Critical properties of the two-dimensional anisotropic Heisenberg model

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While a nonzero spontaneous magnetization m cannot exist in a $d=2$ Heisenberg spin system, it is possible that a phase transition associated with a divergent susceptibility occurs at the Stanley-Kaplan temperature T_c^{SK}. The crossover from this special isotropic case to the anisotropic (Ising) behavior is studied using a Monte Carlo technique. The classical model with Hamiltonian $H=-J\Sigma[(1-\Delta)(S_i^xS_j^x+S_i^yS_j^y)+S_i^zS_j^z]$ on $N\times N$ square lattices with periodic boundary conditions is investigated for $N\leq 100$ and Δ varying from 0.005 to 1. The spontaneous magnetization m, energy, specific heat, longitudinal and transverse susceptibilities, and the self-correlation are determined over a wide temperature range. For weak anisotropy dm/dT decreases nonmonotonically with increasing temperature and deviations from simple spin-wave theory occur at surprisingly low temperatures. Transition temperatures $T_c(\Delta)$ exceed the isotropic value T_c^{SK} predicted by series expansions although the values would also be consistent with $T_c^{SK}=0$ if $T_c(\Delta)\propto|\ln(1/\Delta)|^{-1}$. The asymptotic critical exponent for the order parameter is $\beta=1/8$ for all Δ. The susceptibility data show crossover from $\gamma=1.75$ near $T_c(\Delta)$ to higher values farther from $T_c(\Delta)$. It is shown that finite-size rounding may lead to erroneously large estimates for β and erroneously small estimates for γ. These effects may invalidate some conclusions drawn from experiments on planar systems, too. Accepting the series estimate $k_BT_c^{SK}/J=0.588$ we find that the data are consistent with $T_c(\Delta)-T_c^{SK}\propto\Delta^{1/\phi}$ with $\phi\approx 4$. Assuming power-law behavior we show that our data obey crossover scaling with two-dimensional Heisenberg exponents $\gamma_H\approx 3$, $\alpha_H\approx -2$ in the isotropic limit. The data are also consistent with scaling theory based on the assumption of singularities which are stronger than any power law.

I. INTRODUCTION

The questions concerning magnetism in two dimensions have been a challenge for many years—and still are!—to both theorists and experimentalists. In the anisotropic case, the exact solution of the $S=\frac{1}{2}$ Ising model[1,2] presents an example of a second-order phase transition, where the order parameter (spontaneous magnetization m) behaves as $m\propto|1-T/T_c(1)|^\beta$, $\beta=\frac{1}{8}$ near the critical temperature $T_c(1)$, and the susceptibility χ diverges also with a power law, $\chi\propto|1-T_c(1)/T|^{-\gamma}$, $\gamma=\frac{7}{4}$. In the isotropic Heisenberg model as well as in the XY model and related problems rigorous results owing to Mermin and Wagner[3] and Hohenberg[4] exclude the existence of a nonzero spontaneous magnetization at any nonzero temperature. However, another type of phase transition at a nonzero $T_c(0)$, where the response properties of the system with respect to external fields, etc., change, cannot be ruled out: It was suggested[5,6] on the basis of high-temperature-series extrapolations that χ diverges at $T_c(0)\neq 0$, implying infinite χ for $T<T_c(0)$. This work,[5,6] however, as well as a more recent analysis[7] cannot completely rule out $T_c(0)=0$.

While these extrapolations are based on the assumption of a power-law singularity, Camp and Van Dyke[8] reanalyzed the same series assuming a $\chi=C_1\exp\{C_2[1-T_c(0)/T]^{-\bar{\nu}}\}$ behavior. It is found that this assumption accounts better for the actual behavior of the series-expansion coefficients,[9] especially in the case of the plane rotator (i.e., XY) model; in the Heisenberg case $T_c(0)\neq 0$ and $\bar{\nu}\cong 0.8$ was suggested.[8] Berezinskii[10] and Kosterlitz and Thouless[11] presented theoretical arguments for such a transition (destruction of "topological long-range order"[11]) on the basis of long-wave-length low-temperature approximations in the plane rotator model.[12] While Beresinskii[10] also suggests a phase transition in the Heisenberg case, Kosterlitz and Thouless[11] suggest that no transition occurs.

Substances whose magnetic ordering is (nearly) two dimensional have thus found great experimental attention[13] as expected. A material which is particularly close to the two-dimensional isotropic Heisenberg case seems to be K_2NiF_4, where a ratio (anisotropy energy/exchange energy) $\approx\frac{1}{270}$ is quoted,[14] and the interplanar coupling is still smaller.[14] On the basis of the "universality ideas"[15] one would expect that near T_c the anisotropy should dominate, leading to Ising-like values for the critical exponents. While this expectation is born out reasonably well for the order parameter[14] ($\beta\approx 0.138$), the results[16] for susceptibility ($\gamma\approx 1.0$) and correlation length ($\nu\approx 0.59$) cannot be accounted for by theory: one rather expects a crossover[17] between the Ising values ($\gamma=1.75$) and higher values (the above-mentioned references[7,8] would lead to estimates in the range $2.5\leq\gamma_H\leq\infty$ for the susceptibility exponent of the Heisenberg model).

Clearly the crossover from the ordering anisotropic case to the nonordering isotropic case requires careful theoretical study. It is this problem which will be dealt with in the present paper.

This problem has been studied extensively already, using spin-wave theory,[18,19] Green's-function decoupling,[20,21] series expansions,[20] and Monte Carlo calculations.[19,22]. Spin-wave theories and Green's-function decoupling techniques cannot yield reliable information on critical properties, of course. The available series[20] are very short (five terms)[23] and also the Monte Carlo results[19] refer to extremely small systems (10×10 lattices) and are based on very short Markov chains, thus these results could not give conclusive information on the critical properties either.

In order to study the critical properties of weakly anisotropic Heisenberg magnets we thus made more extensive Monte Carlo calculations, studying $N\times N$ lattices with periodic boundary conditions, continuing earlier studies of three-dimensional systems.[24] We used $N=25$, 50, and 100 in order to estimate the influence of "finite size rounding and shifting"[25] effects on the phase transition. It has been shown in earlier work[24,26] that these effects are rather important, and that they can in fact be accounted for[27,28] by finite size scaling theories.[25] We always use Markov chains with a length of several 100 Monte Carlo steps per spin, which gave reasonable accuracy in spite of the slow convergence observed earlier,[22] which is discussed in the light of the dynamic interpretations of the Monte Carlo process.[28,29] In Sec. II we now describe the method and the model and in Sec. III we summarize the main predictions of the theories enumerated above, while Sec. IV gives our computational results and a detailed comparison with these predictions, and Sec. V contains the conclusions.

II. MODEL AND SIMULATION TECHNIQUE

The model studied is described by the following Hamiltonian[17,23]:

$$H=-J\sum_{ij}[(1-\Delta)(S_i^xS_j^x+S_i^yS_j^y)+S_i^zS_j^z]\ , \tag{1}$$

where $\vec{S}_i$ is a unit vector in the direction of the classical magnetic moment at lattice site i, the sum is extended over nearest-neighbor pairs on the square lattice, J being the exchange constant, and Δ characterizes the amount of (unaxial) anisotropy.

($\Delta=0$ is the isotropic Heisenberg case, $\Delta=1$ the Ising case.) In most experiments[14,15] one has single ion rather than exchange anisotropy, and spin quantum number $S=1$ rather than $S=\infty$, but in the spirit of the universality ideas[15] one expects very similar critical behavior. Since our model is classical (i.e., $S=\infty$) the predictions for an antiferromagnet correspond precisely to those of a ferromagnet, i.e., the magnetization for $J>0$ is equal to the sublattice magnetization for $J<0$, etc.

In the Monte Carlo computer experiments one generates a Markov chain of spin configurations, using suitable transition probabilities. As a starting configuration we always used a completely ordered ferromagnet. The sites of the lattice were considered in turn for a random choice of the orientation of a spin. In order to save computing time, the same procedure is carried out simultaneously using the same random numbers for four lattices at different temperatures. The change in energy δH which would result from this change was calculated from Eq. (1). If $e^{-\delta H/k_BT}$ exceeded a random number ρ in the interval $0<\rho<1$, the change was permitted while otherwise it was rejected. This process is denoted as a "Monte Carlo step" and had to be repeated many times. This procedure corresponds to a numerical solution of the relaxation according to the following master equation for the probability $P(\Omega_1,\ldots,\Omega_i,\ldots,\Omega_{N^2},t)$ of the spin configuration[28,29]

$$\begin{aligned}\frac{d}{dt}P(\Omega_1,\ldots,\Omega_i,\ldots,\Omega_{N^2},t)\\ &=-\sum_{i=1}^{N^2}\int d\Omega_i' W(\Omega_i\to\Omega_i')P(\Omega_1,\ldots,\Omega_i,\ldots,\Omega_{N^2},t)\\ &+\sum_{i=1}^{N^2}\int d\Omega_i' W(\Omega_i'\to\Omega_i)P(\Omega_1,\ldots,\Omega_i',\ldots,\Omega_{N^2},t)\ ,\end{aligned} \tag{2}$$

where Ω_i is the solid angle characterizing $\vec{S}_i$ and the time t has to be measured in Monte Carlo steps per spin. The transition probability $W(\Omega_i\to\Omega_i')$ is in our case given by $\min[\exp(-\delta H/k_BT),1]$. Since W satisfies the detailed balance principle with the probability $P_0\propto e^{-H/k_BT}$ according to the canonic ensemble, Eq. (2) is ergodic by construction. In the Monte Carlo runs one takes averages for any quantities of interest over a number of configurations generated in this way, which thus present time averages of the stochastic model Eq. (2). Convergence problems clearly occur if the non-equilibrium relaxation time characterizing the approach to equilibrium τ_{ne} is very large, since then a large number of initial configurations has to be omitted from the average. Since the treated system is finite, the fluctuations around the equilibrium also affect the accuracy. For example, for the order parameter $\langle m\rangle$ one finds the following error estimate[28,29]:

$$\langle(\delta m)^2\rangle\cong\frac{1}{nN^2}k_BT\chi(1+2\tau_e)\ ,\quad \tau_e/n\ll 1\ , \tag{3}$$

where n is the number of Monte Carlo steps per spin and τ_e the relaxation time of the fluctuations in equilibrium. According to the conventional theory of slowing down one expects $\tau_e=\text{const}\times k_BT\chi$, the constant being of order unity in our units. Thus again a large susceptibility makes it very difficult to obtain results of reasonable precision.

