Finite-size behavior of the Ising square lattice*

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(Received 7 July 1975)

An importance-sampling Monte Carlo method is used to study $N \times N$ Ising square lattices with nearest-neighbor interactions and either free edges or periodic boundary conditions. The internal energy, specific heat, order parameter, susceptibility, and near-neighbor spin-spin correlation functions of the finite lattices are determined as a function of N and extrapolated to the corresponding infinite-system values. The effect of finite size is greater for free edges in all cases. The results agree well with predictions of finite size scaling theory and the shape functions as well as amplitudes of surface contribution terms are determined.

I. INTRODUCTION

Although the properties of the spin-$\frac{1}{2}$ Ising model on an infinite square lattice are well known,[1] the behavior of finite square lattices is less well understood. Some exact calculations have been made[2,3] for the thermal properties on $N \times N$ lattices with periodic boundary conditions (p.b.c.) for $N \leq 64$, but lattices with free edges could be studied only for very small systems ($N \leq 4$). For the magnetic behavior no such information is available for fully finite square lattices. The expected behavior of finite systems has been discussed by Fisher[4] in terms of scaling functions involving the *infinite*-lattice critical exponents. According to this finite-size scaling theory the free energy of an $N \times N$ lattice is given by the scaling ansatz:

$$F(N, T) = N^{-\Psi} \mathcal{F}(N^{\theta} \dot{\epsilon}) , \tag{1.1}$$

with $\Psi = (2 - \alpha)/\nu$, and in terms of the size-dependent "ordering" temperature $T_c(N)$,

$$\dot{\epsilon} = [T - T_c(N)]/T_c(\infty) = \epsilon + \Delta\epsilon(N) , \tag{1.2}$$

$$\epsilon = [T - T_c(\infty)]/T_c(\infty) , \tag{1.3}$$

$$\Delta\epsilon = [T_c(\infty) - T_c(N)]/T_c(\infty) \approx aN^{-\lambda} \quad \text{as } N \to \infty . \tag{1.4}$$

The scaling of the correlation length $\xi \alpha \epsilon^{-\nu}$ suggests $\theta = \nu^{-1}$, so that the size-dependent critical behavior depends upon the scaled variable $x = \dot{\epsilon} N^{1/\nu}$. The calculations of Ferdinand and Fisher[3] show that the thermal properties of $N \times N$ lattices with p.b.c. do obey finite-size scaling, and in this paper we shall study the scaling behavior of other properties. Fisher[4] also predicted that the effect of free-edge boundary conditions is simply to introduce an extra "surface contribution" in the expression for the free energy [Eq. (1.1)]. This surface term should be proportional to N^{-1}. The bulk critical behavior is then modified by a correction term involving a new set of exponents[5,6] α_s, β_s, γ_s, etc. (which involve combinations of infinite-lattice exponents). Using the data for lattices with free edges we shall test the scaling predictions for surface correction exponents and extract the amplitudes of the surface terms. Au-Yang and Fisher[7] have recently shown that these scaling ideas correctly describe the behavior of $N \times \infty$ strips with free edges. For such strips, or for $N \times N$ lattices with p.b.c. in only one direction all surface spins are equivalent and contribute equally to the surface correction. However, lattices with all free edges have corners which may give an additional correction of unknown form and magnitude. It is doubtful that our data will be sufficiently accurate to separate out the corner contributions although for quite small N the effect of the corners may be to increase deviations from the simple scaling form. In any case, the finite-size behavior of the magnetic properties is not known analytically for any boundary conditions and our data should provide the first information in this area.

A complete understanding of these finite-size effects is also quite important from a practical point of view since it will provide a guideline for the interpretation of Monte Carlo data on other more complicated systems.

The method used for these computer "experiments" will be described in Sec. II and the results will be presented in Sec. III. In Sec. IV we shall show how the data obtained for finite systems may be extrapolated to yield infinite-lattice values and shall use the data to test the validity of finite-size scaling theory.

II. MONTE CARLO METHOD

A. Theory and algorithm

The Monte Carlo method was first applied to problems in statistical mechanics by Metropolis

et al.[8] who used it to study the equation of state of a two-dimensional system of hard disks. The technique was modified slightly by Fosdick and coworkers[9] so as to be applicable to Ising-like lattice models and a wide range of studies have followed.[10-12] Since different variations of the method have been used by various workers, we shall briefly describe the procedure which we have followed. (The same approach has been followed in our studies[13] of more complicated Hamiltonians and will not be repeated elsewhere.)

In this importance-sampling Monte Carlo calculation the statistical-mechanical expectation value $\langle A\rangle$ of a property A is estimated by its expectation value over a relatively small sample of the total collection of states of the system. The configurations used for this estimate are chosen so that the probability p_μ of the μth state appearing is related to the importance of its contribution to the expectation value. The estimate $\langle A\rangle_M \approx \langle A\rangle$ is then given by a weighted average over the M states sampled[8,9]:

$$\langle A\rangle_M = \frac{\sum_{\mu=1}^{\mu=M} A_\mu p_\mu^{-1} e^{-E_\mu/kT}}{\sum_{\mu=1}^{\mu=M} p_\mu^{-1} e^{-E_\mu/kT}}, \tag{2.1}$$

where A_μ is the value of A in the μth state and E_μ is the corresponding energy of that state. We have chosen the simplest, although not necessarily optimum, importance-sampling scheme with

$$p_\mu = \frac{e^{-E_\mu/kT}}{\sum_{\mu'=1}^{\mu'=M} e^{-E_\mu/kT}}. \tag{2.2}$$

With this choice the estimate $\langle A\rangle_M$, as given in Eq. (2.1), reduces to the simple arithmetic average

$$\langle A\rangle_M = \frac{1}{M}\sum_{\mu=1}^{\mu=M} A_\mu . \tag{2.3}$$

Since we shall generate each new state from the preceding one (as described below) only the *relative* probability of the two states is needed, i.e.,

$$\rho_{\mu\nu} = p_\mu/p_\nu = e^{-(E_\mu - E_\nu)/kT} \tag{2.4}$$

describes the probability of producing the νth state from the μth one.

We have used this sampling technique to study $N\times N$ Ising square lattices with

$$\mathcal{H} = K_{\rm nn}\sum_{(ij)} \sigma_i\sigma_j , \tag{2.5}$$

where $K_{\rm nn} < 0$ (ferromagnetic), $\sigma_i, \sigma_j = \pm 1$, and (ij) indicates nearest-neighbor nn pairs. Two types of boundary conditions were considered: (i) p.b.c. (periodic boundary conditions), where spins at the start and end of the same row (column) are regarded as nearest neighbors, and (ii) free edges.

Some of the thermodynamic quantities are calculated directly from Eq. (2.1), e.g., the internal energy U, the order parameter (spontaneous magnetization) M, and spin-spin correlation functions $f_{kl} = \langle\sigma_i\sigma_j\rangle$, where spin j has lattice coordinates k, l with respect to spin i. From the fluctuations in these quantities, $(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2$, additional thermodynamic response functions can be determined,[14] e.g., heat capacity C and susceptibility χ:

$$C = \frac{N^2}{kT^2}(\Delta U)^2 = \frac{\partial U}{\partial T}, \tag{2.6}$$

$$\chi = \frac{N^2}{kT}(\Delta M)^2 = \frac{\partial M}{\partial H}, \tag{2.7}$$

where H is a uniform magnetic field. [As shown in Eqs. (2.6) and (2.7) these response functions can also be determined by numerical differentiation of the data as a function of temperature or field.] For an antiferromagnet the simple susceptibility does not diverge but the susceptibility $\chi_{\rm stg}$ of the spins on each *sublattice* ("staggered susceptibility") does. $\chi_{\rm stg}$ can also be determined from fluctuations:

$$\chi_{\rm stg} = \frac{N^2}{kT}(\Delta M_{\rm stg})^2 = \frac{\partial M_{\rm stg}}{\partial H_{\rm stg}}, \tag{2.8}$$

where $M_{\rm stg}$ is the staggered magnetization and $H_{\rm stg}$ the staggered magnetic field.

