Variational and DMRG studies of the frustrated antiferromagnetic Heisenberg $S = 1$ quantum spin chain

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Abstract

In this paper we study a frustrated antiferromagnetic isotropic Heisenberg $S = 1$ quantum spin chain

$$H = \sum_i S_i S_{i+1} + \alpha \sum_i S_i S_{i+2},$$

using a variational ansatz starting from valence bond states and the Density Matrix Renormalization Group. We find both methods to give results in very good qualitative and good quantitative agreement, which clarify the phase diagram as follows: At $\alpha_D = 0.284(1)$, there is a disorder point of the second kind, marking the onset of incommensurate spin-spin correlations in the chain. At $\alpha_L = 0.3725(25)$ there is a Lifshitz point, at which the excitation spectrum is found to develop a particular doubly degenerate structure. These points are the quantum remnants of the transition from antiferromagnetic to spiral order in the classical frustrated chain. At $\alpha_T = 0.7444(6)$ there is a first order phase transition from an Affleck-Kennedy-Lieb-Tasaki (AKLT) phase characterized by non-vanishing string order to a phase which can be understood as a next-nearest neighbor generalization of the AKLT model. At the transition, the
string order parameter shows (to numerical precision) a discontinuous jump of 0.085 to zero; the correlation length and the gap are both finite at the transition. The problem of edge states in open frustrated chains is discussed at length.

75.50.Ee, 75.10.Jm, 75.40.Mg
I. INTRODUCTION

Over the past years, frustrated quantum mechanical systems have met with considerable interest. Research is concentrating on geometrically frustrated systems, where the lattice geometry introduces competing interactions, and on systems, where frustration is directly introduced by interaction, e.g. the additional presence of next-nearest neighbor interactions. Interest in these systems has twofold motivation. There are experimental systems which show geometrical frustration (quasi 1D hexagonal insulators such as CsNiCl$_3$ or effective Kagomé lattices such as SrCr$_{8-x}$Ga$_{4+x}$O$_{19}$); there are also systems frustrated by interaction: A well-known motivation is given by high-$T_c$ superconductors, which exhibit an antiferromagnetic phase. It has been shown early on that doping of these compounds may be mapped to frustrated spin models. Another prominent example is CuGeO$_3$, a one-dimensional $S=1/2$ antiferromagnet with strong competing interactions. On the other hand, there is purely theoretical motivation to study these systems. Taking the classical limit, frustration may introduce rather complex forms of order. Quantum fluctuations will destroy long-range order which may be present in the classical system, if the dimension of the system is low. For one-dimensional quantum systems, order will in general be destroyed even at zero temperature. It is therefore of interest to study which remnants of the classical system survive in the quantum system, and whether there are purely quantum phenomena present. About the simplest frustrated system conceivable is the frustrated Heisenberg isotropic quantum spin chain with antiferromagnetic interactions between nearest and next-nearest neighbors. From the well-established Haldane conjecture it is known that in the limit of a vanishing next-nearest-neighbor interaction there is a fundamental difference between half-integer and integer spin chains. The unfrustrated half-integer spin chain is characterized by almost long-range antiferromagnetic order, with power-law correlations and a critical spectrum $\omega = c(k - \pi)$ at low energies. The integer spin chain has only short-ranged antiferromagnetic order, exponential correlations and a gapped spectrum $\omega = \{c^2(k - \pi)^2 + \Delta^2\}^{1/2}$, where $\Delta$ is the Haldane gap. We may thus expect considerably different behavior also in the frustrated
The case of half-integer spin chains has been extensively studied and is by now well understood.\footnote{10} The case of frustrated isotropic next-nearest neighbor integer spin chains

\[ H = \sum_i S_i S_{i+1} + \alpha \sum_i S_i S_{i+2} \]  

(1)

