Finite-size-scaling estimation of critical exponents in the two-dimensional axial next-nearest-neighbor Ising model

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The magnetic critical exponent of the two-dimensional axial next-nearest-neighbor Ising model is estimated by means of the finite-size scaling of the order parameter. For a finite system without ordering field, this magnitude is computed from the two leading eigenvectors of the transfer matrix. The ferromagnetic-paramagnetic transition temperatures estimated with this method exhibit a small lattice-size dependence. Moreover, they are in good agreement with those obtained using phenomenological renormalization, and also with analytical approximations. The correlation-length critical exponent is calculated by means of phenomenological renormalization. The results found with these numerical techniques indicate that the ferromagnetic-paramagnetic transition of the model seems to be continuous, in contradiction with a previous result obtained using the persistence-length criterion, which indicated that the transition is always first order. We found that the phase transition is first order only when the ratio of the next-nearest-neighbor and nearest-neighbor interactions equals one-half.

I. INTRODUCTION

Systems with competitive interactions have been extensively studied in recent years.[1] The axial next-nearest-neighbor Ising (ANNNI) model[2] is one of the simplest realizations of such systems. The physics underlying this simple model is very rich, including features such as commensurate-incommensurate phase transitions,[3] Lifshitz points,[4] multiphase points with infinite ground-state degeneracy,[5] and disorder lines.[6]

The reduced Hamiltonian of the two-dimensional ANNNI model is defined as

$$-\beta\mathcal{H}=K_0\sum_{m,n}S_{m,n}S_{m+1,n}+K_1\sum_{m,n}S_{m,n}S_{m,n+1}-K_2\sum_{m,n}S_{m,n}S_{m,n+2}\;,$$
$$K_i=J_i/T,\quad J_i>0,\quad S_{m,n}=\mp 1\;, \tag{1}$$

where $\beta=1/T$. The Boltzmann constant is taken to be unity.

The regime of competing interactions $(J_1,J_2>0)$ can be divided into ferromagnetic (small temperature, $X=J_2/J_1<0.5$), paramagnetic (high temperature), and a degenerate phase known as $\langle 2\rangle$ ($X>0.5$, low temperatures); the last phase is characterized by a fourfold degenerate ground state which is a periodic arrangement of two up spins followed by two down spins along the direction of the competitive couplings.

Figure 1 reproduces the phase diagram of the model, obtained by means of phenomenological renormalization (PR) and finite-size scaling (FSS) of the order parameter.[7] In this article we estimate the magnetic and correlation-length critical exponents, and conclude that the ferromagnetic-paramagnetic phase transition of the ANNNI model seems to be continuous. To achieve this purpose we look at the FSS hypothesis according to which the magnetization per spin in a d-dimensional magnetic system of linear dimension N, at the transition point when N is large enough, is expected to behave as

$$m_N\sim N^{(y_h-d)}\;, \tag{2}$$

where y_h is the magnetic critical exponent. However, in a finite system whose Hamiltonian is invariant under spin reversal, the magnetization should vanish identically.

As is well known, this difficulty can be overcome by considering the two-spin correlation function $\langle s_0 s_{\mathbf{r}}\rangle$. In the limit $\mathbf{r}\to\infty$ this quantity approaches the square of the spontaneous magnetization m.

Takano and Saito[8] used the correlation function of a finite system to obtain an estimation of m, and computed y_h in the Ising and three-state Potts model in two dimensions by applying the FSS equation (2). As will be explained in Sec. II, m_N can be found from the two leading eigenvectors of the transfer matrix associated to the system.

The critical exponent y_T of the correlation length ξ was obtained, as usual,[9] from the FSS of ξ at the transition temperature T_c,

$$\xi_N\sim N\;, \tag{3}$$

which in turn implies

$$\left.\frac{\partial(1/\xi_N)}{\partial T}\right|_{T=T_c}\sim N^{(y_T-1)}\;, \tag{4}$$

where T_c is obtained from PR.