The quantities recorded in our simulation were "susceptibility" χ defined above T_c by

$$\chi = \frac{1}{k_B T N^2}\left\langle\left(\sum_i \vec{S}_i\right)^2\right\rangle ,$$

the root-mean-square magnetization $\langle m^2\rangle^{1/2} \equiv N^{-1}(k_B T\chi)^{1/2}$, the transverse susceptibility

$$\chi_\perp = \frac{1}{k_B T N^2}\left[\left\langle\left(\sum_i S_{ix}\right)^2\right\rangle + \left\langle\left(\sum_i S_{iy}\right)^2\right\rangle\right] ,$$

the self-correlation

$$\langle (S_x)^2\rangle = \left\langle \frac{1}{2N^2}\sum_i [(S_{ix})^2 + (S_{iy})^2]\right\rangle ,$$

the energy $\langle E\rangle$ [see Eq. (11) below] and the specific heat per spin $C/k_B = (2J/k_B T)^2(\langle E^2\rangle - \langle E\rangle^2)$.

III. THEORETICAL BACKGROUND

A. Spin-wave predictions

Here we summarize the predictions of first-order spin-wave theory, which are readily obtained by standard techniques.[18,19,30,31] The spin-wave frequencies of an anisotropic spin $\mathcal{S}$ ferromagnetic square lattice with nearest-neighbor interactions J' are

$$\omega_F(\vec{k}) = 2J'\mathcal{S}[2 - (1-\Delta)(\cos k_x + \cos k_y)] , \tag{4}$$

while for the antiferromagnet we have

$$\omega_{AF}(\vec{k}) = 2|J'|\mathcal{S}[4 - (1-\Delta)^2(\cos k_x + \cos k_y)^2]^{1/2} , \tag{5}$$

where the lattice spacing was taken to be unity. From Eq. (4) one obtains for the magnetization per spin ($g\mu_B = 1$, $\hbar = 1$)

$$M = \mathcal{S} - \left(\frac{1}{2\pi}\right)^2 \int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y \frac{1}{e^{\omega_F(\vec{k})/k_B T} - 1} , \tag{6}$$

which gives for $\mathcal{S} \to \infty$, $J'\mathcal{S}^2 = J$,

$$m = \frac{M}{\mathcal{S}} = 1 - \frac{k_B T}{J}\int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y \times \frac{1}{4 - 2(1-\Delta)(\cos k_x + \cos k_y)} = 1 - \frac{k_B T}{J}\frac{1}{2\pi}K(1-\Delta), \tag{7}$$

where $K(x)$ is the elliptic integral of the first kind. Similarly one obtains for the antiferromagnetic sublattice magnetization

$$M_{st} = \mathcal{S} + \tfrac{1}{2} - \frac{1}{2}\left(\frac{1}{2\pi}\right)^2 \int_{-\pi/2}^{+\pi/2} dk_x \int_{-\pi/2}^{+\pi/2} dk_y \times \frac{4|J'|\mathcal{S}}{\omega_{AF}(\vec{k})}\coth\frac{\omega_{AF}(\vec{k})}{2k_B T} , \tag{8}$$

which gives for $\mathcal{S} \to \infty$, $J'\mathcal{S}^2 = J$,

$$m_{st} = \frac{M_{st}}{\mathcal{S}} = 1 - \frac{k_B T}{|J|}\frac{1}{2}\left(\frac{1}{2\pi}\right)^2 \times \int_{-\pi/2}^{+\pi/2} dk_x \int_{-\pi/2}^{+\pi/2} dk_y \frac{4}{4 - (1-\Delta)^2(\cos k_x + \cos k_y)^2} . \tag{9}$$

It is easy to see that Eqs. (7) and (9) are equivalent, as expected in this classical limit, and henceforth we consider the ferromagnetic case only. Since for $\Delta \to 0$ we have $K(1-\Delta) \to \frac{1}{2}\ln(1/\Delta)$, one expects that the spin-wave approximation is valid as long as

$$\frac{k_B T}{|J|} \ll \frac{4\pi}{\ln(1/\Delta)} \equiv \frac{k_B T^{SW}}{|J|} . \tag{10}$$

A similar region of validity for the spin-wave approximation was quoted by Mikeska.[21] It should be noted that for the values of Δ considered here this temperature T^{SW} is of the same order of magnitude as the mean-field critical temperature $T_c^{MF} = 8|J|/3k_B$. Since the actual critical temperature $T_c(\Delta)$ satisfies the relation $T_c(\Delta) \ll T_c^{MF}$, one expects the spin-wave approximation to be a valid description for a broad range of temperatures ($T < 0.5T_c$ in[14,18] K_2NiF_4).

Next we consider the reduced energy

$$\langle E\rangle \equiv \tfrac{1}{2}\{\langle S_z(0,0)S_z(0,1)\rangle + \langle S_z(0,0)S_z(1,0)\rangle + (1-\Delta)[\langle S_x(0,0)S_x(0,1)\rangle + \langle S_x(0,0)S_x(1,0)\rangle + \langle S_y(0,0)S_y(0,1)\rangle + \langle S_y(0,0)S_y(1,0)\rangle]\} , \tag{11}$$

where the arguments of the spins denote their lattice coordinates (the origin being averaged over the lattice). From formulas analogous to those of Watson *et al.*[26]

$$\langle S_x(0,0)S_x(l,m)\rangle = \langle S_y(0,0)S_y(l,m)\rangle = \frac{k_B T}{|J|}\int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \times \frac{\cos(lk_x + mk_y)}{4 - 2(1-\Delta)(\cos k_x + \cos k_y)} \tag{12}$$

and

$$\langle S_z(0,0)S_z(l,m)\rangle = m^2 + O((k_B T/|J|)^2) , \tag{13}$$

one readily obtains using Eqs. (7) and (11)–(13)

$$\langle E\rangle = 1 - k_B T/2|J| , \tag{14}$$

i.e., in first-order spin-wave theory the energy is independent of the anisotropy.[19] From Eq. (12) it is also straightforward to obtain the self-correlation

$$\langle (S_x)^2\rangle = 1 - m \tag{15}$$

and the transverse susceptibility

$$\chi_\perp \equiv \frac{1}{k_B T}\sum_{l,m}|\langle S_x(0,0)S_x(l,m)\rangle + \langle S_y(0,0)S_y(l,m)\rangle| = \frac{1}{2|J|\Delta} . \tag{16}$$

Equations (6)–(16) refer to an infinite system. In finite systems in zero field there is no spontaneous magnetization and thus the spin-wave approximation is mathematically not well defined. A rough estimate of finite-size effects at low temperatures may be obtained, however, by explicitly evaluating the summations which were replaced by integrals in Eq. (6)

$$\frac{1}{\pi^2}\int_0^{\pi} dk_x \int_0^{\pi} dk_y \cdots \to \frac{1}{N^2}\sum_{j=1}^{N}\sum_{l=1}^{N}\cdots \qquad (17)$$

$$\left(k_x = j\frac{\pi}{N}\ ,\ k_y = l\frac{\pi}{N}\right),$$

which are easily evaluated numerically.

B. Crossover scaling predictions

Following standard treatments of crossover scaling for exchange anisotropy,[17,32] we first consider the case where it is assumed that in the isotropic case ($\Delta = 0$) a phase transition occurs at $T_c^{\mathrm{SK}} = T_c(0)$, the divergence of correlation length, susceptibility, etc., being characterized by power-law singularities with exponents ν_H, γ_H, etc. We assume that ordinary scaling laws hold (the exponents β_H and δ_H are then a meaningful characterization for the scaling functions in the presence of a nonzero magnetic field h). Then the crossover scaling hypothesis states for the "susceptibility" $\chi = \chi_\parallel + \chi_\perp$

$$\chi(T,h,\Delta) = \epsilon_0^{-\gamma_H}\tilde{\chi}_0(\epsilon_0\Delta^{-1/\phi}, h\epsilon_0^{-\beta_H\delta_H}) , \qquad (18)$$

where

$$\epsilon_0 = [T - T_c(0)]/T_c(0) , \qquad (19)$$

and ϕ is the crossover exponent. Except for ϕ all unsubscripted exponents are the two-dimensional Ising exponents. The asymptotic behavior of the scaling function $\tilde{\chi}_0(x,y)$ is characterized as follows:

$$\tilde{\chi}_0(\infty,0) = C_H\ ,\quad \tilde{\chi}_0(x,0) = \hat{\chi}_0^{\pm}|x - x_c|^{-\gamma}\ ,\quad x \to x_c\ . \qquad (20)$$

Here C_H denotes the critical amplitude of the susceptibility of the isotropic Heisenberg model, γ is the Ising model susceptibility exponent, $\hat{\chi}_0^{\pm}$ is a constant related to the critical amplitudes of the susceptibility near $T_c(\Delta)$, and x_c is defined by

$$x_c = \Delta^{-1/\phi}\epsilon_{0c} = \Delta^{-1/\phi}[T_c(\Delta) - T_c(0)]/T_c(0)\ ; \qquad (21)$$

note that this implies that the "shift exponent" is given by $1/\phi$

$$T_c(\Delta) - T_c(0) \propto \Delta^{1/\phi}\ . \qquad (22)$$

From Eqs. (18)–(20) one obtains the following relations for the critical amplitude of the susceptibility for $\Delta \neq 0$ $[\chi(T,0,\Delta) = C^{\pm}|1 - T/T_c(\Delta)|^{-\gamma}]$:

$$C^{\pm} = \hat{\chi}_0^{\pm}\Delta^{(\gamma-\gamma_H)/\phi}\,x_c^{-\gamma_H}\ . \qquad (23)$$

Since $\chi_\perp(T,0,0) = \frac{1}{2}\chi(T,0,0)$, we find similarly for the transverse susceptibility

$$\chi_\perp(T,h,\Delta) = \epsilon_0^{-\gamma_H}\tilde{\chi}_{0\perp}(\epsilon_0\Delta^{-1/\phi}\ ,\ h\epsilon_0^{-\beta_H\delta_H})\ , \qquad (24)$$

with $\tilde{\chi}_{0\perp}(\infty,0) = \frac{1}{2}C_H$ but $\tilde{\chi}_{0\perp}(x,0)$ finite at x_c. This immediately yields

$$\chi_\perp(T_c(\Delta),0,\Delta) = x_c^{-\gamma_H}\tilde{\chi}_{0\perp}(x_c,0)\Delta^{-\gamma_H/\phi}\ . \qquad (25)$$