has also attracted considerable interest. Several scenarios and analytical and numerical studies have been proposed, in particular for $S = 1$. Numerical studies\footnote{11,12} seem to indicate that there is no phase transition for any value of frustration. Field theoretical studies\footnote{13,14} predict that there is always a gap for any value of frustration. They indicate a doubly degenerate excitation spectrum beyond $\alpha \approx 0.4$.\footnote{14} On the other hand, it was claimed recently\footnote{15,16} that there is an almost gapless point (to numerical precision) for $\alpha = 0.73(1)$. The situation is thus 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 quantum spin chain (1) with $S = 1$ at $T = 0$. We start with a variational approach based on the Affleck-Kennedy-Lieb-Tasaki (AKLT)\footnote{17,18} model to give analytical predictions. Basically, two ground states are compared to each other, one being the conventional AKLT model, the other an AKLT model which links next-nearest neighbors by singlet bonds (Fig. 1). For further refinement, an ansatz interpolating between these cases is constructed and minimized. Elementary excitations are calculated in a “crackion”\footnote{19,20} picture. On the other hand, we use the Density Matrix Renormalization Group (DMRG)\footnote{5,21} to obtain quantitative results and to check the variational approach. In our DMRG calculations, we typically use $M = 250$ block states in chains up to $L = 380$ sites. This by far exceeds previous calculations\footnote{13,14} in precision. We present calculations of important quantities not considered beforehand and analyze the excitation spectrum carefully. The use of a prediction mechanism\footnote{22} to accelerate the convergence of the exact diagonalization inherent in the DMRG allows us to go up to about $M = 400$ in a $S = 1$ system on a PentiumPro based personal computer while retaining reasonable computing speed. The structure of the
paper is as follows: in section II, we briefly summarize our findings; in section III, we discuss the associated physical scenario in more detail. Sections IV and V present the analytical and numerical calculations.

### II. SUMMARY OF RESULTS

We find that there is an AKLT (Haldane) phase for $\alpha_T < 0.7444(6)$ with a disorder point of the second kind at $\alpha_D = 0.284(1)$ (see Figs. 3 and 2) and a Lifshitz point at $\alpha_L = 0.3725(25)$ (see Fig. 5). The disorder point and the associated Lifshitz point can be understood as the quantum remnants of the phase transition from antiferromagnetic to spiral order in the classical frustrated chain. The AKLT phase can be understood in terms of the conventional $S = 1$ AKLT model (Fig. 1); the associated string order parameter is nonzero (Fig. 6), corresponding to hidden order linked to the breaking of a discrete $Z_2 \times Z_2$ symmetry in the chain. The string order parameter shows a maximum of $0.4397(1)$ at $\alpha = 0.3375(25)$ close to the disorder point, and disappears with a discontinuous jump of about $0.085$ at $\alpha_T = 0.7444(6)$. The gap rises monotonically to a maximum $\Delta = 0.82(1)$ at $\alpha = 0.40(1)$, then drops monotonically (Fig. 7). Just before the disorder point, the correlation length drops steeply (in all probability, with infinite slope close to the disorder point) to reach a minimum of $\xi_D = 1.20(2)$ exactly at the disorder point, and rises slowly and monotonously beyond (Fig. 3). The real-space correlations are purely antiferromagnetic below the disorder point, but incommensurate above (Fig. 2). The change in the wave vector $q$ is discontinuous at the disorder point (Fig. 4). The bulk excitations for $\alpha > \alpha_L$ are characterized by a pairwise degeneracy of states of equal spin, but different parity. This degeneracy is not present for $\alpha < \alpha_L$. The variational approach predicts the Lifshitz point at $\alpha_{\text{var}}^L = 0.32$ and a gap maximum at $\alpha = 0.38$ with $\Delta_{\text{var}}(0.38) = 0.97$, and the presence of the AKLT phase up to $\alpha_{\text{var}}^T = 0.75$ (or $\alpha_{\text{var}}^T = 0.81$, depending on the approach).

Beyond $\alpha_T = 0.7444(6)$, we can characterize the system by a next-nearest neighbor generalization of the AKLT-model, taking all odd and all even numbered spins separately.
and defining the usual AKLT-model on each subchain (Fig. 1). Defining a conventional string order parameter on each subchain, we find this string correlator to decay exponentially on a scale much longer than the bulk correlation length for $\alpha$ greater than about 1 (Fig. 3). As the $Z_2 \times Z_2$ symmetry is not broken in the total chain, the string correlator is not an order parameter, but its very slow decay shows it characterizes well the NNN-AKLT phase. The gap increases with frustration. In the $\alpha \to \infty$ limit, it tends towards the unfrustrated value $\Delta = 0.41050(2) \alpha$ due to the chain decomposition. The correlation length first decreases; in the large frustration limit it tends towards twice the unfrustrated value, $\xi = 12.04$, due to the doubling of the lattice spacing in the decomposed chains. The bulk excitations retain the pair structure mentioned above.

At the transition point $\alpha_T = 0.7444(6)$ we measure the correlation length to saturate to $\xi_T \approx 18$ on the AKLT side of the transition, clearly excluding a critical or near-critical point as conjectured before. We find the bulk excitation gap to be $\Delta_T \approx 0.10$. On the NNN-AKLT side the correlation length is longer, and might be divergent. In both phases we can identify close to the transition edge states that are remnants of the other phase. This together with the discontinuous jump of the string order parameter by $\approx 0.085$, about 20 percent of its maximal value, leads us to classify this point as a first-order transition. This is in accordance with the predictions of the variational approach, predicting a (too big) gap of $\Delta_{\text{var}}^{\alpha_T} = 0.325$.

