

# First Order Transition in the Frustrated Antiferromagnetic Heisenberg $S = 1$ Quantum Spin Chain

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We study a frustrated Heisenberg  $S = 1$  quantum spin chain with next-nearest neighbor (NNN) coupling  $\alpha$  using a variational ansatz and the density matrix renormalization group. We find as quantum remnants of the phase transition in the classical chain a disorder point at  $\alpha_D = 0.284(1)$  and a Lifshitz point at  $\alpha_L = 0.3725(25)$ . Our main finding is a first-order transition from an Affleck-Kennedy-Lieb-Tasaki (AKLT) phase to a NNN generalization of the AKLT phase at  $\alpha_T = 0.7444(6)$ . At the transition, string order jumps discontinuously by  $\approx 0.085$  to 0; correlation length and gap are finite. [S0031-9007(96)01843-1]

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In recent years, classical and quantum frustrated systems in low dimensions have been extensively studied, motivated by both experiment and their role as a theoretical testbed: Frustrated systems show rich behavior, but many conventional techniques meet with considerable difficulty [1]. The Heisenberg isotropic quantum spin chain with antiferromagnetic interactions between nearest and next-nearest neighbors (NNNs) are about the simplest frustrated quantal system, and thus of central interest. From the well-established [2] Haldane conjecture [3] it is known that in the limit of no frustration there is a fundamental difference between half-integer and integer spin chains. We may thus expect significantly different behavior also in the frustrated chains.

Frustrated half-integer spin chains have been extensively studied and are by now well understood [4]. Frustrated next-nearest neighbor integer spin chains have also attracted considerable interest. Several scenarios and analytical and numerical studies have been proposed, in particular, for  $S = 1$ . Numerical studies [5] seem to indicate that there is no phase transition for any value of frustration. Field theoretical studies [6,7] predict that there is always a gap for any value of frustration. On the other hand, it was claimed recently [8] that there is an (almost) gapless point for a  $\alpha = 0.73(1)$ . Thus the situation is obscure; there is no agreement whether there is a phase transition in the chain and, if so, of which order.

In this work we study the phase diagram of a frustrated antiferromagnetic isotropic Heisenberg  $S = 1$  quantum spin chain

$$H = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} + \alpha \sum_i \mathbf{S}_i \mathbf{S}_{i+2} \quad (1)$$

at  $T = 0$ . We find a disorder point of the first kind for  $\alpha_D = 0.284(1)$ , a quantum remnant of the phase

transition in the classical model. Our main result is that there is a first-order transition at  $\alpha_T = 0.7444(6)$  with a discontinuous jump in the string order and a finite correlation length. The emerging picture is thus substantially different from the frustrated  $S = \frac{1}{2}$  chain.

We start with an analytical approach [9] based on the Affleck-Kennedy-Lieb-Tasaki (AKLT) [10] model, as a guideline for the numerical results presented below. Basically, two ground states are compared: one being the conventional AKLT model, the other a NNN-AKLT model which links next-nearest neighbors by singlet bonds (Fig. 1). These two ground states arise naturally if one considers the unfrustrated  $\alpha = 0$  limit, known to be well described by the AKLT model, and the  $\alpha \rightarrow \infty$  limit, where the chain decomposes into two unfrustrated subchains. Comparing ground-state energies, we obtain a naive (but surprisingly good) estimate for the transition point  $\alpha_T^{\text{var}} = \frac{3}{4}$ . The elementary excitations in the AKLT phase can be studied in a soliton approach in the spirit of Ref. [11]. The dispersion law of the soliton excitation for  $\alpha < 0.75$  is given by

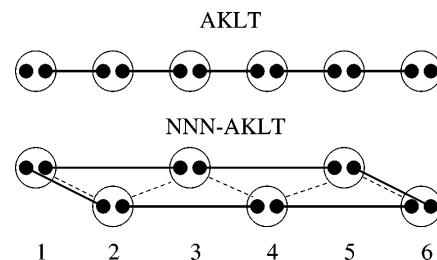


FIG. 1. Schematic representation of the AKLT model and the NNN-AKLT. Circles are spin-1 sites, a dot is a spin  $\frac{1}{2}$ , and fat links are singlet bonds between spins. Note the free spin  $\frac{1}{2}$  at each end of the open AKLT chain. In the NNN-AKLT model, the chain is indicated by dashed lines.

$$\begin{aligned} \varepsilon(k) = & \frac{14}{9} + \frac{26}{27}\alpha + \frac{160\alpha - 18}{27} \cos(k) \\ & - \frac{14}{9} \alpha \cos(2k) \\ & + (2 - 26\alpha/3) \frac{3 + 5 \cos(k)}{5 + 3 \cos(k)}. \end{aligned} \quad (2)$$

