-1} e^{-ikr} \Gamma(r), \tag{12}$$

where

$$k = \frac{2\pi l}{N}, \; l \in Z. \tag{13}$$

To study 80×10 lattices we used 50 000 MCS/s after equilibrating over 20 000 MCS/s; for 160×20 lattices we used 40 000 MCS/s to reach thermal equilibrium and 50 000 MCS/s to compute averages. In several cases we made longer runs, near T_c, to reduce the effect of critical fluctuations and critical slowing down; for the 80×10 lattice we used 70 000 MCS/s after equilibrating over 20 000, and for the 160×20 lattice we used 100 000 MCS/s and 50 000 MCS/s, respectively. Unless stated otherwise, all results reported here correspond to the 160×20 lattice.

To calculate averages we only used the results of one

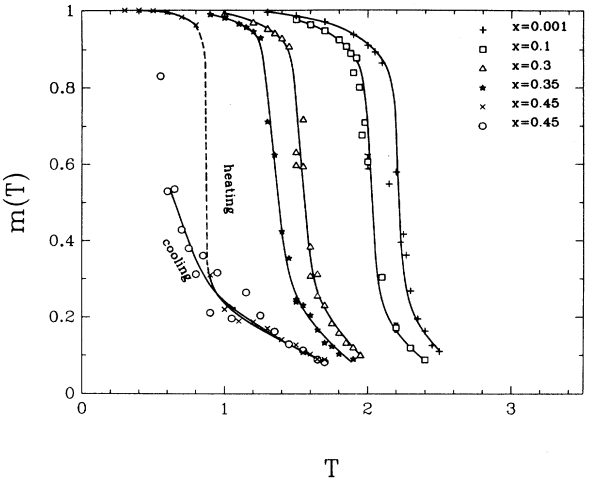


FIG. 1. Magnetization curves for some typical values of x. For $x = 0.45$ hysteresis is shown; a discontinuity is clearly seen in the corresponding heating curve. Note the unstable character of the cooling curve. Unless stated otherwise, all lines are merely a guide to the eye.

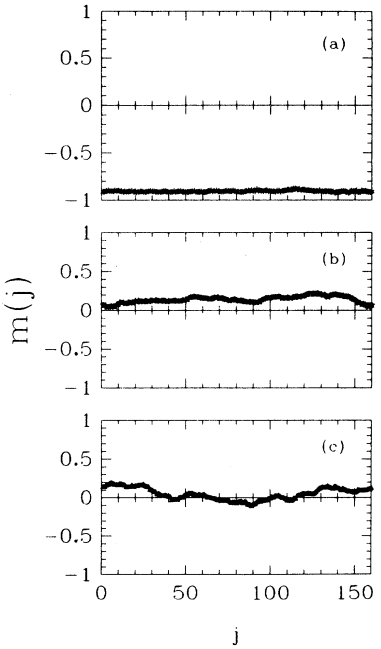


FIG. 2. Profiles of column magnetization for three values of temperature: (a) $T = 1.45$, (b) $T = 1.55$, (c) $T = 1.85$ (i.e., low T, T_c region, high T).