The process of determining these quantities via Eqs. (2.1) and (2.6)–(2.8) begins with the choice of an initial spin configuration for the system as a whole. The computer program is constructed so as to allow initialization to a perfectly ordered ferromagnetic or antiferromagnetic configuration, or if desired to start with the last spin configuration generated in the preceding calculation. The program then proceeds through the lattice considering each spin (in order) as the "reference" spin for a spin-flip trial. Using a preconstructed table which identifies the nearest neighbors of each spin in the lattice, the program counts the net number of nearest neighbors which are aligned parallel to the reference spin. A second preconstructed table is then used to look up the probability factor $\rho_{\mu\nu}$ corresponding to that particular nearest-neighbor arrangement. (In the case of free edges those spins which lie on the boundary are given a fictitious neighbor, or for corner spins two fictitious neighbors, lying outside the surface. This fictitious neighbor has spin value 0 and therefore does not contribute to the spin sums or energy, but its existence allows the identical procedure to be used for surface spins as for interior spins.) If $\rho_{\mu\nu} > 1$ the reference spin is overturned; otherwise a random number r is chosen from a set of random numbers generated uniformly in the interval from

0 to 1 and compared with $\rho_{\mu\nu}$. If $r<\rho_\mu$, the reference spin is overturned. Regardless of the outcome of this procedure the spin-flip trial is considered completed, and the program proceeds to the next spin, where the same process is then repeated. We have adopted the definition of the time scale in which one complete pass through the entire lattice constitutes one Monte Carlo (MC) step per spin. (For the sampling scheme in which the reference spin is chosen randomly,[15] 1 MC step per spin was simply N^2 spin-flip trials. The number of spin trials per MC step is the same in our procedure but because the reference spins are not chosen in the same way the dynamical behavior will not be identical.) After each MC step the desired properties of the resultant configuration are determined and stored until they are later used to compute the averages [i.e., Eqs. (2.1) and (2.6)–(2.8)]. After a specified number of MC steps (usually between 10 and 100) subaverages are determined for the "group" of states and printed out. The first few states generated are strongly correlated with the initial state and are not truly representative of the "equilibrium" properties of the system. The first 50–200 MC steps are therefore discarded and *not* used in computing averages. After the desired number of groups have been generated the program computes final averages and then repeats the calculation at another temperature. The resultant table of printout provides a "control chart" for the time development of the system properties.

The program, written in FORTRAN, required about 500 μsec per spin trial (including the time needed for determining the averages) on a CDC 6400. For the calculations on systems with free edges no spin-spin correlations were calculated and the program was modified so as to keep track of changes in internal energy and order parameter as the spin flips occurred. With this change and additional use of logical statements the running time was reduced to about $\frac{1}{4}$ of the above. Several calculations made with an almost identical program required about 35 μsec per trial on the IBM 370/168 at the KFA Jülich.

B. Error analysis

One limitation on the accuracy of our data is due to the limited fraction of the total number of states which can be sampled. If the process were truly stochastic the experimental standard deviation would decrease as $M^{-1/2}$, where M is the number of MC steps. Near the ordering temperature, however, the (critical) fluctuations become quite large and very many MC steps are needed to reduce the absolute error. The number of states generated was chosen to yield an accuracy of at least 1% in the internal energy (as determined from test runs) and was from 2 to 5 times larger near T_c. (As we shall see shortly, the desired sample size cannot be determined from simple statistical considerations alone.) For p.b.c. data the maximum number of MC steps which were kept for the averages decreased from 10^4 for $N=4$ to 2×10^3 for $N=10$ and 5×10^2 for $N=60$. (Each data point was, however, taken at least twice from two separate starting configurations.) In the case of free edges the reduced running time allowed us to increase the number of MC steps per data point and as many as 2×10^4 states were generated for $N=10$ and 1.5×10^3 for $N=60$. Points near T_c were computed three or four times from different initial states.

In addition to this error caused by finite sampling, a rather more subtle error is introduced through the time correlations between successive configurations.[16] One obvious result of this correlation is the finite relaxation time which the system requires to reach equilibrium from the initial state. (By equilibrium we refer to the circumstance in which the properties of a sequence of states can be described by normal thermal fluctuations from expectation values.) This relaxation effect is perfectly normal and its effect can be eliminated simply by discarding the first few configurations generated. Near T_c the initial state chosen for each calculation was one which had been generated at a nearby temperature and whose properties were within thermal-fluctuation distance from the new expectation value. For this reason the relaxation to equilibrium in our experiments is not a serious problem. A much more insidious error is produced by time correlations which exist even after the system has seemingly reached equilibrium. The worst possible result of this is to allow the system to be trapped in a metastable state with a relaxation time which may be long compared to our observation (or sampling) time. In general, however, coarse time correlation effects (simple relaxation or oscillations) can be readily found through inspection of the control charts. Even if such gross effects do not occur, successive states are nonetheless not wholly independent and standard statistical error analysis no longer applies. In principle, the true errors associated with the static properties can be determined by studying the dynamics of the model. Such a study is both extremely time consuming and complicated to analyze.[16] In practice, then, it is preferable to estimate the actual errors associated with the Monte Carlo data for static properties using a "coarse-graining" or "time-smoothing" scheme.[17,18] As we have already mentioned, the

total number of M Monte Carlo steps is broken up into M_p groups of successive sequences of p steps each (i.e., $M = pM_p$). Coarse-grained (or time smoothed) averages are calculated for each group of configurations:

$$A_s = \frac{1}{p} \sum_{s\text{th group}} A_\mu . \tag{2.9}$$

The variance of these coarse-grained values is given by

$$V_p = \frac{p}{M_p - 1} \sum_{s=1}^{s=M_p} (A_s - \langle A \rangle_s)^2 . \tag{2.10}$$

(V_1 is the variance which is calculated using simple statistics, i.e., assuming uncorrelated data.) As p becomes large the correlation between successive coarse-grained data points becomes small; in the limit $p \to \infty$, $V_p \to V_\infty$ gives the true error. (Since the number of coarse-grained data points decreases with increasing p the error in the estimate for V_p increases.) The ratio V_∞ / V_1 is what Friedberg and Cameron called the statistical inefficiency (SI) which estimates how much larger a sample is actually needed to produce a true error equal to the V_1 calculated from the original sample. With this approach the errors can be readily understood and it is not necessary to be concerned further with the effect of time correlations on the static properties.

Poor random-number quality could also give rise to undesirable correlation effects or to incorrect probability distributions. For this reason the CDC 6400 system random-number generator was carefully tested. Test runs were made on different blocks of random numbers and the first four moments of the generated distributions were determined. The mean was never more than 0.6% (and usually much less) from the ideal value of 0.5, and the other moments, as well as skewness and kurtosis were in excellent quantitative agreement with values for a perfectly ideal distribution. The autocorrelation never exceeded 2×10^{-3}. The random numbers for the IBM 370/168 were produced by two generators with different seeds, one of which filled a table and the other which drew from the table. The characteristics of the resultant distribution were also close to ideal.[19]

C. Test simulation

As a test of the accuracy of the data and coarse-graining error estimates, Monte Carlo data for $N = 4$, p.b.c., and 10^4 MC steps were compared with the exact values. Table I shows internal-energy results for both the completely stochastic model (run B) as well as for the case in which the "reference" spins are chosen in sequence (run A). Both sets of data agree rather well with the analytic values although in both cases the simple standard deviations, calculated under the assumption of uncorrelated data, are often too small. On the other hand, the coarse-grained error estimates $\sigma'_{\langle u \rangle}$ are almost always larger than the actual errors. The maximum ratio $(\sigma'_{\langle u \rangle}/\sigma_{\langle u \rangle})^2$ [which is equal to the statistical inefficiency (SI) described in Sec. II B] is 2.5 for run A and a surprisingly large 4.3 for run B. In run B, however, after 1 MC step some spins had been considered more than once and others not at all. Successive configurations are then more closely correlated than if all spins had been given the opportunity to flip. (This effect should be reduced somewhat for larger systems.) Even though our sampling technique differs from that used by Friedberg and Cameron,[18] the SI's are quite similar. Since the fluctuations will be even greater in larger systems the time

TABLE I. Comparison of Monte Carlo data and analytic values of the reduced internal energy per spin for an $N = 4$ square lattice with p.b.c.

kT/K_{nn}	$\langle U/U_0 \rangle_{\text{anal}}$	$\langle U/U_0 \rangle_A$ [a]	σ [b]	σ' [b]	$\langle U/U_0 \rangle_B$ [b]	σ [b]	σ' [b]
1.087	0.997 24	0.997 47	0.000 26	0.000 26	0.997 36	0.000 26	0.000 42
1.449	0.980 06	0.978 41	0.000 76	0.000 86	0.980 89	0.000 73	0.001 37
1.811	0.926 93	0.927 40	0.001 46	0.002 08	0.924 71	0.001 50	0.002 96
2.173	0.819 21	0.816 45	0.002 36	0.003 76	0.814 67	0.002 34	0.004 87
2.536	0.675 08	0.675 57	0.002 85	0.004 46	0.671 57	0.002 83	0.005 89
2.898	0.540 69	0.541 85	0.002 90	0.004 33	0.532 22	0.002 92	0.005 83
3.260	0.438 73	0.437 28	0.002 85	0.003 99	0.435 34	0.002 77	0.005 13
3.622	0.366 35	0.361 40	0.002 60	0.003 78	0.370 79	0.002 67	0.004 46

[a] Run A was made by going through the lattice in order. Run B was made by choosing the reference spin randomly.