A similar procedure may be carried through for the order parameter m,

$$m(T,h,\Delta) = \epsilon_0^{\beta_H}\tilde{m}_0(\epsilon_0\Delta^{-1/\phi}\ ,\ h\epsilon_0^{-\beta_H\delta_H})\ ; \qquad (26)$$

since the isotropic spontaneous magnetization $m(T,0,0)$ vanishes identically we have to require that $\tilde{m}_0(x,0) \to 0$ as $x \to \infty$ as well as $\tilde{m}_0(0,y) \to 0$ as $y \to 0$, of course. On the other hand we have

$$\tilde{m}_0(x,0) = \hat{m}_0(x_c - x)^{\beta}\ ,\quad x \to x_c^-\ , \qquad (27)$$

where β is the Ising-model order-parameter exponent. This yields

$$m(T,0,\Delta) = \hat{m}_0 x_c^{\beta_H}\Delta^{(\beta_H-\beta)/\phi}\{[T_c(\Delta) - T_c(0)]/T_c(0)\}^{\beta}\ , \qquad (28)$$

i.e., the critical amplitude $B(\Delta) \propto \Delta^{(\beta_H-\beta)/\phi}$. Similar arguments for the specific heat yield

$$C(T,H,\Delta)/k_B = |\epsilon_0|^{-\alpha_H}\tilde{C}_0(\epsilon_0\Delta^{-1/\phi}\ ,\ h|\epsilon_0|^{-\beta_H\delta_H})\ . \qquad (29)$$

In analogy to Eq. (20) we require

$$\tilde{C}_0(\pm\infty,0) = A_H^{\pm}\ ,\quad \tilde{C}_0(x,0) = \hat{C}_0^{\pm}|x - x_c|^{-\alpha}\ ,\quad x \to x_c\ . \qquad (30)$$

The $\pm$ sign refers to amplitudes above and below $T_c(0)$ or $T_c(\Delta)$, respectively. The prediction for the specific-heat amplitudes is $[C(T,0,\Delta) = A^{\pm}|1 - T/T_c(\Delta)|^{-\alpha}]$

$$A^{\pm} = \hat{C}_0^{\pm}x_c^{-\alpha_H}\Delta^{(\alpha-\alpha_H)/\phi}\ . \qquad (31)$$

More care is required in the discussion of the self-correlation. Since the renormalization-group analysis proved the following structure for the Fourier transform $G(\vec{k})$ of the correlation function[33]:

$$G(\vec{k}) = G_0k^{-2+\eta} + G_1(k)\epsilon^{1-\alpha} + G_2(k)\epsilon^1 + \cdots\ ,$$
$$k \to 0\ ,\quad \epsilon = T/T_c - 1 \to 0\ ,\quad k\epsilon^{-\nu} \to \infty \qquad (32)$$

and assuming that $G(\vec{k})$ is regular in ϵ outside of this scaling limit, one expects the following behavior from an integration of Eq. (32) over the Brillouin zone:

$$\langle (S_x)^2\rangle = \tfrac{1}{3} + \epsilon_0^{1-\alpha_H}\tilde{f}_0^{(0)}(\epsilon_0\Delta^{-1/\phi}\ ,\ h\epsilon_0^{-\beta_H\delta_H})$$
$$+ \epsilon_0^1\tilde{f}_0^{(1)}(\epsilon_0\Delta^{-1/\phi}\ ,\ h\epsilon_0^{-\beta_H\delta_H}) + \cdots\ . \qquad (33)$$

The term ϵ_0^1 has to be included in the analysis, since α_H—if such a phase transition exists at all in the Heisenberg model—is probably strongly negative, and thus $\epsilon_0^{1-\alpha_H}$ is not the leading temperature dependence. The critical value of the self-correlation follows from symmetry. Since $\tilde{f}_0^{(0)}(x,0)$

and $\tilde{f}_0^{(1)}(x, 0)$ should be finite (and nonzero) at $x = x_c$, one immediately predicts

$$[\langle(S_x)^2\rangle - \tfrac{1}{3}]_{T_c(\Delta)} = x_c^{1-\alpha_H}\tilde{f}_0^{(0)}(x_c, 0)\Delta^{(1-\alpha_H)/\phi} + x_c\tilde{f}_0^{(1)}(x_c, 0)\Delta^{1/\phi} + \cdots . \quad (34)$$

This rather conventional scaling analysis has to be modified, however, if the correlation length ξ_H diverges exponentially fast[8,10–12] instead of following a power law, however. Kosterlitz suggested[12] that scaling relations remain valid, however, if $\epsilon_0^{-\nu_H}$ is replaced by ξ_H. Thus we rewrite Eq. (18)

$$\chi(T, h, \Delta) = \xi_H^{\tilde{\gamma}_H}\,\overline{\chi}_0(\xi_H^{-1}\Delta^{-1/\tilde{\phi}}\;,\; h\xi_H^{\tilde{\beta}_H\delta_H}) , \quad (35)$$

where in the case of power-law singularities

$$\tilde{\gamma}_H = \gamma_H/\nu_H\;,\quad \tilde{\phi} = \phi/\nu_H\;,\quad \tilde{\beta}_H = \beta_H/\nu_H\;,\quad \tilde{\alpha}_H = \alpha_H/\nu_H\;.$$

If instead of power-law singularities we have[8,10–12]

$$\xi_H = \hat{\xi}_H \exp(c\,\epsilon_0^{-\bar{\nu}}) , \quad (36)$$

where c is a constant and $\bar{\nu}$ is a new exponent; ν_H, γ_H, β_H, ϕ, and α_H become meaningless, but $\tilde{\alpha}_H$, $\tilde{\beta}_H$, $\tilde{\gamma}_H$, δ_H, η_H, and $\tilde{\phi}$ are still meaningful exponents. It is easy to see that one then obtains for the shift of T_c from $\xi_H^{-1}\Delta^{-1/\tilde{\phi}} = x_c'$ that

$$[T_c(\Delta) - T_c(0)]/T_c(0) = \{c/[\ln(\hat{\xi}_H x_c'\Delta^{1/\tilde{\phi}})^{-1}]\}^{1/\bar{\nu}} , \quad (37)$$

i.e., a complicated logarithmic behavior. But one still obtains rather simple amplitude predictions: Eqs. (23), (25), (28), (31), and (33) are replaced by

$$C^{\pm} \propto \Delta^{-\tilde{\gamma}_H/\tilde{\phi}}\;,\quad \chi_\perp(T_c(\Delta), 0, \Delta) \propto \Delta^{-\tilde{\gamma}_H/\tilde{\phi}}\;,$$
$$B(\Delta) \propto \Delta^{\tilde{\beta}_H/\tilde{\phi}}\;,\quad A^{\pm} \propto \Delta^{-\tilde{\alpha}_H/\tilde{\phi}}\;, \quad (38)$$
$$[\langle(S_x)^2\rangle - \tfrac{1}{3}]_{T_c(\Delta)} \propto \Delta^{-\tilde{\alpha}_H/\tilde{\phi}}\;.$$

If $\tilde{\alpha}_H$, $\tilde{\gamma}_H$, and $\tilde{\phi}$ have finite values, these amplitude predictions still imply simple power laws. In the case where $\tilde{\phi}$ would turn out to be zero, but $\tilde{\alpha}_H$, $\tilde{\beta}_H$, and $\tilde{\gamma}_H$ are nonzero, it may be recommended to use a scaling representation which is intermediate between Eqs. (18) and (35), i.e.,

$$\chi(T, h, \Delta) = \xi_H^{-\tilde{\gamma}_H}\,\overline{\chi}_0(\epsilon_0\Delta^{-1/\phi}\;,\; h\xi_H^{\tilde{\beta}_H\delta_H}) . \quad (39)$$

In this case one would retain a simple power law for the shift exponent [Eq. (22)], while one would get power-law predictions for the logarithms of the amplitudes instead of for the amplitudes themselves, e.g.,

$$\ln\chi_\perp(T_c(\Delta), 0, \Delta) = \ln[\xi_H^{\tilde{\gamma}_H}\,\overline{\chi}_{0\perp}(x_c, 0)] + c\tilde{\gamma}_H x_c^{-\bar{\nu}}\Delta^{-\bar{\nu}/\phi}. \quad (40)$$

If $T_c(0) = 0$ it may be that either one of these possibilities [Eqs. (18), (35), or (39), respectively] still holds, if $T_c(0)$ in the denominator of Eqs. (19), (21), (28), and (37) is replaced by $T_c^{\rm MF}$, for instance.

It will be one of the main objectives of the present investigation to determine if the data can be consistently interpreted in terms of at least one of these scaling analyses, and to extract estimates for the corresponding exponents.

IV. RESULTS OF COMPUTER EXPERIMENTS

A. Raw data and their analysis

In view of the difficulties reported previously[19,22] in two-dimensional Heisenberg systems concerning the accuracy of the Monte Carlo method, it seemed important to consider the time correlations between subsequent configurations (cf. Sec. II). In Fig. 1 we show some raw data on $m_z(t) = (1/N^2)\sum S_i^z(t)$ as a function of t. Simple inspection of such plots already shows the problems involved: Subsequent values of $m_z(t)$ are indeed strongly correlated, and the correlation time exceeds the associated values of $k_BT\chi$ distinctly, especially for small Δ. Thus the conventional theory of slowing down seems particularly bad in this case, although all these data are far away from the respective critical point.[34] A possible interpretation is that the relaxation becomes quite slow already in the vicinity of $k_BT/J \approx 1$, i.e., in the vicinity of the mean-field critical temperature, where the probability factor for spin flips, $e^{-\delta H/k_BT}$, may already be very small in unfavorable cases.

Another effect limiting the accuracy of our investigation was the occurrence of "metastable states" with strong magnetization in the x (or y) direction below $T_c(\Delta)$. Owing to the symmetry of the Hamiltonian [Eq. (1)] such a transverse magnetization should average to zero much quicker than $m_z(t)$.[35] However, if such a state occurred its lifetime turned out to be too large to observe its decay. Such states were found for $\Delta = 0.02$ and for $N = 25$, but not for $N = 50$ or 100; for $\Delta = 0.01$ they occurred at some temperatures both for $N = 25$ and 50, while the results for $N = 100$ remained unaffected. For $\Delta = 0.005$, even some of the data for $N = 100$ were affected, and still larger systems would be required to obtain more reliable results. In such metastable states the energy was very close to the equilibrium value, while the values of root-mean-square magnetization, self-correlation and, of course, transverse susceptibility were erratic. It is unclear to us if these states have to be interpreted in terms of domain-wall-like or vortexlike[11] excitations, and clearly a more detailed study of these effects would be desirable. Nevertheless, the situation is in general *much* more favorable than in the fully isotropic case, where no spontaneous magnetization exists and thus the susceptibility and therefore fluctuations are extremely large at low temperatures. For nonzero Δ and N not very small a spontaneous magnetization is metastable at low temperatures, and

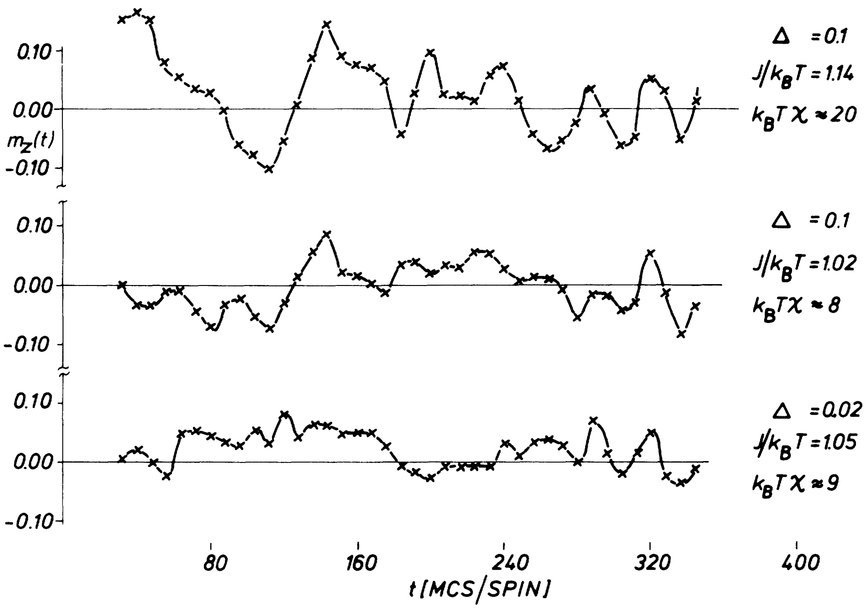

FIG. 1. Raw Monte Carlo data of the z component of the magnetization plotted vs time [in units of Monte Carlo steps (MCS) per spin]. The curves through the points are only guides to the eye. Three runs with different values of Δ or J/k_BT are shown. Magnitude of the fluctuations of $m_z(t)$ determines $\chi_{\parallel}$, the susceptibility with respect to the z direction.

therefore fluctuations are much smaller.