### III. PHYSICAL SCENARIO

We now proceed to expound the physical scenario briefly outlined above. The physics of the frustrated $S = 1$ quantum spin chain is entirely determined by the parameter $\alpha$. We find two phases, namely the AKLT ($Haldane$) 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 $\alpha_T$. 
A. The AKLT Phase

The point $\alpha = 0$ corresponds to a nearest-neighbor Heisenberg quantum spin chain. It is well established by now\textsuperscript{5,6} that at $\alpha = 0$ the above model has a finite correlation length of $\xi = 6.03(2)$, a Haldane gap $\Delta = 0.41050(2)$, and is characterized by a so-called string order parameter\textsuperscript{24,26}

$$O_\pi^z(i, j) = \langle S^z_i (\exp \sum_{k=i+1}^j i\pi S^z_k) S^z_j \rangle$$

which measures the hidden order of the $S = 1$ Heisenberg chain, which is due to a broken $Z_2 \times Z_2$ symmetry.\textsuperscript{22} Its numerical value\textsuperscript{6} is $O_\pi^z = \lim_{|i-j| \to \infty} O_\pi^z(i, j) = 0.374325096(2)$. There is a very intuitive description of this point provided by the Affleck-Kennedy-Lieb-Tasaki model:\textsuperscript{17,18} each $S = 1$ spin is decomposed into a symmetric sum of two $S = 1/2$ spins (Fig. 1). Each of the $S = 1/2$ spins is linked to one of the neighboring $S = 1/2$ spins by a singlet bond. The adequacy of this description is established by the fact that the AKLT model shows the same hidden order characterized by a string order parameter\textsuperscript{24,26} $O_\pi^z = 4/9$, has a gap to the first bulk excitation, and a finite correlation length. One of the most striking predictions of the AKLT model verified by the Heisenberg chain is the presence of two effectively free $S = 1/2$ spins at the right and left end of an open chain. This gives rise to a low-lying edge excitation triplet, the so-called Kennedy triplet, which degenerates with the ground state singlet in the thermodynamic limit.\textsuperscript{27}

We argue that for $\alpha_T < 0.7444(6)$ the AKLT model provides an adequate description and a good starting point for a variational description of the spectrum. This is corroborated by the observation that the string order parameter is non-zero throughout this phase (Fig. 6), and peaks at $0.4397(1)$, very close to the AKLT value of $4/9$. It drops to zero discontinuously at the phase transition, and is thus an adequate order parameter for this phase. The results obtained by the variational approach starting from the AKLT model are in a qualitative agreement with the numerical findings: We observe a gap maximum at $\alpha = 0.40(1)$ with $\Delta = 0.82(1)$, which is predicted at $\alpha = 0.38$ with $\Delta^{\text{var}} = 0.97$ by the variational approach.
Predicted and observed gap curve are in reasonable agreement (Fig. 7). Let us however note at this point that we do not find the intermediate drop of the gap Pati et al. observe at $\alpha \approx 0.5$, but rather observe a monotonous drop of the gap. For a (rather technical) explanation of the disagreement, which can be traced to the appearance of parasitical edge states which were not taken completely into account, we refer to Section V.

In the region where the string order parameter peaks, numerical and variational ground state energies agree very well, and the general behavior of the ground state energy is well predicted by the variational approach (Fig. 10).

The shift in the structure function peak away from $\pi$ (explained below) is predicted variationally at $\alpha_{var}^L = 0.32$ and found numerically at $\alpha = 0.3725(25)$. However, in the variational approach the peak shifts to $q = \pm 2\pi/3$ as $\alpha$ approaches the transition point, and then drops discontinuously to $\pm \pi/2$, whereas we observe numerically that $q$ smoothly decreases from $\pi$ to $\pi/2$ with increasing $\alpha$. Here, the variational approach is too simplistic. It is no use comparing correlation lengths: The matrix product states of the AKLT model notoriously underestimate correlation lengths.

We conclude by remarking that we clearly observe the Kennedy triplet numerically, as a $S_{total} = 1$ end excitation with odd parity (abbreviated in the following as $1-\bar{1}$), degenerating with the 0+ ground state. The first bulk excitation is then given by the lowest 2+ state. We have also calculated the spectrum in a chain where a spin $\frac{1}{2}$ was added at each end, binding the free spins and lifting the degeneracy. Then the ground state is given by the lowest 0− state, and the first bulk excitation by the lowest 1+ state. The findings of both procedures are in excellent agreement. In an open chain, there is for $\alpha > \alpha_D$ a low-lying 1+ edge excitation in addition to the Kennedy triplet, which we will identify as a precursor of the NNN-AKLT phase below.
B. The Disorder Point in the Frustrated Spin Chain

In a previous work 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 second kind, a well-defined concept arising in classical statistical mechanics. Let us briefly review the physical properties of such a disorder point without mathematical details; for such details, we refer to the previous work and the references cited therein.