[b] σ is the standard deviation of $\langle U/U_0 \rangle$ obtained assuming uncorrelated data. σ' is the standard deviation obtained using the coarse-grained technique described in the text. Values of the standard deviation which are too small to account for the discrepancy with the analytic values are underlined.

TABLE II. Comparison of Monte Carlo data and analytic values for the order parameter for an $N=4$ square lattice with p.b.c.

kT/K_{nn}	$\langle\|M\|\rangle_{\text{anal}}$	$\langle\|M\|\rangle_{\text{anal}}$	σ [a]	σ' [a]	SI
1.087	0.998 59	0.998 71	0.000 18	0.000 88	23.1
1.449	0.988 98	0.988 24	0.000 56	0.003 03	29.6
1.811	0.954 65	0.955 54	0.001 20	0.004 66	15.0
2.173	0.873 45	0.870 46	0.002 20	0.011 29	26.4
2.536	0.752 07	0.752 27	0.002 85	0.014 10	24.3
2.898	0.631 03	0.632 70	0.003 20	0.013 74	18.7
3.260	0.536 05	0.535 99	0.003 16	0.014 90	22.5
3.622	0.468 04	0.469 40	0.003 05	0.010 30	11.1

[a] σ is the standard deviation obtained assuming uncorrelated data and σ' is obtained using the coarse-graining technique described in the text. Standard-deviation estimates which are too small to account for the actual errors are underlined.

correlations should lead to much larger SI's near T_c. The repeated, independent calculation of a given data point several times from different starting configurations should then yield less correlated data than a single long chain of states.

Comparison between MC order-parameter data and exact values is made in Table II. The agreement is quite good although the SI values are quite high. This is not unreasonable, however, since the energy determines the spin-flip process and states with different magnetizations may have identical energies.

This simulation not only shows the high accuracy which may be obtained but also provides one last check on the correctness of the program.

III. RESULTS

A. Thermal properties

Internal-energy data, normalized by $U_0 = N^2 K_{nn}$, are shown for a wide range of lattice sizes in Fig. 1. The results for lattices with p.b.c. are only slightly affected by the variation in lattice size outside of a relatively narrow region about the infinite-lattice critical temperature. In contrast, the internal energy for lattices with free edges shows a distinct size dependence even for the largest lattices ($N=60$ and 100). The qualitative difference in these curves with respect to the p.b.c. data is due to the "broken bonds" at the surface which make the ground-state energy per spin size dependent. The temperature variation of the SI for the p.b.c. internal-energy data is shown for several lattice sizes in Fig. 2. As expected the maximum in the SI grows with increasing lattice size; the variation depends on a relatively low power of N in the range of sizes studied. It is clear then (as had been concluded from studies[15,16] of the dynamics of the stochastic Ising model) that studies of the critical behavior of very large lattices will be hindered not only by large fluctuations but also by these time correlation effects.

Specific-heat values were determined from the fluctuations in the internal energy [see Eq. (2.6)], and their temperature variation is shown in Fig. 3. The data for p.b.c. with $N=4$, 8, and 32 compare favorably with the curves representing exact results[3] and show no signs of the systematic deviations as had earlier results of Yang.[20,21] The more extensive (and more accurate) data for lattices

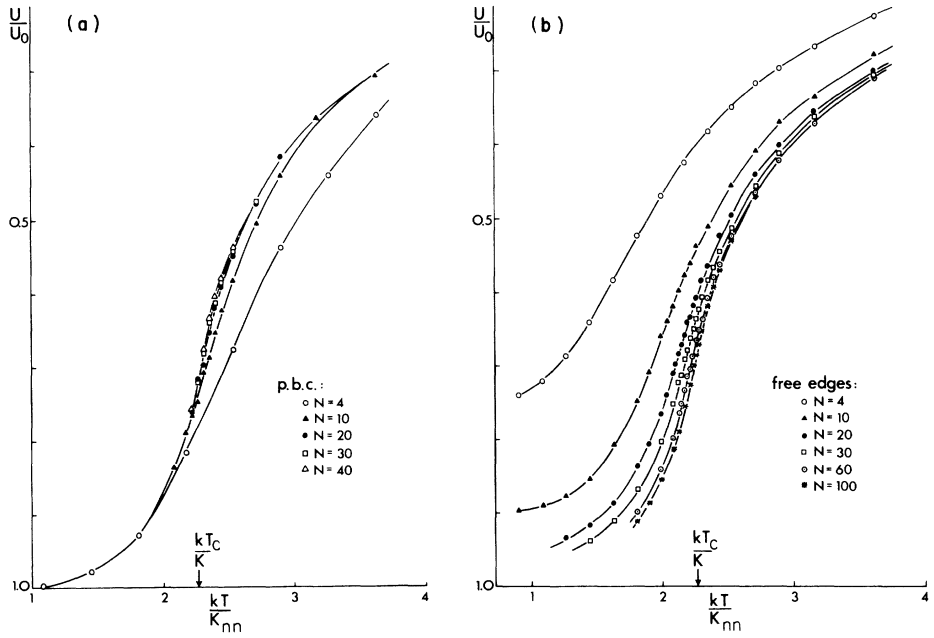

FIG. 1. Temperature variation of the internal energy for $N \times N$ lattices. The arrows show the infinite-lattice T_c.

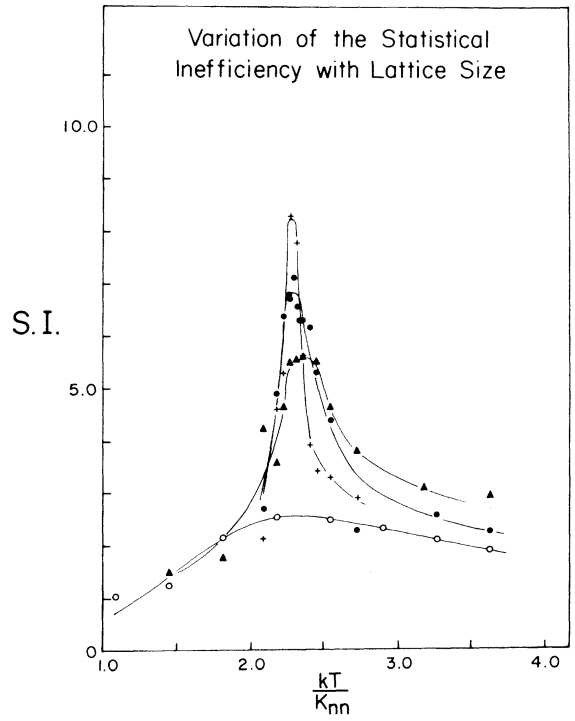

FIG. 2. Size dependence of the statistical inefficiency [Eq. (2.10)]: $N=4$, O; $N=10$, ▲; $N=20$, ●; $N=50$, +. The infinite lattice T_c is $kT/K_{nn}=2.269$.

with free edges[22] are qualitatively similar, although the maxima are lower than for p.b.c. and the positions of the maxima are shifted more (and in the opposite direction) with decreasing lattice size. In both cases the specific-heat data agreed with curves obtained from numerical differentiation of the U-vs-T curves shown in Fig. 1.

B. Magnetic properties

The order-parameter data[22] for both types of boundary conditions are shown in Fig. 4 along with exact infinite-lattice curves. Because the entire lattice may overturn within the course of an experiment, we have plotted the expectation value of the absolute value of the order parameter $|M|$ $(=\langle|M|\rangle)$ to make the direction of the order parameter unimportant. For p.b.c. the "tail" at high temperatures is pronounced, but for $T<T_c$ and $N\geq 10$ the order parameter is virtually independent of lattice size to within just a few percent of the infinite-lattice critical temperature $T_c(\infty)$. In contrast the size dependence of the free-edge data is quite pronounced even well below $T_c(\infty)$. For example, even the data for $N=100$ lie clearly below the $N=\infty$ curve for $T=0.8T_c(\infty)$.

