Critical properties of the spin-1 Heisenberg chain with uniaxial anisotropy

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We use finite-size scaling to determine the critical properties of spin-1 chains with uniaxial single-ion anisotropy D. A phase diagram is obtained in the (D,Δ) plane, where Δ is the strength of the interaction in the direction of the single-ion anisotropy. Critical exponents are estimated.

I. INTRODUCTION

One-dimensional quantum-spin systems have been studied widely in the past. These models were originally proposed with the hope of giving a better understanding of the magnetic properties of matter by restriction to one dimension, where theoretical efforts can often be taken to a high level of analysis, sometimes even yielding exact solutions which can then be used as test cases for approximate methods employed in the study of the more realistic three-dimensional case. However, because of the absence of long-range order[1] of one-dimensional systems with short-range interactions, except possibly at zero temperature, there are some fundamental differences between their two- and three-dimensional analogs. Today, many examples of (quasi-)one-dimensional quantum-spin systems are known,[2] some of which, relevant to this paper, will be mentioned below. Such compounds usually have a phase transition at very low temperatures, where higher-dimensional ordering sets in. Therefore, the investigation of such models is in no way a mere academic task.

In this paper, we present a finite-size-scaling study of the $T=0$ properties of the spin-1 nearest-neighbor Heisenberg model with uniaxial and single-ion anisotropy defined by the Hamiltonian

$$H=-J\sum_{l=1}^{N}(S_l^xS_{l+1}^x+S_l^yS_{l+1}^y+\Delta S_l^zS_{l+1}^z)+D\sum_{l=1}^{N}(S_l^z)^2 . \tag{1.1}$$

Either periodic boundary conditions (PBC's), or free-boundary conditions (FBC's) are imposed. In the former case, one sets $\vec{S}_{N+1}=\vec{S}_1$, while in the latter, one considers a system of $N+1$ particles.

For $S=\frac{1}{2}$, the last term in (1.1) reduces to a constant and H is exactly integrable.[3] The phase behavior with respect to varying the strength of the uniaxial anisotropy Δ is well understood in this case.[4] For $\Delta>1$, the ground state ψ_0 is ferromagnetic, i.e., $M=\pm\frac{1}{2}$, where

$$M=\left\langle\frac{1}{N}\sum_{l=1}^{N}S_l^z\right\rangle .$$

At $\Delta=1$, where ψ_0 is $(2N+1)$-fold degenerate, a first-order transition occurs to the planar phase with order parameter $M=0$ for $\Delta<1$. The ground state is nondegenerate for $-1<\Delta<1$, with a gapless excitation spectrum and algebraically decaying two-spin correlation functions. At $\Delta=-1$, a gap again opens up with an essential zero, leading to an exponential decay of the correlations. The ground state is now doubly degenerate and reduces to the Néel state for $\Delta\to-\infty$, the antiferromagnetic Ising model. The staggered magnetization,

$$M_S=\left\langle\frac{1}{N}\sum_{l=1}^{N}(-1)^lS_l^z\right\rangle ,$$

is nonzero for $\Delta<-1$ and can be interpreted as the order parameter of this "Néel phase," thus we have

$$\lim_{\Delta\to-1}M_S\sim\exp[-\pi^2/2\sqrt{(1+\Delta)}] , \tag{1.2}$$

and there is an infinite-order phase transition from the Néel to the planar phase at $\Delta=-1$.

However, for $S=1$, model (1.1) has so far received very little attention. This may be partly due to the fact that this model cannot be diagonalized with the methods developed in Refs. 5 and 6. However, since (1.1) with $S=1$ has been used to explain the properties of $CsNiCl_3$, $RbNiCl_3$, $RbFeCl_3$, and $CsNiF_3$,[7] there is a need to study this case from the experimental side as well. Since spin-wave theory has been used to determine the quantities relevant for the experiment,[8] an independent check of this approximation seems appropriate.

Luther and Scalapino[9] (LS) studied the case $\Delta=0$ as a particular representation of the two-dimensional (2D) planar model,[10] and concluded that it will undergo a phase transition driven by varying the strength of the single-ion anisotropy D, corresponding to the temperature of the 2D planar model. They find a critical strength $D_c>0$, below which the transverse susceptibility stays infinite with an exponent η decreasing with decreasing D and $\eta=1/\sqrt{8}$ at D_c. den Nijs[11] claims that a corrected version of the LS theory would produce the accepted value of $\eta=\frac{1}{4}$ (Ref. 10) at D_c. Jullien and Pfeuty[12] performed finite-cell calculations for $\Delta=0$, and found strong evidence for a transition at some finite D_c with a gap opening with an essential zero for $D>D_c$ and a gapless phase for $0\le D\le D_c$.

Recently, Botet and Jullien[13] have used finite-chain numerical calculations to determine the $T=0$ phases for antiferromagnetic ($\Delta<0$) exchange and $D=0$. They conjecture a drastically different behavior than for $S=\frac{1}{2}$ with a

new phase occurring between the gapless planar and the Néel regimes. The Heisenberg antiferromagnet ($\Delta=-1$) is in this new phase, which is characterized by a singlet ground state and a finite gap. The transition to the Néel phase is predicted to be continuous, and estimates of the critical exponents are given. These results are consistent with recent work by Haldane,[14] who contends, on the basis of a mapping of the one-dimensional Heisenberg antiferromagnet onto the nonlinear $O(3)$-σ model is the continuum limit, that the $T=0$ properties for even half-integer spins differ fundamentally from odd half-integer spins. Bonner and Müller,[15] however, performed a finite-chain analysis of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg Ising chain, which shows similar behavior to its spin-1 counterpart. They conclude that the behavior of the spin-1 Heisenberg antiferromagnetic remains questionable. Blöte[16] has studied the ground state of small antiferromagnetic Heisenberg chains for s between $\frac{1}{2}$ and 3 in order to extract the scaling behavior as a function of spin. The numerical predictions for the specific heat of (1.1) obtained via extrapolation of finite-system data by de Neef and de Jonge[17] and Blöte[18] have been compared to experiments on many occasions.[19]

While preparing this paper, we received a copy of what was then unpublished work from Botet *et al.*,[20] in which results on the ground-state properties of (1.1) as obtained by finite-size scaling are reported. Our conclusions about the different phases are basically the same as those of these authors, but we have carried out a more careful study in the ferromagnetic regime.

From this list of work, it seems evident that a major part of research on spin-1 chains has relied on numerical calculations. For completeness, some of the approximate analytical approaches to this problem should also be mentioned: Linear[21] and nonlinear[22] spin-wave theories have been used to calculate the spin-wave dispersion of (1.1) in the ferromagnetic phase, where long-range -order is present. Mead and Papanicolaou[23] calculated, among other things, the ground-state energy using a variational approximation. Recently, de Alcantra Bonfim and Schneider[24] used a path-integral approach to map (1.1) onto the isotropic two-dimensional classicaly XY model, allowing them to discuss the critical properties. It should also be mentioned that explicit examples of exactly integrable spin-1 chains have been constructed by taking extreme anisotropy limits of certain two-dimensional statistical models.[25] However, these examples always terminate with more complicated interactions than the Hamiltonian (1.1). It is an intriguing fact that, although (1.1) is exactly integrable for $S=\frac{1}{2}$, this Hamiltonian cannot be treated with the same methods for $S=1$.