The exponent y_T may be read off from the slopes of the curves $N/\xi_N(T), N'/\xi_{N'}(T)$ at their intersection point, namely, at $T=T_c$,

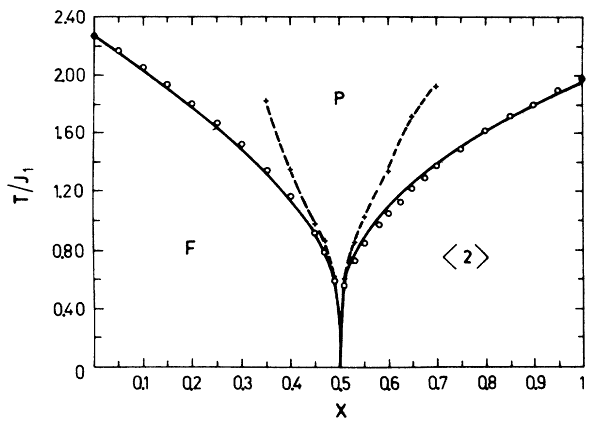

FIG. 1. Phase diagram of the ANNNI model, for $J_0=J_1$. Solid lines represent analytical calculations using the Müller-Hartmann and Zittartz approximation. The circles denote our estimation of the transition temperatures obtained through the FSS of the order parameter and PR. The symbols F and $\langle 2\rangle$ indicate the ordered phases. The paramagnetic (P) region has some internal structure (dashed line). Size effects are negligible on the lower transition line and very difficult to estimate along the second transition line.

$$Y_T=\frac{\ln\left[\left.\frac{\partial(N/\xi_N)/\partial T}{\partial(N'/\xi_{N'})/\partial T}\right|_{T=T_c}\right]}{\ln(N/N')}\ , \tag{5}$$

where N and N' are two different lattice sizes.

II. THE MAGNETIC CRITICAL EXPONENT

We use an Hermitian (real) representation of the transfer matrix $\hat{T}$ of a lattice of $M\times N$ sites with periodic boundary conditions.[10] Then $\hat{T}$ can be written as

$$\hat{T}=V_0^{1/2}V_H V_1 V_2 V_0^{1/2}\ , \tag{6}$$

where the V's are $2^N\times 2^N$ matrices given by

$$\begin{aligned} V_H&=\exp\left[H\sum_n \sigma_n^x\right],\\ V_1&=\exp\left[K_1\sum_n \sigma_n^x\sigma_{n+1}^x\right],\\ V_2&=\exp\left[-K_2\sum_n \sigma_n^x\sigma_{n+2}^x\right],\\ V_0&=(2\cosh K_0)^N(\tanh K_0)^{\hat{\mathcal{N}}}\ .\end{aligned} \tag{7}$$

σ_n^x is the Pauli spin matrix for the site n in an arbitrary row, H the reduced magnetic field, N the number of columns, and $\hat{\mathcal{N}}$ is the row number operator which written in terms of spin raising and lowering operators is simply

$$\hat{\mathcal{N}}=\sum_n \sigma_n^+\sigma_n^-\ . \tag{8}$$

This enables us to compute its eigenvectors by means of the Lanczos scheme.[11] As is explained in Ref. 10, this represents a significant saving of computer time.

Following Ref 12, the correlation function for two spins located on sites (m,n) and $(m+P,n')$ is expressed as

$$\langle S_{m,n}S_{n+P,n'}\rangle=\frac{\sum_i\sum_j \langle j\,|\,V_0^{1/2}\sigma_n^x V_0^{-1/2}\,|\,i\rangle\langle i\,|\,V_0^{1/2}\sigma_{n'}^x V_0^{-1/2}\,|\,j\rangle\lambda_i^P\lambda_j^{(M-P)}}{\mathrm{Tr}\hat{T}^M}\ , \tag{9}$$

where the double sum runs over an orthogonal basis in which $\hat{T}$ is diagonal, λ_j is the eigenvalue corresponding to the $|\,j\rangle$ eigenstate, and M is the number of rows.

As $M\to\infty$, Eq. (9) reduces to

$$\langle S_{m,n}S_{m+P,n'}\rangle \xrightarrow[M\to\infty]{} \sum_i \langle \psi_1\,|\,V_0^{1/2}\sigma_n^x V_0^{-1/2}\,|\,i\rangle\langle i\,|\,V_0^{1/2}\sigma_{n'}^x V_0^{-1/2}\,|\,\psi_1\rangle\left[\frac{\lambda_i}{\lambda_1}\right]^P\ , \tag{10}$$

where $|\,\psi_1\rangle$ is the eigenvector corresponding to the maximum eigenvalue λ_1.