The gap does not disappear at the transition point [ $\Delta^{\text{var}}(\alpha = 0.75) \approx 0.325$ ], indicating a first-order phase transition (or absence of a phase transition). In the NNN-AKLT phase (Fig. 1) the soliton dispersion can be obtained from (2) by  $\alpha \rightarrow 0$ ,  $k \rightarrow 2k$ , and scaling the expression by  $\alpha$ . This description is perhaps too crude, for example, at  $\alpha = 0.75$  the energy per spin of the completely dimerized valence bond state is exactly the same as that of the AKLT and NNN-AKLT configurations. We have constructed a variational wave function in higher matrix dimensions interpolating smoothly between the AKLT, NNN-AKLT, and the completely dimerized state. We find results in reasonable agreement with the naive findings just presented; the main feature is that though the discontinuity at the transition is less distinct, and the transition point shifted to  $\alpha \approx 0.81$ , the transition is still found to be first order [9].

To obtain quantitative results, we use the density matrix renormalization group (DMRG) [12], typically using  $M = 250$  block states in chains up to  $L = 350$ . This by far exceeds previous calculations [8] in precision. We present calculations of important quantities not considered beforehand and analyze the excitation spectrum carefully. The use of a prediction mechanism [13] to accelerate the exact diagonalization in the DMRG allows us to perform all calculations on a PentiumPro based personal computer at good computing speed. The DMRG is particularly adapted to the problem, as it allows us to treat large systems and is not plagued by quantum Monte Carlo's negative sign problem. We have calculated a number of low-lying states, including their magnetization, to distinguish between edge and bulk excitations in open chains, spin-spin correlations, and the string order parameter. It should be mentioned that our results do not verify some observations obtained by Pati *et al.* [8] using the DMRG, namely, the local drop in the gap at  $\alpha \approx 0.5$ , and their gap data at the transition. This difference in results going beyond finite size effects may be explained by the presence of parasitic edge excitations which were not taken completely into account in Ref. [8].

Numerically, we find two phases, namely, the AKLT (the Haldane) and the NNN-AKLT phase, and three special points in the phase diagram, the disorder point  $\alpha_D$ , the Lifshitz point  $\alpha_L$ , and the transition point  $\alpha_T$ .

The AKLT phase for  $\alpha_T < 0.7444(6)$  is characterized by the string order parameter [14]

$$\mathcal{O}_\pi^z(i, j) = \left\langle S_i^z \left( \exp \sum_{k=i+1}^j i\pi S_k^z \right) S_j^z \right\rangle \quad (3)$$

measuring the *hidden order* of the  $S = 1$  Heisenberg chain due to a broken  $Z_2 \times Z_2$  symmetry. This gives rise to the Kennedy edge excitation triplet, which is degenerate with the ground state singlet in the thermodynamic limit [15]. We clearly observe the Kennedy triplet numerically, as a  $S_{\text{tot}} = 1$  boundary excitation with odd parity (abbreviated in the following as  $1^-$ ), degenerate with the  $0^+$  ground state. The first bulk excitation is given by the lowest  $2^+$  state.

The string order parameter is nonzero throughout this phase (Fig. 2), peaks at  $0.4397(1)$  very close to the AKLT value of  $\frac{4}{9}$ , and drops to zero discontinuously at the phase transition. The gap results obtained by the variational approach starting from the AKLT model are in reasonable agreement with the numerical findings (Fig. 3).

The most remarkable feature of this phase is the disorder point. In a previous work [16] by one of us (U. Sch.) it was shown that the relationship between the antiferromagnetic Heisenberg model and the AKLT model for  $S = 1$  can be understood within the framework of a *disorder point of the first kind*, a well-defined concept in classical statistical mechanics [17]. It basically arises in a disordered phase linked by continuous transitions to two ordered low-temperature phases with different forms of order. In the case of the frustrated antiferromagnetic Heisenberg quantum spin chain, there is no ordered zero-temperature phase [18]. However, the quantum spin- $S$  chain at  $T = 0$  can be mapped to a classical spin chain at  $T \neq 0$ . It is known [19] that, at least for the unfrustrated Heisenberg model, the relationship  $T \propto 1/S$  holds. The classical spin chain at finite temperatures is disordered due to the Mermin-Wagner theorem [18], but ordered at  $T = 0$ . The  $T = 0$  classical spin chain

