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# Ground-state properties of a spin-1 antiferromagnetic chain

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A finite-cell-scaling analysis of the spin-1 antiferromagnetic Heisenberg-Ising chain, shows that the ground-state properties are completely different than in the spin-$\frac{1}{2}$ case. Between the $XY$ gapless phase and the doublet ground-state Néel phase, it appears, in an extended range of the anisotropy ($0 \lesssim \lambda \lesssim 1.18$) a characteristic Heisenberg-phase with a nonmagnetic singlet ground state, nonzero gap, and exponential decay of the correlation functions.

Quantum spin chains are of current interest, both experimentally and theoretically.[1] Experimentally, a number of crystals are investigated, in which the magnetic ions are arranged in chains with strong intrachain and small interchain interactions. Theoretically, these are the simplest many-body models in which quantum effects play an essential role. In particular the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg-Ising chain, defined by the Hamiltonian

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

shows a particular transition in the ground state at $\lambda = 1$, with an "essential singularity," which has been widely studied in the past.[2]

The Heisenberg system, with $\lambda = 1$, shares the same properties as the whole $0 \leqslant \lambda \leqslant 1$ region where the system is gapless, without long-range order, and with power-law decay for the ground-state spin-correlation functions. For $\lambda > 1$, the system has a doublet ground state with a nonzero gap, a spontaneous staggered $z$ magnetization and an exponential behavior for the ground-state correlations. A naive conclusion would be to trust these results for large spins.

In this Communication, we consider the spin-1 antiferromagnetic Heisenberg-Ising chain. This model (with an extra uniaxial anisotropy term of the form $DS_i^{z2}$) is experimentally realized in the compounds $CsNiCl_3$ and $RbNiCl_3$.[3] We report on exact numerical calculations done on finite cells. From a scaling analysis of our results we show unambiguously that the ground-state properties of (1) are completely different in the spin-1 case than in the spin-$\frac{1}{2}$ case. The most spectacular result is that the isotropic, $\lambda = 1$, Heisenberg case belongs to an extended phase in $\lambda$ ($0 \lesssim \lambda \lesssim 1.18$) characterized by a nonmagnetic singlet ground state, a nonzero gap, and an exponential decay of the spin-correlation functions. In contrast with the spin-$\frac{1}{2}$ case, there is no transition in the ground state at the Heisenberg point $\lambda = 1$. There is instead a change of symmetry of the first excited state. The predictions of Haldane[4] about the different behaviors of integer and half-integer spin chains are here completely confirmed. Moreover, the locations, the exponents of the transitions, and the behavior of the spin-correlation functions have been estimated.

We have considered finite rings of $N$ sites ($N$ even) with periodic boundary conditions. The following symmetries have been used to reduce the size of the matrices: the conservation of $\Sigma^z = \sum_i S_i^z$ and total wave vector $K$, the right-left ($\rho = \pm 1$) and spin reverse ($\sigma = \pm 1$) symmetries. Even so, the larger matrix was of order 1728 for $N = 12$ and we have used the Lanczös algorithm[5] to compute the energies and wave functions of each ground state in the different subspaces of any symmetry. We have observed that the ground state of the chain is always a singlet corresponding to $\Sigma^z = 0$, $K = 0$, and $\rho = \sigma = +1$. For $\lambda > 1$, the first excited state is a singlet corresponding to $\Sigma^z = 0$, $K = \pi$, and $\rho = \sigma = -1$ while for $\lambda < 1$ it is a doublet corresponding to $\Sigma^z = \pm 1$, $K = \pi$, $\rho = -1$. The crossing of the first excited state at $\lambda = 1$, for any finite $N$, is expected from the extra symmetry (spin rotation invariance) of the Heisenberg case.

The most significant results of our calculations are summarized in Figs. 1 and 2. More details (in particular the ground-state energies) will be given elsewhere.[6] Figure 1 reports the results for the gap $G_N$ between the two lowest states of the chain in terms of "scaled gaps" $NG_N$ as a function of $\lambda$. Figure 2 reports the results for the correlation functions in the ground state, between two opposite spins on the ring, defined as

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

where $n = N/2$. The result is obviously independent of the site $i$. In the following we will suppose that the behavior of the correlation functions with $n$, when $n = N/2 \to \infty$, reflects their behavior with distance in the infinite system. (This is the case for systems where the exact solution is known.)