The paper is organized as follows: Section II starts with a description of the computer used to diagonalize the Hamiltonian exactly by machine for a small number of particles. Some results on ground-state energies are then reported. In Sec. III we recall the hypothesis of finite-size scaling and phenomenological renormalization-group theory. These methods are then used in Sec. IV to locate the boundaries of the different ground-state phases of the Hamiltonian in the parameter plane (D,Δ). In Sec. V we present some results concerning the critical exponents.

II. NUMERICAL METHODS AND GROUND-STATE ENERGIES

A. Methods of diagonalization

For a finite system of N spins, the problem of calculating the energy levels of Hamiltonian (1.1) reduces to the diagonalization of a $(2s+1)^N\times(2s+1)^N$ matrix, where s is the magnitude of the spin. This was first done for $s=\frac{1}{2}$ by Bonner and Fisher,[26] who then estimated ground-state and thermodynamic properties for $|\Delta|>1$ by careful extrapolation to the infinite system. One can use direct products of single-spin states as basis states, which can take three values for $s=1$: $|+\rangle$, $|0\rangle$, and $|-\rangle$. The Ising and single-ion anisotropy parts of (1.1) are then diagonal in this basis. By classifying the states by the value of $S^z=\sum_{l=1}^{N}S_l^z$, the Hamiltonian splits up into $2N+1$ blocks of magnitude I_M, where M is the value of S^z of a given class of states

$$I_M=\sum_{k=0}^{\left[\frac{N-|M|+2}{2}\right]-1}\frac{N!}{k!(k+|M|)!(N-2k-|M|)!}\,, \tag{2.1}$$

$$\sum_{M=-N}^{N}I_M=3^N\,.$$

A further reduction in matrix size can be achieved if PBC's are imposed. By using translational invariance, each state is then also classified by a wave number $k=2\pi l/N$, $l=0,1,2,\ldots,N-1$. The diagonalization was then performed numerically within a given subspace (M,k). Our computer (IBM 3083) allowed us to take $N=10$ at the most.

If one wants to obtain information about larger systems, one has to use a different algorithm. For example, it is easy to show that, given any initial state $\psi_0^{(0)}$, the sequence

$$E_0^{(n+1)}=\frac{\langle\psi_0^{(n)}|H|\psi_0^{(n)}\rangle}{\langle\psi_0^{(n)}|\psi_0^{(n)}\rangle},\quad \psi_0^{(n)}=H\psi_0^{(n-1)} \tag{2.2}$$

in the limit $n\to\infty$ tends to the energy of H, which has the largest absolute value.

It is also evident that the off-diagonal matrix elements of H all have the same value, $-J$. By subtracting a positive constant c from the diagonal elements of H one can also force them to be negative. This then ensures that the eigenvector $|\psi_0\rangle$, obtained by iterating (2.2) infinitely many times, is the ground state. Writing

$$|\psi_0\rangle=\sum_{\mu}c_\mu|\psi_\mu\rangle\,, \tag{2.3}$$

where $\{|\psi_\mu\rangle\}$ is the basis introduced above, all c_μ must have the same sign as a consequence of the Perron-Frobenius theorem. Thus, by applying this algorithm to $\underline{H}-c\mathbb{1}$ in any subspace (M,k), one obtains the unique ground state $|\psi_0\rangle$ of (M,k) and the ground-state energy E_0 to arbitrary accuracy. The rate of convergence is determined by the next-largest eigenvalue. The advantage of this method is that one does not have to store the entire matrix $\underline{H}$, but only two vectors for the iteration, at the ex-

pense of not obtaining the entire spectrum of H.

For $k=0$ or π, we have also exploited the reflection symmetry of H. Each state is then characterized by an additional quantum number $u=\pm 1$, according to its behavior under reflection.

With this algorithm, we were able to calculate ground-state energies for $N=14$ within a reasonable amount of time. Also, it is not difficult to calculate correlation functions once the ground state is known to sufficient accuracy.

B. Ground-state energies

As a program check, we compared the finite N ground-state energies E_N for the Heisenberg antiferromagnet ($\Delta=-1$, $D=0$) to calculations published by Blöte[16] and found agreement to all digits quoted in his paper for $N\leq 10$. Blöte fits the data on finite systems to three parameters to obtain the ground-state energy $E_G(s)$ of the infinite system for spin values between $\frac{1}{2}$ and 3. One of the forms he uses is

$$\tilde{E}_N(s)=E_G(s)+\alpha/N^{\beta}\,, \tag{2.4}$$

where $\tilde{E}_N(s)$ denotes the ground-state energy per spin of the N-spin system of magnitude s, suitably normalized,

$$\tilde{E}_N(s)=E_N(s)/JNs^2\,. \tag{2.5}$$

In Table I we have listed $\tilde{E}_N(s)$ and $\beta(N)$, N even, for $s=\frac{1}{2}$ ($6\leq N\leq 18$) and $s=1$ ($2\leq N\leq 14$). The finite-size-scaling properties of these two cases appear to be strikingly different. For $s=\frac{1}{2}$, β is almost independent of N, and seems to converge to 2. In fact, $\beta=2$ has been used by Bonner and Fisher[26] to extrapolate their data to the thermodynamic limit. For $s=1$, however, β is strongly N dependent and, moreover, seems to diverge for $N\to\infty$. This suggests that exponential behavior is more appropriate for the finite-size corrections to E_G in the large-N limit. This is a first example of a sensitive spin dependence in the strong quantum limit of small spin values.

Next, we calculated the ground-state energies for the Heisenberg ferromagnet ($\Delta=1$) with varying single-ion anisotropy $D>0$. This is of interest both experimentally, because (1.1) was used for $(\Delta,D)=(1,0.38)$ to explain experiments on $CsNiF_3$,[7] and theoretically, since many approximate ground-state calculations have been performed for this range of parameter values. Figure 1 shows a comparison of our extrapolated ground-state energies with the results obtained by (i) semiclassical calculation,[27] (ii) three-term $1/s$ expansion,[28] and (iii) variational bound calculations.[23] We expect the estimates from the finite-size data to be accurate to 1% for all D values. Something very interesting is revealed by Fig. 1: Calculations (i)—(iii) are essentially based on a rather sophisticated spin-wave approximation. We see that they yield more or less reasonable results for small D, where spin-wave theory is expected to be a good approximation. It is even striking that the ground-state energy calculated from the three-term $1/s$ expansion agrees to within 1% with our extrapolated values up to $D=1$. For larger D, all theories overestimate the true ground-state energy E_0 since it can easily be shown that E_0 must be a monotonically increasing function of D, which approaches 0 as D goes to infinity. Why then does spin-wave theory break down for larger D? We propose that there are other excitations besides the spin waves, which become more and more important as D is increased, and eventually determine the structure of the ground state. However, since we are studying a quantum system with a nontrivial ground state, it is not easy to identify the nature of these excitations.