A disorder point can arise if a system exhibits two ordered low-temperature phases with differently broken symmetries, e.g. an antiferromagnetically ordered phase and a spiral phase with a generally incommensurate wave number $q$ and if these phases are linked to the disordered high-temperature phase by continuous phase transitions. It is intuitively clear that in the disordered phase there will be remaining short-range correlations of the type found in the adjacent ordered phases. Moving across the phase diagram, one expects to find a line in the disordered phase separating regions with the two different types of correlations, a so-called disorder line. As the correlations are short-ranged, the correlation function peak in momentum space (in $S(q)$) starts moving from, say, $q = \pi$ to a general $q$ not exactly at the disorder line, but at a different line, the so-called Lifshitz line, somewhere in the incommensurate-correlation region. The two lines join in the multicritical point, where the two ordered phases and the disordered phase meet.

The remarkable fact is that such disorder lines, throughout a variety of substantially different physical systems, can be classified into two types with a number of well-defined physical properties.

Typical properties of a disorder line of the second kind (the one found here) are:

- Moving through parameter space on a path characterized by a parameter $\gamma$ across a disorder line at $\gamma_0$, the correlation length $\xi(\gamma)$ exhibits an infinite slope on the commensurate side at $\gamma_0$. On the incommensurate side, the slope is typically finite:
The correlation length may, but need not have a local minimum at $\gamma_0$.

- The real space correlation function changes from a commensurate to an incommensurate wave number $q(\gamma)$ on the disorder line. The function of the wave number $q(\gamma)$ has a singular derivative at $\gamma_0$ on the incommensurate side

$$\left. \frac{dq}{d\gamma} \right|_{\gamma_0;C} = 0 \quad \left. \frac{dq}{d\gamma} \right|_{\gamma_0;IC} = \infty \quad (4)$$

and evolves as

$$(q(\gamma) - q(\gamma_0)) = (\gamma - \gamma_0)^\sigma \quad (5)$$

for small $\gamma - \gamma_0$.

- At $\gamma_0$, there is a *dimensional reduction* of the real space correlation function. This means that comparing the correlation function to an Ornstein-Zernike correlation function

$$\langle S(0)S(x) \rangle \propto e^{-x/\xi}/r^{(d-1)/2} \quad (6)$$

the underlying problem seems to have a lower dimension than the original physical problem, i.e. $d < 1 + 1$ here.

In the case of the frustrated antiferromagnetic Heisenberg quantum spin chain, there is no ordered zero-temperature phase. However, the quantum spin chain at zero temperature may be mapped to a classical spin chain at finite temperature. From the non-linear sigma model it is known that at least for the unfrustrated Heisenberg model the temperature $T$ of the classical chain is linked to the quantum spin $S$ by

$$T \propto 1/S \quad (7)$$
The classical spin chain at finite temperatures is disordered due to the Mermin-Wagner theorem, but it is ordered at $T = 0$. Reconsidering the arguments at the beginning of this section, replacing temperature by inverse spin, one sees that the $T = 0$ classical spin chain provides the required commensurate and incommensurate ordered low-temperature phases.

In the case of the relationship between the AKLT model and the antiferromagnetic Heisenberg chain, one has to consider a general bilinear-biquadratic spin chain as the simplest generalized Hamiltonian containing both models; it actually shows a phase transition between an ordered commensurate and an ordered incommensurate phase in the classical limit. The disorder point in that case, which was identified as the AKLT model, is thus a quantum remnant of the classical phase transition.

For a classical frustrated antiferromagnetic Heisenberg chain, there is a similar phase transition. For $\alpha < \alpha_c = 0.25$, the chain is antiferromagnetically ordered:

$$\langle S_0 S_x \rangle \propto \cos qx$$

with $q = \pi$. For $\alpha > \alpha_c$, there is spiral order

$$\langle S_0 S_x \rangle \propto \cos q(\alpha)x$$

with

$$q(\alpha) = \arccos(-1/4\alpha).$$

In analogy to the bilinear-biquadratic spin chain, we may therefore predict the presence of a disorder point for a certain $\alpha_D$, exhibiting the same properties as listed above. Indeed, we can identify an $\alpha_D = 0.284(1)$, which meets the above criteria to numerical precision. Correlations become incommensurate in real space at this point (see Fig. 2). The wave number $q$ for $\alpha > \alpha_D$ (Fig. 4) obtained from fits to a two-dimensional Ornstein-Zernike correlation function