Figure 2 shows data for the root-mean-square magnetization for three anisotropies, and Fig. 3 shows corresponding curves for the energy $\langle E\rangle$. Both diagrams indicate that rather precise smooth curves could be obtained, which show distinctly the change as Δ is varied. For the sake of clarity the other data for $\Delta = 0.05$, 0.02, and 0.005, which look quite similar, have been omitted. While distinct finite-size effects are seen in the curves for $\langle m^2\rangle^{1/2}$, the finite-size effects on $\langle E\rangle$ were too small to be observed. In Fig. 2 we included spin-wave asymptotes for $\Delta = 0.01$, calculated from Eqs. (7) or (17), respectively. While on the basis of Eq. (10) we had expected that spin-wave theory should be safely valid for $T < 0.1T^{\text{SW}}$, i.e., $T < 0.4T_c$, or $k_B T/J \lesssim 0.27$ since $k_B T^{\text{SW}}/J \cong 2.73$, it turns out that dramatic deviations occur at much lower temperatures! A similar result can be seen in Fig. 3, where the spin-wave asymptote [Eq. (14)] should fit to the data for all Δ at low temperatures, while in fact the spin-wave asymptote agrees only with the data for $\Delta = 0.01$. In the previous investigation of Patterson and Jones[19] the size of the systems was too small ($N = 10$) and the accuracy too poor, and therefore these deviations were overlooked.

In order to study this surprising effect in more detail, we present our low-temperature data on

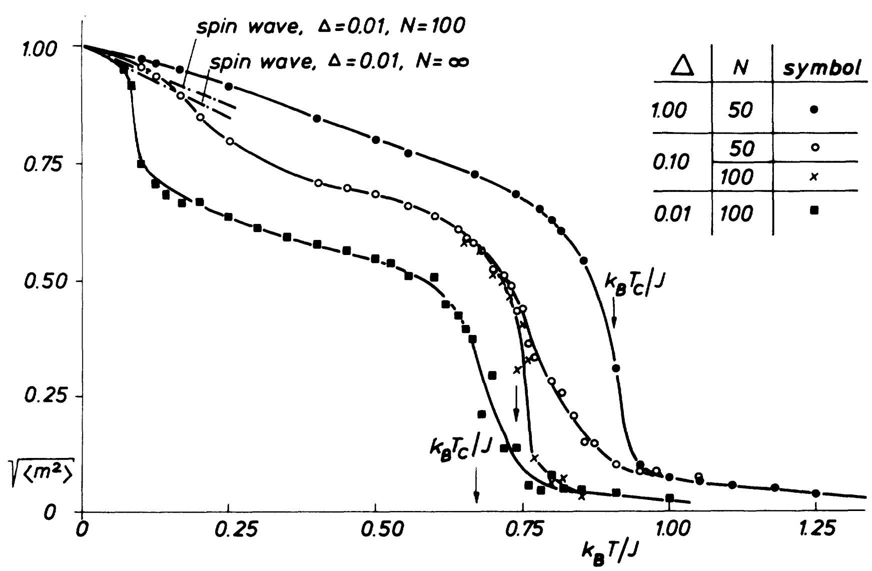

FIG. 2. Root-mean-square magnetization $\langle m^2\rangle^{1/2}$ plotted vs temperature, for three values of Δ. In the case of Δ = 0.1 data both for $N = 50$ and $N = 100$ are shown. Arrows denote our best estimates for $T_c(\Delta)$ of an infinite system. Full curves drawn are only guides to the eye.

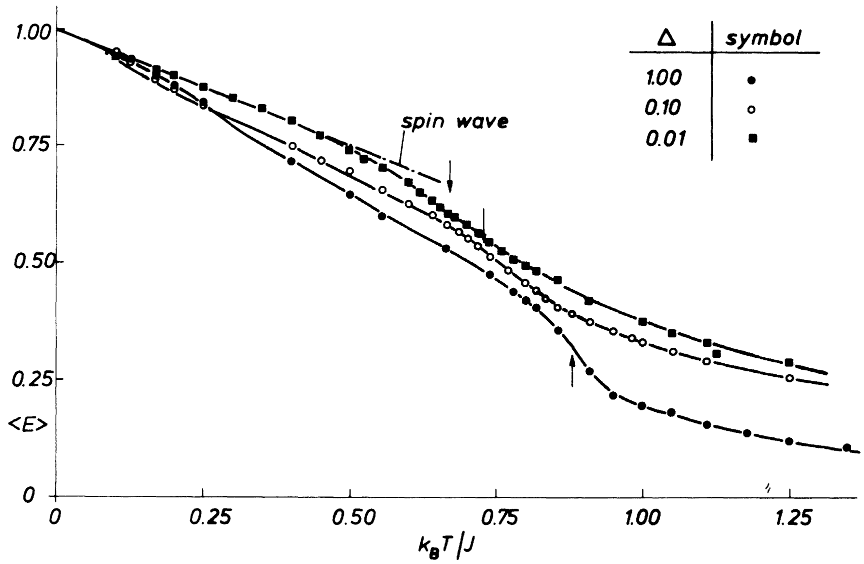

FIG. 3. Energy plotted vs temperature for $N = 50$, $\Delta = 0.1$ and $N = 100$, $\Delta = 0.01$. Note that the error bars of these results are in most cases much smaller than the size of the points. Arrows denote the estimates for $T_c(\Delta)$.

expanded scales in Fig. 4. While the temperature where the first deviations occur is shifting only very slowly to smaller values for $\Delta \to 0$, the amount of deviation at larger temperatures increases very drastically. These deviations are not only unexpected from the theoretical point of view[18,21] but they are also not in accord with the experimental observations in K_2NiF_4. Hence we speculate that these strong deviations are a peculiarity of the classical limit, where also the deviation of $\langle m \rangle$ from unity increases much faster (i.e., $\propto k_B T$) than in the quantum case $\{= \frac{1}{2}\pi(k_B T/4J) \times \exp[-(16\Delta J/S)/k_B T]\}$. Thus a renormalization of spin-wave frequencies owing to interaction effects may become important much earlier.[36] A theoretical study of spin-wave interaction effects in these classical magnets seems highly desirable, but it is outside the scope of the present paper.

Next we turn to the critical properties of the systems considered. Since our simulations were made for finite systems of moderate size, a sharp phase transition cannot occur and rounding effects must be accounted for. These effects also introduce some uncertainty even in the estimates of the critical temperature $T_c(\Delta)$. Figures 5 and 6 illustrate our procedures to determine $T_c(\Delta)$ for two cases, $\Delta = 1$ and $\Delta = 0.1$. The self-correlation, energy, and specific heat are plotted versus temperature. Both $\langle (S_x)^2 \rangle$ and $\langle E \rangle$ can be obtained with very high precision, especially for not very small values of Δ, and within the accuracy of our simulation they are not affected by finite size. This fact is in accord with Ising $S = \frac{1}{2}$ studies.[27] In the Ising case $\Delta = 1.0$ we also used some general series expansions[37] to obtain the result for the zero-field susceptibility $(K = J/k_B T)$

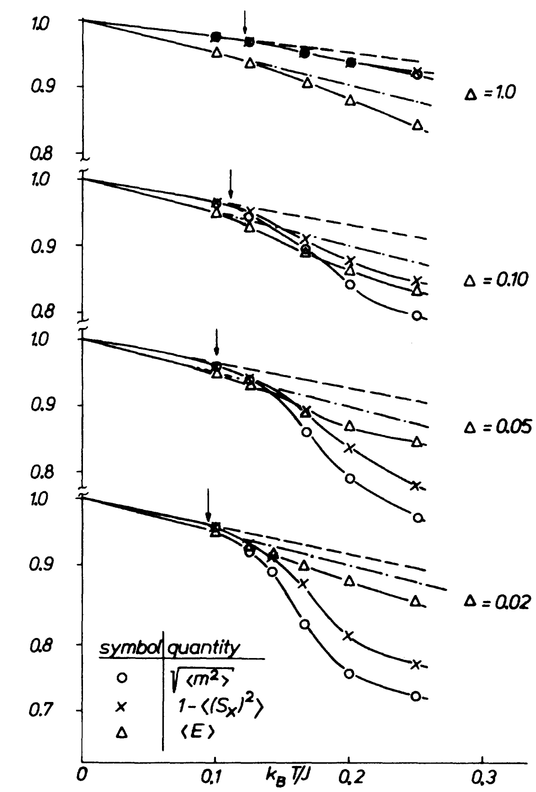

FIG. 4. Root-mean-square magnetization, self-correlation, and energy plotted vs temperature in the spin-wave region. Four values of Δ are shown. Dash-dotted curve represents Eq. (14), the broken line represents Eqs. (7) and (17). All points refer to $N = 50$. Note that the spin-wave predictions for m and $1 - \langle (S_x)^2 \rangle$ coincide [Eq. (15)]. Arrows denote the temperature where the first deviations from the spin-wave theory occur. This is also roughly the temperature where the Monte Carlo results for $\langle m^2 \rangle^{1/2}$ and $1 - \langle (S_x)^2 \rangle$ start to disagree.