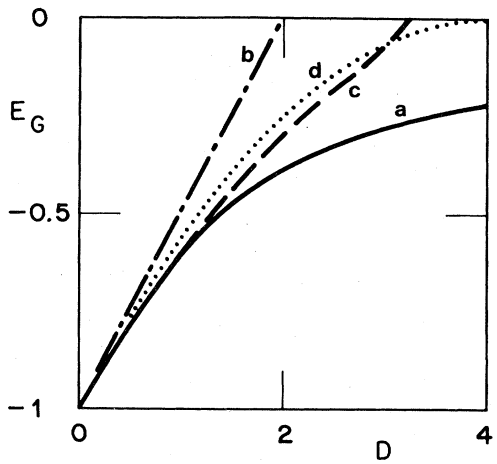

FIG. 1. Ground-state energy for Hamiltonian (1.1) with $\Delta=1$: (a) extrapolated finite-chain result; (b) semiclassical bound; (c) three-term $1/s$ expansion; (d) variational bound.

III. FINITE-SIZE SCALING AND PHENOMENOLOGICAL RENORMALIZATION

Finite-size scaling (FSS), formulated several years ago by Fisher,[29] has been used increasingly in many ways to

TABLE I. Ground-state energies and exponent β (see text) of the Heisenberg antiferromagnetic chain $(\Delta,D)=(-1,0)$ for $s=\frac{1}{2}$ (left three columns) and $s=1$ (right three columns).

	$s=\frac{1}{2}$			$s=1$	
N	$\tilde{E}_N(s)$	$\beta(N)$	N	$\tilde{E}_N(s)$	$\beta(N)$
6	3.737 034		2	4.0	
8	3.651 093	2.102	4	3.0	2.615
10	3.612 357	2.065	6	2.872 474	2.428
12	3.591 594	2.046	8	2.834 239	2.528
14	3.579 171	2.034	10	2.818 826	2.710
16	3.571 148	2.027	12	2.811 593	2.940
18	3.565 666		14	2.807 876	

extrapolate the information available from a finite, or partially infinite, system to the thermodynamic limit. The phenomenological renormalization (PR), introduced by Nightingale,[30] is a consequence of the finite-size-scaling idea. It has yielded remarkable results for the critical behavior of various models.[31] It has also been applied to quantum-spin systems,[32] where, in analogy to the transfer-matrix formalism, one considers strips of finite width with one infinite dimension. We shall first describe the concepts of FSS and PR, and then explain how we apply these methods to our quantum system.

In order to be definite, we consider "two-dimensional" systems consisting of infinite strips of finite width N. We let one parameter, T (the temperature), be varied, and assume that in the thermodynamic limit $N\to\infty$, the system has a continuous phase transition at a critical temperature T_c. For a physical quantity Q, this implies typically that in the infinite system

$$Q_\infty(T)\sim |T-T_c|^{-\omega}, \tag{3.1}$$

while $Q_N(T)$ cannot have any singularity for any finite N. But with increasing N, the singularity of Q starts to develop. The basic FSS hypothesis is that a scaling function F_Q exists such that

$$Q_N(T)\sim Q_\infty(T)F_Q(N/\xi_\infty(T)), \tag{3.2}$$

where $\xi_\infty(T)$ is the correlation length in the infinite system. Since $Q_N(T)$ is an analytic function even at T_c, F_Q has to compensate the singularities of Q_∞ and ξ_∞ at T_c. If

$$\xi_\infty(T)\sim |T-T_c|^{-\nu}, \tag{3.3}$$

then F_Q must behave like

$$F_Q(z)\sim z^{\omega/\nu} \text{ for } z\to 0. \tag{3.4}$$

It follows that at T_c, $Q_N(T)$ depends on N as a power law,

$$Q_N(T_c)\sim N^{\omega/\nu}. \tag{3.5}$$

In fact, any derivative of Q_N with respect to T must be regular at T_c, which can be expressed by stating that

$$Q_N(T)\sim N^{\omega/\nu}G_Q(N^{1/\nu}(T-T_c)), \tag{3.6}$$

where G_Q is a scaling function which is regular at T_c. When one considers a phase transition of infinite order, i.e., let $\nu\to\infty$ in (3.3), one usually expresses critical exponents in terms of the correlation length,

$$Q_\infty(T)\sim[\xi_\infty(T)]^\omega \text{ at } T_c. \tag{3.7}$$

It then follows from (3.2) that

$$Q_N(T_c)\sim N^\omega. \tag{3.8}$$

It is evident that the FSS hypothesis allows the calculation of critical properties of a given model to be carried out in many different ways, for instance, by examining the scaling properties of various physical quantities. Phenomenological renormalization[30] is one such way, and it has been shown[31] to be most successful for systems with a continuous phase transition. One starts by calculating the correlation length $\xi_N(T)$ for a strip of width N. Scaling this system by a factor of L implies a scaling transformation for the correlation length

$$\xi_N(T)=L\xi_{N/L}(T_{L,N}). \tag{3.9}$$

The equation

$$T_{L,N}=T_{L,N}(T) \tag{3.10}$$

can be interpreted as a renormalization transformation. Note that a fixed point of (3.10) does not imply singular behavior of the correlation length, since two different functions appear in (3.9). However, the N dependence in Eq. (3.10) is expected to be weak. This expectation is justified in view of the FSS hypothesis.[33] These considerations suggest the following procedure to calculate the critical temperature T_c. Define $T_c(N,M)$ by

$$\xi_N(T_c)/N=\xi_M(T_c)/M \tag{3.11}$$

and extrapolate the results to the thermodynamic limit. Another way to calculate T_c is to search for power-law behavior in N; see (3.5). One considers three scripts of width N, M, and P, and obtains $T_c(N,M,P)$ as the solution of

$$\frac{\ln[Q_M(T_c)/Q_N(T_c)]}{\ln[Q_p(T_c)/Q_M(T_c)]}=\frac{\ln(M/N)}{\ln(P/M)}. \tag{3.12}$$

The advantage of this method is that one can obtain T_c^0 by examining several different physical quantities Q, and has, therefore, an internal consistency check. The critical exponents can then be obtained by using (3.5) or (3.8) and

$$\frac{\omega}{\nu}=\frac{\ln[Q_N(T_c)/Q_M(T_c)]}{\ln(N/M)}. \tag{3.13}$$

For an algebraic phase transition, ν can be determined from

$$1+\frac{1}{\nu}=\ln\left[\frac{d\xi_N}{dT}(T_c)\Big/\frac{d\xi_M}{dT}(T_c)\right]\Big/\ln(N/M), \tag{3.14}$$

which follows from (3.2) with $Q=d\xi/dT$.

For more general cases (transition of infinite order), Roomany and Wyld[34] have given a direct way to determine the Callen-Symanzik β function from finite-size data. The functional form of the β function then determines the critical behavior of ξ at T_c. The Roomany-Wyld approximants to the β function in our notation are given by

$$\frac{\beta_{N,M}(T)}{T}=\frac{\ln[M\xi_M(T)/N\xi_N(T)]}{\ln(N/M)[1+(1/2T)d/dT]\ln[N\xi_N(T)M\xi_M(T)]}. \tag{3.15}$$

Our notation has so far been based on the cases most often treated in the literature, namely, the application of FSS and PR to the transfer matrix of two-dimensional classical problems. How can one now apply these concepts to a one-dimensional quantum Hamiltonian?