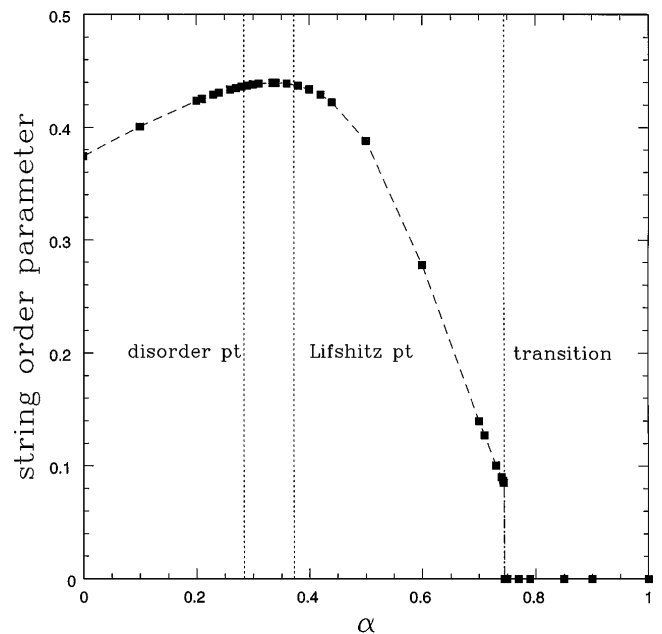


FIG. 2. String order parameter  $\lim_{|i-j| \rightarrow \infty} \mathcal{O}(i, j)$ .

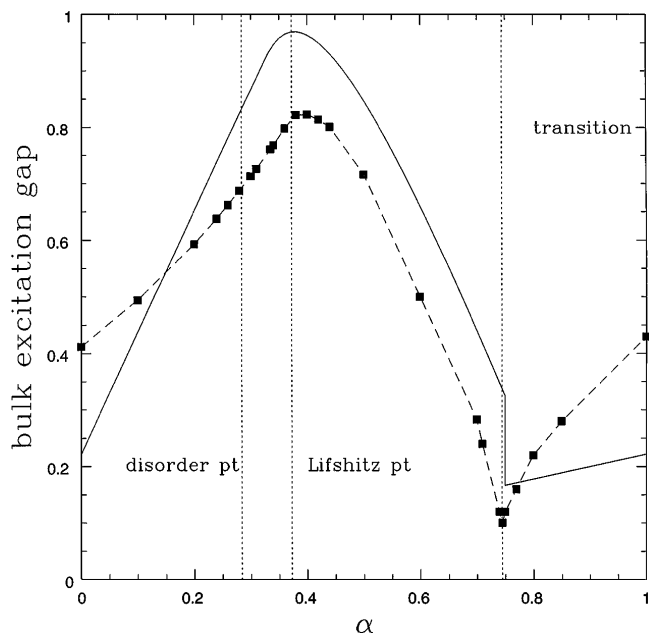


FIG. 3. Bulk excitation gap  $\Delta(\alpha)$ . The precision is  $\approx 0.02$  at the transition, better elsewhere. As shown values, lower bounds were chosen. Solid line: analytical result.

provides the required ordered low-temperature phases. For  $\alpha < \alpha_c = 0.25$ , the chain is antiferromagnetically ordered; for  $\alpha > \alpha_c$ , there is spiral order  $\langle \mathbf{S}_0 \mathbf{S}_x \rangle \propto \cos q(\alpha)x$  with  $q(\alpha) = \arccos(-1/4\alpha)$ . Indeed, we can identify an  $\alpha_D = 0.284(1)$ , which meets the criteria of a disorder point to numerical precision: Correlations become incommensurate in real space at this point; the wave number  $q(\alpha)$  for  $\alpha > \alpha_D$  shows the expected singular behavior; the correlation length  $\xi$  shows a minimum of  $\xi \approx 1.20$  and a very steep slope for  $\alpha < \alpha_D$ , probably infinite.

For  $0.37 < \alpha < 0.375$  we find the associated Lifshitz point, defined by the emergence of a two-peak structure in the  $S(q)$  structure function, with maxima at  $q_{\max} \neq \pi$ . The small difference in the location of the Lifshitz point in Ref. [8] is an effect of the smaller precision and system size studied there. At the Lifshitz point, we see the development of a *doubly degenerate* structure of the excitation spectrum, already predicted by Allen and Sénéchal [7] and in agreement with Eq. (2): The lowest  $2^-$  state is degenerate with the  $2^+$  state. Classically, the two degenerate states correspond to spin waves  $\cos qx$  (even parity) and  $\sin qx$  (odd parity). Variationally, the Lifshitz point is predicted at  $\alpha \approx 0.325$ . Note that, above  $\alpha_D$ , there is a low-lying  $1^+$  edge excitation in the open chain, a precursor of the transition. This explains the difference in gap curves between Ref. [8] and us.