$$\langle S_0 S_x \rangle \propto \cos q(\alpha)x \frac{\exp(-x/\xi(\alpha))}{\sqrt{x}}$$
shows the expected singular behavior; the singularity is roughly square-root-like. Figure 3 shows a minimum of $\xi \approx 1.20$ at this point, and a very steep slope of $\xi$ for $\alpha < \alpha_D$. It is numerically not infinite but clearly much bigger than the slope on the incommensurate side. We are not able to show the dimensional reduction at the disorder point numerically; at very small correlation lengths, it is hard to distinguish between purely exponential and mixed exponential-power law behavior. At the disorder point, it seems easier to obtain a purely exponential fit to the correlation function; but the data does not seem precise enough that we would want to make a definite statement here.

In the case of the AKLT disorder point this identification was easily possible due to the analytically known properties of its ground state. As all other data ties in extremely well into a very plausible physical scenario, we are convinced that our identification is correct.

For $0.37 < \alpha < 0.375$ we find the associated Lifshitz point, where the $S(q)$ structure function develops a two-peak structure (see Fig. 5). There is no particular behavior of the structure function at the disorder point apart from a maximal broadening due to the minimum in $\xi$. This point has already been found by Pati et al.\textsuperscript{15,16} to be at 0.39(1). As we have investigated longer chains at higher precision, we consider our result to be more precise. In any case, this minor disagreement has no direct physical implications.

The particular feature of the Lifshitz point is the development of a \textit{doubly-degenerate} structure of the excitation spectrum. Let us remark that the existence of two fundamentally different spectra has already been predicted by Allen and Sénéchal;\textsuperscript{14} they had numerical data suggesting that spectra switch at $\alpha \approx 0.4$.

Let us consider closed chains (all statements in the following are for chains of \textit{even} length). In the AKLT phase, a closed chain can be simulated numerically by adding a spin $\frac{1}{2}$ at each chain end, \textit{as long as the energy to excite the bonds of these spins to the chain exceeds the bulk gap energy}. We find numerically for this modified chain:

- $\alpha < \alpha_L$: The ground state is given by the lowest 0− state. The first bulk excitation is given by the lowest 1+ state, which does not degenerate with the lowest 1− state.
• $\alpha > \alpha_L$: At the Lifshitz point, the lowest 1+ state degenerates with the lowest 1− state, which was higher in energy in the single-state spectrum. This corresponds to the double peak structure evolving in $S(q)$: classically speaking, the two degenerate states correspond to spin waves $\cos qx$ (even parity) and $\sin qx$ (odd parity). The ground state is still given by the lowest 0− state.

These observations can be reproduced in unmodified open chains, if edge excitations are excluded from the spectrum (see Figs. 12 and 13, discussion in Section V).

Let us briefly discuss the behavior of the gap and the string order parameter. As can be seen from figures 7 and 6, the maximum of neither is associated with one of the two special points just discussed. This is no surprise in the case of the gap, which has no particular relationship to the disorder point phenomenon. The maximum of the string order parameter lies at $0.33 < \alpha < 0.335$, clearly separated from the disorder point. In our previous study we found the maximum of the string order parameter to be at the disorder point. This was however a particular feature due to the identification of the AKLT point as the disorder point in the bilinear-biquadratic $S = 1$ spin chain. As the string order parameter is particularly adapted to the AKLT model, it showed its maximum there. In our present study, the disorder point need not be (and obviously is not) associated with the frustrated Hamiltonian “closest” to the AKLT model in a generalized coupling space.

C. The Next-Nearest Neighbor AKLT Phase

In the limiting case $\alpha = \infty$, the frustrated chain decomposes into two unfrustrated chains on the even and odd sites. Each of these chains can be adequately described by the conventional AKLT model. We thus use the next-nearest neighbor AKLT model as shown in Fig. 1 as starting point for our argumentation. Observe that in an open chain, there are two free $S = \frac{1}{2}$ spins at each chain end, which we link up by nearest-neighbor singlet bonds. There are therefore no free end spins, and the ground state of an open chain is not degenerate. This can be verified numerically. The low-lying bulk excitation
spectrum retains its doubly-degenerate structure. The ground state energy per site should asymptotically behave as \( E_0(0)\alpha \), where \( E_0(0) \) is the ground state energy of the unfrustrated chain. Fig. 11 shows that the asymptotic behavior is already reached for intermediate \( \alpha \), lending support to our variational ansatz. We expect an excitation gap of \( \Delta(\alpha) = \Delta(0)\alpha \) in the \( \alpha \to \infty \) limit. Our numerical calculations (Fig. 7) show that the asymptotic behavior of the gap is already approached for intermediate \( \alpha \), lending further support to the variational ansatz. The observed gap exceeds the asymptotically expected gap, as it costs more energy to excite a chain which is still (weakly) linked to the other one.