The magnetic susceptibility obtained from the order-parameter fluctuations is shown in Fig. 5. {Because all calculations were made in zero field it is not possible to compare these data with $\Delta M/\Delta H$ [see Eq. (2.7)].} As with the specific heat, both the magnitude as well as the position of the maximum depend upon lattice size. An additional complication and source of error is introduced here through the tendency of the entire lattice to overturn (even below T_c) during the course of a calculation. Although such a reversal is immaterial for the determination of the specific heat or order parameter ($\langle|M|\rangle$ is calculated), the susceptibility may be greatly affected. $\langle M\rangle$, which is needed for the calculation of χ, may be quite small if such a reversal occurs, whereas $\langle|M|\rangle$ would still be large. Two runs could therefore yield quite similar estimates for $\langle|M|\rangle$ but vastly different susceptibilities [see Eq. (2.7)]. This effect is less

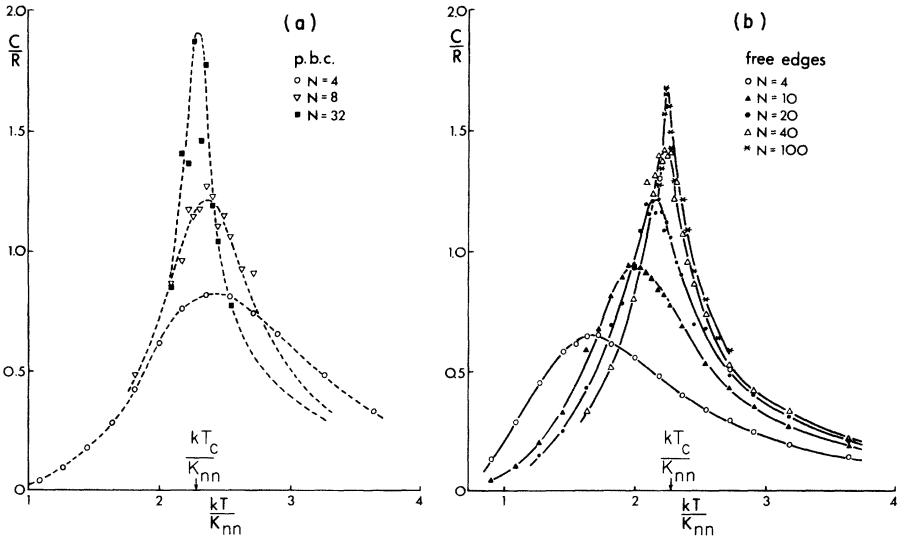

FIG. 3. Temperature depenence of the specific heat. The dashed curves in (a) are the exact curves of Ferdinand and Fisher (Ref. 3). $kT_c(\infty)/K_{nn}=2.269$.

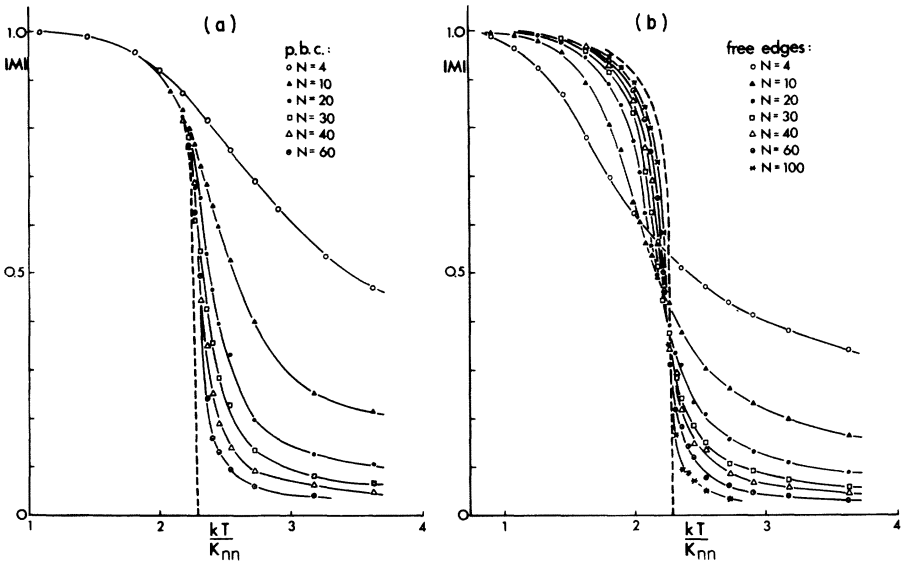

FIG. 4. Temperature variation of the order parameter. The dashed lines represent the exact $N=\infty$ curve (Ref. 1).

pronounced in very large lattices for which the characteristic time, i.e., number of Monte Carlo steps, associated with a reversal is long compared to the observation time. The effect is also more important in lattices with p.b.c. for which "droplets" of overturned spins on the edge of a lattice can grow in both directions. This aid to reversal is absent in the free-edge case.

The staggered susceptibility has also been calculated for several different size lattices with p.b.c. The data are compared with the infinite-lattice result in Fig. 6. This figure is somewhat less impressive than the preceding one since the susceptibility never diverges and the dependence on lattice size is relatively mild. Both fluctuations and size dependence are much more pronounced above T_c than below. Nonetheless for $N \geq 20$ the averages of the data for different N agree well with the infinite-lattice curve. Even the qualitative behavior of smaller lattices is characteristic of an

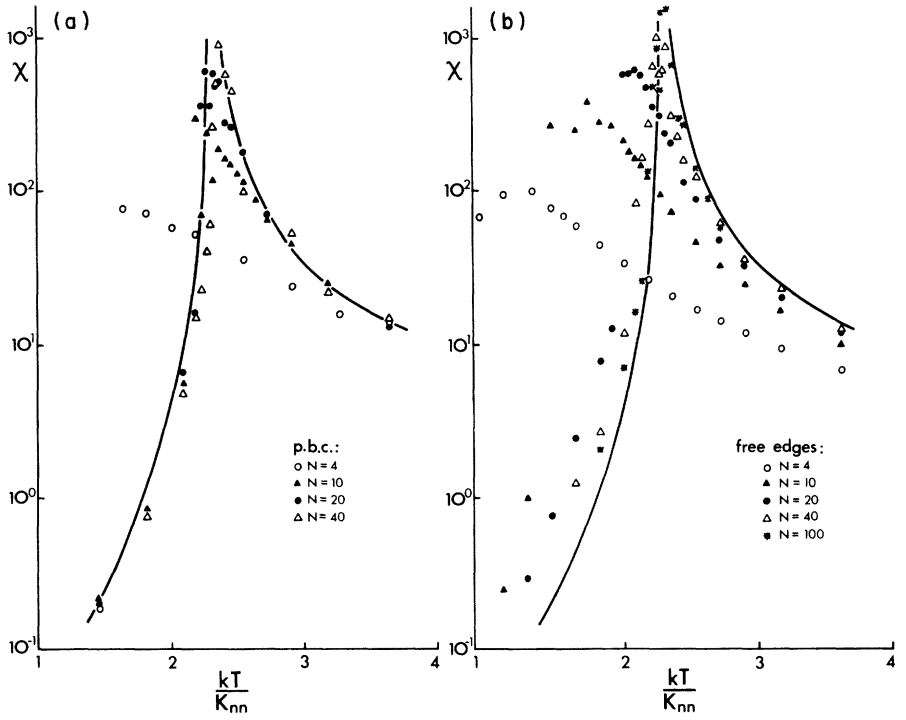

FIG. 5. Temperature variation of the susceptibility. The solid curves are exact for an infinite lattice (Ref. 23).

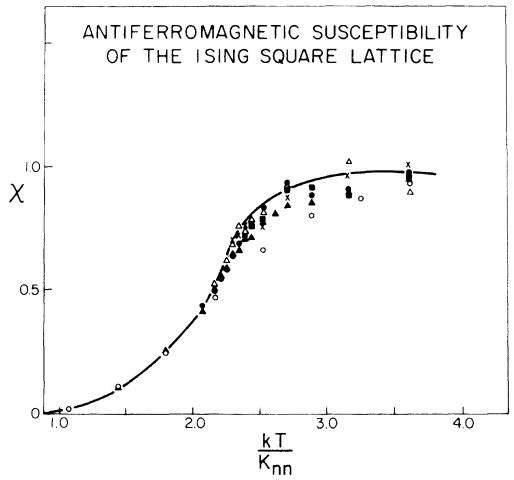

FIG. 6. Temperature variation of the staggered (antiferromagnetic) susceptibility. The solid line gives the infinite-lattice result (Ref. 24): $kT_c(\infty)/K_{nn} = 2.269$.

Ising antiferromagnet with a broad maximum lying clearly above the critical temperature.