In an open chain in the NNN-AKLT phase, there are two free  $S = \frac{1}{2}$  spins at each chain end, which we link up by nearest-neighbor singlet bonds. The ground state of an open chain is thus unique, which we can verify numerically. The low-lying bulk excitation spectrum retains its

doubly degenerate structure. Ground-state energy, excitation gap and correlation length approach their asymptotic behavior,  $E_0(\alpha) = \alpha E_0(0)$ ,  $\xi(\alpha) = 2\xi(0)$ , and  $\Delta(\alpha) = \alpha\Delta(0)$ . Asymptotic behavior is slower to set in for  $\xi$  and  $\Delta$ : The gap is slightly bigger, as it costs more energy to excite a subchain still coupled to the other subchain;  $\xi$  is correspondingly smaller than expected.

The remaining central question is how the change from the AKLT to the NNN-AKLT phase at  $\alpha_T = 0.7444(6)$  can be characterized.

We observe a finite gap  $\Delta(\alpha)$  (Fig. 3) at the transition. This fact is obscured by the presence of parasitic low-lying states corresponding to edge excitations, which have to be excluded. The minimal gap is small,  $\Delta \approx 0.10$ , to be compared with a variational prediction of  $\Delta = 0.325$ . The correlation length (Fig. 4) increases on both sides of the transition, but remains clearly finite on the AKLT side ( $\xi \approx 18$ ), whereas it becomes very long on the NNN-AKLT side, such that a divergence cannot be as clearly excluded. This behavior is not compatible with a second-order transition.

Our main argument in favor of the first-order transition is the clearly discontinuous disappearance of the string order parameter (Fig. 2) at  $\alpha_T = 0.7444(6)$ . We observe numerically a jump of 0.085 (20% of its maximum value) between  $\alpha = 0.74375$  and  $\alpha = 0.7450$ . Up to  $\alpha = 0.74375$ , the string order parameter decays almost linearly; at this point the slope increases about sixty times. It appears extremely unlikely that there is a crossover from this linear behavior to an extremely strong power-law decay (as in a continuous transition).

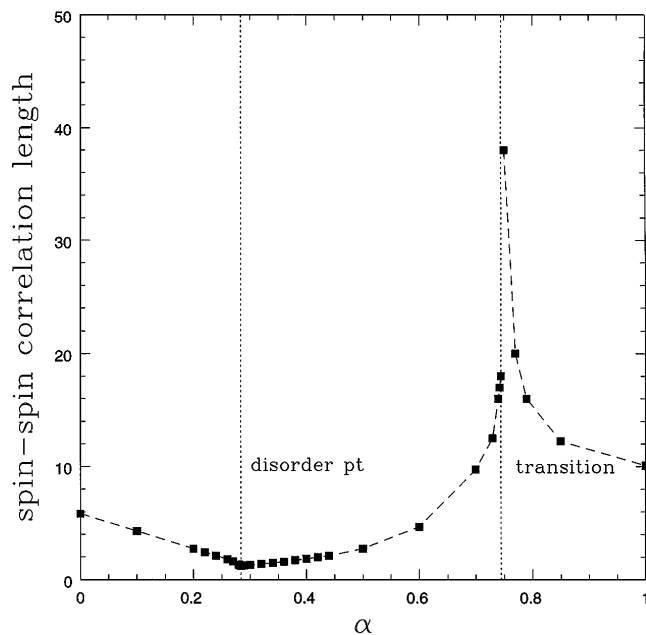


FIG. 4. Spin-spin correlation lengths  $\xi$ . They are systematically underestimated by the DMRG. At the transition the error is maximal, but will, generously estimated, not exceed 20%.

A first-order transition would be most neatly identified by a discontinuous derivative of the ground-state energy per spin. Numerically, we find it very difficult to clearly identify such a discontinuity. Though the correlation length is finite, it is long enough to suggest a rather soft first-order transition.

We are therefore led to locate a first-order phase transition at  $\alpha_T = 0.7444(6)$ , in very good agreement with the naive analytical prediction  $\alpha_T^{\text{var}} = 0.75$ .

To summarize, we can devise a clear and coherent picture of a frustrated  $S = 1$  isotropic Heisenberg spin chain. Its behavior is fundamentally governed by the underlying classical model, characterized by a phase transition from an antiferromagnetic to a spiral ordered phase, reflected by the presence of a disorder point and a Lifshitz point. The classical transition is thus not linked to the first-order transition found at  $\alpha_T = 0.7444(6)$ , which is a pure quantum effect. We argue that there is a first-order phase transition because the underlying physical change is the doubling of the lattice spacing, which is not a typical breaking of a symmetry group in a continuous phase transition. We therefore suggest that there is a whole first-order transition *line* in the  $\alpha - \delta$  plane, if one includes a  $[1 + (-1)^i \delta]$  alternation in the nearest-neighbor interaction in (1). Assuming the transition line to be characterized by vanishing string order, we suggest it should be identified with the  $(BC)$  line in Fig. 3 of Ref. [8], which probably means that our NNN-AKLT phase is smoothly connected with the dimerized phase.

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