In the following, we assume there is no external ordering field H applied to the system. Then the Hamiltonian is invariant under spin reversal, and the eigenvectors of the transfer matrix can be classified into even and odd, i.e., $\hat{T}$ commutes with $(-1)^{\hat{\mathcal{N}}}$. A further simplification of the asymptotic behavior of the correlation function can now be done.

Since $|\,\psi_1\rangle$ is an even state and the operator $V_0^{1/2}\sigma_n^x V_0^{-1/2}$ changes parity, Eq. (10) can be written

$$\langle S_{m,n}S_{n+P,n'}\rangle \xrightarrow[P\to\infty]{} \langle \psi_1\,|\,V_0^{1/2}\sigma_n^x V_0^{-1/2}\,|\,\psi_2\rangle\langle \psi_2\,|\,V_0^{1/2}\sigma_{n'}^x V_0^{-1/2}\,|\,\psi_1\rangle\left[\frac{\lambda_2}{\lambda_1}\right]^P\ , \tag{11}$$

where $|\,\psi_2\rangle$ denotes the eigenstate corresponding to the second largest eigenvalue λ_2 of the transfer matrix. Now consider the thermodynamic limit, i.e., $N\to\infty$. In that case some care must be taken but Eq. (11) is still true.

As is well known, at a critical point, λ_2 approaches λ_1 implying a divergence of the correlation length,

$$\xi=\left[\ln\left[\frac{\lambda_1}{\lambda_2}\right]\right]^{-1}\ . \tag{12}$$

The degeneracy of λ_1 and λ_2 for $T<T_c$ means that the correlation function given in Eq. (11) yields a finite asymptotic value,

$$\langle S_{m,n}S_{m+P,n'}\rangle \xrightarrow[P\to\infty]{} \langle\psi_1|V_0^{1/2}\sigma_n^x V_0^{-1/2}|\psi_2\rangle\langle\psi_2|V_0^{1/2}\sigma_{n'}^x V_0^{-1/2}|\psi_1\rangle \ . \quad (13)$$

If $x<0.5$ (ferromagnetic ground state), the square of the spontaneous magnetization m is given by

$$m^2=\langle\psi_1|V_0^{1/2}\sigma_n^x V_0^{-1/2}|\psi_2\rangle\langle\psi_2|V_0^{1/2}\sigma_{n'}^x V_0^{-1/2}|\psi_1\rangle \quad (14)$$

for any election of n and n'.

If $X>0.5$ ($\langle 2\rangle$ ground state) at low temperatures, the spontaneous magnetization vanishes identically. However, it is possible to look at any of the four sublattices obtained by keeping one every four columns. In this case the (sublattice) magnetization is nonzero and may be calculated through Eq. (14) by selecting $n'=n+4k$ ($k=0,1,2,\ldots$).

For a finite system (finite N), the right-hand side of Eq. (14) may be considered as an estimation of the order parameter provided N is taken large enough. Moreover, m_N is expected to behave according to Eq. (2), i.e., to obey FSS.

III. RESULTS

In this work we have used lattice sizes up to $N_{max}=12$ and studied the case $K_0=K_1$. This can be achieved in a relatively fast way using the Lanczös scheme and the method described in Ref. 10.

A. $X<0.5$

Two methods can be used to determine y_h.[8] The first one uses T_c as a data, which can be obtained for instance from PR. Once T_c is known, y_h is estimated from the FSS of m_N.

In the second method T_c itself is determined from the FSS of m_N. Provided the FSS equation (2) holds for three different values N_1, N_2, and N_3 at $T=T_c$, then T_c and y_h can be determined simultaneously from the equation

$$g(T_c,N_1,N_2)=g(T_c,N_2,N_3)=d-y_h \ , \quad (15)$$

where g is the scaling function defined as

$$g(T,N,N')=-\frac{\ln[m_N(T)/,m_{N'}(T)]}{\ln(N/N')} \ . \quad (16)$$

The first equality of Eq. (15) gives T_c and the second one gives y_h.

Figures 2(a) and 2(b) show the convergence of our estimation of $d-y_h$ for $X=0$ (Ising model) and $X=0.45$, respectively. It can be seen that convergence is faster for the first procedure. The convergence is improved in both methods when smaller values of X are considered.