C. Spin-spin correlations

For lattices with p.b.c. both row spin-spin correlations $f_{k0} = |\langle\sigma_i\sigma_j\rangle|$ [where spin j has coordinates $(k,0)$ with respect to spin i] with $k \leq 10$, and diagonal spin-spin correlations f_{kk} with $k \leq 3$ were calculated. Both f_{10} and f_{01} were determined and any discrepancy between the two was an indicator of insufficient sampling. Results for different lattice sizes are shown over a wide temperature range in Fig. 7. Because of the p.b.c. the maximum distance along a row from any spin is $\frac{1}{2}N$ and more-distant-neighbor correlations do not exist in small systems. For example, f_{80} (Fig. 7) does not exist for $N<16$. As might be expected the dependence on lattice size is more pronounced for the more-distant-neighbor correlations, particularly not too far above T_c where the correlation length becomes roughly comparable to system dimensions.

IV. DISCUSSION

A. Extrapolation to infinite-lattice behavior

1. Internal energy

For p.b.c. the asymptotic size dependence of the internal energy is known to be[3] exponential:

$$U(N) - U(\infty) \propto e^{[-\Gamma(T)N]}, \tag{4.1}$$

where $\Gamma(T)$ is proportional to the inverse correlation length $\kappa(T)$. The data are shown as a function of N^{-1} in Fig. 8 for a relatively broad temperature range. Using Eq. (4.1) and $\Gamma(T) \sim 0.7\kappa(T)$ (as we shall see later in this section) we have fitted the asymptotic N dependence of the data in Fig. 8 with good success at all temperatures except $kT/K_{nn} = 2.264$. This temperature is extremely close to $T_c(\infty)$ and the errors in the Monte Carlo data are the greatest. In addition, the asymptotic size dependence at this temperature is not reached until $N \gg 60$. For T outside the range $0.95T_c(\infty)$–$1.15T_c(\infty)$ the effect of extrapolation is virtually negligible. Within this region where extrapolation effects are observable, even the assumption of a variation which is linear in N^{-1} yields infinite-lattice estimates which are correct to better than 1% accuracy.

For lattices with free edges, however, the effect of finite size is both more pronounced and in the opposite direction. The asymptotic size dependence is clearly linear in N^{-1}, as would be expected from the surface contribution. The dominance of this term is not surprising since we have already seen in the p.b.c. case that the bulk N dependence is relatively small and a substantial fraction of the spins lie on the surface. For $N=10$ 36% of the spins are surface spins and even for $N=100$ the surface contribution (~4%) is not completely negligible.

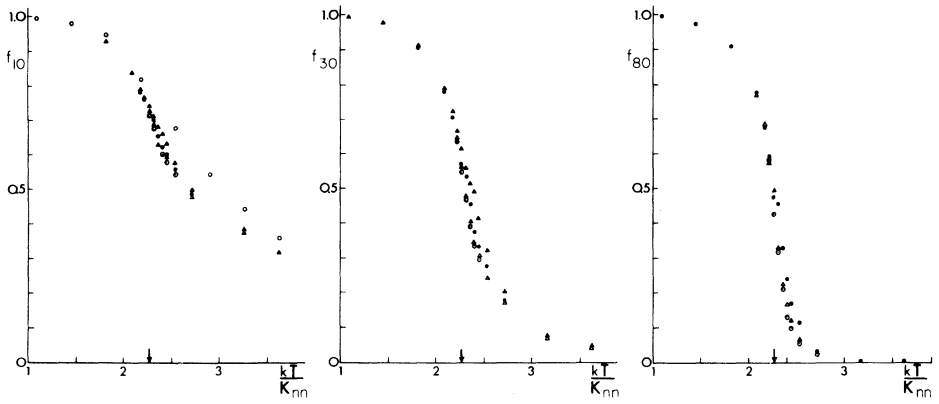

FIG. 7. Temperature variation of spin-spin correlation functions for $N\times N$ lattices with p.b.c. f_{k0}: $N=4$, ○; $N=10$, ▲; $N=20$, ●; $N=40$, △; $N=60$, ⊙. The arrows show $T_c(\infty)$.

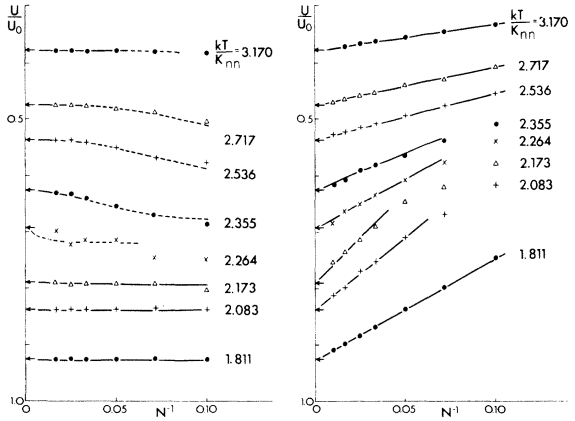

FIG. 8. Extrapolation of internal-energy data to infinite lattice size. For p.b.c. (on the left-hand side) the curves are fitted to the data assuming an asymptotic size variation with $[U(\infty)-U(N)] \propto e^{-N\Gamma(T)}$, where $\Gamma(T)$ is proportional to the inverse correlation length. For free edges on the right-hand side the curves are linear in N^{-1}. $kT_c(\infty)/K_{nn} = 2.269$. The arrows give the exact $N=\infty$ values (see Ref. 1).

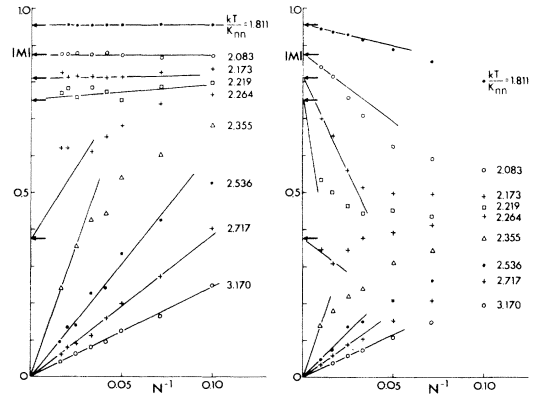

FIG. 9. Linear extrapolation of the order-parameter data to $N=\infty$: p.b.c. data to the left-hand side, free-edge data to the right-hand side. The arrows give exact infinite-lattice values (see Ref. 1). $kT_c(\infty)/K_{nn} = 2.269$.

2. *Order parameter*

The extrapolation of the order-parameter data to $N=\infty$ is depicted in Fig. 9. In both cases the asymptotic size dependence is linear in N^{-1} except very close to $T_c(\infty)$. Below T_c, however, the size correction terms are of opposite sign for different boundary conditions. In addition, the magnitude of the size dependence is much greater for lattices with free edges and the asymptotic dependence is not reached until N is quite large. For p.b.c. all of the data outside the interval $0.98T_c(\infty)$–$1.02T_c(\infty)$ extrapolate quite accurately. Within this interval the extrapolation breaks down and (as we shall see in Sec. IV B) the size dependence is dominated by a "critical" $N^{-1/8}$ variation. For free edges the size dependence close to $T_c(\infty)$ is even more complicated. (This will also be discussed in Sec. IV B.)

3. *Ordering temperature*

The definition of the pseudo-ordering temperature of a finite lattice is not wholly unambiguous. The most common (and perhaps most physical) definition[2-4,7,25] is to associate the maximum in the specific heat, or equivalently the point of maximum slope in internal energy, with $T_c(N)$. Using this definition we have plotted the variation $T_c(N)$ vs N^{-1} for both sets of boundary conditions in Fig. 10. Our p.b.c. data for large N lie slightly above the exact asymptotic dependence found by Ferdinand and Fisher.[3] This systematic difference is probably due to subjective prejudice in locating the inflection point in the internal energy and is both small and well within our error bars. [A linear best fit to our data yields an estimate for $T_c(\infty)$ which is correct to better than 0.5%.] The linear dependence in N^{-1} is consistent with Eq. (1.4) with $\lambda = 1$. Since $\nu = 1$ for the square lattice this result gives no hint as to whether $\lambda = 1$ or $\lambda = \nu^{-1}$ (see Ref. 4) in general. The amplitude of the free-edge size dependence $a = +1.25 \pm 0.04$ [see Eq. (1.4)] is much larger than the p.b.c. value[3] $a = -0.36$. For comparison we note that Ferdinand and Fisher esti-

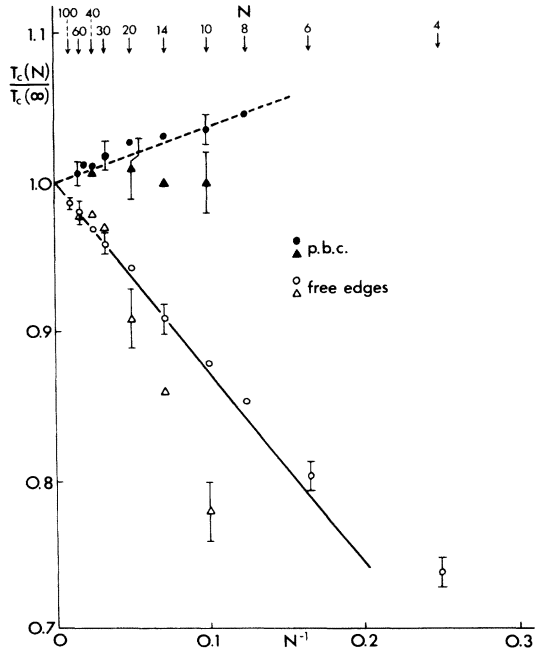

FIG. 10. Extrapolation of $T_c(N)$ vs N^{-1}. The circles give the temperatures at which C_{max} occur, the triangles are for χ_{max}. $kT_c(\infty)/K_{nn} = 2.269$. The dashed line is the *asymptotic* specific-heat behavior for p.b.c. (Ref. 3).

mated the free-edge value $a = 1.35 \pm 0.08$ from results on very small $N \times N$ lattices and Au-Yang and Fisher[7] have recently shown that $a = 0.893$ for infinitely long strips N spins wide.

