Finite-size-scaling study of the spin-1 Heisenberg-Ising chain with uniaxial anisotropy

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Finite-cell calculations (up to $N=12$ spins) have been performed on the spin-1 Heisenberg-Ising chain with an uniaxial anisotropy, $\mathscr{H}=\sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2]$. From a scaling analysis of the gap between the ground state and the first excited state, a phase diagram has been drawn in the (λ,D) plane and the transition lines between the "ferromagnetic," "X-Y," "singlet-ground-state," and "antiferromagnetic" phases have been estimated for the infinite-N system. One of the most important results is that a singlet-ground-state phase with a nonzero gap exists in an extended range of λ and D values including the Heisenberg point $\lambda=1$, $D=0$, in contrast with the spin-$\frac{1}{2}$ case. Moreover, for $\lambda\simeq 1$, the gap decreases with increasing positive anisotropy D, goes through a minimum, estimated to be zero, and then increases with D.

I. INTRODUCTION

The ground-state properties of the Heisenberg-Ising chain

$$\mathscr{H}=\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z) \tag{1}$$

are well known in the case of $S=\frac{1}{2}$ spins.[1] Between the doublet-ground-state ferromagnetic (F) and antiferromagnetic (AF) phases, there exists, for $-1<\lambda<1$, a peculiar X-Y phase, characterized by a gapless ground-state and power-law decay of the spin-correlation functions. The AF transition at $\lambda=1$ is characterized by an "essential singularity," the gap, and the z-magnetization opening like $\exp[-1/(\lambda-1)^{1/2}]$ for $\lambda>1$, while the ferromagnetic transition at $\lambda=-1$, which corresponds to a simple crossing of levels, has first-order character.

Since the semiquantitative analytical predictions by Haldane[2] that properties for integer spin must differ qualitatively from those for half-integer spin, there is a need for studying larger spin cases. We have already presented[3] some results on the Heisenberg-Ising chain in the spin-1 case which confirm unambiguously Haldane's predictions. We have established that, between the gapless X-Y phase and the doublet-ground-state AF phase, there exists, for an extended range of λ values ($0\lesssim\lambda\lesssim 1.18$) containing the AF Heisenberg point $\lambda=1$, a new phase characterized by a nonmagnetic singlet ground state, nonzero gap, and exponential decay of the spin-correlation functions. The singlet-doublet transition at $\lambda\sim 1.18$ has a regular second-order character while the X-Y—singlet transition is an essential singularity located near $\lambda\simeq 0$.

In the present paper we give details of this study and extend it to the case with a uniaxial anisotropy. Thus we report on the finite-cell-scaling analysis of the full spin-1 Hamiltonian

$$\mathscr{H}=\sum_i [S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \lambda S_i^z S_{i+1}^z + D(S_i^z)^2] \tag{2}$$

in the entire range of λ and D parameters. The $(S_i^z)^2$ anisotropic term which is obviously meaningless in the spin-$\frac{1}{2}$ case, becomes essential in larger spin cases and must be considered both for experimental and theoretical reasons.

Experimentally, the full Hamiltonian (2) has been used to interpret the magnetic properties of a number of crystals in which the magnetic ions are arranged in chains with strong intrachain and small interchain interactions.[4] In the spin-1 case, the Hamiltonian (2) has been explicitly used to explain the properties of antiferromagnetic $CsNiCl_3$, $RbNiCl_3$, and $RbFeCl_3$ compounds.[5] A simple spin-wave theory has been used in that case.[6] However, in such approximative treatments the gap is strictly equal to D while it will be shown here that the gap may have another origin with a nontrivial variation with D.

Theoretically, the introduction of the anisotropic term $D(S_i^z)^2$ is of interest through the equivalence between one-dimensional (1D) quantum models and two-dimensional (2D) classical models.[7] For $\lambda=0$ it has been shown that Hamiltonian (2) is a truncated Hamiltonian formulation of the classical X-Y model in two dimensions.[8] Through this equivalence the parameter D plays the role of the temperature in the classical model. This equivalence has been confirmed by numerical finite-cell calculations on Hamiltonian (2) (with $\lambda=0$) (Ref. 9) which confirms the existence of a line of fixed points up to a classical value $D_c\simeq 0.4$, where an essential singularity occurs as in the Kosterlitz-Thouless[10] transition of the classical equivalent. This result is consistent with other calculations.[11]

The present study can be considered as an extension of both $\lambda=0$ (Ref. 9) and $D=0$ (Ref. 3) previous investigations. One of our main motivations is to locate the phase boundary of the X-Y phase in the (λ,D) plane. This phase extends up to $D=0.4$ for $\lambda=0$ (Ref. 9) while it seems to terminate near $\lambda\gtrsim 0$ for $D=0$.[3]

In Sec. II we present the results for the ordering of the low-lying levels. Then in Secs. III and IV we give the scaling analysis of the respective gaps between the ground state and the first excited state. In Sec. IV we analyze the correlation functions and a conclusion is given in Sec. V.