Figure 3 shows the dependence of $d-y_h$ with X and N. Convergence is rather poor when $X>0.3$ and can be improved by using T_c (N_{max}) as obtained from PR [see Fig. 2(b)].

A similar result is obtained for the critical exponent of the correlation length $\nu=1/y_T$, which is estimated through Eq. (5). This is shown in Fig. 4 where it also can be been that convergence turns out to be poor for $X>0.3$.

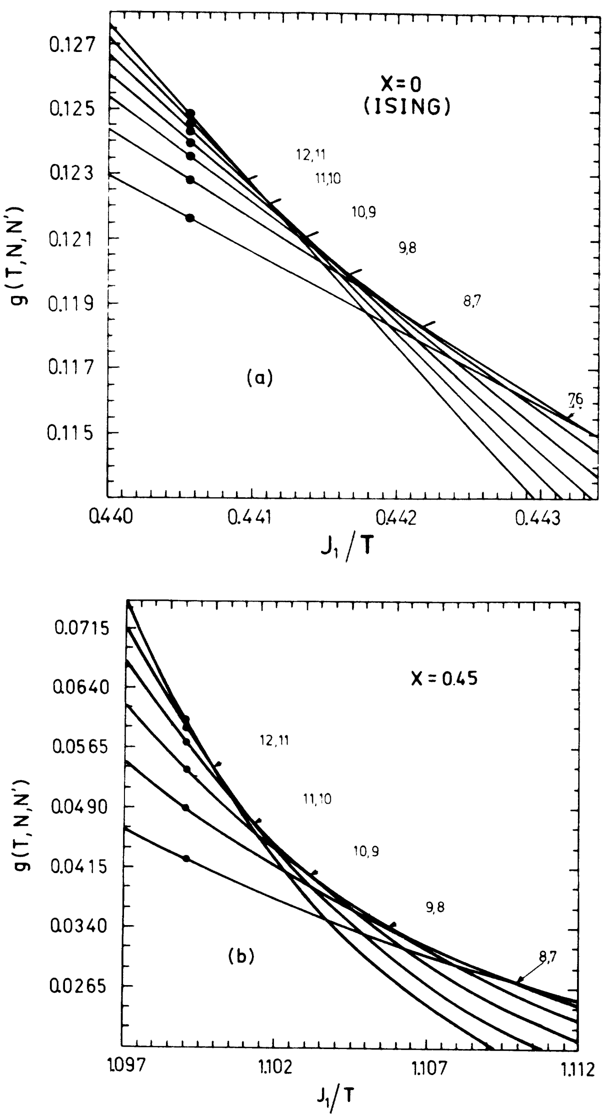

FIG. 2. Scaling function $g(T,N,N')$ vs J_1/T for different values of N and N'. The arrows indicate the points used for the estimations of both $d-y_h$ and T_c by means of Eq. (15). The dots represent the convergence of the estimation of $d-y_h$ using T_c as data obtained from PR. In (a) we show results for $X=0$ (Ising model) which exhibit a faster convergence than those for (b) $X=0.45$.

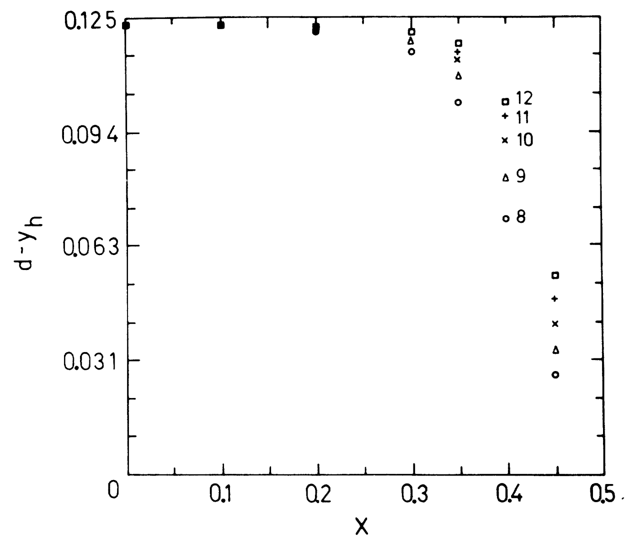

FIG. 3. $d-y_h$ as a function of X for different lattice widths.