Alternatively, however, one could associate $T_c(N)$ with the maximum of the zero-field susceptibility. Using this definition one obtains distinctly different values (see Fig. 10) at least for small and intermediate N values. Because of the relatively large errors associated with these estimates we cannot tell whether the asymptotic size dependence, i.e., for *very* large N, is the same as for the specific-heat maxima or whether $\lambda > 1$ for the susceptibility peak. In their MC calculation for $N = 110$ lattices Stoll and Schneider[26] found susceptibility maxima at $\sim 1.01 T_c(\infty)$ for both p.b.c. and free edges. In any case for $N < 30$ the difference between the two values is of the same magnitude as the shift of T_c itself.

4. *Spin-spin correlations*

The correlation functions should approach their infinite-lattice values exponentially as described by Eq. (4.1) with $\Gamma(T) = p\kappa(T)$. The data were analyzed by making plots of $\ln[f_{k0}(N) - f_{k0}(\infty)]$ vs N for various estimates of $f_{k0}(\infty)$. The resultant plots seem to have $N = 0$ intercepts which vary as k^{-1} so we show a plot of the reduced difference $\ln(\Delta f_{k0}/k)$, where $\Delta f_{k0} = [f_{k0}(N) - f_{k0}(\infty)]$ for one temperature in Fig. 11.

The data for large N are extremely difficult to analyze since even very small errors in $f_{k0}(N)$ or in estimates for $f_{k0}(\infty)$ are magnified when taking the difference between the two. All of the $T > T_c$ correlation-function size dependences can be fitted by this exponential dependence with $p = 0.7 \pm 0.2$. This can be compared with the value $p = 2$ which Au-Yang and Fisher[7] found for Ising strips. For $T < T_c$ virtually no size dependence was observed except very close to $T_c(\infty)$. Note, however, that the reduced correlation function $(f_{k0} - \langle M \rangle^2)$ would have a more complicated size dependence just below $T_c(\infty)$ than would either individually. The extrapolated $(N = \infty)$ estimates for the spin-spin correlations are shown in Fig. 12. For $T > T_c$ the correlations clearly approach M^2 asymptotically as $k \to \infty$ for all temperatures except $kT/K_{nn} = 2.264$, which is so close to $T_c(\infty)$ that the asymptotic region has not yet been reached. In all cases the diagonal correlations lie on the smooth curves drawn through the row correlation values. This isotropic decay for small k agrees with the conclusion of Kadanoff.[27,28]

Our extrapolated correlation values were used to estimate the temperature dependence of the inverse correlation length $\kappa(T)$. For $T > T_c$ and $\kappa r \gg 1$ the spin-spin correlation should be de-

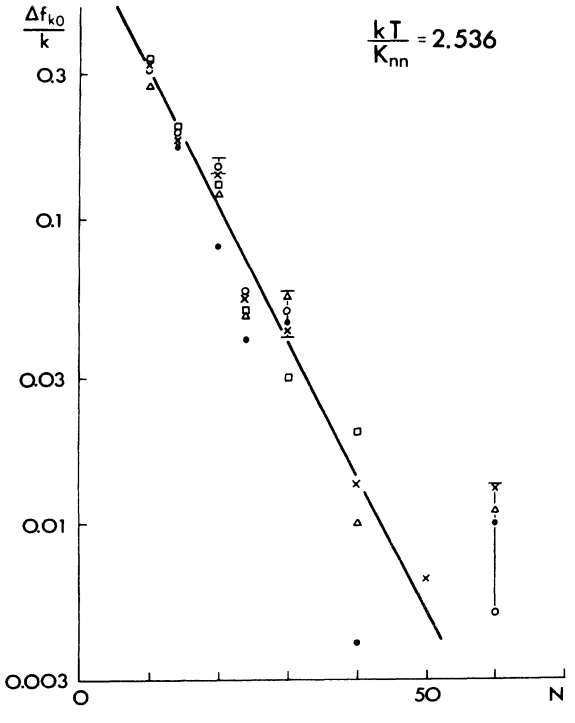

FIG. 11. Variation of $\ln(\Delta f/k)$ vs N, where $\Delta f = f_{k0}(N) - f_{k0}(\infty)$ for $kT/K_{nn} = 2.536$. The solid line is the best fit with slope equal to 0.104 and $k = 2, \circ$; $k = 3, \times$; $k = 4, \triangle$; $k = 6, \bullet$.

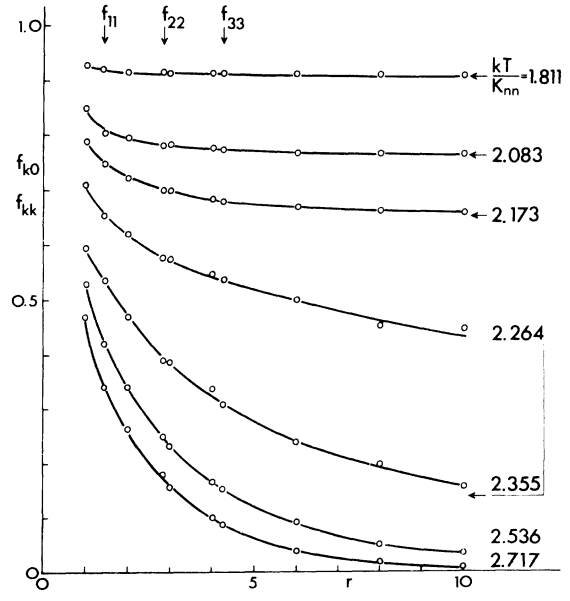

FIG. 12. Variation of row and diagonal spin-spin correlations with r. The circles are the extrapolated $N = \infty$ values. The arrows on the right-hand side give $M^2(T)$.

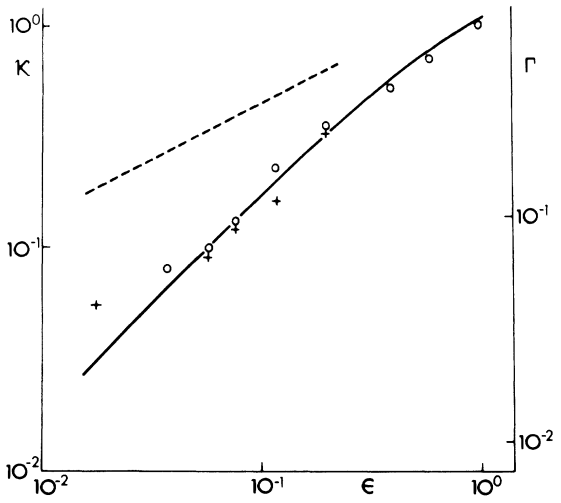

FIG. 13. Variation of $\kappa(T)$ and $\Gamma(T)$ vs ϵ. The scale on the left-hand side is for κ (○) and the scale on the right-hand side is for Γ (+). Actual $N=\infty$ variation of κ, ——; Bethe approximation for κ, ---(see Ref. 28).

scribed by[27,28]

$$f(r) = D_+ \kappa^{-1/4} e^{-\kappa r}/r^{1/2}, \tag{4.2}$$

where r is the distance between spins whose correlation is being considered. In our notation $r=k$ for the row correlations. Plots of $\ln(r^{1/2} f_{k0})$ vs r should then show asymptotically linear behavior (for large k) with slope κ and intercept $\ln(D_+ \kappa^{-1/4})$. The κ values resulting from these plots are compared with the known infinite-lattice variation[27] in Fig. 13. The accuracy of the Monte Carlo estimates is generally quite good and supplies a much better result than most approximate theories. (The Bethe-approximation curve[28] is shown for comparison.) For $\kappa \lesssim 0.1$ the requirement that $\kappa r \gg 1$ cannot be fulfilled from our data and reliable estimates cannot be made. For comparison we have also plotted in Fig. 13 the mean estimates for $\Gamma(T)$ which were determined from the extrapolations of the spin-spin correlation functions. The general agreement between the two functions is quite good although the scale factor p between $\Gamma(T)$ and $\kappa(T)$ cannot be determined with great accuracy: $p = 0.7 \pm 0.2$. [Here too the estimate for $\Gamma(T)$ at the smallest ϵ value is inaccurate, in this case because the N dependence of the correlation functions is so slow.]