II. DETERMINATION OF THE GROUND STATE AND CROSSINGS BETWEEN LOW-LYING LEVELS

We have diagonalized numerically the full Hamiltonian (2) for finite rings of N spins with periodic boundary conditions for even values of N up to 12. Most of the results presented here are restricted to $N \leq 10$, only few results with $N=12$ will be reported. To reduce the size of the matrix to be diagonalized, it has been essential to consider the symmetries. First, we have used the conservation of the z projection of the total spin $\Sigma^z = \sum_i S_i^z$ which takes integer values from $-N$ up to $+N$. We have also taken into account the conservation of the total wave vector K, which takes values $2\pi n/N$ with n as an integer varying from 0 up to $N-1$. Second, we have considered the right-left ($\rho = \pm 1$) and the spin-reverse ($\sigma = \pm 1$) symmetries. Note that the spin-reverse symmetry is only useful to reduce the matrices in the $\Sigma^z = 0$ subspaces; in other cases, it only tells us that Σ^z and $-\Sigma^z$ subspaces are degenerate. The largest matrix to be diagonalized was of the order 1728 for $N=12$ (subspace $\Sigma^z = \pm 1$). To handle such large matrices we have used the Lanczös algorithm[12] which appeared to be very powerful, giving the ground-state energy in each subspace of given symmetry with great accuracy (error within 10^{-7}).

Let us present the results concerning the ordering of the low-lying eigenstates first. We have observed, for any finite N, that the ground state for the whole chain is either the singlet ground state of the subspace $\Sigma^z=0, K=0, \sigma=\rho=+1$, or the fully ferromagnetic doublet state $\Sigma^z = \pm N, K=0, \sigma=\rho=+1$ of energy $N(D+\lambda)$. It has never been the ground state of a subspace of an intermediate value of Σ^z. We have numerically determined, in the (λ, D) plane, the line corresponding to the crossing between the $\Sigma^z=0$ and $\pm N$ ground states. This line only slightly varies with N for $N=6,8,10$. The estimated infinite-N limit of this line is represented by curve 1 in Fig. 1. On the left-hand side of this line (region I), the ground state of the chain is ferromagnetic with the largest possible z magnetization, while on the right-hand side of this line (regions II, III, and IV) the ground state is a $\Sigma^z=0$ singlet ground state. Since this line corresponds to a crossing of levels with a jump of the z magnetization, it corresponds to a first-order phase transition in the infinite-N system.

The asymptotic large-D behavior of line 1 could have been expected from general consideration on Hamiltonian (2) by considering the X-Y part smaller than the λ and D parts. For D large and positive we recover the asymptotic line $D=-\lambda$ corresponding to the crossing between the singlet state $|0,0,\ldots,0\rangle$ at energy 0 and the ferromagnetic doublet $|\pm 1, \pm 1, \ldots, \pm 1\rangle$ at energy $N(\lambda + D)$. For D large and negative the curve 1 becomes asymptotically tangent to the axis $\lambda=0$ and varies as $\lambda \sim -4/D^2$. This can be understood by considering that for D large and negative the ground state is mostly constructed from the $S^z = \pm 1$ doublets on each site. The $S^z=0$ states, highly excited (at energy $|D|$ above the doublets), can be treated in second-order perturbation leading to an effective Heisenberg-Ising Hamiltonian of spin $\frac{1}{2}$ with an effective coupling constant proportional to $1/D^2$.

In order to be more precise in the region to the right of line 1, where the ground state is the $\Sigma^z=0$ singlet, we have also determined the crossings between the first excited states. In region II the first excited state is a $\Sigma^z = \pm 1$ doublet. In region III the first excited state is a $\Sigma^z=0$ singlet but with different symmetries than the ground state ($K=\pi, \rho=\sigma=-1$). In region IV the first excited state is a $\Sigma^z = \pm 2$ doublet. The boundary lines 2 (between regions II and III), 3 (between regions III and IV), and 4 (between regions II and IV) have been determined for $N=6,8,10$ and the estimated extrapolation for $N \to \infty$ are represented by dashed curves in Fig. 1. Note that in general these lines do not represent phase transitions except if the gap between the ground state and the first excited state tends to zero when $N \to \infty$. We will present now the study of the different gaps in each region II, III, and IV.

III. BOUNDARY BETWEEN THE SINGLET-GROUND-STATE PHASE AND THE NÉEL DOUBLET-GROUND-STATE AF PHASE

In this section we focus our attention on region III of Fig. 1, where the two lowest levels of (2) are both singlets of $\Sigma^z=0$ subspaces. By analyzing the gap G_{00}^N between these two lowest levels one can observe that it tends to zero exponentially with N for large λ values, it behaves as a power law $G_{00}^N \sim N^{-z}$ with $z \simeq 1$, for large N, only along a given line in the (λ, D) plane, while to the left of this line it seems to tend to a nonzero constant value. This is a strong indication that a second-order phase transition occurs on this line in the infinite-N system, the vanishing gap corresponding to the divergence of the correlation length in the equivalent classical model. To determine more precisely this transition line, we have postulated that $z=1$ at the transition (this is justified by the quantum-classical equivalence) and we have proceeded as in the

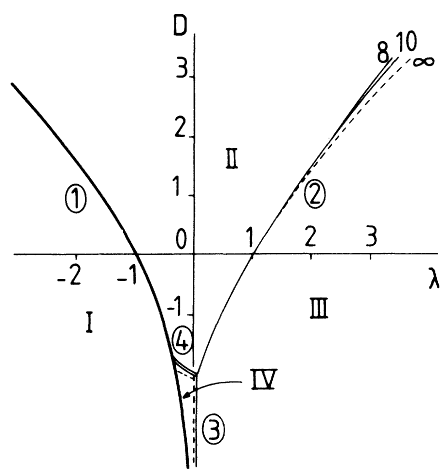

FIG. 1. Thick solid line 1 separates the ferromagnetic region I where the ground state is the doublet $\Sigma^z = \pm N$ from the other regions (II, III, IV) where the ground state is a singlet $\Sigma^z=0$. In regions II, III, and IV the first excited state is, respectively, a doublet $\Sigma^z = \pm 1$, a singlet $\Sigma^z=0$, and a doublet $\Sigma^z = \pm 2$. Crossing lines 2, 3, and 4 have been determined up to $N=10$ and extrapolated for $N \to \infty$ (dashed lines).