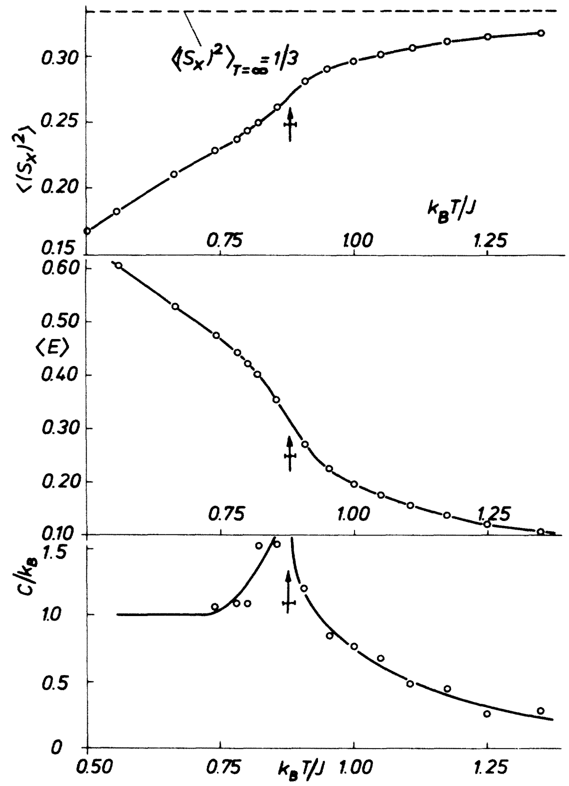

FIG. 5. Self-correlation, energy, and specific heat plotted vs temperature for $\Delta = 1.0$ (Ising case). Arrows show our best estimate for $T_c(\Delta)$; the accuracy of this estimate is also indicated. Curve drawn in the case of the specific heat is consistent with graphical differentiation of the energy. All data points refer to $N = 50$.

$$k_B T\chi = \tfrac{1}{3}\left(1 + \tfrac{4}{3}K + \tfrac{4}{3}K^2 + \tfrac{1144}{675}K^3 + \tfrac{3476}{2025}K^4 + \tfrac{4577473}{2381400}K^5 + \cdots\right). \qquad (41)$$

Owing to an extremely strong even-odd oscillation the series does not allow any precise determination of $T_c(1)$, it only suggests that $T_c(1) = 0.91 \pm 0.05$, consistent with the Monte Carlo estimate $T_c(1) = 0.88 \pm 0.01$. In view of this fact no attempt was made to obtain similar series for $\Delta \neq 1$.

It is evident from Fig. 6 that the scatter in the specific-heat data is extremely large, and thus this quantity could not be used for any conclusion whatsoever concerning the predictions of Sec. III. It is evident, however, from Fig. 3 that the anomaly in the slope of the $\langle E\rangle$ vs T curves vanishes as $\Delta \to 0$, which is in accord with both Eqs. (31) and (38), if α_H or $\tilde{\alpha}_H$ are negative. In the case $\Delta = 0$, where extensive series (up to 10 terms in K) are available, Ritchie and Fisher[7] proposed a rounded rather than singular specific-heat peak. This suggestion is certainly consistent with our results. This vanishing anomaly in $\langle E\rangle$ and $\langle (S_x)^2\rangle$ makes our estimates of $T_c(\Delta)$ increasingly uncertain as $\Delta \to 0$, but there we still have the check provided by the order parameter and the susceptibility to be shown below. Figures 7–12 show the critical behavior of the order parameter and susceptibility. The susceptibility data exhibited rather strong scatter, similar to the specific heat, but nevertheless, owing to the very pronounced singularity meaningful exponent estimates could be obtained. Since the susceptibility data used were in most cases not closer to $T_c(\Delta)$ than 10%, finite-size effects were unimportant, and averages over $N = 25$, 50, and 100 were made. The data for the order parameter, on the other hand, were much more precise but affected by finite-size effects even far below T_c, especially if Δ was small. Figure 7 shows that for the range of values for Δ and N studied, the magnetization was consistent with an $1/N$ extrapolation. We do not expect that this behavior remains valid as $\Delta \to 0$, of course: for

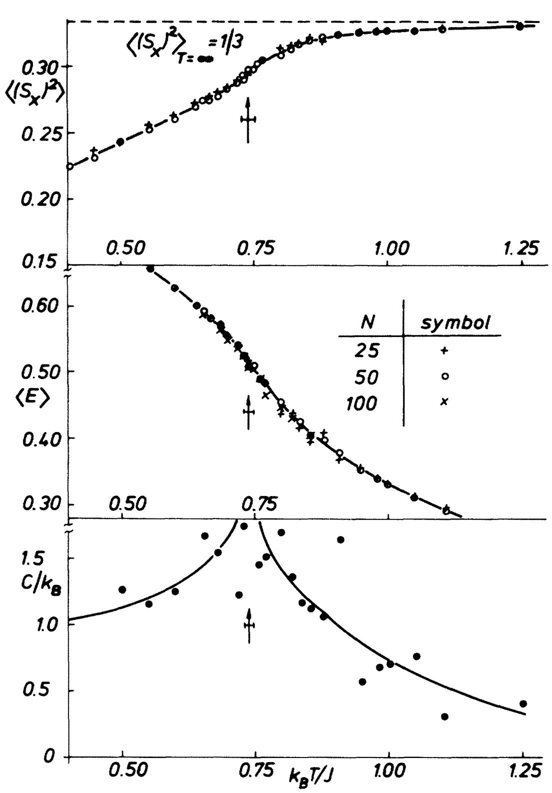

FIG. 6. Self-correlation, energy, and specific heat plotted vs temperature for $\Delta = 0.1$ and various N (in the case of the specific heat, the points are averages over $N = 25, 50$, and 100 at each temperature, since the scatter of the data points did not indicate any systematic finite-size effect.) Curves drawn through the points for the energy and self-correlation are only guides to the eye, while the curve for the specific heat is obtained from graphical differentiation of the energy. Arrows show our best estimate for $T_c(\Delta)$ and its accuracy.

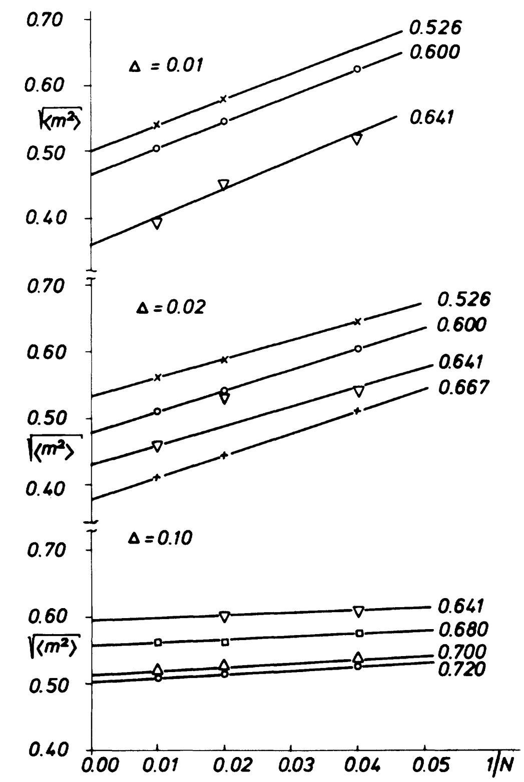

FIG. 7. Root-mean-square magnetization plotted vs inverse linear dimension for three values of Δ. Parameter of the curves is the temperature k_BT/J.

$\Delta = 0$ $\langle m^2\rangle$ may vary as $\propto N^{-x}$, with $0 < x < 1$. Resulting estimates[10] for $\langle m^2\rangle$ in this case are somewhat smaller than the values obtained for $\langle m^2\rangle$ in the case $\Delta \neq 0$ at the temperatures $k_BT/J \gtrsim 0.3$. Therefore the accuracy of the critical amplitudes

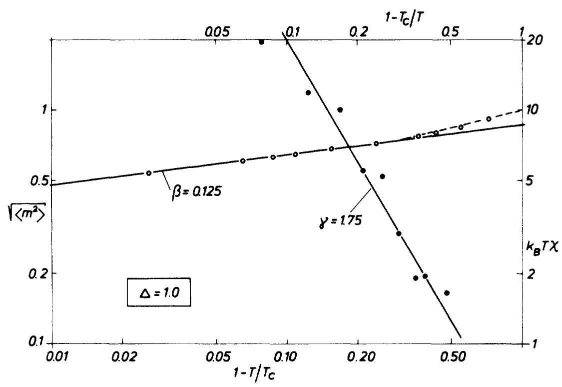

FIG. 8. Log-log plot of magnetization (open circles) and susceptiblity (full circles) above T_c for $N = 50$ and $\Delta = 1.0$. (The four points of the susceptibility closest to T_c are averages of $N = 50$ and 100.) Note that the upper temperature scale refers to the susceptibility and the lower one to the magnetization. Temperature variables are chosen such that correction terms are rather small.

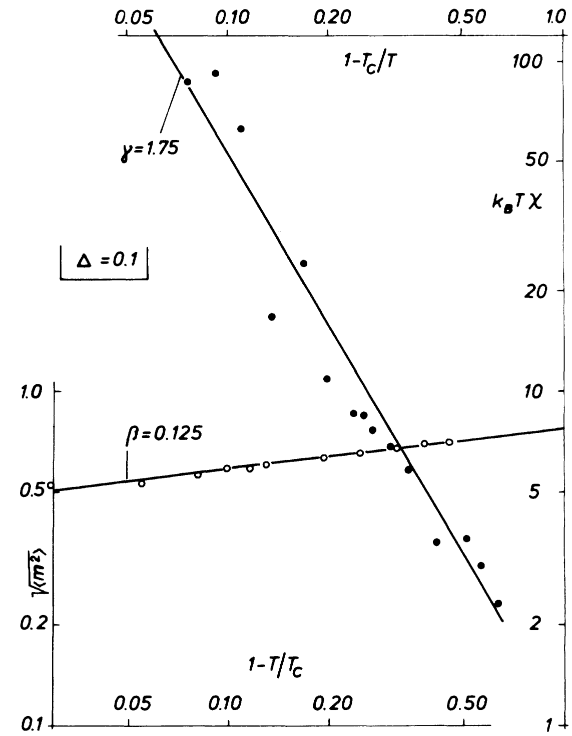

FIG. 9. Log-log plot of magnetization (open circles) and susceptibility (full circles) (above T_c) for $\Delta = 0.1$. Susceptibility points are averages over $N = 25$, 50, and 100. (The scatter of the points for individual N is about twice as large and not systematic.)