For a classical model, the correlation length ξ can be

calculated from the two largest eigenvalues, λ_0 and λ_1, of the transfer matrix by[35]

$$\xi = 1/\ln(\lambda_1/\lambda_0) . \tag{3.16}$$

The FSS hypothesis then states that, if ξ_N denotes the correlation length of a finite system of size N, then, at criticality, ξ_N must scale with system size as

$$\xi_N \sim N . \tag{3.17}$$

If a quantum Hamiltonian H is obtained from the τ-continuum limit[36] of the transfer matrix $\underline{T}$ of a classical system, i.e., if formally

$$\underline{T} = e^{\tau H} , \tag{3.18}$$

then, we infer from (3.16) and (3.17) that the gap N between the ground and first excited states of H of a finite system must scale as

$$\omega_N \sim 1/N \tag{3.19}$$

when the corresponding classical system is at its critical temperature. This means physically that time scales in the same way as space. The temperature in the classical model usually enters in the parameters of the quantum Hamiltonian.

Generally, in a quantum system, the zero-temperature critical behavior is determined by the absence of an energy gap between the ground and first excited states.

Assuming translational invariance, one can express the relation between the vanishing of the gap ω and wave number q by

$$\omega \sim q^z \text{ as } q \to 0 , \tag{3.20}$$

and z is called the dynamical critical exponent.[37] For a finite system of size N, the smallest nonzero q is equal to $2\pi/N$. It is therefore reasonable to expect the gap ω_N to behave like

$$\omega_N \sim 1/N^z . \tag{3.21}$$

Since the Hamiltonian (1.1) has not been shown to be related to a classical model in the above-mentioned sense, we must check that $z=1$ whenever the gap exhibits power-law behavior in N in order to have justification for using FSS and PR for an estimate of critical exponents.

IV. PHASE BOUNDARIES

A. Symmetries of the ground and first excited states

For all N investigated, the ground state is either a singlet with $S^z=0$ or the ferromagnetic doublet with $S^z=\pm N$. There is a line in the (D,Δ) plane, where a discontinuous jump occurs between these two ground-state symmetries. Since M is the order parameter of our system, this jump is a first-order phase transition from the ferromagnetic to the planar phases. We have determined numerically the line of this transition by implicitly solving the equation

$$E^N_{0,\,M=0}(D,\Delta) = E^N_{0,\,M=N}(D,\Delta) . \tag{4.1}$$

Here, $E^N_{0,M}$ denotes the ground state of an N-spin system with magnetization M. There is very little N dependence along the entire line. The extrapolation to the thermodynamic limit is shown in Fig. 2. Of course, the curve must go through the isotropic Heisenberg ferromagnetic, $(D,\Delta)=(0,1)$, where one has a $(2N+1)$-fold degenerate ground state, $E^N_{0,M}$, which is the same for all allowed values of M. For large D, the curve approaches asymptotically the straight line $\Delta=D$, which is the transition point in the absence of the x and y components of the interaction. Second-order perturbation theory in this strong-coupling regime yields an approximate solution of (4.1),

$$D = \tfrac{1}{4}[\Delta + (9\Delta^2 - 16)^{1/2}] . \tag{4.2}$$

In the limit $D \to -\infty$, the line $\Delta=0$ is the asymptote. We find numerically that

$$D \approx -1/2\Delta \text{ as } D \to -\infty . \tag{4.3}$$

We define the planar regime by that part of the (D,Δ) plane for which the order parameter M of the ground state is equal to zero. In this case, it is of interest to determine to which subspace (M,k,u) the first-excited state ψ_1 belongs. We find three possibilities:

$$\begin{aligned} &\text{(i)} \quad \psi_1 \in (\pm 1, 0, +1) \text{ doublet} , \\ &\text{(ii)} \quad \psi_1 \in (0, \pi, -1) \text{ singlet} , \\ &\text{(iii)} \quad \psi_1 \in (\pm 2, 0, +1) \text{ doublet} . \end{aligned} \tag{4.4}$$

The planar regime is thus divided into three parts, (i)–(iii), whose extrapolated boundaries have also been drawn in Fig. 2. The isotropic Heisenberg antiferromagnetic $(D,\Delta)=(0,-1)$ lies on the boundary line between (i) and (ii), since the doublet of (i) becomes degenerate with the singlet of (ii) to build a triplet excitation with lowest energy above the ground state for all values of N. The straight line $D=-\Delta$ is the asymptote for this boundary in the limit $D \to +\infty$, which can easily be seen by comparing the energy of the Néel state $E_N = -N(D-\Delta)$ to the state ψ_0, which is characterized by $S^z_l \mid \psi_0\rangle = 0$ for all

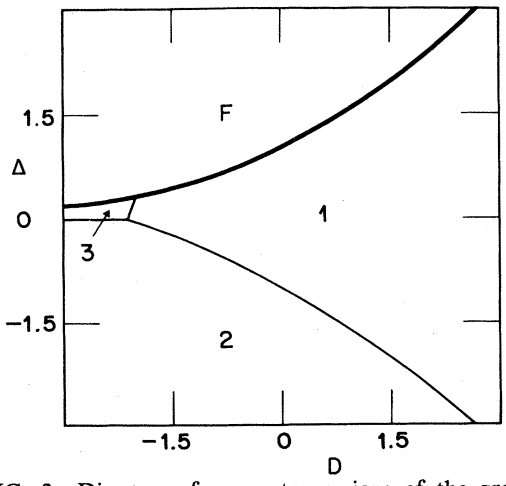

FIG. 2. Diagram of symmetry regions of the ground and first excited states. The thick solid line separates the region of the ferromagnetic ground state F from the region of the planar ground state with $M=0$, where 1, 2, and 3 denote the different symmetries of the first excited state; see (4.4).

l, and has energy 0. The boundary between (i) and (iii) is of less interest and has only been included for completeness.

B. Phase boundaries for $\Delta > 0$

Knowing to which symmetries the ground and first excited states belong, we can now use the finite-size-scaling methods to determine the behavior of the energy gap as a function of the size N and the Hamiltonian parameters D and Δ. In Fig. 3 we have plotted the function

$$R_N(\Delta,D)=\frac{(N+1)\omega_{N+1}(D,\Delta)}{N\omega_N(D,\Delta)} \tag{4.5}$$

for $N=9$ in the planar regime and for $\Delta \geq 0$. The gap $\omega_N(D,\Delta)$ is defined by

$$\omega_N(D,\Delta)=E_1^N(\Delta,D)-E_0^N(\Delta,D)\ , \tag{4.6}$$

where E_1^N and E_0^N are the first excited and the ground-state energies, respectively. A remarkable behavior can be seen from Fig. 3; there is a region in the (D,Δ) plane where R_N is almost constant and equal to 1. This feature becomes even more pronounced when N is increased to larger values. Therefore, the points in this region are fixed points in the sense of (3.13), where we have already identified ω with ξ^{-1}, which is reasonable since $R_N=1$ implies that $z=1$ [see (3.2)]. This figure then gives clear evidence of the existence of a gapless phase with $z=1$. It can also be seen that R_N starts to increase with D for sufficiently large D. In the limit $D\to\infty$, we have

$$R_N(\Delta,D)\to(N+1)/N \quad \text{as } D\to\infty\ , \tag{4.7}$$

because in the absence of interaction, the gap $\omega_N=1$ for all N. Fixing the exchange energy $J\Delta$ in the z direction, one therefore expects a transition to take place at some finite $D_c(\Delta)$, separating the small-D gapless phase from the large-D finite-gap phase.