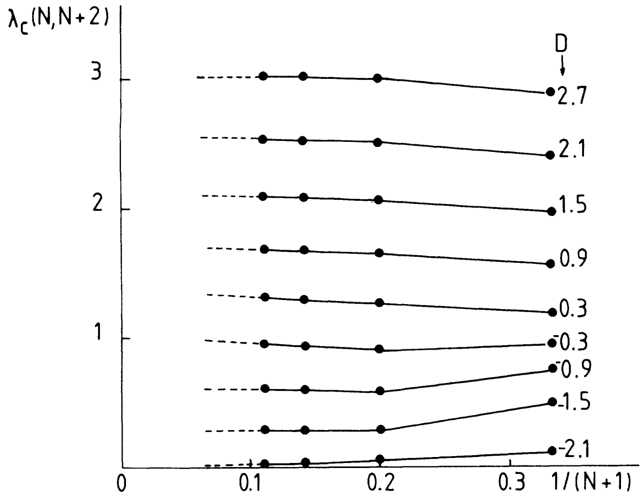

FIG. 2. Fixed point $\lambda_c(N,N+2)$ of the phenomenological renormalization-group equation for the gap G_{00}^N for different D values.

phenomenological renormalization-group method[13] by comparing successive sizes. Let us define an implicit renormalization-group transformation which transforms λ into λ' for a given constant D value after a size transformation $N \rightarrow N+2$,

$$(N+2)G_{00}^{N+2}(\lambda',D) = NG_{00}^{N}(\lambda,D) . \tag{3}$$

The N-dependent fixed point $\lambda_c(N,N+2)$, which corresponds to the successive crossings of the "scaled" gap $NG_{00}^N(\lambda,D)$, has been plotted as a function of $1/(N+1)$ in Fig. 2 for several D values. One observes that these critical values extrapolate quite well to a given line $\lambda_c(D)$ represented by curve a in Fig. 3. The same procedure except for fixed λ and varying D would have given exactly the same answer. In fact, it can be shown that the successive curves in the (λ,D) plane which correspond to the crossings of the successive scaled gaps $NG_{00}^N(\lambda,D)$ and $(N+2)G_{00}^{N+2}(\lambda,D)$ are converging nicely to curve a when $N \rightarrow \infty$. Line a cuts the λ axis at the point $\lambda \simeq 1.18$, $D=0$ already found[3] and the D axis at the point A ($\lambda=0$, $D \simeq -2.1 \pm 0.1$). For large λ values curve a becomes superimposed to line 2 and they become asymptotic to the $\lambda = D$ direction. This asymptotic direction could have been found by a simple analysis of Hamiltonian (2) with a vanishing X-Y part: It corresponds to a crossing between the $\Sigma^z=0$ state $|0,0,0,\dots\rangle$ of energy 0 and $\Sigma^z=1$ Néel doublet of components $|+-+-\cdots\rangle$ and $|-+-+\cdots\rangle$ of energy $N(D-\lambda)$. From this reasoning it is expected that the second-order phase transition on line a transforms into a first-order phase transition for $\lambda \rightarrow \infty$. It would be very interesting to know if this transformation occurs at a given point on curve a for finite λ or only asymptotically when $\lambda \rightarrow \infty$. If this transformation occurs at a finite point of curve a this point must necessarily correspond to the junction between lines a and 2. It is, however, very difficult, due to the numerical uncertainties, to locate precisely the junction between lines a and 2. A more clear conclusion comes from the analysis of the exponent ν which tells how the correlation length diverges at the transition.

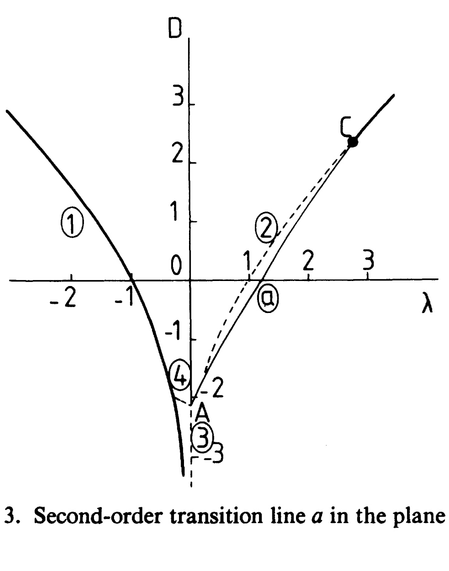

FIG. 3. Second-order transition line a in the plane (λ,D).