$B(\Delta)$ of the order parameter deduced from the extrapolated data becomes increasingly uncertain as $\Delta \to 0$. It seems reasonable to assume, however, that $\langle m^2\rangle$ decreases monotonically as $\Delta \to 0$ and as $N \to \infty$. Then the subtle simultaneous crossover in the behavior of $\langle m^2\rangle$ as a function of N and Δ cannot account for the difficulties with the spin-wave approximation. On the contrary, it might be that the discrepancies between the spin-wave results and the true behavior for $N \to \infty$ are even larger. These finite-size effects on the magnetization are much more pronounced than the corresponding effects in the three-dimensional calculations.[24,26] Probably, this effect could be reduced by use of the "self-consistent effective field boundary conditions"[38] which were rather successful in three dimensions,[38] but the large amount of additional computing time which a thorough study would require prevented us from using this method in the present investigation.

Figure 8 gives log-log plots for magnetization and susceptibility for the Ising limit ($\Delta = 1.0$). Using the value for T_c quoted above, the order parameter fits very well to $\beta = \frac{1}{8}$, and also the susceptibility data are consistent with $\gamma = 1.75$. The same result is obtained for $\Delta = 0.1$ (Fig. 9), indicating that the system still behaves rather anisotropically. For $\Delta = 0.05$ and in particular for $\Delta = 0.02$ (Fig. 10) it is seen that the slope of the susceptibility is distinctly larger for intermediate temperatures ($\gamma_{eff} \approx 2.2$ for $0.2 \lesssim \epsilon = 1 - T_c/T \lesssim 0.6$), while closer to T_c a changeover to $\gamma = 1.75$ occurs. The temperature difference where the changeover occurs becomes smaller as Δ decreases [at $\Delta = 0.01$ (Fig. 11) it is probably close to $\epsilon = 0.1$], but the lack of sufficient data points for $\epsilon < 0.1$ prevents us from making a definite statement concerning the variation of the susceptibility critical amplitude with Δ, to check out Eqs. (23) or (38), respectively. In any case the data are qualitatively consistent with crossover theories of this type, and disagree with the statement of Mikeska's Green's-functions treatment,[21] that for small Δ the susceptibility above T_c is essentially unaffected by the anisotropy.

From Figs. 7–11 it is seen that the order-parameter exponent is $\beta = \frac{1}{8}$—using the critical temperatures determined above—in all cases. The finite size (outside a narrow region around T_c) affects the critical amplitude rather than the exponent (Fig. 10). An extrapolation of the amplitudes

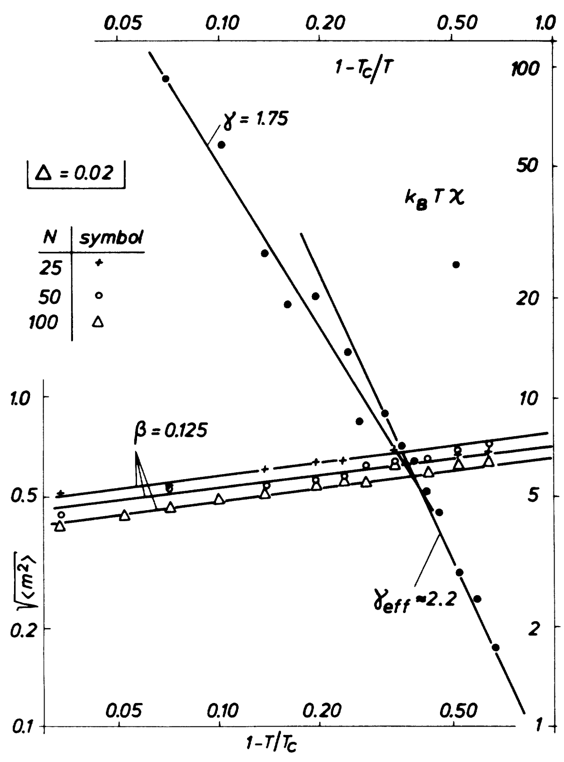

FIG. 10. Log-log plot of magnetization and susceptibility (above T_c) for $\Delta = 0.02$. Susceptibility points are averages over $N = 25$, 50, and 100, since again no systematics were detected in the scatter, while the order parameter points are shown for each individual N.

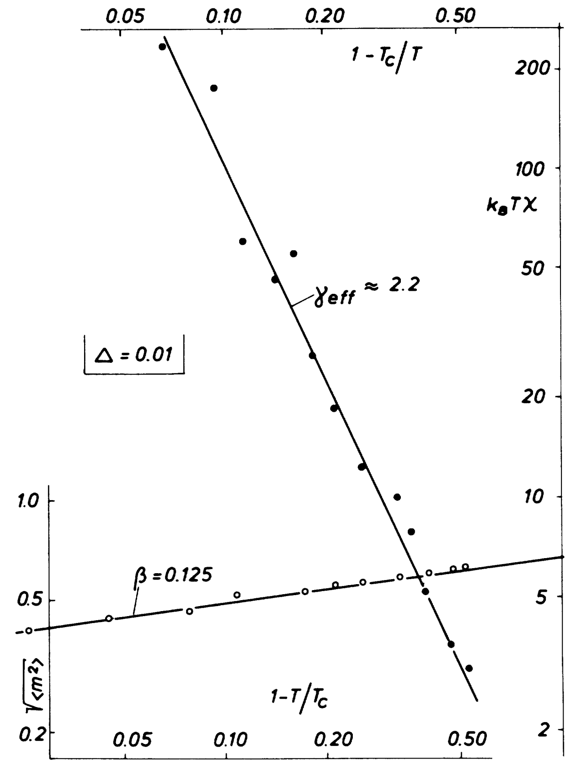

FIG. 11. Log-log plot of magnetization (open circles) and susceptibility (full circles) (above T_c) for $\Delta = 0.01$. Susceptibility points are averages over $N = 50$ and 100, the order parameter points refer to $N = 100$.

similar to Fig. 7 gave final estimates for $B(\Delta)$, to be discussed below. Owing to finite-size rounding the data points usually start to lie distinctly above the straight lines at values of $\epsilon = 1 - T/T_c \approx 0.03$.

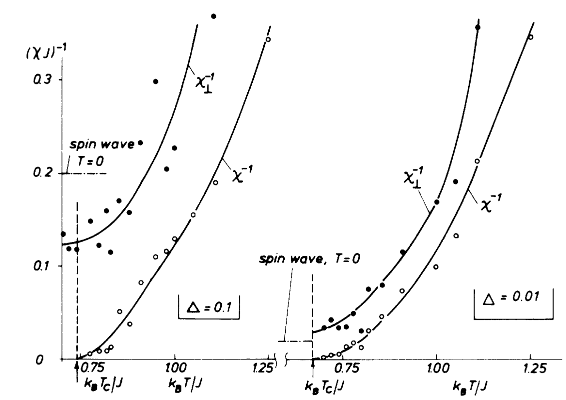

FIG. 12. Inverse total susceptibility χ^{-1} and inverse transverse susceptibility $\chi_\perp^{-1}$ plotted as a function of temperature for $\Delta = 0.1$ and 0.01. All data points are averages over $N = 25$, 50, and 100. Spin-wave asymptotes are calculated from Eq. (16). Below T_c for most temperatures this averaging over N was not possible, owing to the mentioned "metastability effects" for $N = 25$ or 50, and therefore most data for $\chi_\perp^{-1}$ below T_c are omitted.

In Fig. 12 we then compare the temperature dependence of the total susceptibility and the transverse susceptibility for $\Delta = 0.1$ and 0.01 (the curves for $\Delta = 0.02$ and 0.05 are similar). While for $T \gg T_c$ the temperature dependence of χ^{-1} and $\chi_\perp^{-1}$ are quite similar, $\chi_\perp^{-1}$ remains nonzero at T_c, as expected. For the values of Δ studied here $\chi_\perp^{-1}(T_c(\Delta))$ and $\chi_\perp^{-1}(T=0)$ have about the same order of magnitude.

B. Comparison with experiment

The computer simulation uses a classical system and thus only a semiquantitative comparison with experimental systems—which are quantum systems—is possible. This difference is irrelevant with respect to exponent estimates, of course. It must be stressed that our results are not in perfect agreement with the experiments in[14,16] K_2NiF_4 and other layered magnets.[13] First of all the order-parameter exponent quoted is distinctly larger, $\beta = 0.138$,[14] or even $\beta \approx 0.15$–0.18.[13] This is usually interpreted in terms of an admixture of the three-dimensional behavior.[13,14] It turns out, however, that this is not the only possible explanation, since rounding phenomena may lead to a similar effect. This is seen in our data if we treat T_c as an adjustable parameter of our order-parameter curve. We could then fit our data up to much higher temperatures until the "tail" in Fig. 2 becomes important. This is illustrated in the lower part of Fig. 13, where for $\Delta = 0.1$, T_c was shifted upwards about 3%, and now for $\epsilon > 0.003$ (instead of $\epsilon > 0.03$ as in Fig. 9) a nice fit to a power law is obtained for $N = 100$, with $\beta_{eff} = 0.16$. This result is clearly meaningless, of course, since for $N = 50$ a different shift would be needed, and we feel that from our other data (Fig. 6) we can exclude such a high T_c safely. It fits nicely to such

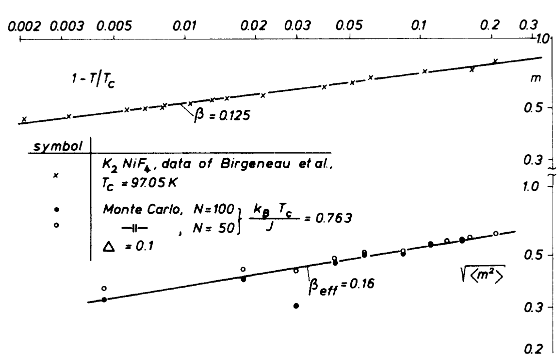

FIG. 13. Log-log plots of the order parameter of K_2NiF_4 taken from Birgeneau *et al.* (Ref. 14) (upper part) and of Monte Carlo data for $\Delta = 0.1$, in order to show that by shifting T_c one can fit the experimental data to $\beta = \frac{1}{8}$, and on the other hand, the computer simulation data to $\beta^{eff} \approx 0.16$.

an interpretation that near the real T_c (i.e., near $\epsilon = 0.03$ in Fig. 13, lower part) we observe the largest statistical fluctuations.[39] The same explanation may account for the anomalously high exponents determined experimentally. For example, in K_2NiF_4 $T_c = 97.23$ K was chosen[14] and then the region of the rounding was $\epsilon = 2 \times 10^{-4}$. However, using the tabulated data[14] with a $T_c = 97.05$ K (Fig. 13) shows that the data points are now quite consistent with $\beta = 0.125$, but rounding sets in at $\epsilon = 2 \times 10^{-3}$. These data for K_2NiF_4 have perhaps the highest resolution of all experimental data[13] to date. For other systems where the resolution is worse or the rounding more pronounced, a similar analysis would give even larger shifts in the estimate for β. Of course, we do not imply that one may select T_c arbitrarily to obtain a value of β one desires, but rather we imply that the uncertainties may be larger than usually assumed.