For the calculation of the critical exponents, it is of great importance to determine $D_c(\Delta)$ as accurately as possible from the finite-chain data available. This task turned out to be very difficult, because, for fixed Δ, there is an entire line of fixed points; the exponent z varies only slightly around 1, and the end point of this line is not easily obtained in the thermodynamic limit. Guided by the experience gained from the study of the spin-$\frac{1}{2}$ XXZ model, which is exactly soluble and shows features similar to our Hamiltonian, we finally settled for a method shortly to be described.

As mentioned in Sec. III, one can determine D_c by extrapolating the approximate critical D values $D_c(N,M,P)$ obtained by solving (3.14) for a physical quantity Q, which is singular at D_c. Since the gap ω is such a quantity, we can define

$$S_{N,M,P}(\Delta,D)\equiv\frac{\ln[\omega_N(\Delta,D)/\omega_M(\Delta,D)]\ln(M/P)}{\ln[\omega_M(\Delta,D)/\omega_P(\Delta,D)]\ln(N/M)}$$
$$=\frac{z(\Delta,D,N,M)}{z(\Delta,D,M,P)}\ , \tag{4.8}$$

and look for solutions $D_c(\Delta)$, for which $S_{N,M,P}(\Delta,D_c(\Delta))=1$. Figure 4 is a plot of $S_{N,N-1,N-2}(\Delta,D)$ for $N=10$, $\Delta=0.6$, and $0\leq D\leq 2$. This function is always less than 1 and there is no solution to the above equation. The same holds true if one chooses other values for N,M,P. But there is a maximum $D_{\max}$ close to $D=0.8$, for which $S\approx 0.9985$. This maximum indicates that one obtains the best power-law approximation,

$$\omega_N=A/N^z\ , \tag{4.9}$$

for the three N values considered. The fact that $S<1$ means that $z(N)$ is always a decreasing function of N for the sizes considered,

$$z(M)<z(N) \quad \text{for } M>N\ . \tag{4.10}$$

One also sees from Fig. 4 that for $D>D_{\max}$, S starts to decrease dramatically, indicating a different scaling behavior in this range. We have determined $D_c(\Delta)$ by extrapolating $D_c(N,\Delta)$ obtained as the solution of

$$\frac{\partial S_{N,N-1,N-2}(\Delta,D)}{\partial D}=0\ , \tag{4.11}$$

for N between 7 and 14. In the Appendix we describe several methods for extrapolating finite-N data to the thermodynamic limit $N\to\infty$.

Because of the very irregular N dependence of $D_{\max}$ for

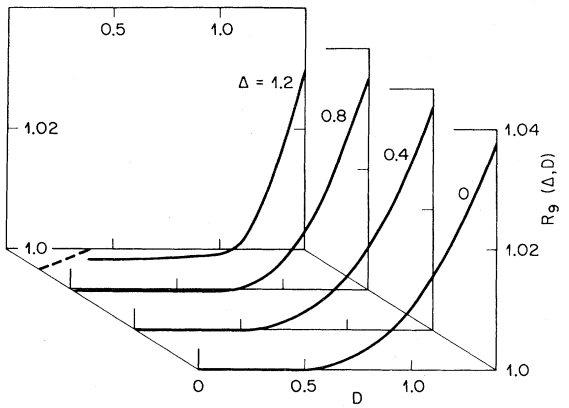

FIG. 3. Function $R_N(\Delta,D)$ [Eq. (4.5)] for $N=9$. The dashed line denotes the transition to the ferromagnetic ground state.

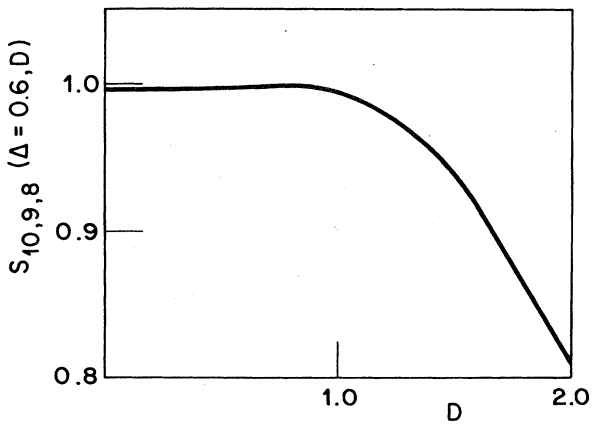

FIG. 4. The function $S_{N,M,P}(\Delta,D)$ [Eq. (4.8)] for $\Delta=0.6$ and $N,M,P=10,9,8$.

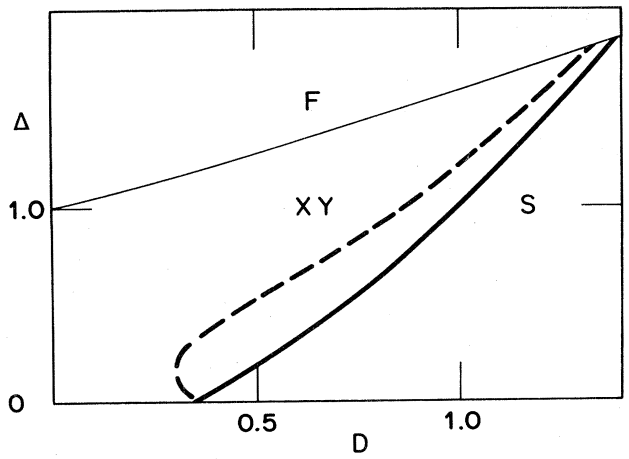

FIG. 5. Lines of the transition from the gapless phase XY to the singlet ground-state phase with gap S for $\Delta \geq 0$ as predicted by (4.11) (thick solid line) and the phenomenological renormalization (3.13) (dashed line). Upper thin solid line denotes transition to the ferromagnetic ground-state region F.

small sizes and Δ close to 0, it turned out to be useful to have data available for N up to 14. The extrapolated curve $D_c(\Delta)$ is shown in Fig. 5 together with the line of the first-order transition to the ferromagnetic phase.

We believe that by using this method to determine $D_c(\Delta)$, we have eliminated the leading corrections to finite-size scaling for our system. This claim can be substantiated by looking at the critical couplings $D_c^2(\Delta)$ that would be obtained by a naive application of the basic equation (3.13) following from PR. We believe this curve to be wrong for the following reasons:

(i) The phenomenological renormalization applied to the antiferromagnetic transition of the spin-$\frac{1}{2}$ XXZ model, which is known to be exactly at $\Delta_c = -1$, would yield an estimate $\Delta_c \approx -0.4$. As in our case, this is well within the region of Δ, where the XXZ model is known to be gapless. The use of (4.11) yields estimates $\Delta_c(N)$ which can easily be extrapolated to $\Delta_c = -1$.