In the phenomenological renormalization-group method[13] one can define a N-dependent exponent, $\nu(N,N+2)$, by linearizing the renormalization-group equation (3) near the fixed point $\lambda_c(N,N+2)$ for each constant-D value. It is now important to note that D has been taken constant since, in principle, different results would have been obtained, for finite N, by varying D instead of λ. This exponent $\nu(N,N+2)$ can be numerically obtained through

$$\nu(N,N+2) = \frac{\ln[(N+2)/N]}{\ln[(N+2)G_{00}'^{N+2}/(NG_{00}'^{N})]} , \tag{4}$$

where $G_{00}'^{N}$ designs the partial derivative of G_{00}^N with respect to λ. $\nu(N,N+2)$ has been plotted as a function of $1/(N+1)$ in Fig. 4 for different D values. In a large range of D values ($-1.5 \lesssim D \lesssim 1.5$), $\nu(N,N+2)$ seems to converge quite well to the same asymptotic value,

$$\nu \simeq 1.2 \pm 0.1 ,$$

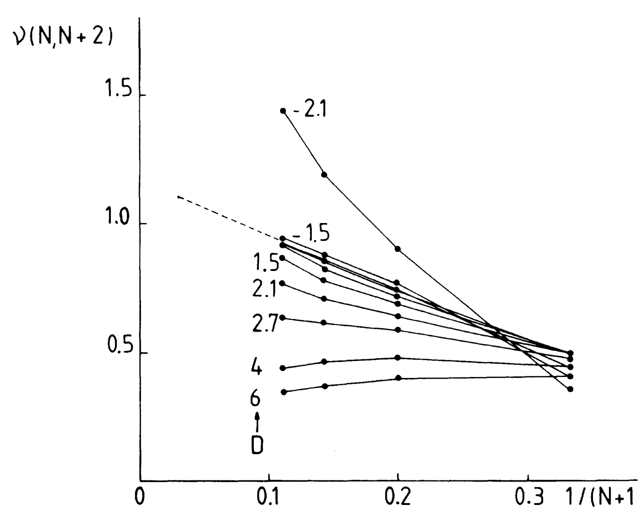

FIG. 4. Exponent $\nu(N,N+2)$ of the phenomenological renormalization-group equation for the gap G_{00}^N plotted as a function of $1/(N+1)$ for different D values.

which is consistent with the value $\nu \simeq 1.3 \pm 0.2$ already reported in the case $D=0$.[3] However, we observe deviations for large negative and large positive D values. These deviations can be more clearly analyzed in another plot given in Fig. 5 where we have plotted $\nu(N,N+2)$ as a function of D, for different pairs of successive sizes $(N,N+2)$. One can see that when N increases, $\nu(N,N+2)$ presents a much more pronounced plateau suggesting strongly that, in the infinite-N system, ν becomes independent of D in a large range of D values, as already found from Fig. 4. Note that this result justifies *a posteriori* that we could have taken D constant to evaluate ν. The same analysis, but with varying D and constant λ, would have given the same limiting value $\nu \simeq 1.2$ for $N \to \infty$ in the range $0 \lesssim \lambda \lesssim 2.5$. This result for ν implies that the gap closes as $(\lambda_c - \lambda)^s$ (fixed D) or $(D-D_c)^s$ (fixed λ) with $s = \nu z \simeq 1.2 \pm 0.1$.

In Fig. 5 one can see a marked crossover, $\nu(N,N+2)$ becoming suddenly very large, when D becomes negative and approaches the point A ($\lambda=0, D\simeq -2.1$). This crossover becomes more and more pronounced when N increases. This suggests that, if ν is constant along the line a in the infinite-N system, it becomes suddenly infinite at point A. In fact, $\nu=\infty$ means that, at this point, the gap closes more quickly than any power law as it is expected for an essential singularity. This result is consistent with the fact that, at this point, the second-order line a merges into the boundary of the X-Y phase which corresponds to an essential singularity as it will be seen below. Another deviation can be seen in Fig. 5, but for positive large-D values. Now it seems that, instead of converging to $\nu \simeq 1.2$, ν converges to zero for sufficiently large-D values. Even if this step is less pronounced than above it is also more and more marked when $N \to \infty$. One can estimate $D \simeq 2.3$ the value above which $\nu(N,N+2)$ starts to tend to zero when $N \to \infty$. The fact that $\nu=0$, i.e., $s=\nu z=0$, means that the gap could have a discontinuity. This suggests strongly that at a given point ($\lambda \simeq 2.75, D \simeq 2.3$) (point C in Fig. 3) the second-order phase transition transforms into a first-order phase transition. Then this point C must correspond to the point where line a joins line 2.

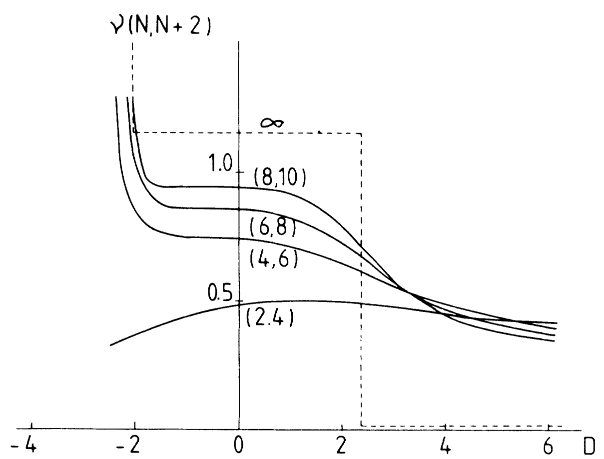

FIG. 5. Exponent $\nu(N,N+2)$ of Fig. 4 plotted as a function of D for different pairs of size $(N,N+2)$. Its estimated extrapolation for infinite N is represented by the dashed curve.