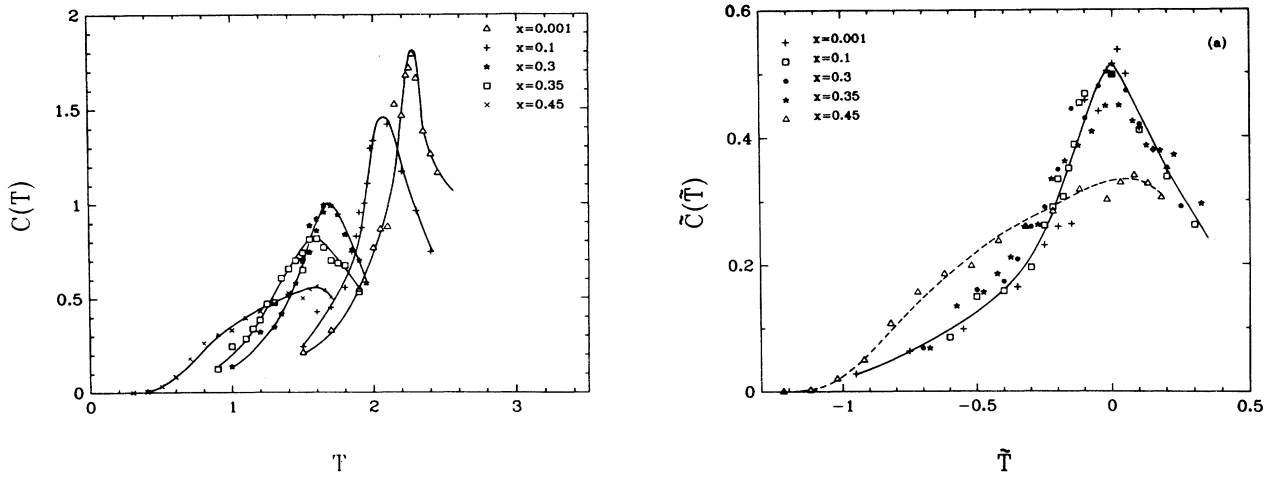
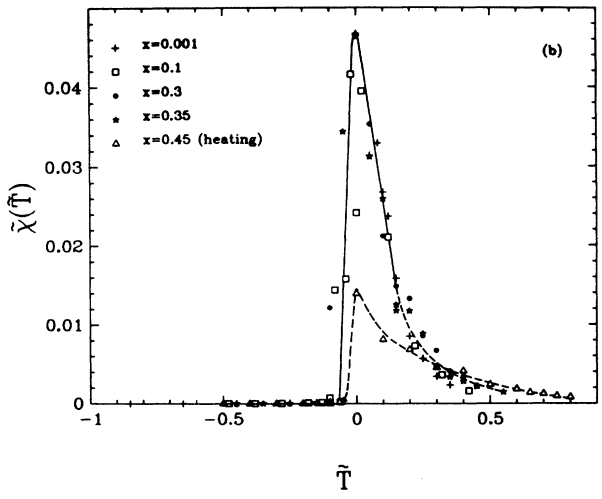


FIG. 3. Specific-heat curves for several values of x.

every P Monte Carlo steps per spin. We took P to be typically 100, 200, and 400; the values of the computed quantities obtained for $P = 100$ were highly stable for quantities (as total magnetization, energy per site, etc.) that are not fluctuations themselves. This was checked for all the runs, which allows us to consider data obtained with $P = 100$ as statistically independent.

We started from a complete ordered lattice (heating) or from a randomly chosen one (cooling). Then we changed T, using as initial configuration for the next run with $T \pm \Delta T$, the last configuration obtained at temperature T.

The spins were mainly updated by sweeping the lattice orderly along the rows; we also made some runs sweeping along columns and randomly, finding a high agreement among them. We also tried different random-



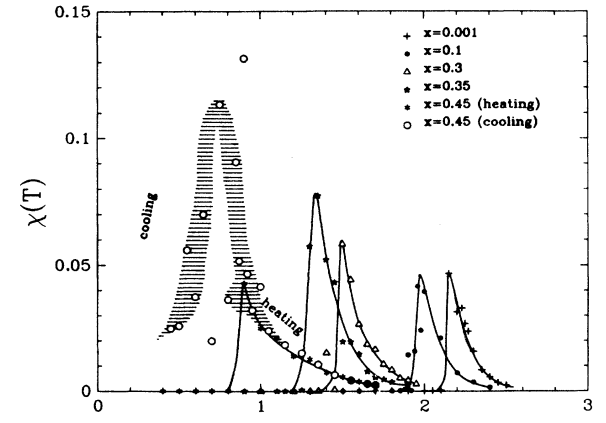


FIG. 4. Susceptibility curves for some typical values of x. Due to the presence of metastable states, no meaningful curve can be drawn for the cooling run for $x = 0.45$; the shaded region attempts to indicate the probable shape of the corresponding curve.