(ii) Careful extrapolation of $z(D,\Delta,N)$ as a function of N shows that z can have a minimum in N and increase again for larger sizes. This is never the case for $N \leq 14$, but results obtained for the spin-$\frac{1}{2}$ XXZ model indicate that this really can happen. This point is crucial in our case, since at $D_c(N,\Delta)$, we always have $z < 1$.

(iii) Later, we shall report the results for the critical exponent γ of the transverse susceptibility χ_{xx}. We now want to mention that by solving (4.11) using χ_{xx} instead of the gap, we obtain a critical line which almost superimposes $D_c(\Delta)$. Within the errors emanating from extrapolation to the thermodynamic limit, one can state that the two lines are identical.

C. Phase diagram for $\Delta < 0$

There are two reasons why we have chosen to present the results for antiferromagnetic exchange $\Delta < 0$ in a separate subsection. First, the behavior of the gap seems to be very different from the ferromagnetic case. Second, the size-scaling behavior of all physical quantities is such that, in this case, one cannot go beyond a qualitative characterization of the phase properties. Nevertheless, it seems that this part of the parameter plane exhibits some very interesting features. This can be seen from Fig. 6, where we plotted the curves obtained by solving the equations

$$z(\Delta,D,N,N+2)=1 \tag{4.12}$$

for $N=4,6,8$ in Fig. 6(a). Similar curves actually have already been published by Botet *et al.*,[20] but we obtained them independently. In Fig. 6(b) we plotted the curves obtained by solving

$$\frac{\partial S_{N+2,N,N-2}}{\partial \Delta}=0 \quad \text{and} \quad \frac{\partial^2 S_{N+2,N,N-2}}{\partial \Delta^2}<0\,, \tag{4.13}$$

where $S_{N+2,N,N-2}(D,\Delta)$ is defined by (4.8) and was used to obtain the phase boundary in the ferromagnetic region. Sizes N of Fig. 6(b) are $N=8,10,12$. For $D \geq 0.4$, there are actually additional maxima for $N=10,12$ and for $\Delta > 0$; these almost coincide with the line of maxima for $N=8$ drawn in Fig. 6(b).

There is a fingerlike shape to the curve in Fig. 6(a) for positive D values. Moreover, the behavior with increasing N suggests that these "fingers" might actually collapse into a single line in the thermodynamic limit. However, we can only obtain weak support of this conjecture from extrapolating the finite-chain data, because the size dependence is very irregular even when one considers only even N. Figure 6(b) also reveals the existence of a line which is in good agreement with the fingerlike curves of Fig. 6(a). This agreement is very different from the ferromagnetic region, where we found a considerable difference between estimates derived from (4.12) and from derivatives of S with respect to D.

It is clear from the data that the gapless phase extends into the antiferromagnetic part of the (D,Δ) plane only in a very small region indicated by the fingerlike curves of Fig. 6(a) and, most probably, there is only a single line with vanishing energy gap. Where then does the gapless phase terminate as one approaches the antiferromagnetic region? One can again obtain a partial answer to this question by comparing the behavior of the curves of Figs.

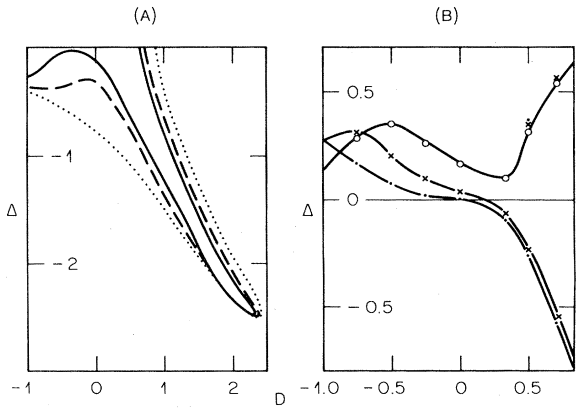

FIG. 6. (a) Curves obtained by solving (4.12) for $\Delta \leq 0$ with $N=4$ ($\cdots$), 6 ($- - -$), and 10 (——). (b) Curves obtained by solving (4.13) with $N=8$ (○), 10 (×), and 12 (●).

6(a) and 6(b). From Fig. 6(a), one can see that for $-1.0 \leq D \leq 0.4$, the transition must be very close to $\Delta=0$ in Fig. 6(b). For sufficiently large D values ($D \geq 0.4$) and for sufficiently N ($N \geq 10$), one obtains two maxima of $S_{N+2,N,N-2}(D,\Delta)$; one for $\Delta>0$ and one for $\Delta<0$. For $D \leq 0.35$, only one maximum remains. This will agree well with Fig. 6(a), if one associates the lines of maxima for $\Delta<0$ and $D>0.4$ with the "fingers" of Fig. 6(a). The other lines of maxima for $\Delta>0$ and $D>0.4$ should then converge to the boundary between the gapless and large-D phase already determined in Sec. IV B (see Fig. 5). However, we have used the derivative of $S_{N+2,N,N-2}(D,\Delta)$ with respect to D and not Δ. This is nicely satisfied for $D \geq 0.6$, where one obtains good agreement of the extrapolated values with the results of Sec. IV B. For $0.35 < D < 0.6$, the size dependence of the curves in Fig. 6(b) is rather erratic and no extrapolations are possible.

For $D \leq 0.35$, where only one maximum for each N considered is present, one can again reasonably extrapolate the data and find that the true transition line must be close to the D axis. The curves of Figs. 6(a) and 6(b) are actually complementary for $-1.0 < D < 0.35$, because in Fig. 6(a) the D axis is approached from negative values of Δ, while in Fig. 6(b) it is approached from positive ones.

In summary, we find that for almost the entire antiferromagnetic region $\Delta<0$, the ground state is separated by a gap from the first excited states. Although it is impossible to exactly locate the phase boundaries, it seems that the boundary to the gapless phase is very close to the D axis. Both Figs. 6(a) and 6(b) support this view.

These results finally lead us to propose the phase diagram depicted in Fig. 7. We have a gapless phase for low-valued D and $\Delta>0$ which terminates along the line a,

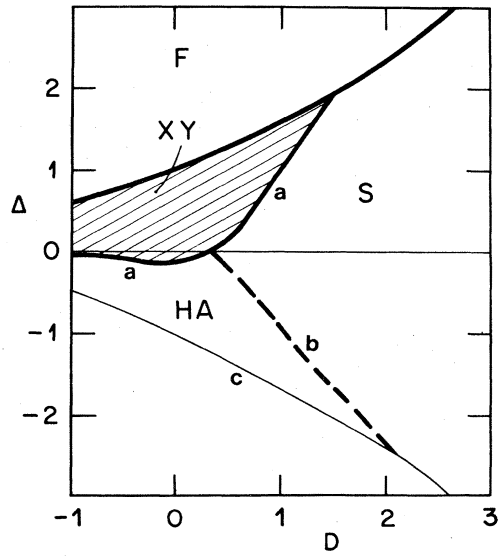

FIG. 7. Phase diagram of Hamiltonian (1.1). Lower thin solid line c denotes change of symmetry of the first-excited state. Hatched area denotes gapless phase XY. Line a denotes boundary of the gapless phase in the planar region. The dashed line b, along which (1.1) is also gapless, separates the region above c into two phases S and HA, where HA contains the Heisenberg antiferromagnet $(\Delta,D)=(-1,0)$. F denotes the region of the ferromagnetic ground state.

where the lower part of this line is somewhat uncertain, but surely close to the D axis. At $(D,\Delta)\approx(0.35,0)$, a line b emerges in the antiferromagnetic region, along which the Hamiltonian is also gapless. We have not examined the gap beyond the lower thin line c in Fig. 7, which indicates the change of symmetry of the first-excited state. For this part of the (D,Δ) plane we refer to the very recent work of Botet *et al.*,[20] who carefully investigated the transition to the Néel phase occurring in this region.