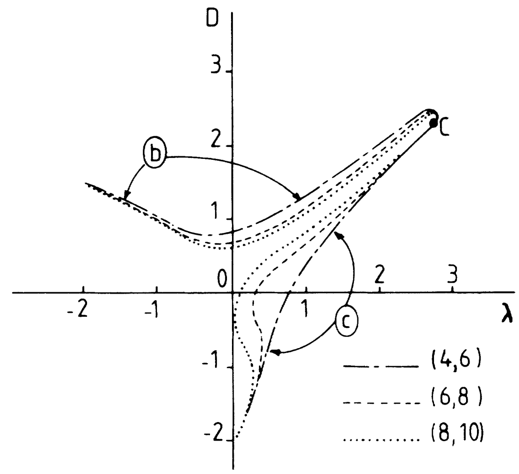

FIG. 6. Lines in the (λ,D) area where the successive scaled gaps NG_{01}^N and $(N+2)G_{01}^{N+2}$, for sizes $(N,N+2)$, are equal. Dashed-dotted, dashed, and dotted lines correspond, respectively, to sizes (4,6), (6,8), and (8,10).

IV. BOUNDARY OF THE X-Y PHASE

Let us now consider region II, where the ground state is the $\Sigma^z=0$ singlet and the first excited state is the $\Sigma^z=1$ doublet. We have performed the same analysis as in the preceding section with the gap G_{01}^N between these two states. Here it seems that the gap varies as $1/N$ in a large region and fits quite well a behavior such as

$$G_{01}^N \sim G_{01}^\infty + A/N$$

with G_{01}^∞ very small. The X-Y phase is the region where it can be estimated that G_{01}^∞ is zero. The N^{-1} term observed outside of the X-Y phase is probably due to the fact that we are always well below the large-size crossover towards an exponential behavior. In Fig. 6 we have drawn the lines in the (λ,D) plane where the successive scaled gaps NG_{01}^N and $(N+2)G_{01}^{N+2}$ are equal for $N=4,6,8$. These curves converge less rapidly than above and it is more difficult to estimate the line of transition in the infinite system. As before we have calculated the index $\nu(N,N+2)$ for λ fixed and D varying along part b of the line and for D fixed and λ varying along part c: The results are, respectively, reported in Figs. 7 and 8. It is clear from

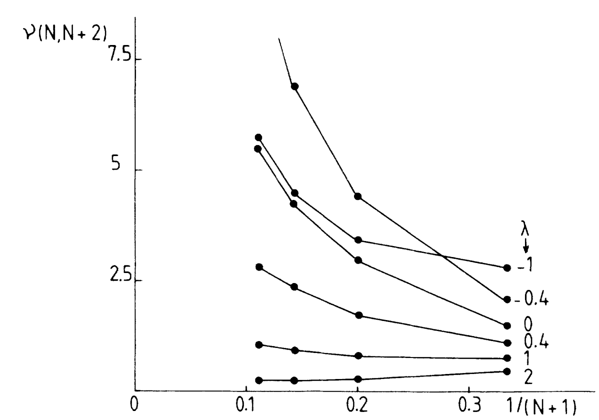

FIG. 7. Exponent $\nu(N,N+2)$ of the phenomenological renormalization-group equation for the gap G_{01}^N, calculated when crossing line b of Fig. 6 at different constant-λ values.

Fig. 7, that, if the curve b has a definite limit when $N \to \infty$, the exponent ν would be infinite on this line suggesting strongly that this line of transition corresponds to an essential singularity as already found for $\lambda = 0$ and $D \simeq 0.4$.[9] In Fig. 8 the divergence of $\nu(N,N+2)$ when $N \to \infty$ is less clear since in the range $-0.3 \lesssim D \lesssim 0.3$ the curves show a change of curvature. But the extrapolated value found for ν would be so large in that case ($\nu \simeq 15$) that it is reasonable to also predict an essential singularity along the limiting curve corresponding to part c.

A very strange behavior is observed in the range $0 \lesssim \lambda \lesssim 2.5$ where parts b and c of the curve have a finger-like shape which seems to stay up to $N \to \infty$. In that range of λ values the successive scaled gaps NG_{01}^{N} and $(N+2)G_{01}^{N+2}$ are crossing in two neighboring points. Moreover, the finger-shaped edge corresponds nicely to the point C where line a, determined in the preceding section, becomes first order. From this analysis we are tempted to conclude that in the infinite system there exists a tiny X-Y region, perhaps reduced into a single line, terminating at point C. This X-Y region would be between the "Heisenberg" singlet-ground-state phase (containing the Heisenberg AF point $\lambda = 1, D = 0$) and the large-D singlet-ground-state phase. Also difficult is to estimate the limiting curve corresponding to part c in the range $-2.1 < D < 0$. In Fig. 9 we give two possible phase diagrams for the infinite-N system where the X-Y phase is represented by the area with the solid lines. In both cases the boundary of the X-Y phase cuts the ferromagnetic first-order transition line at a given point B ($\lambda \sim -1.8$, $D \sim 1.35$). The two following problems remain difficult to clarify according to our calculations.