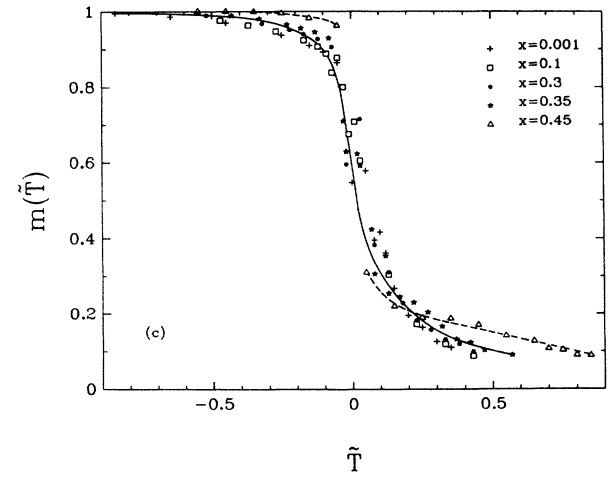


FIG. 5. Reduced specific heat (a), susceptibility (b), and magnetization (c). It is clear that all curves but those for $x = 0.45$ follow a single law.

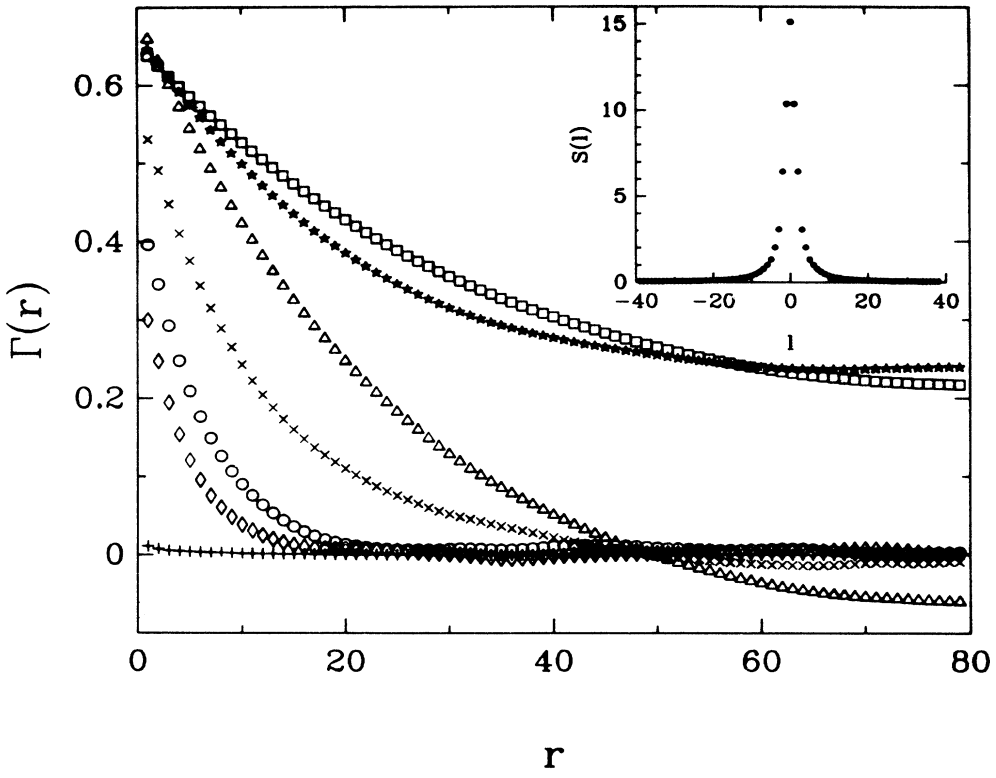


FIG. 6. Correlation function for $x = 0.3$ and different values of temperature: (+) $T = 1.45$; (□) $T = 1.5$; (⋆) $T = 1.55$; (△) $T = 1.6$; (×) $T = 1.7$; (o) $T = 1.8$; (◇) $T = 1.9$. The inset shows a typical structure factor curve for $T = 1.75$. Structure factor curves near T_c are very sharply peaked, resembling a δ function. As T increases the curves become wider and smaller.

number generators[10] and seeds, in order to discard any misleading result that might be induced by them. To get the results shown here we needed the equivalent of several thousand hours of CPU time on a μ-VAX II.[11]

III. ANALYSIS OF RESULTS

Magnetization data for different values of x is shown in Fig. 1. It can be seen that the $m(T)$ curves are continuous and show no hysteresis for $x < 0.4$ but for $x = 0.45$ we already found a discontinuity and hysteresis, which suggest that the transition is becoming first order. This change in the character of the transition has also been obtained in previous works,[2,6,4,5] although there are some numerical discrepancies related to the actual value of x where it takes place. Note, however, that we do not find a sharp peak in the corresponding specific-heat results (see below).