The conclusion that the experimental fitting T_c procedures possibly underestimated rounding phenomena is confirmed, if we interpret the experimental rounding phenomena also in terms of a characteristic length L_R, on which the crystal is basically ideal (perhaps mean distance between point defects, dislocations, or other inhomogeneities). For then one would argue that rounding occurs when the correlation length ξ exceeds this length L_R. In three-dimensional magnetic crystals, analysis of the specific-heat data revealed[40] that rounding (i.e., deviation from the *true* asymptotic form) occurs at $\epsilon \approx 10^{-3}$ or even larger values of ϵ, even if the log-log plots for smaller ϵ looked well behaved. This result would imply that $L_R \approx \xi_0 \epsilon^{-\nu} \approx 100$ lattice constants, putting $\xi_0 \approx 1$ and $\nu \approx \frac{2}{3}$. There is no reason to assume that L_R is much larger for a crystal with two-dimensional magnetic ordering. Even in the Ising limit one would then expect ($\xi_0 \approx 1$, $\nu = 1$) that rounding occurs for $\epsilon < 10^{-2}$. For nearly isotropic systems one probably has $\xi_0^{eff} \approx 1$, $\nu^{eff} \approx 2$,[41] which would imply that rounding occurs for $\epsilon < 10^{-1}$! Surprisingly enough, in K_2NiF_4 below T_c this estimate is clearly too pessimistic, as seen from Fig. 13, although the experimental data on the correlation length and susceptibility above T_c could possibly be interpreted in terms of such a rounding off. Here for $0.02 < \epsilon < 0.2$ an exponent $\gamma^{eff} \approx 1$ was found for the susceptibility,[16] while for larger ϵ the effective exponent would be much larger. The other choice $T_c = 97.05$ K would not change this estimate, of course. Obviously we cannot give a completely convincing explanation for this experiment on the basis of our model calculations. We mention only as a speculation the following possibilities: (i) The phase transition in K_2NiF_4 cannot be accounted for by the simple model Eq. (1). (ii) The round-

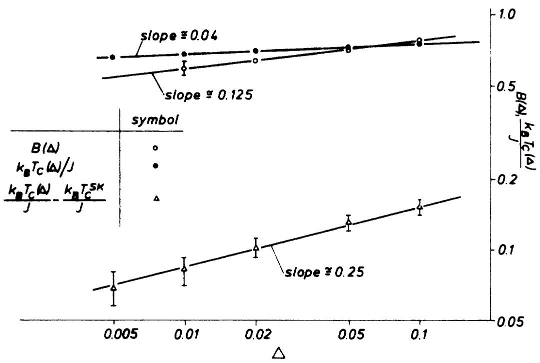

FIG. 14. Log-log plot of the order-parameter critical amplitude $B(\Delta)$ and the critical temperature $k_B T_c(\Delta)/J$ vs Δ. For $\Delta = 0.005$ a meaningful estimate for $B(\Delta)$ was impossible, since reliable data for the order parameter were available for $N=100$ only, and thus any extrapolation to $N\to\infty$ as in Fig. 7 could not be done. Error bars are shown if they exceed the size of the dots. No error estimate was taken into account for the value of T_c^{SK}, and a possible systematic error in $B(\Delta)$ owing to a nonlinear variation of $\langle m^2\rangle$ with $1/N$ is also neglected.

ing phenomena are strongly asymmetric with respect to T_c, with little rounding below T_c, and much rounding above T_c. Fitting power laws to functions which are rounded off would of course lead to exponent estimates which are too low. Such an asymmetry would require a very strong asymmetry in the critical amplitude of the correlation length, since one must approach the same finite value of ξ at T_c from both sides. (iii) The wave-vector-dependent susceptibility for $\epsilon < 0.2$ deviates strongly from the Ornstein-Zernike form, and thus the data analysis of Ref. 16 would be incorrect. On the other hand, in the rather anisotropic case of K_2CoF_4 ($\Delta\approx 0.3$)[13] Ising exponents have been found, consistent with our results for $\Delta = 0.1$ and 1.0. Owing to the slower increase of the correlation length in that material, one expects that rounding phenomena are much less important than in highly isotropic substances.

C. Comparison with crossover scaling analysis

In Fig. 14 log-log plots are given for the Δ dependence of the order-parameter amplitude $B(\Delta)$ and the critical temperature $k_B T_c(\Delta)$. It is seen that the slope of the $k_B T_c(\Delta)$ vs Δ curve is very small; if $k_B T_c(0)=0$—i.e., no phase transition of the Stanley-Kaplan type[6]—$T_c(\Delta)$ would vanish with Δ roughly logarithmically. If we accept the value $k_B T_c/J = 0.588$ quoted by Ritchie and Fisher, the data again fit to a straight line but now with a slope of 0.25, which has to be identified as $1/\phi$ if Eq. (22) applies.

In Fig. 15 the critical value of the transverse susceptibility and the reduced self-correlation are shown in a similar way. Note that these results—as well as the results for $B(\Delta)$—are independent of T_c^{SK}, they depend on the correct choice of $T_c(\Delta)$ only. It is interesting to note that the variation $(\chi_\perp^{-1})_{T_c(\Delta)} \propto \Delta^{0.65}$ is slower than the variation in the spin-wave regime [Eq. (16)]. With respect to $B(\Delta)$ a variation with $\ln(1/\Delta)$ as suggested by Mikeska[21] cannot be ruled out, although a power law seems to be more probable. Note also that Mikeska's Green's-function treatment[21] does not lead to any shift of T_c, which is clearly incorrect. The Green's-function treatment of Dalton and Wood,[7] which implies that $T_c(\Delta)\propto(\ln 1/\Delta)^{-1}$, cannot be ruled out, however.

In order to check the consistency of our data with the high-temperature series[7] more directly, we plot our susceptibility data vs $1 - T_c^{SK}/T$ in Fig. 16 where T_c^{SK} was taken from the analysis of Ritchie and Fisher;[7] accepting that their values $k_B T_c^{SK}/J = 0.588$ and[7] $\gamma_H = 3$ would lead to a critical amplitude of about $C_H \approx 0.52$ for the susceptibility. It is seen that the data points fit quite closely to the resulting straight line for temperatures in the range from $0.6 > 1 - T_c^{SK}/T > 0.2$, where χ itself changes by $1\frac{1}{2}$ decades, without adjustable parameters being available. Adjusting the critical amplitude to $C_H \approx 0.6$ would produce an even better fit. Close to T_c^{SK} deviations occur; the departure from the asymptotic curve sets in earliest (i.e., for largest ϵ) for the largest Δ values. The deviations are expected, of course, since owing to the shift of T_c, χ diverges at a higher temperature than T_c^{SK} for $\Delta\neq 0$. Thus our data are consistent both with the series expansions[6,7] and with a power-law singularity. Thus accepting Eqs. (22), (25), (28), and (34), we obtain $\gamma_H/\phi = 0.65$, $(\beta_H - \beta)/\phi = 0.125$, $1/\phi = 0.25$, and thus $\gamma_H \approx 2.6$, $\beta_H \approx 0.62$, $\alpha_H \approx -1.85$, $\nu_H \approx 1.9$, $\delta_H \approx 5.2$, and $\eta_H \approx 0.65$, if scaling is invoked. Alternatively, if from the series[7] we use $\gamma_H \approx 3.0$ together with $\gamma_H/(\beta_H - \beta) = 5.2$, we obtain $\beta_H \approx 0.7$, $\alpha_H \approx -2.4$, $\nu_H \approx 2.2$,

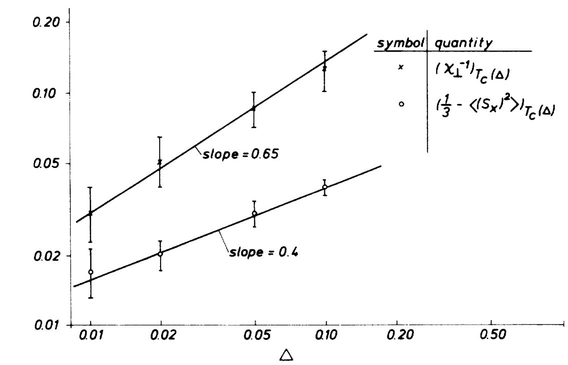

FIG. 15. Log-log plot of the inverse transverse susceptibility $\chi_\perp^{-1}$ and the reduced self-correlation $\frac{1}{3} - \langle (S_x)^2\rangle$, both taken at $T_c(\Delta)$.

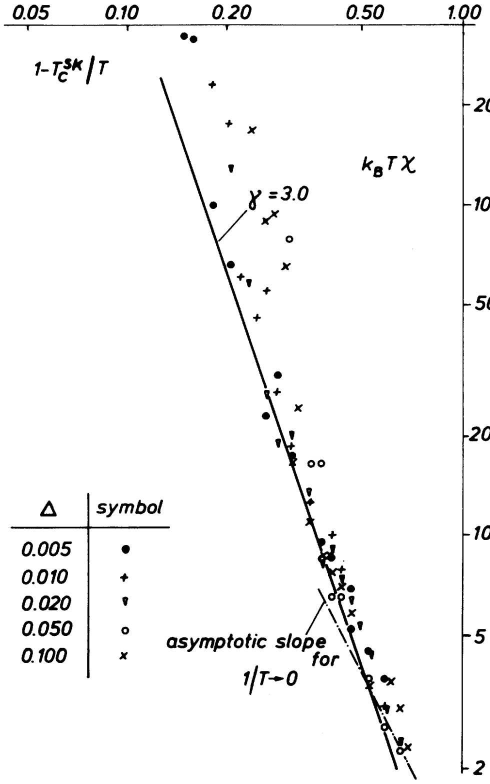

FIG. 16. Log-log plot of the susceptibility data for various Δ vs the distance from the Stanley-Kaplan transition temperature. The lines are obtained from the analysis of Ritchie and Fisher (Ref. 7).

$\delta_H\approx5.3$, and $\eta_H\approx0.64$. Choosing the slopes slightly differently we could obtain simple rational numbers for β_H, γ_H, and ϕ, and using scaling relations to determine the other exponents, we could have as well

$$\alpha_H=-2\pm0.4\,,\quad \beta_H=\tfrac12\pm0.2\,,\quad \gamma_H=3\pm0.5\,,\qquad(42)$$
$$\delta_H=7\pm2\,,\quad \eta_H=\tfrac12\pm0.2\,,\quad \nu_H=2\pm0.4\,,\quad \phi=4\pm0.6\,;$$

this is a tentative speculation, of course. We have not used the estimate for $\frac13-\langle(S_x)^2\rangle\sim\Delta^{0.4}$, since a competition between the two powers $\Delta^{(1-\alpha_H)/\phi}\approx\Delta^{0.75}$ and $\Delta^{1/\phi}\approx\Delta^{0.25}$ is to be expected [Eq. (34)].