(i) Is the X-Y region reduced to a single line [DC in Fig. 9(b)] for $\lambda > 0$?

(ii) Is the boundary strictly superimposed with the D axis between D and A?

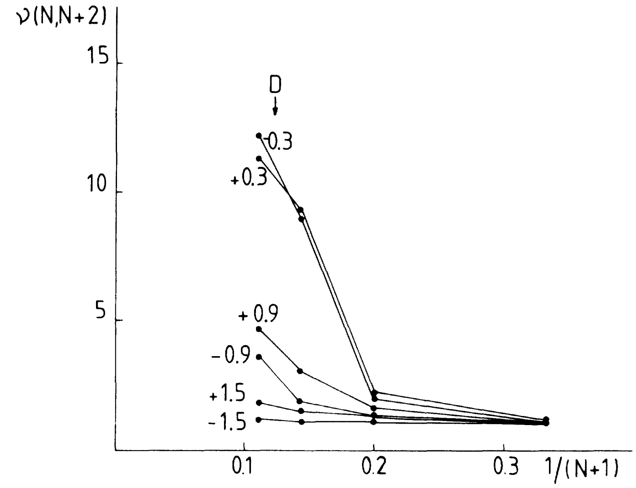

FIG. 8. Exponent $\nu(N,N+2)$ of the phenomenological renormalization-group equation for the gap G_{01}^{N}, calculated when crossing line c of Fig. 6 at different constant-D values.

To complete the phase diagram below point C, it remains to elucidate what happens in region IV of Fig. 1 where the two lowest states are the $\Sigma^z = 0$ singlet and the $\Sigma^z = \pm 2$ doublet. As above we have studied the gap G_{02}^{N} between these two states. In Fig. 10 we have drawn the lines in the (λ, D) plane where the successive scaled gaps NG_{02}^{N} and $(N+2)G_{02}^{N+2}$ are equal, for $N = 4,6,8$. These lines converge to the lines 3 and 4 of Fig. 1 when $N \to \infty$. The analysis of the exponent ν would show that, again, these lines correspond to essential singularities. Thus region IV with its vanishing gap corresponds also to an X-Y phase. One could say that region IV corresponds to a spin-$\frac{1}{2}$—like X-Y phase while the dashed area of Fig. 11 corresponds to a regular spin-1 X-Y phase.

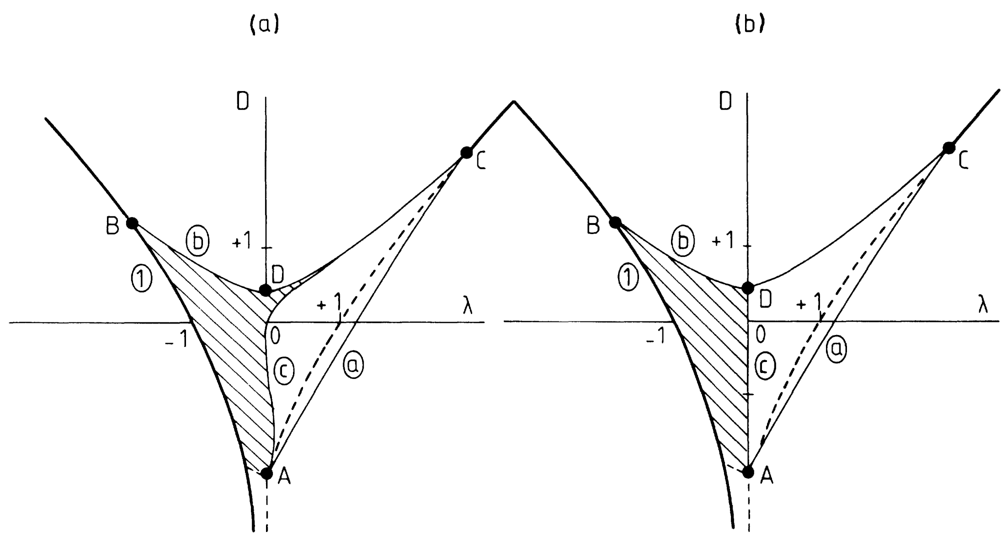

FIG. 9. Two possible estimations of the shape of the boundary of the X-Y phase in the (λ, D) plane for $N \to \infty$. X-Y phase (dashed area) is separated from the ferromagnetic phase by the first-order transition line 1, from the high-D singlet-ground-state phase by the essential singularity line b, and from the Heisenberg singlet-ground-state phase by the essential singularity line c.

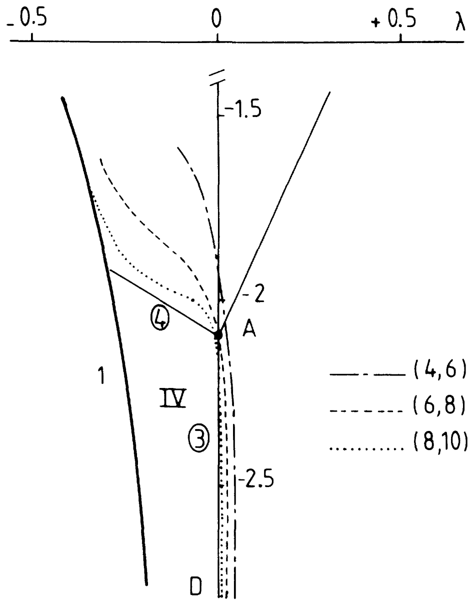

FIG. 10. Lines in the (λ,D) plane where the successive scaled gaps NG_{02}^{N} and $(N+2)G_{02}^{N+2}$, for sizes $(N,N+2)$, are equal. Dashed-dotted, dashed, and dotted lines correspond, respectively, to sizes (4,6), (6,8), and (8,10).