Three typical profiles of m_j are shown in Fig. 2. We can see that they do not show any modulation at all.

In Ref. 7 some m_j profiles were shown exhibiting modulation for $T \sim T_c$. To further check this point we tried runs using the same number of steps as in that work (4000 MCS/s after equilibrating over 1600 MCS/s), obtaining similar profiles. Therefore we believe that those modulations arise from the fact that the number of steps used is too small. A similar behavior to the one shown in Fig. 2 was found for all the studied values of x.

In general, errors in $m(T)$ curves have been calculated, as usual, considering data as statistically independent, according to the technique referred to in Sec. II B.

The specific-heat results shown in Fig. 3 indicate that the curves become wider and less sharply peaked as we

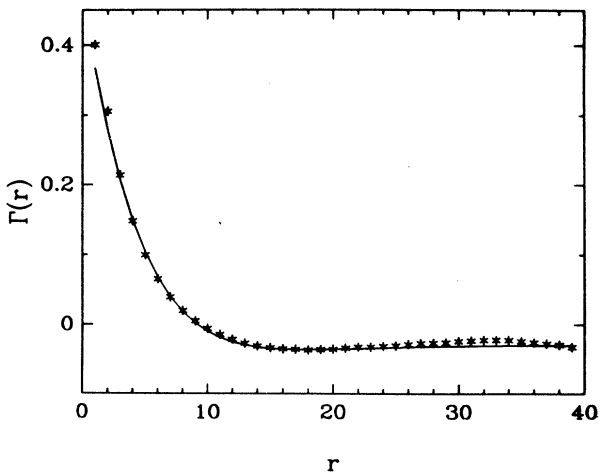


FIG. 7. Data points for the 80×10 lattice, $x = 0.3, T = 1.92$, fitted with the law given by Eq. (18) (solid line) with $\lambda = 0.2, k = 0.09, \varphi = 0.4, A = 0.55, B = -0.03$, which gives a period of approximately 70 lattice sites.

approach $x = 0.5$. As mentioned before, we could not observe the expected sharply peaked maximum characterizing the first-order transition shown by $m(T)$ curves for $x = 0.45$, perhaps because it is necessary to sweep it with even smaller ΔT steps.

Errors in specific-heat curves were estimated from repeated runs starting from different initial configurations, using different random-number generators or seeds; in some cases we also compared cooling and heating runs. Our data can be considered accurate within ±5% (10% near T_c).

Small anomalies that could have been considered as additional small peaks proved to be due to the sensitiveness of specific heat to critical fluctuations and to critical slowing down. To be sure that this was the case, we ran these points again using a greater number of MCS/s; alternatively, we ran all the conflicting temperatures again using smaller ΔT steps. In both cases we found that these small peaks were corrected.

Susceptibility results are shown in Fig. 4. As in the previous quantities, it is possible to see that the $x = 0.45$ curve is qualitatively different from the others.

We have found that the results of the specific heat, susceptibility, and magnetization for $x < 0.45$ show some degree of scaling. Using $\tilde{T}(x) = T - T_c(x)$ we were able to reduce all specific-heat curves to a single one. The same behavior was found for χ and m. The corresponding laws are (see Fig. 5)

$$\tilde{C}(\tilde{T}(x)) = w_c(x)\, C(T - T_c(x)), \tag{14}$$

$$\tilde{\chi}(\tilde{T}(x)) = w_\chi(x)\, \chi(T - T_c(x)), \tag{15}$$

$$\tilde{m}(\tilde{T}(x)) = m(T - T_c(x)), \tag{16}$$

where

$$w_c(x) = 0.3 + \tfrac{2}{3}x, \tag{17}$$

$$w_\chi(x) = 1 - \tfrac{3}{2}x. \tag{18}$$

To study microscopic details of the model we found it interesting to calculate the correlation function and the related structure factor. Correlation function curves for different values of T are shown in Fig. 6 for one particular value of x.