In the limit of very strong frustration, we expect also a correlation length which is twice the unfrustrated correlation length, due to the doubling of the lattice spacing: \( \xi(\alpha \to \infty) = 12.04 \). For the correlation length we observe numerically a drop away from the transition point to a plateau of \( \xi \approx 10 \) at \( \alpha \approx 2 \), with an increase of \( \xi \) for larger \( \alpha \). The correlation length is smaller than asymptotically expected, corresponding to the too large gap. We cannot make any statement on the large-\( \alpha \) behavior, as the DMRG precision becomes insufficient.

Let us now address the question whether there is an order parameter characterizing this phase in analogy to the conventional string order parameter in the AKLT phase. Considering the next-nearest neighbor AKLT model, the natural generalization of the string order parameter is given by

\[
G^z(\pi)(i, j) = \langle S^z_i \exp \sum_{k=i+2,...}^{k<j} i\pi S^z_k S^z_j \rangle, \tag{12}
\]

where \( i \) and \( j \) are both even (odd), i.e. on the same subchain. At least for \( \alpha = \infty \), this must be a good order parameter.

We observe numerically that \( G \) vanishes in the AKLT phase with a decay length substantially shorter than the spin-spin correlation length. In the NNN-AKLT phase it does not exhibit a finite value for \( |i - j| \to \infty \) (consider Fig. 9). The decay can be very well fitted to an exponential; a power-law decay is excluded for the values we have considered. In contrast to the conventional string order parameter, our generalization is thus not an
order parameter. However, it does characterize the nature of this phase in accordance with our analytical model: above $\alpha \approx 1$, the decay lengths are typically much longer than the associated spin-spin correlation lengths: for $\alpha = 2$, the ratio is already of the order of 10. We argue that the difference to the Haldane phase is given by the restoration of the $Z_2 \times Z_2$ symmetry on the chain, as characterized by the disappearance of the conventional string order parameter. In the AKLT picture this is graphically represented by the two nearest-neighbor singlet bonds at the chain ends. In the finite frustration case, we characterize the symmetry on each subchain as “almost” broken: obviously it is broken on the isolated subchains; but the coupling between the subchains (weaker with increasing $\alpha$) restores the symmetry on a length scale much longer than the system correlation length. The following simple picture can help to illustrate this phenomenon physically: the difference between our AKLT phase and the exact AKLT state is that in the AKLT phase there exist bound pairs of solitons in the hidden (string) order, and the same applies to the subchains in our NNN-AKLT phase, but now there is a nonzero probability of having a bound pair with solitons sitting on different subchains, which destroys the long-range string order inside subchains on the scale which is roughly the mean distance between soliton pairs. For the Heisenberg point, variational studies indicate that this mean distance is about 60 lattice sites. However, we have no argument at the moment concerning the $\alpha$ dependence of this length scale. Further work is necessary to fully understand this phenomenon.

D. The First Order Phase Transition at $\alpha = 0.7444(6)$

The remaining question is how the change from the AKLT to the NNN-AKLT phase at $\alpha = 0.7444(6)$ can be characterized. Basically, we have to decide between (i) no transition, but a gradual change; (ii) a first-order phase transition; (iii) a continuous phase transition. Let us recall that in the related bilinear-biquadratic $S = 1$ quantum spin chain there is a continuous phase transition on the incommensurate side of the disorder point at the Lai-Sutherland point. In the following, we want to discuss our numerical and analytical
evidence which definitely excludes a critical point and thus a continuous phase transition, and clearly indicates a first-order transition. Let us first present the raw data.

In the AKLT phase below the transition, we observe a finite correlation length peaking at the transition with a value of $\xi \approx 18$ (see Fig. 8). This data, obtained from chains of $L \leq 380$, clearly excludes a continuous phase transition, which would require a divergent correlation length on both sides of the transition. In the NNN-AKLT phase, the correlation length is much longer. Immediately above the transition, our numerical data does not allow the extraction of a reasonable correlation length. We can thus not decide whether it is finite or divergent at the transition in the NNN-AKLT phase. This behavior corresponds to a pronounced peak in the structure function, but there is no particular behavior of the peak location $q$. Apart from the exclusion of a continuous phase transition, the apparent discontinuity in the correlation length strongly suggests a first order transition.