For $\lambda > 1$, our results are consistent with a sec-

 

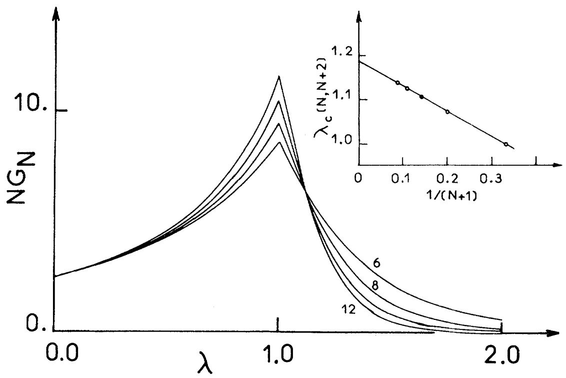


FIG. 1. Plot of the scaled gap $NG_N$ as a function of $\lambda$ for $N=6$, 8, 10, and 12. (For clarity, the cases $N=2$ and 4, which can be obtained analytically, have been omitted.) In inset is shown $\lambda_c(N,N+2)$ vs $1/N$ (see text).

ond-order phase transition in the infinite system ($N\rightarrow\infty$), for a given critical value $\lambda_c$ larger than 1. This transition corresponds to a closing of the gap and appearance of a staggered $z$ magnetization when increasing $\lambda$. A simple log-log plot of $G_N$ vs $N$ shows that the gap follows a power-law behavior of the type $G_N \sim N^{-z}$ only around $\lambda \sim 1.15$ with $z \sim 1$, while it behaves exponentially below and above this $\lambda$ value. We can reasonably assume that the dynamical exponent $z$ is strictly equal to 1 at the transition.[7] Then a scaling analysis, as done in the "phenomenological renormalization group"[8] can be developed by comparing successive sizes. An implicit renormalization-group transformation which transforms $\lambda$ into $\lambda'$ after a size rescaling from $N$ to $N+2$ is defined by

$$(N+2)G_{N+2}(\lambda')=NG_N(\lambda) \quad .$$

The $N$-dependent fixed-point $\lambda_c(N,N+2)$ (which corresponds to the successive crossings of the scaled gaps of Fig. 1) has been plotted as a function of

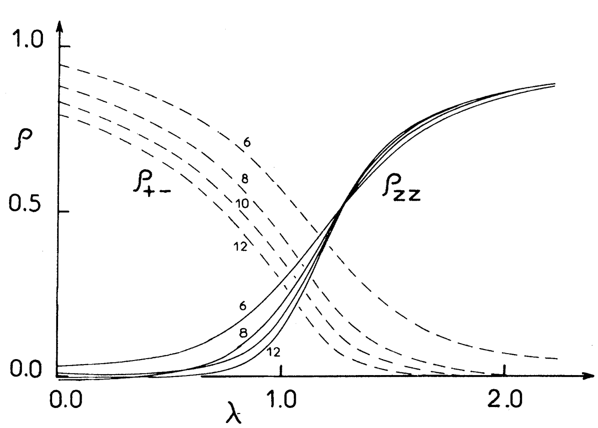


FIG. 2. Plot of the correlation functions: $\rho_{+-}=(-1)^n\langle S_i^+S_{i+n}^-\rangle$ and $\rho_{zz}=(-1)^n\langle S_i^zS_{i+n}^z\rangle$, where $n=N/2$, as a function of $\lambda$ for $N=6$, 8, 10, and 12.

$1/(N+1)$ in inset of Fig. 1. The extrapolation to $N\rightarrow\infty$ gives an estimate for the location of the transition in the infinite system: $\lambda_c=1.18\pm0.01$. The corresponding exponent $\nu$ which tells how the coherence length $\xi$ diverges at the transition ($\xi \sim |\lambda-\lambda_c|^{-\nu}$) can be calculated by linearizing near $\lambda_c(N,N+2)$:

$$\nu(N,N+2)=\frac{\ln[(N+2)/N]}{\ln[(N+2)G'_{N+2}/(NG'_N)]} \quad ,$$

where $G'_N$ and $G'_{N+2}$ are the derivatives of the gap, with respect to $\lambda$, taken at $\lambda_c(N,N+2)$. The results extrapolated to infinite $N$ gives the following estimate for $\nu$ in the infinite system:

$$\nu=1.3\pm0.2 \quad .$$

This analysis is consistent with a gap closing as $G\sim(\lambda_c-\lambda)^s$ in the infinite system with $s=\nu z \sim 1.3\pm0.2$.

Similarly a log-log analysis of the $z$-$z$ correlation function shows that $\rho_{zz}$ follows a power law of the type $\rho_{zz}(n)\sim n^{-\eta_z}$ for large $n$, around $\lambda\sim1.18$. Taking $\lambda_c$ as determined above, one gets $\eta_z=0.23\pm0.03$. A scaling analysis of the correlation function yields $\nu=1.2\pm0.2$ consistent with the value coming from the scaling of the gap. This analysis implies an opening of the staggered magnetization $m_z=\lim_{N\rightarrow\infty}\rho_{zz}^{1/2}$ at $\lambda_c$ of the form $m_z\sim(\lambda-\lambda_c)^\beta$ with $\beta=\nu\eta_z/2=0.17\pm0.05$. Moreover, in a large range of $\lambda$ values above $\lambda_c$, we observe that $\rho_{zz}$ converges exponentially very quickly giving a good precision for the behavior of the staggered magnetization which is very well fitted by the formula $m_z=[1-(\lambda_c/\lambda)^\alpha]^{1/6}$ with $\alpha=2.067$.