B. Scaling analysis of finite-size behavior

Finite-size scaling theory has been tested for a variety of thin films[4,29,30] but relatively little has been done on *fully* finite two-dimensional Ising models. The success of the theory has been demonstrated for the thermal properties of square lattices with p.b.c. but no comparable analysis exists for other properties or for lattices with free edges. Using the data described previously we shall now carry out a more complete analysis in terms of Fisher's finite-size scaling theory.[4] The basic scaling ansatz described in the Introduction [see Eq. (1.1)] was formulated in terms of the temperature deviation from the *shifted* ordering temperature, i.e., $\dot{\epsilon} \propto T - T_c(N)$ as in Eq. (1.2). Since $T_c(N)$ is not known exactly (and as described in Sec. IV A3 is not even unambiguously defined) the use of $\dot{\epsilon}$ introduces another source of error into the analysis. We therefore prefer to use the alternative formulation[4]

$$F(N,T) = N^{-\psi} \mathcal{F}^0(N^{\theta}\epsilon), \tag{4.3}$$

where the shape function $\mathcal{F}^0$ is asymptotically the same as $\mathcal{F}$ [see Eq. (1.1)] for *large* values of the argument and ϵ is known exactly.

1. Scaling for lattices with p.b.c.

The scaling relation for the order parameter is given by[4]

$$M = N^{-\beta/\nu} X^0(\epsilon N^{1/\nu}), \tag{4.4}$$

where X^0 is a function of $x = \epsilon N^{1/\nu}$ only, and β and ν are the exponents for the infinite square lattice. The success of this relation can be tested by plotting $MN^{\beta/\nu}$ vs x. This plot has the advantage that, assuming scaling is obeyed, it graphically defines the shape function $X^0(x)$. In Fig. 14 we show such a finite-size scaling plot of the order-parameter data for $10 \leq N \leq 60$. The data lie on a single smooth curve for temperatures both above and below $T_c(\infty)$ and clearly validate finite-size scaling. For large N, and thus large x, the infinite-lattice

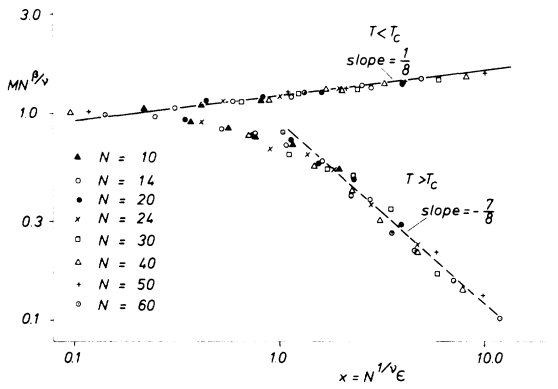

FIG. 14. Finite-size scaling plot for the order parameter for lattices with p.b.c. Data for $N=10$, ▲; $N=14$, ○; $N=20$, ●; $N=24$, ×; $N=30$, □; $N=40$, △; $N=50$, +; $N=60$, ⊙. For $T<T_c$ the solid line is $1.22\,x^{1/8}$; for $T>T_c$ the dashed line is $0.92\,x^{-7/8}$.

critical behavior must be asymptotically reproduced. Inspection of Eq. (4.4) shows that

$$X^0(x) \approx Bx^{\beta} \tag{4.5}$$

for very large x, where B is the critical amplitude for the infinite-lattice order parameter. The straight line through the $T < T_c(\infty)$ data in Fig. 14 describes Eq. (4.5) with *no* adjustable parameters. The asymptotic behavior is obeyed over a surprisingly large range, i.e., large x means $x \gtrsim 0.2$. For smaller x finite-size "rounding" becomes important and below $x = 0.1$ the data approach the constant value $X^0(0) = 1.00 \pm 0.04$. (Additional data not shown in Fig. 14 are available down to $x = 0.02$.) This rounding means that close to $T_c(\infty)$ the order-parameter size dependence is dominated by an $N^{-\beta/\nu} = N^{-1/8}$ variation. This result explains the extrapolation difficulties encountered near $T_c(\infty)$ in Fig. 9.

Above $T_c(\infty)$ the large-x shape function must reproduce the N^{-1} decay of the order parameter to zero as $N \to \infty$. From Eq. (4.4) it is obvious that $X^0(x) \propto x^{1-\beta}$ for large x. (The amplitude is not predicted theoretically.) The straight line through the $T > T_c$ data in Fig. 4 fits the large-x behavior quite well with an amplitude $B^+ = X^0(x)/x^{1-\beta} = 0.90 \pm 0.05$.

The scaling behavior of the susceptibility was analyzed in terms of χT with the scaling relation

$$\chi T = N^{\gamma/\nu} Y^0(x), \tag{4.6}$$

where $x = \epsilon N^{1/\nu}$ below T_c and $x = \epsilon' N^{1/\nu}$ above T_c,[31] where $\epsilon' = |1 - T_c(\infty)/T|$. In similar fashion to the order-parameter treatment it can be shown that the large-x behavior of the shape function is given

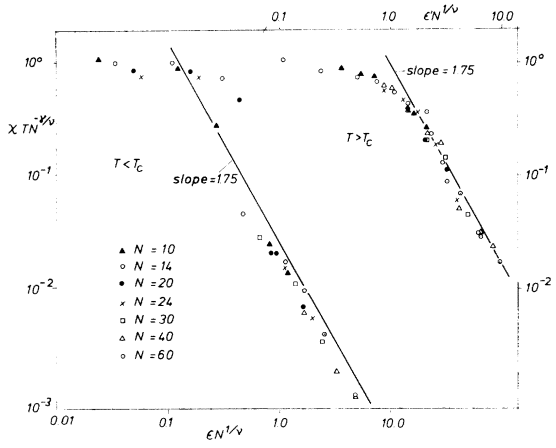

FIG. 15. Finite-size scaling plot for the susceptibility of lattices with p.b.c. For $T < T_c$, $\epsilon = |1 - T/T_c|$ and the solid line is $C^- x^{-7/4}$, with $C^- = 0.0255$ (see Ref. 22). For $T > T_c$, $\epsilon' = |1 - T_c/T|$ and the solid line is $C^+ x^{-7/4}$, with $C^+ = 0.963$ (Ref. 23).

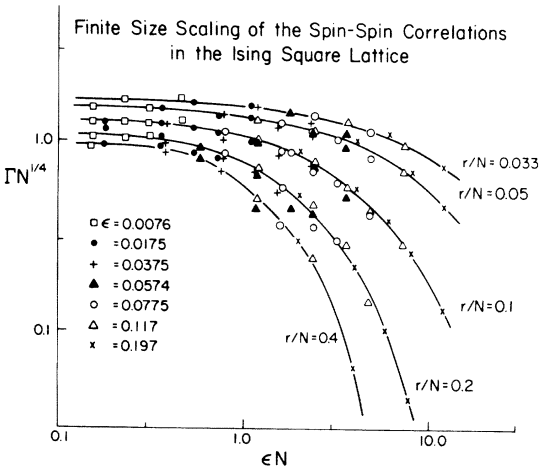

FIG. 16. Finite-size scaling plot for the spin-spin correlations. Data are for $10 \leq N \leq 60$.

by

$$Y^0(x) = C^{\pm} x^{-\gamma}, \quad x \to \infty, \tag{4.7}$$

where $C^{\pm}$ are the susceptibility amplitudes of the critical power law for the $N = \infty$ susceptibility above and below T_c. Finite-size scaling plots of the susceptibility both above and below T_c are shown in Fig. 15 along with the theoretically predicted behavior; cf. Eq. (4.7) (with *no* adjustable constants). The scaling of the susceptibility is quite good with excellent agreement with the predicted asymptotic form above T_c. Below T_c there is a small systematic error which would appear to be outside of our experimental error estimates. As $x \to 0$ $Y^0(x)$ approaches the constant value 1.0 ± 0.1.