In Ref. 7 modulations found were suggested to be a consequence of strong modulated correlations, which set in gradually with increasing temperature. In order to find out whether there is any modulation in our correlation data we tried to fit it with the following law:

$$\Gamma(r) = A\, e^{-\lambda r} \cos(kr + \varphi) + B. \tag{19}$$

Figure 7 shows one of the best fits achieved for a particular value of x. The value of $k \simeq 0.09$ found, gives a period of about 70 lattice sites, which is of the order of the lattice size. For our biggest system (160×20) it was even more difficult to find correlation curves that might have any modulation. This result is in agreement with the structure factor curves, which have, in general, a peak centered in $k = 0$ (see Fig 6).

The analysis of the correlation function data also gave

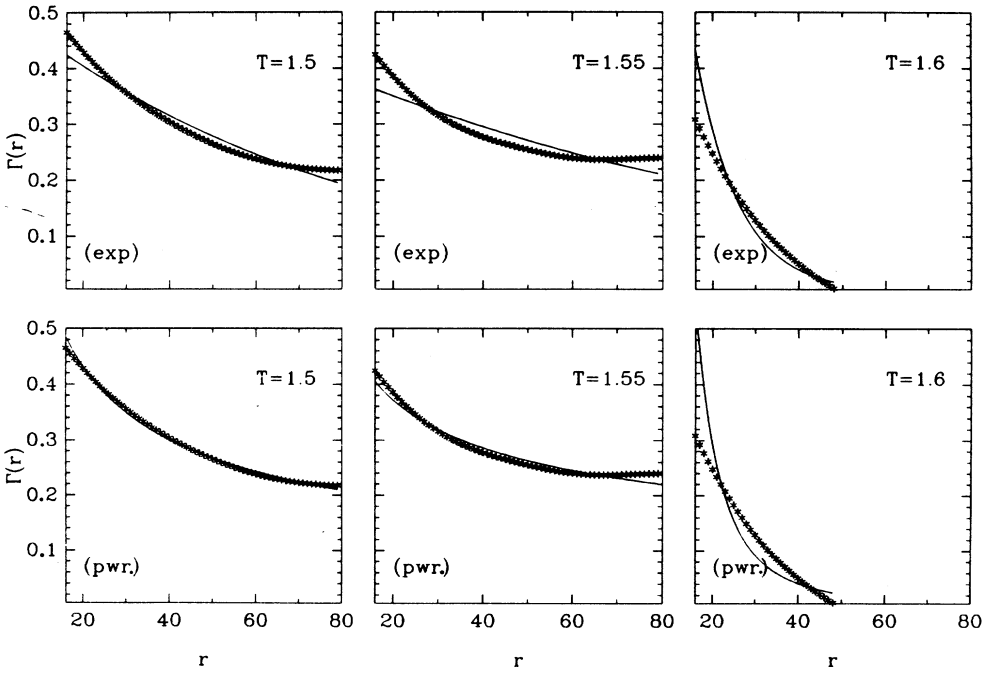


FIG. 8. Critical temperature determination using exponential and power-law fittings of the correlation functions, for $x = 0.3$. For $T = 1.5$ and 1.55 the power law gives a better least-squares fit. For $T = 1.6$ the best fit is given by the exponential.

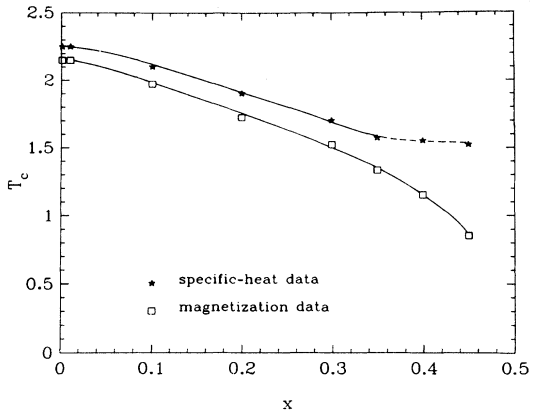


FIG. 9. Phase diagram for $x < 0.5$. The behavior of the critical line obtained from the specific-heat data near $x \simeq 0.4$ can be related to the change of the shape of the corresponding $C(T)$ curves.

us an alternative way of estimating T_c. We fit some curves (those in the expected T_c region) with a power law and an exponential law (see Fig. 8). We found one or, at most, two contiguous temperatures whose corresponding curves follow a power law with minimum error (as expected for T_c). We think that T_c obtained in this way is accurate within $\Delta T = 0.05$. The transition temperature obtained in this form is similar to T_c obtained from susceptibility and magnetization data. As usual, the specific-heat critical temperature is slightly higher. Figure 9 shows the phase diagram for the studied region, obtained from our data.