The fingerlike shapes of Fig. 6(a) are not in contradiction to the single line proposed in Fig. 7, because, for any finite N, the function $z(D,\Delta,N,N+2)$ has to be analytic in D and Δ. Therefore, the curve $z(D,\Delta,N,N+2)=1$ can never separate into two curves at a point in the (D,Δ) plane, and the only possibility they have is to follow as closely as possible the line of Fig. 7, turning around it and following it again on the other side, which is exactly what happens.

V. CRITICAL EXPONENTS

Having determined the phase boundaries, we can now calculate the critical exponents ν and γ, where ν refers to the power of the divergence of the correlation length, and γ to the transverse susceptibility χ_{xx}, defined by

$$\chi_{xx}=\frac{2}{N}\sum_{\lambda}\left|\left\langle\lambda\left|\sum_{l}S_l^x\right|0\right\rangle\right|^2\Big/(\omega_\lambda-\omega_0)\ . \tag{5.1}$$

$\langle\lambda|$ denotes the eigenvectors of Hamiltonian (1.1) with energy ω_λ, and $|0\rangle$ is the ground state. In most cases, for λ we have taken only the lowest excited state which yields a very small difference from the true value of χ_{xx}. The critical exponents were then calculated with the methods described in Sec. III.

A. Ferromagnetic region

Using (3.16) we calculated ν_{NM} along the transition line $D_c(\Delta)$ (Fig. 5) for $M=N-1$ and derivatives taken with respect to D. In Table II the values for $\nu_{N,N-1}$ are listed for N between 4 and 12 and $\Delta=0.6$. The trend is the same along the entire line $D_c(\Delta)$. One can see that ν does not converge to a finite value. Therefore, we conclude that the correlation length ξ diverges faster than any power in $D-D_c(\Delta)$. To obtain a more precise idea about the divergence of ξ, we used the β-function approximants (3.17) for $M=N-1$, and fitted them to the following form for $\xi \sim 1/\omega$:

$$\omega \sim \exp[-A(D-D_c)^{-\sigma}]\ . \tag{5.2}$$

Values for $\sigma_{N,N-1}$ are also listed in Table II for $\Delta=0.6$. One can see that when the form (5.2) is correct, one clearly gets a nonzero value for σ. But it is impossible to determine σ precisely because it strongly depends on the width of the interval of D values chosen to carry out a least-squares fit of the β function. A, D_c, and σ in (5.2) have been fitted.

Assuming ν to be infinite, we evaluated γ by using (3.8) and also listed it in Table II for $\Delta=0.6$. The convergence seems to be very good in this case and one can give a precise estimate of $\gamma=1.7495\pm0.001$. These good conver-

TABLE II. Critical exponents ν, σ, and γ as a function of N for $\Delta=0.6$.

N	$\nu_{N-1,N}$	$\sigma_{N-1,N}$	$\gamma_{N-1,N}$
4	6.58	0.03	1.7741
5	6.49	0.06	1.7629
6	6.54	0.12	1.7576
7	6.63	0.17	1.7548
8	6.73	0.21	1.7531
9	6.83	0.23	1.7520
10	6.93	0.28	1.7513
11	7.03	0.35	1.7508
12	7.14	0.41	1.7505

gence properties hold for all Δ and one always obtains $\gamma=1.75$ to very good precision. In fact, extrapolating the lines $\gamma(D,\Delta,N,N+1)=1.75$ leads to a curve $D_c(\Delta)$ which almost superimposes the curve previously found in Sec. IV B.

We have so far determined the exponent ν to be infinite and σ in (5.2) to be nonzero. Furthermore, γ has been found to be equal to 1.75 with very good precision along the entire line $D_c(\Delta)$. These findings suggest that the transition taking place along $D_c(\Delta)$ for $\Delta>0$ belongs to the universality class of the two-dimensional classical XY model studied by Kosterlitz and Thouless.[10] These authors predict $\sigma=\frac{1}{2}$, which is not excluded by our results. For $\Delta=0$, evidence for the above conjecture has already been presented by Luther and Scalapino,[9] den Nijs,[11] and by Jullien and Pfeuty.[12] The Hamiltonian (1.1) for $\Delta=0$ is only a truncated version of the $O(2)$ model, which has been shown by Hamer and Barber[38] and Roomany and Wyld[34] to belong to the same universality class as the 2D XY model. Recently, de Alcantra Bonfim and Schneider[24] mapped the spin-1 chain (1.1) onto the 2D isotropic XY model in the critical region, and therefore anticipated our results.

In the region where the gap vanishes, the spin-spin correlation function is expected to fall as a power of the distance between the spins,

$$\langle S_0^x S_l^x \rangle \sim |l|^{-\eta(D,\Delta)} . \tag{5.3}$$

From the scaling law[10]

$$\gamma=2-\eta , \tag{5.4}$$

we infer that $\eta=0.25$ along $D_c(\Delta)$ independent of Δ. In the gapless region, η usually decreases when D is decreased and tends to zero when one approaches the line of the first-order transition to the ferromagnetic ground state. But when Δ approaches zero, it appears that η varies very slightly with D and is always close to 0.25. At the point $(D,\Delta)=(0.38,1)$, expected to describe $CsNiF_3$, we obtain $\eta=0.11$.

B. Antiferromagnetic region

In the antiferromagnetic region we have to investigate the single transition line b in the $D>0$ and $\Delta<0$ quadrant (Fig. 7) and the boundary to the gapless phase a. For the single transition line b, we determined $\nu_{N,N-2}$ by evaluating it at the lines $z(\Delta,D,N,N-2)=1$ of Fig. 6(a). We always took that side of the "finger" which is the continuation of the curve $z(\Delta,D,N,N-2)=1$ from the ferromagnetic region. In Table III we have listed $\nu_{N,N-2}$ for N beween 6 and 14 and $\Delta=-1.0$. It seems that ν tends to a finite value for $N\to\infty$. This trend is observed along the entire line b, although it becomes less evident that ν converges to a finite value when Δ is close to zero. Unfortunately, evaluating ν on the other side of the "finger" yields different, but also finite, results.