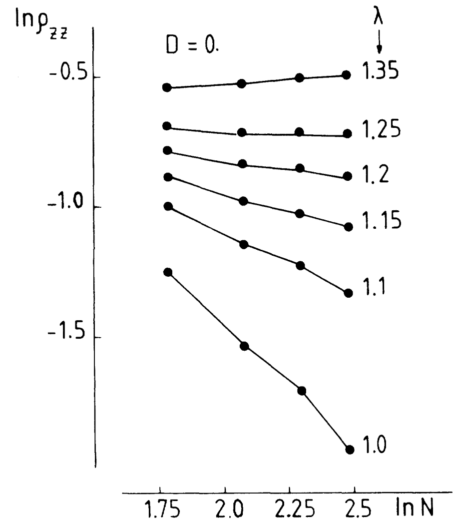

FIG. 11. Plot of $\ln\rho_{zz}$ vs $\ln N$ for $D=0$ and different λ values.

V. CORRELATION FUNCTION

We have calculated, at a few points on the plane (λ,D) in the antiferromagnetic region $\lambda>0$, the following correlation functions between two opposite spins on the ring:

$$\rho_{+-}=(-1)^n\langle S_i^+S_{i+n}^-\rangle\ ,\quad \rho_{zz}=(-1)^n\langle S_i^zS_{i+n}^z\rangle \qquad (5)$$

with $n=N/2$. Since we have used periodic boundary conditions the result is independent of the site i. The sign $(-1)^n$ has been introduced in order to obtain positive quantities in the antiferromagnetic region. The angular brackets mean that the expectation value has been taken in the $\Sigma^z=0$ singlet ground state of the chain. We will implicitly suppose that the dependence of correlation functions with n, for finite systems of $N=2n$ spins when $N\to\infty$, is the same as their dependence with distance between spins in the infinite-N system. This is the case for systems where the exact solution is known. These calculations of the correlation functions were more difficult than those for the gap for two reasons: First, we need the eigenvector (and not only the eigenvalue) to calculate the expectation value in the ground state, and, second, due to $N/2$ odd-even oscillations in ρ_{zz}, we were obliged to go up to $N=12$ to get significant results on the asymptotic behavior.

Let us discuss the results on ρ_{zz} first. There is a clear change of behavior on line a. To the right of this line ρ_{zz} tends to a constant value when $n=N/2\to\infty$. The limiting value $\rho_{zz}=m^2$ can be interpreted as the square of the staggered z magnetization in the antiferromagnetic phase. On the contrary, to the left of this line ρ_{zz} tends quickly to zero with $n=N/2$. By analyzing ρ_{zz} in a log-log plot one can show that ρ_{zz} follows a power-law behavior of the type $\rho_{zz}(n)\sim n^{-\eta_z}$ just on line a. An example is given in Fig. 11 where one can see that the slope of $\ln\rho_{zz}$ vs $\ln N$ is rapidly varying when crossing the curve a by increasing λ at a constant-D value (here $D=0$). The even-odd oscillations do not allow us to obtain η_z with very good precision. However, taking $\lambda=1.18$ for $D=0$, one can estimate $\eta_z=0.23\pm0.03$. The same analysis done for different D values shows that η_z does not vary along this line a. The value of η_z implies an opening of the staggered z magnetization of the type $m_z\sim(\lambda-\lambda_c)^{\beta}$ (for fixed D) or $m_z\sim(D_c-D)^{\beta}$ (for fixed λ) on the right-hand side of line a with an exponent $\beta=\nu\eta_z/2\simeq0.17\pm0.04$.

The results for ρ_{+-} are more difficult to interpret since everywhere $\rho_{+-}\to0$ when $n=N/2\to\infty$. In fact, one must expect that ρ_{+-} follows a power-law behavior of the type $\rho_{+-}\sim n^{-\eta_{+-}}$ for $n=N/2\to\infty$, in the entire X-Y region, with a varying η_{+-} exponent, while it must follow an exponential behavior in the singlet-ground-state regions where the gap is nonzero. However, it is not possible to determine the boundary of the X-Y region by using this criterion since, if the gap is nonzero but very small, we observe always power-law behavior. It would be necessary to reach much larger cells to hope to see the crossover towards an exponential behavior. This is illustrated in Fig. 12 where one observes always straight lines in a log-log plot on the right of the frontier $\lambda\simeq0$ of the X-Y phase. However, one can observe that the value $\eta_{+-}=0.25$ predicted by Haldane[2] at the frontier of the X-Y phase is very well recovered. For $\lambda=0$ and $D=-0.4$, 0, and 0.4, one obtains, respectively, $\eta_{+-}=0.245\pm0.007$, $\eta_{+-}=0.248\pm0.007$, and $\eta_{+-}=0.255\pm0.007$. This confirms the fact that the frontier of the X-Y phase must be almost close to the D axis. However, even if the precision is quite good here, these results do not allow us to distinguish between the two possibilities of phase diagram [Figs. 9(a) and 9(b)] especially concerning the finger-shaped part DC of the diagram. One can see in Fig. 9 that for $D=0.4$, η_{+-} varies very slowly with λ.