We do not have enough information to make a serious finite-size study of our results. Nevertheless, there are several comments that can be made related to this point.

The size dependence of T_c for a particular value of x can be seen in Fig. 10. The critical temperature found from the specific heat has only a weak dependence on the size of the lattice, and it increases a little with x. This leads us to think that our lattice size is big enough to study the system from this simulation.

The structure factor proved to be somewhat more size dependent: for the 160×20 lattices it is just a single peaked curve, centered around $k = 0$, while for 80×10 lattices it has two peaks at $k = \pm\frac{\pi}{N}$ (predicting a long-wavelength modulation).

As mentioned before, the importance of using a lattice as big as possible was also seen while checking the independence of results on the updating method. In fact, when updating by columns the 80×10 lattice, we needed more steps to reach thermal equilibrium than those required when updating by rows; this was not the case for the 160×20 lattice.

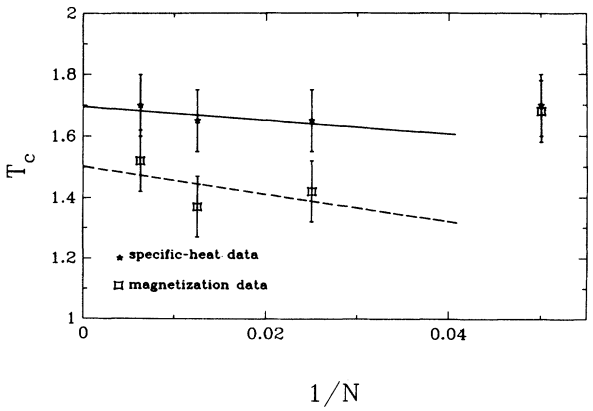


FIG. 10. Size dependence of T_c for $x = 0.3$.

IV. SUMMARY

We performed a Monte Carlo simulation on the 2D "2+4" model, obtaining the phase diagram for $x < 0.5$, along with macroscopic (magnetization, energy, specific heat, suceptibility) as well as microscopic (correlation functions, structure factor) quantities of the system. Our results show no modulation in this region of the x parameter, although we carefully looked for them not only in the column magnetization but also in the correlation function and structure factor. The fact that these modulations show up in short runs points out that to get a correct picture of this model one needs longer Monte Carlo sequences than in other Ising-like systems. This is especially true as one approaches $x \simeq 0.5$, as in the well-known case of the ANNNI model. We also found that the use of big enough lattices is an important point to this end.

The system exhibits a change in the character of the phase transition (from continuous to discontinuous) as x becomes greater than 0.4. Magnetization data clearly show hysteresis in heating and cooling runs. Scaling laws found for $x < 0.45$ give support to the idea that for these values of the ratio of the interaction constants, the system has only quantitative changes as a function of x.

From the technical point of view, we found it useful to obtain the critical temperature studying the asymptotic dependence with distance of the correlation function.

For $x > 0.5$ the situation is, of course, very different. The ground state itself shows a modulation, and has a different (higher) degeneracy.[12] In this case the main result is the already mentioned nonexistence of incommensurate phases.[3] Hence, a Monte Carlo simulation should be rather oriented to the study of the kinetics of the wall domains. Work in this direction is in progress.

ACKNOWLEDGMENTS

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[10] *Applications of the Monte Carlo Method in Statistical Physics*, Vol. 36 of *Topics in Current Physics*, edited by K. Binder (Springer-Verlag, Berlin, 1984), p. 3.
[11] Results for the 160×20 system were obtained using a Definicon DSI-020 card, which is about 2.5 times faster than a μ-VAX II.
[12] The $x > 0.5$ region is of no interest for the lipid bilayer system, because of physical reasons (see Ref. 7). The $\langle 3\text{-}1 \rangle$ modulation, moreover, is not adequate to represent the bilayer, because of both its wavelength and symmetry.