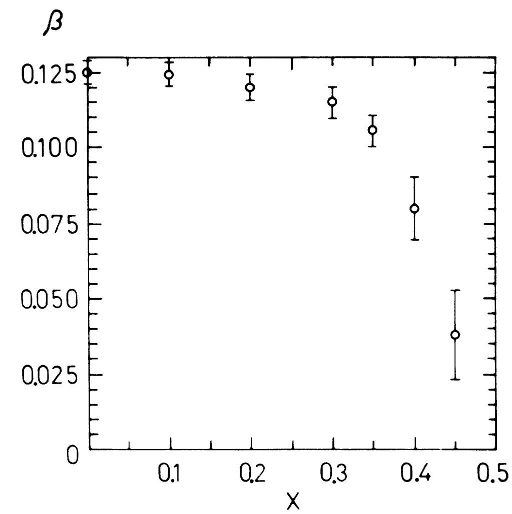

FIG. 5. Magnetization critical exponent β as a function of X. The error bars represent the sensitivity of β to small changes (less than 1%) in the transition temperatures.

Convergence could be improved using extrapolation procedures found in the literature.[13] Unfortunately, the use of such convergence acceleration techniques requires a reasonable number of terms in the original sequence [requirement fulfilled in calculations involving transfer matrix on two-dimensional systems or quantum Hamiltonians in (1 + 1) dimension]; moreover, the terms must be of relatively high numerical precision to avoid round-off problems.

In our case, numerical accuracy reaches 0.001% but it seems not to be accurate enough to avoid convergence unstability.[14] We have estimated the magnetization critical exponent through the hyperscaling equation $\beta=(d-y_h)\nu$.

Figures 5 and 6 show β and ν, respectively, and their sensitivity to small changes (less than 1%) in the transition temperatures which is represented by the error bars. It can be seen that sensitivity is minimum at $X=0$ (Ising model) where β and ν deviate less than 0.1% from their exact values.

B. $X>0.5$

In this case, N is restricted to be 4,8,12, . . . , due to the ground-state structure and periodic boundary conditions. Hence, we have been unable to use the second method. ($N=4$ seems to be too small to be considered, and $N=16$ demands a great amount of memory storage.[15])

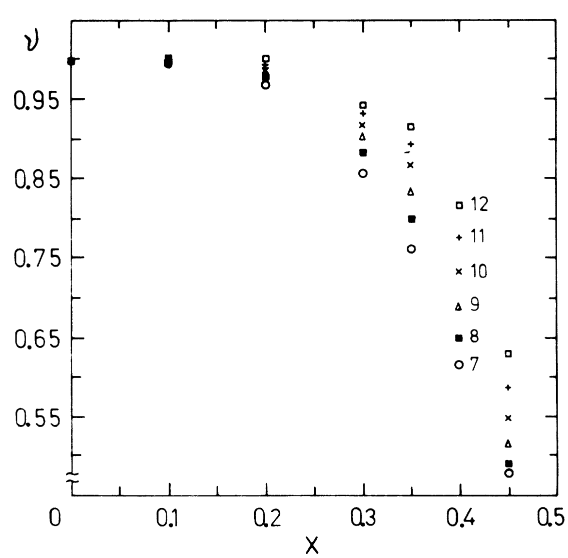

FIG. 4. Critical exponent of the correlation length, ν, as a function of X for different lattice widths.

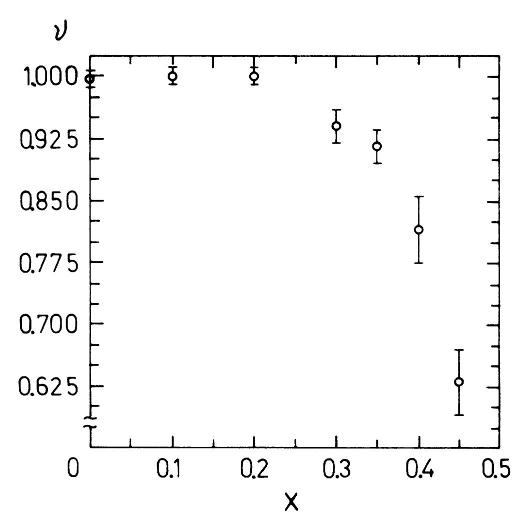

FIG. 6. Correlation length critical exponent ν as a function of X. The error bars denote the sensitivity of ν to small changes (less than 1%) in the transition temperatures.