We stress the fact, however, that divergencies which are stronger than power laws can by no means be excluded. This is seen in Fig. 17, where we replot the data of Fig. 16 such that Eq. (36) would yield a straight line. We use $\bar\nu=0.8$ following Camp and van Dyke,[8] but keep $k_BT_c/J=0.588$ since Ref. 8 refers to the triangular lattice. It is seen that this form fits the data equally well, and is in fact numerically not too different from a power law for a broad range of values of χ. Replotting $T_c(\Delta)-T_c^{SK}$ from Fig. 14 in the appropriate logarithmic form leads to a reasonable straight line as well. If we would accept Eq. (38), we would obtain $\tilde\gamma_H/\tilde\phi=0.65$, $\tilde\beta_H/\tilde\phi=0.125$, $-\alpha_H/\tilde\phi=0.4$, i.e., Eq. (42) would be replaced by

$$\delta_H=6.2\,,\quad \eta_H=0.55\,,\quad \gamma_H=\beta_H=\nu_H=-\alpha_H=\phi=+\infty\,.\qquad(43)$$

$\tilde\phi$, $\tilde\gamma_H$, $\tilde\beta_H$, and $\tilde\alpha_H$ cannot be determined independently. Since the above values for their ratios do not satisfy the relation $\tilde\gamma_H/\tilde\beta_H+2=\tilde\alpha_H/\tilde\beta_H$, it must be concluded that probably $\langle(S_x)^2\rangle-\frac13$ is again strongly affected by correction terms. Note, however, that Eq. (43) would disagree with recent renormalization group treatments.[42]

V. CONCLUSIONS

The main results of this investigation can be summarized as follows: (i) The Monte Carlo

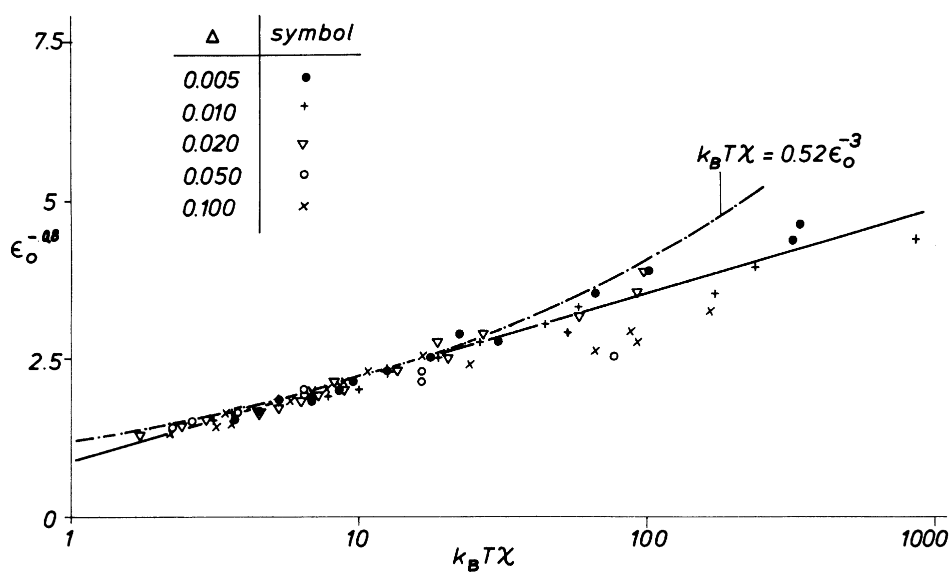

FIG. 17. Semilog plot of $\epsilon_0^{0.8}$ vs $k_BT\chi$, where $\epsilon_0=1-T_c^{SK}/T$ and data for various values for Δ are shown. The dash-dotted curve represents an ordinary power-law prediction as obtained from Ritchie and Fisher (Ref. 7).

method can be applied with moderate amount of computing time to the two-dimensional Heisenberg model even in the case of very weak anisotropy. This is in contrast to the fully isotropic case, in zero field, where the large relaxation times associated with the large susceptibility do not allow accurate studies[22,43] unfortunately [cf. Eq. (3)]. A significant improvement in the accuracy of our exponent estimates would require going to smaller Δ values and larger lattices and longer Markov chains. We estimate that substantial improvement would require at least 10^2 as much computing time as used here (which was equivalent to 35 h at an IBM 370/168 machine). (ii) Conventional spin-wave theory is valid only for $T/T_c(\Delta) \lesssim 0.15$ in the range of Δ values studied, in contrast to both theoretical predictions[18] $T/T_c(\Delta) \lesssim 0.50$ and experimental results on K_2NiF_4.[14]

Since $k_B T_c(\Delta)/J$ is quite small, this early breakdown of the spin-wave approximation is rather unexpected. (iii) For all values of Δ studied the order parameter is well described by an exponent $\beta \approx \frac{1}{8}$ for $T \lesssim T_c(\Delta)$, while above $T_c(\Delta)$ we find susceptibility exponents $\gamma \approx 1.75$ [or larger effective values farther away from $T_c(\Delta)$]. In no case do we obtain $\gamma \approx 0.8-1.0$ as in the K_2NiF_4 and K_2MnF_4 experiments.[16,13] While we present arguments that rounding phenomena may have been underestimated in this experiment (and in related other experiments, too), it seems less probable that these experimental results can entirely be attributed to these rounding effects. Thus the implication might be that the phase transition of K_2NiF_4 is seriously affected by terms not included in the simple Hamiltonian [Eq. (1)]. It is interesting to note that in our model the transverse susceptibility (Fig. 12) behaves qualitatively similar to the three-dimensional case. Since in the experiment[16] a considerable uncertainty concerning $\chi_\perp$ occurred, it is hoped that these results may be helpful in a reanalysis of the experimental data. (iv) The critical temperatures $T_c(\Delta)$ are shifted to lower values as Δ decreased. If $T_c(0)=0$, the shift is certainly not stronger than logarithmic while if one accepts the Stanley-Kaplan transition temperature $T_c(0) = T_c^{SK}$ one finds a variation $T_c(\Delta) - T_c(0) \propto \Delta^{1/\phi}$ with $\phi \approx 4$. In the latter case the singularities in the isotropic limit must be either power laws with rather large exponents ($\gamma_H \approx 3$; $\alpha_H \approx -2$), or even exponential singularities ($\gamma_H = -\alpha_H = \infty$). Our data are in both cases qualitatively consistent with crossover scaling theories.[17,44] For $T \gtrsim 1.2\, T_c^{SK}$ our susceptibility data are independent of Δ for small Δ and in good numerical agreement with the series expansions for $\Delta = 0$.[5,7] The quantitative difference between $\gamma_H \approx 3$ and ∞, however, is quite small in this regime (Fig. 17).

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Noted added in proof. The experimental aspects of the phase transition in K_2NiF_4 have been reanalyzed very recently (R. J. Birgeneau, private communications; J. Als-Nielsen, R. J. Birgeneau, H. J. Guppenheim and G. Shirane, unpublished); this reanalysis sheds new light on the question why in Ref. 16 exponents $\gamma \approx 1$, $\nu \approx 0.5$ were obtained. It turns out that the treatment of the transverse susceptibility in Ref. 16 was probably erroneous, and that this fact is the main reason for the discrepancies between theory and experiment, and not an inappropriate treatment of rounding phenomena. In fact, using $T_N = 97.22$ K and a Gaussian distribution of subsystem T_N, s with $\sigma = 0.08$ K, it was possible (R. J. Birgeneau, private communication) to obtain an internally consistent fit to both the order parameter and susceptibility data with Ising exponents $\beta = \frac{1}{8}$ and $\gamma = \frac{7}{4}$. This supports our conclusion that an ideal system would not appear to have the anomalous exponents reported in Ref. 16 over any range of temperature. Of course, it is clear that experimentally neither the precise extent nor precise nature of the rounding is known and it is well possible that the finite size rounding discussed earlier is as effective in "broadening" the transition as internal variations of crystal composition. Note also that recent renormalization group treatments (G. Grinstein and A. Luther, unpublished) indicate that randomly spaced impurities do *not* lead to any rounding of a second-order phase transition.

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[34]See Eq. (3) and subsequent discussion. In studies of the two-dimensional $S=\frac{1}{2}$ Ising model it turned out that $k_B T\chi$ and τ_e are comparable for $T > T_c$, apart from temperatures extremely close to T_c, while $\tau_e \gg k_B T\chi$ for $T < T_c$. See, for example, E. Stoll, K. Binder, and T. Schneider, Phys. Rev. B 8, 3266 (1973).

[35]Since N is finite,

$$\lim_{\tau\to\infty}[1/(\tau-\tau_0)]\int_{\tau_0}^{\tau} m_s(t)=0$$

in our simulation. Below $T_c(\Delta)$ τ is by far too large to observe this result in practice, if one starts the simulation with $m_s(0)=1$, however.

[36]This would be in contrast to the usual expectation that spin-wave theory works best in the classical case. While these deviations are surprising in view of Eq. (10), they are less surprising in view of the more cautious statement that the spin-wave approximation is valid for $T < 0.2\ T_c$ (see, e.g., P. W. Anderson, in *Solid State Physics*, edited by E. Seitz and D. Turnbull (Academic, New York, 1963), Vol. 14, p. 99 (1962). On the other hand it is conceivable that these deviations are a consequence of the finite size of our systems. This possibility seems less probable to us, however. We expect that the deviations become more drastic for $N\to\infty$ than seen in Fig. 4 (see Fig. 7 and subsequent discussion). It should also be noted that the "magnetization" calculated from spin-wave theory is $\langle m\rangle$, while the "magnetization" calculated from the computer experiment is $\langle m^2\rangle^{1/2}$. A possible difference between these two quantities can hardly account for the discrepancies, however, since $\langle m^2\rangle \geq \langle m\rangle^2$, while our results for the magnetization are significantly *smaller* than the spin-wave results. This problem clearly requires further study, notably since no such discrepancies have been detected in experiments (Ref. 14) so far.

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[43] In order to test the prediction $\langle m^2 \rangle \propto N^{-k_B T/\pi J}$ which follows from the work of Berezinskii (Ref. 10), we made some runs for $N = 25$ and 2500 Monte Carlo Steps per spin for $k_B T/J = 0.1$, 0.2, 0.3, and 0.4; while $\langle E \rangle$ was well behaved the results for $\langle m^2 \rangle$ gave an erratic nonmonotonic variation with temperature.

[44] Our crossover analysis assumes $\beta_H = 0$ and a vanishing magnetization amplitude for $\Delta = 0$. We think that this behavior is more plausible than the suggestion of Y. Imry, G. Deutscher, D. J. Borgman, and S. Alexander [Phys. Rev. A 7, 744 (1973)] that the nonexistence of spontaneous order is reflected in a zero or negative value for β_H. This suggestion is also less consistent with our data.