We observe a finite gap $\Delta(\alpha)$ (Fig. 7) everywhere in the same range. This fact is obscured by the presence of parasitic low-lying states corresponding to edge excitations, as explained in Section V. The minimal gap is rather small, $\Delta \approx 0.10$, to be compared with a variational prediction of $\Delta = 0.325$. At the transition, the precision of the gap is not too high; estimates we give are at the lower bound. In the AKLT phase, the observation of a finite gap ties in with the observation of a finite correlation length. The case of the NNN-AKLT phase we will discuss below.

Our main argument in favor of the first order transition is the clearly discontinuous disappearance of the string order parameter (Fig. 5). We observe numerically a jump of 0.085 (20 percent of its maximum value) between $\alpha = 0.74375$ and $\alpha = 0.74500$. Up to $\alpha = 0.74375$, the string order parameter decays almost linearly; at this point the slope increases about sixtyfold. We think it is therefore extremely unlikely that there is a crossover from this linear behavior to an extremely strong power-law decay (as in a continuous transition), but identify this behavior as a discontinuous jump.

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 at least in the AKLT phase, it is long enough to suggest a rather soft first-order transition. The presence of degenerate edge states at the transition further obscures the numerical data.

Another characteristic feature of a first-order transition is the so-called level crossing: at the transition, the energy of one of the two ground states involved drops below the other one. Typically, certain wave function symmetries change at the transition, and close to the transition, in each phase there should be a trace of the ground state of the other phase. Considering the non-local order parameter, one may not expect that the symmetry changed is revealed in a change of parity or the total spin of the ground state, two quantities we control. Actually, the ground state is 0+ in both phases. But its degeneracy changes from 4 (AKLT) to 1 (NNN-AKLT), indicating the change of some more complex wave function symmetry.

We propose the following physical scenario at the transition, which is strongly supported by our numerical data, and which gives a mechanism for the first-order transition:

- **Below** the transition, in the AKLT phase, we find a 1+ edge excitation (see Section V, Figs. [12] and [13]), which degenerates with the ground state at the transition. This edge excitation is a precursor state of the transition: In the 0+, 1− and 1+ state we observe that the center of the chain is characterized by an exponential decay of correlations. We say it is in the bulk phase, which is just the AKLT phase. Close to the transition the chain ends, however, belong to a different edge phase: as we calculate spin-spin correlations symmetrized around the center, this is evidenced by a clear change in the spin-spin correlation function. For longer chains at fixed α, we find that the bulk region grows, but not the edge region, showing that we are in fact dealing with an end effect. We call this a pseudo coexistence of phases: though they coexist on the finite chain, the edge phase is not extensive; in the thermodynamical limit it is just a boundary effect, so there is no true coexistence. We may however consider the chain ends as a nucleation center for the new phase: we suppose this is because the open
chain ends allow a lowering of energy by replacing an AKLT chain with free end spins by two chains, whose free end spins can be bound by singlets, which lower the energy. We identify the edge phase with the NNN-AKLT phase, because its influence exists only close to the transition and the string order parameter does not develop a finite long-range value in the edge phase. At the transition the AKLT bulk phase, whose correlation length is finite all the way, is pushed out entirely, as the NNN-AKLT edge phase becomes extensive. At this point, the $0^+$, $1^+$ and $1^-$ states are degenerate (to numerical precision). The bulk excitation of the AKLT phase has a finite gap up to the transition.

- **Above** the transition, in the NNN-AKLT phase, there is no bulk-edge separation in the ground state. There is a low-lying $1^\pm$ pair of states (almost) degenerate with the ground state at the transition, emerging as low-lying excitations. The magnetization is concentrated in the chain ends, shifting towards the center, as the energy cost of this excitation approaches that of a NNN-AKLT bulk excitation. Calculating increasing chain lengths for fixed $\alpha$, the magnetization remains at the chain ends. These excitations must thus be classified as edge excitations, until the gap between $1^\pm$ and $0^+$ becomes of the order of the bulk gap between $2^\pm$ and $1^\pm$. We observe the following interesting phenomenon: Up to the discontinuous jump, the string order parameters as calculated in the $0^+$ and the $1^\pm$ states agree to numerical precision, excluding the edge regions. After the transition, the string order decays fast to zero in the $0^+$ ground state, but remains non-zero in the bulk of the $1^\pm$ states much longer before decaying. With increasing $\alpha$ (as the excitation wanders into the bulk) the decay behaviour approaches that of the $0^+$ state, and the string order starts fluctuating strongly. The effect disappears at $\alpha \approx 0.80$. The correlation length observed in the center region ties in well with the AKLT correlation length just below the transition.

We suggest, on the above grounds, that those $1^\pm$ states are the trace of the old AKLT ground state in the new phase, however, “polluted” by parasitic edge excitations.
Then, the described spectrum behavior is consistent with the level crossing picture and with all the other data indicating the first order transition. Assuming that the spin wave velocity does not diverge at the transition, our gap curve would suggest that the correlation length is finite on the NNN-AKLT side of the transition also.