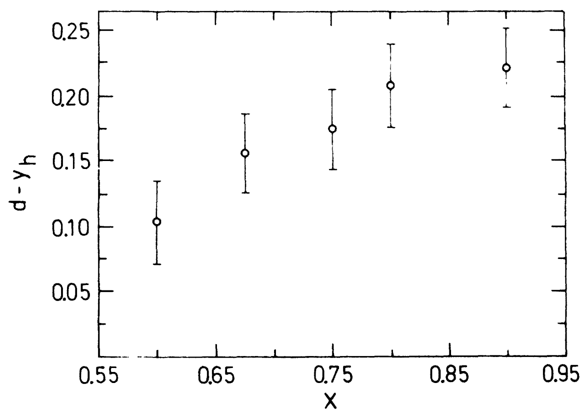

FIG. 7. $d-y_h$ for $X>0.5$. In this case we were restricted to using only two lattice widths ($N=8$ and 12), due to the ground-state structure. The error bars, denoting the sensitivity of $d-y_h$ with the transition temperature localization, indicate that for a more reliable estimation, higher values of N should be considered.

Figure 7 shows rough estimations of $d-y_h$, obtained with $N=8$ and 12. The transition temperature T_c was estimated using PR. The error bars indicate as before the sensitivity of $d-y_h$ to be small variation (less than 1%) in T_c.

C. Transition temperatures

In contrast with the sensitivity of the critical exponents β and ν with the lattice size, we have found that the transition temperatures determined with PR and the FSS of the magnetization exhibit a small lattice-size dependence. Both procedures give approximately the same numerical values of T_c. However, the agreement with analytical calculations, such as those which use the Müller-Hartmann and Zittartz[16] approximation, is quite satisfactory. For instance, Hornreich *et al.*[17] give for $X<0.5$, the following expression of the ferromagnetic-paramagnetic transition line:

$$\sinh(2K_0)\sinh(2K_1-4K_2)=1 \ . \quad (17)$$

For $X>0.5$, Kroemer and Pesch[18] have found via surface energy calculations that the $\langle 2 \rangle$-paramagnetic transition line is given by

$$2K_0=\ln\left[\frac{1-\exp(-4K_2)}{[1-\exp(-K_1-2K_2)][1-\exp(K_1-2K_2)]}\right] . \quad (18)$$

Figure 1 shows Eqs. (17) and (18) for $K_0=K_1$ together with PR and FSS results. The agreement among these methods is remarkable.

IV. CONCLUSIONS

Results for $X<0.5$ admit any of the following interpretations.

(i) The model has always an Ising-like behavior, in which case our results are simply showing an increase of the size dependence as $X\to 0.5$.

(ii) The system is always nonuniversal, but for $X\lesssim 0.2$ it is numerically very hard to distinguish this from an Ising-like behavior.[19]

(iii) Lastly, it could be that the system is Ising-like for $X\lesssim 0.2$ and nonuniversal for $X\gtrsim 0.2$. In this case, however, there should have to be some extra indication of this behavior in the phase diagram, which is not apparent in our results.

To summarize, we do not have conclusive evidence on this subject. Nevertheless, our results are useful to show that as $X\to 0.5$ it is observed that $y_n\to 2=d$ implying a first-order transition.[20] Note that convergence for $d-y_n$ obtained with the first method described before is accurate enough [see Fig. 2(b)] to consider $y_h\to d$.

In a previous work[10] the present authors employing a criterion associated with the persistance length[21] found that the phase transition seems to be first order for all $X\neq 0$, while this work indicates that for $X<0.5$ the system undergoes a continuous phase transitions.

This contradiction leaves an open problem related to the application to first-order transitions of criteria well verified for continuous transitions. We think, in particular, that the use of the persistence-length criteria needs further clarification. Results for $X>0.5$ are less relevant, because we were limited by computing considerations to use results for $N=8$ and $N=12$ only.[15]

ACKNOWLEDGMENT

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