We have listed the exponent ν as obtained by extrapolation of $\nu_{N,N-2}$ to the thermodynamic limit for various values of Δ in Table IV. Although we do not claim high accuracy, we believe that qualitatively we have obtained the correct picture. ν seems to decrease from infinity at $(\Delta,D)=(0,0.35)$ to 0 at $(\Delta,D)\approx(-2.6,2.4)$, where line b of Fig. 7 joins line c of change of symmetry of the first excited state. Therefore, we conjecture that line b is the line of an ordinary algebraic phase transition with a continuously varying exponent ν.

The calculation of the exponent γ/ν from χ_{xx} also reveals that

$$\eta=2-\gamma/\nu \tag{5.5}$$

varies along line b. We have listed η in Table IV, where one sees that η increases from 0.25 at $(\Delta,D)=(0,0.35)$ to about 0.64 at $(\Delta,D)=(-2.0,1.75)$.

Let us now look at boundary a for the gapless phase. There are some problems in determining the critical exponents in this case. First, we can no longer let D be the parameter which is varied and used to take the derivative of the gap to obtain ν, because the transition line is expected to be almost parallel to the D axis. Second, because we are unable with our system sizes to locate the transition with reasonable accuracy, we can only give a crude estimate of the exponent η.

We have calculated ν by taking derivatives with respect to the exchange anisotropy Δ, and it then assumes that ν diverges in the thermodynamic limit. Furthermore, η seems to be close to 0.25 along the transition line. This follows from the fact that η varies little on the D axis $(\Delta=0)$ and is always close to 0.25 there, and that we expect the transition to take place at $\Delta\approx0$ for all $D>-1$. This behavior at line a has also been found by Botet *et al.*[20] and supports a conjecture of Haldane,[14] who predicts a phase transition from the gapless region into the "antiferromagnetic" phase with a gap opening with an essential singularity close to the D axis, and the transverse correlation function decaying with an exponent $\eta=\frac{1}{4}$ at

TABLE III. Critical exponent ν as a function of N for $\Delta=-1.0$.

$\Delta=-1.0$	
N	$\nu_{N,N-2}$
6	0.811
8	0.933
10	1.069
12	1.179
14	1.249

TABLE IV. Estimates of ν and η for various $\Delta<0$.

Δ	ν	η
0	∞	0.25
−0.5	3.2	0.31
−1.0	1.5	0.38
−1.5	0.6	0.48
−2.0	0.3	0.64

the transition. This then implies that the isotropic Heisenberg antiferromagnet $(\Delta,D)=(-1.0,0)$ lies within this "antiferromagnetic" phase, and its ground is therefore separated by a gap from the lowest excited levels, and its correlations decay exponentially with distance. Such behavior is very different from the $s=\frac{1}{2}$ case, where the Heisenberg antiferromagnetic is rigorously known to be gapless.

VI. CONCLUSIONS

In this work, we have studied the critical properties of the spin-1 Heisenberg chain with uniaxial anisotropy by using finite-size scaling. We have found evidence for a phase transition for ferromagnetic interaction $\Delta>0$, which occurs along a line $D_c(\Delta)$ in the (D,Δ) plane and seems to belong to the universality class of the two-dimensional planar model. However, severe problems arose in determining the critical couplings $D_c(\Delta)$, which could only be resolved by a comparison to the spin-$\frac{1}{2}$ XXZ model, which is amenable to an exact solution and shows similar phase behavior. We believe therefore that a straightforward application of finite-size scaling does not accurately locate the transition for $\Delta>0$.

For antiferromagnetic coupling $\Delta<0$, we found a nonzero energy gap almost everywhere except on line b of Fig. 7, along which a phase transition with continuously varying critical exponents ν and η seems to occur. Because of the irregular scaling properties for $\Delta<0$, unfortunately we cannot go beyond a qualitative characterization of the phase behavior.

It is interesting to observe that the behavior of the spin chains defined by (1.1) is very different for integer and half-integer spins.

First, we find strong numerical evidence that supports the conjectures of Haldane[14] and Botet *et al.*[13,20] concerning the existence of an intermediate phase between the XY and Néel phases, which *only* exists for integer spins. This conjecture can be further strengthened by a trivial extension of a proof of Lieb *et al.*,[39] who show that the Heisenberg antiferromagnet does not have an energy gap for $s=\frac{1}{2}$. This proof can easily be extended to all half-integer values of s, but does not hold for integer s.

Second, we have looked at the behavior of the energy gap as a function of $D>0$, and for $|\Delta|<1$ and $s=\frac{3}{2}$. A finite-size-scaling analysis yields the result that there is no gap anywhere in this region, and therefore, there are no transitions of the kind we found for $s=1$ in this case. Such behavior can be expected for $D\to\infty$, because then one effectively reduces the spin to $s=\frac{1}{2}$.

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APPENDIX

In this Appendix we describe some methods we used to extrapolate our finite-size data to the thermodynamic limit.

Let Q be any physical quantity of the infinite system. An obvious way to determine Q from the finite-size approximants Q_N is to write

$$Q_N=\sum_{l=0}^{N_T-1}\alpha_l(1/N)^l\,, \tag{A1}$$

where N_T is the number of different system sizes for which one has calculated Q_N. Then

$$Q=\alpha_0\,. \tag{A2}$$

This approach supposes that Q is an analytic function of $1/N$ around $1/N=0$ (or $N=\infty$), which unfortunately is in contradiction to the finite-size-scaling hypothesis whenever Q becomes critical. However, there are cases where Q remains an analytic function of N even at the critical point, which of course requires the critical exponent of Q to be an integer.

For example, the energy gap ω_N behaves like

$$\omega_N=\tan(\pi/4N) \tag{A3}$$

at the critical point of the $s=\frac{1}{2}$ transverse Ising model,[40] which is analytic at $1/N=0$.

One might also expect the critical exponents themselves to have an analytic N dependence. A check for the usefulness of the method is to calculate Q by taking different N values in (Al), which should yield the same results. A second method we used is to solve the equation

$$Q_N=Q+A/N^{\alpha} \tag{A4}$$

for Q, A, and α by taking three different N values, which allows for a real exponent α. This method turned out to be useful for the ground-state energy where the infinite-system estimate is almost independent of N.

Finally, we mention a method recently introduced in this context by Hamer and Barber.[41] Using it, one implements a one-parameter family of sequence transformations invented by Van den Broeck and Schwartz.[42] Given a sequence of values Q_N which converge to some limiting value $Q=\lim_{N\to\infty}Q_N$, one forms a table of approximants to Q denoted by $[N,L]$, where

$$[N,0]=Q_N\,, \tag{A5}$$

and the $(L+1)$th column of approximants is generated from the Lth and $(L-1)$th columns via the formula

$$\frac{1}{[M,L+1]-[M,L]}+\frac{\alpha}{[M,L-1]-[M,L]} = \frac{1}{[M+1,L]-[M,L]}+\frac{1}{[M-1,L]-[M,L]}, \quad \text{(A6)}$$

with the auxiliary condition $[M,-1]=\infty$. For $\alpha=1$, Wynn's[43] ϵ algorithm for generating the Padé table is recovered, while for $\alpha=0$ the transformation is equivalent to an iterated Aitken-Shanks table.[44] We used this method mostly with $\alpha=1$ or 0. Other α's do not usually yield very different estimates in the cases where convergence seems to be good.

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