All this scaling analysis around $\lambda=\lambda_c\sim1.18$ is consistent with the recent theory of Haldane[4] who predicted a transition with $\eta_z=\frac{1}{4}$ at a given $\lambda_c$ larger than 1. Moreover we have been able to give more details on the transition by estimating $\lambda_c$ and other exponents like $\beta$ and $\nu$. This transition which corresponds to a change of nature of the ground state from singlet to doublet is similar to the transition in the ground state of transverse Ising model[9] and has nothing to do with the transition observed at $\lambda=1$ in the spin-$\frac{1}{2}$ Heisenberg-Ising chain.[2] However, our exponents $\nu$ and $\beta$ seem closer to $\nu=\frac{4}{3}$ and $\beta=\frac{1}{6}$ than the values $\nu=1$ and $\beta=\frac{1}{8}$ of the one-dimensional transverse Ising model.

For $\lambda<1$, the situation is quite different and the scaling analysis is more difficult there. One can see on Fig. 1 that in an extended range ($0<\lambda\lesssim0.2$) the scaled gaps are quite superimposed so that $G$ seems to behave as $1/N$. Similarly, in the same region, the $\rho_{+-}$ correlation function tends to zero as $n^{-\eta_{+-}}$, for large $n$ with $\eta_{+-}$ varying only slightly with $\lambda$. This is a typical situation where an essential singularity or a line of fixed points is present.[10] Any attempt to analyze the results by the phenomenological renormalization-group method gives a quasi-infinite $\nu$ exponent at the transition.[11] It is really difficult to locate precisely the termination of the line where an essential singularity takes place. A simple analysis of the gap of the type $G = G^{\infty} + A/N$ yields $G^{\infty} \sim 0$ up to $\lambda \lesssim 0.1$ suggesting that the termination is certainly smaller than $\lambda = 0.1$. Haldane[4] predicted such a line of fixed points terminated by a transition point at which $\eta_{+-} = \frac{1}{4}$. Here, we suggest that the essential singularity takes place strictly at $\lambda = 0$, since at this point we find $\eta_{+-} = 0.248 \pm 0.005$, which includes the predicted value with a good precision. For $\lambda \sim 0.1$, $\eta_{+-} \sim 0.260$ is already significantly larger than $\frac{1}{4}$. The fact that we observe power-law behaviors for both $G$ and $\rho_{+-}$ up to $\lambda \sim 0.2$ comes perhaps from the fact that the gap is so small in this region that it would be necessary to reach very large cells to observe the crossover to an exponential behavior. Assuming an essential singularity at $\lambda = 0$ and searching a behavior of the kind $G \sim A \times \exp(-B/\lambda^{\sigma})$,[12] one can estimate $\sigma = 0.30 \pm 0.05$.

Between the essential singularity and the transition at $\lambda_c$ the chain has a nonmagnetic singlet ground state with a nonzero gap and exponential behavior for the correlation functions. More precisely, in the Heisenberg case $\lambda = 1$, we have obtained a good fit by the form suggested by Haldane[4]:

$$\rho_{+-} = 2\rho_{zz} = An^{-1/2}\exp(-Kn) + Bn^{-2}\exp(-2Kn)$$

with $K \sim 0.07$, $A \sim 1.2$, and $B \sim -3$.

So, the antiferromagnetic spin-1 Heisenberg chain, with its finite gap and exponential decay for the correlations, has completely different ground-state properties than in the spin-$\frac{1}{2}$ case. The particular Heisenberg symmetry at $\lambda = 1$ is here characterized by a simple crossing, accompanied by a change of the symmetry, of the first excited level. This causes an abrupt change in the slope $dG/d\lambda$ for the variation of the gap with the anisotropy which could have interesting experimental consequences (for example, in optical experiments when varying anisotropy).

The study has been completed in presence of an uniaxial anisotropy $DS_i^{z2}$ and the results will be reported soon.[6] As expected, when increasing $D$, the gap increases and the singlet ground-state phase is enlarged [$\lambda_c$ increases and the essential singularity disappears around $D \sim 0.4$ (Ref. 13)]. The presence of a nonzero gap in a large range of $\lambda$ and $D$ values could explain why a simple spin-wave theory done on the same Hamiltonian seems to apply quite well to spin-1 compounds.[14] However, in the spin-wave approximation, the gap is strictly equal to $D$ while here it already exists for $D = 0$ and has a quite complicated behavior with respect to $\lambda$. This could explain the discrepancies between the different estimations given for $\lambda$ and $D$ in these compounds.[3,14] Even if the extension to larger spins is more difficult we expect to extend the same study to the case of spins $\frac{3}{2}$ and 2. We hope that the present work will stimulate further exact theoretical investigations to check our conclusions concerning the locations of the transitions and the values of the various exponents. The study of antiferromagnetic chains with arbitrary spins will certainly be the subject of an increasing interest in the near future.

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