The finite-size behavior of the spin-spin correlation between two sites a distance r apart, $f(r, \epsilon)$, is slightly more complicated in that the scaling relation involves *two* scaling variables:

$$f(r, \epsilon) = N^{-2\beta/\nu} G^0(rN^{-1}, \ \epsilon N^{1/\nu}), \tag{4.8}$$

where G^0 is a two-dimensional shape function. This surface is traced out by plotting $fN^{2\beta/\nu} = fN^{1/4}$ vs $x = \epsilon N = \epsilon N^{1/\nu}$ for a range of constant r/N values. The results[33] shown in Fig. 16 indicate that the scaling relation 4.8 is fulfilled. For small x the shape function for each r/N value approaches a constant. Since $f \propto r^{-1/4}$ for $T = T_c$, this implies that $G^0(r/N, 0) = (r/N)^{1/4}$. This prediction is borne out quite well by the data in Fig. 16.

2. *Scaling for lattices with free edges*

The scaling relations given by Eqs. (4.4) and (4.6) (as well as the equivalent one for the specific heat) remain valid for lattices with free edges; however, the asymptotic form for the shape func-

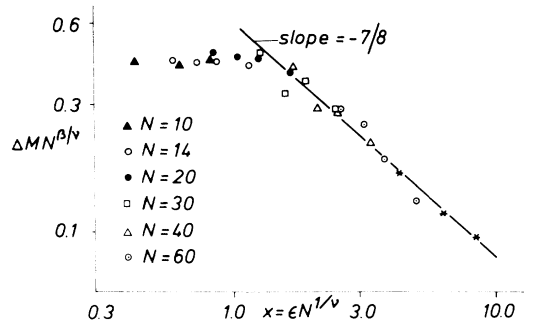

FIG. 17. Finite-size scaling plot for the correction to the bulk finite-size order-parameter behavior for lattices with free edges. $\Delta M = M - B\epsilon^{1/8}$, with $B = 1.22$. The solid line is the best fit assuming the asymptotic scaling form $B_s x^{\beta_s}$, with $\beta_s = \beta - \nu = -7/8$, and yields $B_s = 0.60$.

tion includes a surface correction term, e.g.,[4]

$$X^0(x) = Bx^{\beta} + B_s x^{\beta_s}, \tag{4.9}$$

where β_s is a new exponent which according to scaling is given by $\beta_s = \beta - \nu$. A simple scaling plot of the order parameter, i.e., $MN^{\beta/\nu}$ vs x, showed that scaling was obeyed. The surface correction term was extracted by taking the difference $\Delta M = M - B\epsilon^{\beta}$ and plotting $\Delta M N^{\beta/\nu}$ vs x. [Note that $\Delta M N^{\beta/\nu} = X^0(x) - Bx^{\beta}$.] The results are shown in Fig. 17. Although the data are rather precise, small errors are magnified in this plot since ΔM is generally small. Figure 17 shows that the correction term (which we attributed to the surface) does scale and the asymptotic form, for $x \gtrsim 1.5$, is consistent with the scaling value $\beta_s = -\frac{7}{8}$ and an amplitude $B_s = 0.60 \pm 0.05$. Within experimental error $B = 2B_s$, and there is no theoretical guide to help us decide whether or not this is coincidence or has physical significance.

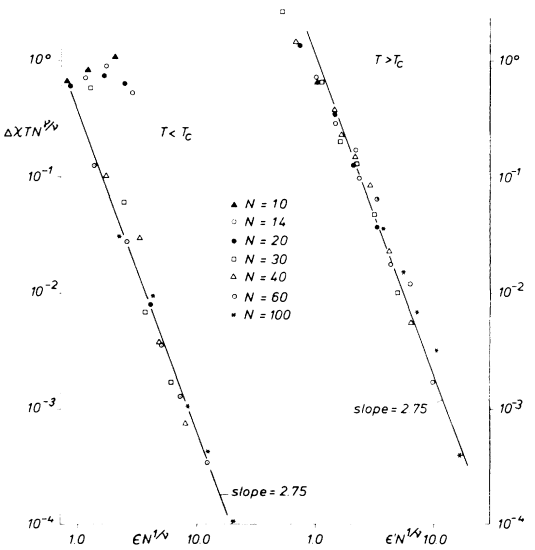

FIG. 18. Finite-size scaling plot for the correction to the bulk finite-size susceptibility behavior for lattices with free edges. For $T < T_c$, $\Delta\chi T = \chi T - C^- \epsilon^{-7/4}$, with $C^- = 0.0262$, and for $T > T_c$, $\Delta\chi T = \chi T - C^+ \epsilon'^{-7/4}$, with $C^+ = 0.963$. The solid lines are best fits assuming the asymptotic scaling form $C_s^{\pm} x^{\gamma_s}$ with $\gamma_s = \gamma + \nu = 11/4$. The resultant amplitudes are $C_s^- = 0.35$ and $C_s^+ = 1.1$.

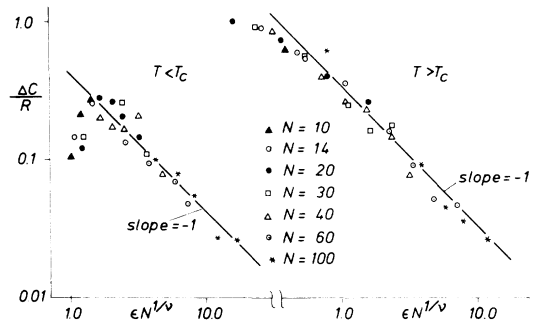

FIG. 19. Finite-size scaling plot for the correction to the bulk finite-size specific-heat behavior for lattices with free edges. $C/R = A^{\pm} \ln \epsilon + A'$, where $A^{\pm} = 0.4945$ and $A' = -0.306$. The solid line is a best fit to the data assuming the asymptotic scaling form $A_s^{\pm} \epsilon^{-\alpha_s}$, with $\alpha_s = \alpha + \nu = 1$. The resultant amplitudes are $A_s^- = 0.42$ and $A_s^+ = 0.33$.

Identical analyses were carried out for the corrections to the susceptibility and specific-heat scaling shape functions. In Fig. 18 we show $\Delta\chi T N^{\gamma/\nu}$ vs x for temperatures above and below $T_c(\infty)$. The solid lines have slope 2.75 corresponding to the scaling prediction $\gamma_s = \gamma + \nu$. The data are fitted quite well by this exponent with correction amplitudes $C_s^- = 0.35 \pm 0.10$ and $C_s^+ = 1.1 \pm 0.3$. The asymptotic form seems to describe the data well for $x \gtrsim 2.0$.

The correction to the specific heat is plotted in Fig. 19. The large-x data are well fitted by the scaling exponent $\alpha_s = \alpha + \nu$ and amplitude $A_s^- = 0.42 \pm 0.08$ and $A_s^+ = 0.33 \pm 0.06$. Within experimental error these two values are identical. The correction for a single surface for an infinite system[3] is symmetric about T_c, $A_s^{\pm} = 0.140$. The above analysis for the specific heat should be viewed with some caution since the higher-order corrections are probably not neglible for the values of x which we have taken to define the asymptotic region.

V. SUMMARY AND CONCLUSION

The results presented here show that the Monte Carlo method yields quantitatively precise information about the properties of $N \times N$ Ising square lattices. Even more important is the result that the data obtained on lattices which are small enough to be studied without using excessive amounts of computer time can be reliably extra-

polated to $N=\infty$ except in a very narrow region about T_c. This conclusion should be equally valid if more-distant-neighbor coupling or a magnetic field is introduced. In three dimensions the accuracy should be even better.[25,34] In addition, finite-size scaling theory has been verified for magnetic properties as well as the thermal behavior for both p.b.c. and free edges. For p.b.c. the asymptotic large-x scaling region is reached for rather small values of x and even lattices as small as 10×10 can be used to help determine the scaling shape functions. The scaling predictions for the surface correction exponents are found to be in excellent agreement with the free-edge data. The power-law behavior of the correction terms are valid for $x \gtrsim 1.0$. The success of finite-size scaling theory shows quite clearly that Monte Carlo data, even for medium size lattices, can be used to study the asymptotic critical behavior for infinite systems.

ACKNOWLEDGMENTS

We wish to thank Dr. K. Binder, Dr. M. H. Lee, Dr. J. E. Rives, and Dr. D. Stauffer for helpful suggestions and comments. We also wish to thank the IFF of the KFA Jülich for their hospitality during the latter portion of this work. The author is also grateful to the Alexander von Humboldt Foundation for its support and the Universität des Saarlandes for its hospitality during the preparation of this manuscript.

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*Supported in part by the NSF.

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