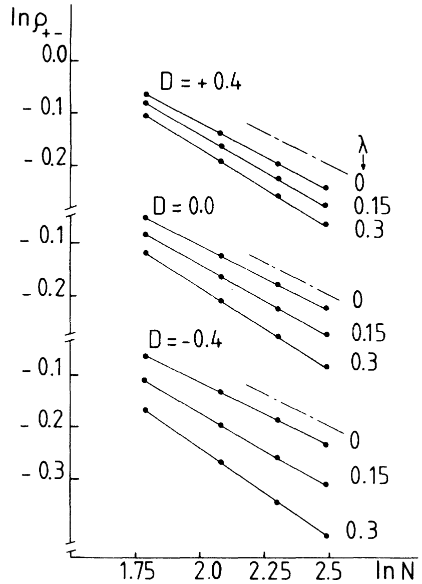

FIG. 12. Plot of $\ln\rho_{+-}$ vs $\ln N$ for $D=0.4$, 0, -0.4, and $\lambda=0$, 0.15, and 0.3. The slope $-\frac{1}{4}$ is indicated by the dashed-dotted lines.

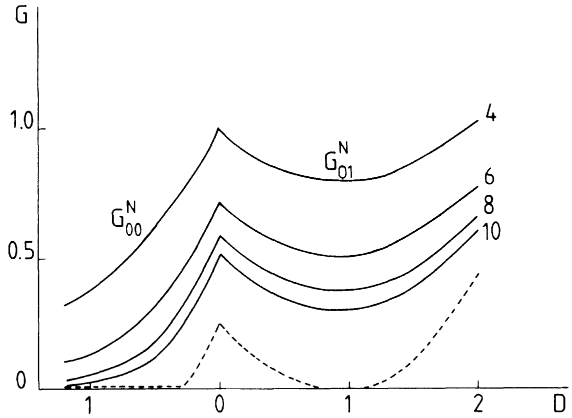

FIG. 13. Variation of the gap with the single-site anisotropy parameter D in the Heisenberg case ($\lambda=1$). Estimated gap for the infinite-N system is represented by the dashed curve.

VI. CONCLUSION

By studying the lowest states of Hamiltonian (2) for finite chains (up to $N=12$), we have been able to construct a complete $T=0$ phase diagram in the plane (λ,D) (Fig. 9). We have been able to extend the boundaries of the singlet-ground-state Heisenberg phase in the presence of a uniaxial anisotropy D. We recall that this new phase which includes the AF Heisenberg point ($\lambda=+1, D=0$) is characteristic of integer spin chains and would not exist in the half-integer case. To its right, for large AF anisotropy of the coupling, this Heisenberg phase is bounded by the Néel-type AF phase through a second-order transition line (line a in Fig. 9). When crossing this line the singlet ground state changes into a doublet ground state and a staggered spontaneous magnetization appears in the z direction. The exponents of the transition ($\nu\simeq1.2$, $\beta\simeq0.17$) have been estimated. To its left, when the anisotropy of the coupling becomes ferromagnetic ($\lambda<0$), the Heisenberg phase is bounded by the X-Y phase through an essential singularity line. When approaching this line from the Heisenberg phase the gap closes more quickly than any power law. We have not been able to determine more precisely the shape of this transition line. It would be interesting to know if it exactly superimposes the D axis. Here some analytical studies could help. In particular, knowing the classical equivalent of the λ term one could study its influence on the existence of the Kosterlitz-Thouless transition. If the hypothesis of Fig. 9(b) is true the Kosterlitz-Thouless phase would disappear for $\lambda>0$ while it would stay for $\lambda<0$.

Another result is the existence of a tiny X-Y phase, perhaps reduced to a single line, separating the Heisenberg phase to the singlet-ground-state phase for large single-site anisotropy. In contrast with what we could expect (and what we announced in Ref. 3) the gap between the singlet ground state and the bottom of the continuum is not simply enlarged when applying a positive uniaxial anisotropy. This gap starts to decrease first, goes through a minimum which is estimated to be zero here, and then increases again. This suggests that the large-D phase and the Heisenberg phase which look quite similar (singlet ground state with a nonzero gap) are in fact of different natures. This point also must be elucidated in further studies.

As a conclusion we give in Fig. 13 the behavior of the gap when applying the D parameter on the Heisenberg antiferromagnet ($\lambda=1$). The estimated gap in the infinite system is represented by the dashed curves. One sees clearly in this figure the difference between the behavior of the G_{00} gap when crossing line a and the behavior of the G_{01} gap when crossing the part DC of the phase diagram. The gap for $D=0$ is quite large, about one-quarter of the coupling parameter; the same value is recovered for $D\simeq1.7$, i.e., for an anisotropy parameter almost twice as large as the coupling constant. This might have important experimental consequences and we think that the physical interpretation of the behavior of a spin-1 chain such as $CsNiCl_3$ and $RbNiCl_3$ might be different. If a gap exists the magnetic susceptibility must tend to zero, after passing through a maximum, when lowering the temperature, while it would saturate as $T\rightarrow0$ in the gapless case. Also, the gap could be seen in the spin-wave spectrum by neutron-diffraction experiments.

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