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 \( \alpha_T^{\text{var}} = 0.75 \) (see next section).

In the following we discuss in more detail our variational and numerical approaches.

**IV. ANALYTICAL RESULTS: VARIATIONAL APPROACH TO THE FRUSTRATED SPIN CHAIN**

In the following we are presenting our variational calculations. Such calculations are very useful to understand the nature of the ground state and the excitations of quantum systems, and even get a quantitative estimate of energies. However, strictly speaking, no variational result can be considered a strong argument, as far as the nature or very existence of a phase transition is concerned. Nevertheless, in many cases a variational study of the ground state and the elementary excitations, while looking for the possible points where the gap closes, turns out to be useful and gives an important hint of the actual system behavior. For example, variational studies of the solitonic excitations in the \( S = 1 \) chain\(^{20,34-36}\) allow one to reproduce qualitatively the structure of the phase diagram in the presence of anisotropies, biquadratic exchange, and an external magnetic field; a variational study of the Shastry-Sutherland-type\(^{37}\) solitons in the dimer order qualitatively captures the picture of the transition from the dimerized to the nondimerized phase.\(^{38}\) Therefore we will present here the variational results for frustrated \( S = 1 \) chain as arguments complementing the numeric findings. The good agreement between the physical assumptions underlying the variational ansatz and the numerical results shows that we capture essential parts of the physics of the frustrated \( S = 1 \) chain.
A. Ground State and Elementary Excitations: A Naive Approach

In the most naive way, one can attempt to describe the ground state of the frustrated $S = 1$ chain as being the AKLT state below an $\alpha_{T}^{\text{var}}$ and NNN-AKLT state above. The ground state energy per spin $E_{0}$ then would be $E_{0}^{\text{AKLT}} = -4/3 + 4\alpha/9$ in the AKLT phase and $E_{0}^{\text{NNN}} = -4\alpha/3$ in the NNN-AKLT phase, which gives a rough (but surprisingly good, see Fig. 10) estimate for the transition point $\alpha_{T}^{\text{var}} = \frac{3}{4}$.

The elementary excitations in the AKLT phase then can be studied in a soliton approach in the spirit of Refs. 19,20. Technically this is most easily done in the matrix product states formalism. Let us briefly summarize the results. The AKLT state can be represented in the form of a trace over the matrix product

$$|\text{AKLT}\rangle = \text{Tr}(\prod_{i=1}^{N} g_{i}), \quad (13)$$

where

$$g_{i} = \frac{1}{\sqrt{3}} \begin{pmatrix} |0\rangle_{i} & -\sqrt{2}|+\rangle_{i} \\ \sqrt{2}|-\rangle_{i} & -|0\rangle_{i} \end{pmatrix} \quad (14)$$

is a 2×2 matrix composed of the spin states of the $i$-th site. The soliton ("crackion," in the terminology of Fath and Solyom) state $|C^{\mu}_{n}\rangle$, describing the soliton in the string order located at the $n$-th site and having $S^{z} = \mu$, $\mu = 0, \pm 1$, can be written as

$$|C^{\mu}_{n}\rangle = \text{Tr}(\prod_{i=1}^{n-1} g_{i}(\sigma^{\mu}g_{n}) \prod_{i=n+1}^{N} g_{i}), \quad (15)$$

where $\sigma^{\mu}$ denotes the Pauli matrices in the spherical basis. Physical excitations with a definite momentum can be easily constructed as $|C^{\mu}(k)\rangle = \sum_{n} e^{ikn}|C^{\mu}_{n}\rangle$, and their dispersion is

$$\varepsilon^{\mu}(k) = \frac{\langle C^{\mu}(k)| (\hat{H} - E_{0}) |C^{\mu}(k)\rangle}{\langle C^{\mu}(k) | C^{\mu}(k) \rangle}. \quad (20)$$

The averages can be calculated using the transfer matrix technique (see Refs. 40,41), and finally, after a simple but lengthy calculation, one arrives at the following formula for the dispersion law of the soliton excitation at $\alpha < 0.75$:
\[ \varepsilon^{\mu}(k) = \frac{14}{9} + \frac{26}{27} \alpha + \frac{160\alpha - 18}{27} \cos(k) - \frac{14}{9} \alpha \cos(2k) \\
+ (2 - 26\alpha/3) \frac{3 + 5\cos(k)}{5 + 3\cos(k)} \]
(16)

Because of the isotropy of the problem, all three branches with different \( \mu \) are degenerate.

A few typical dispersion curves at different values of \( \alpha \) are displayed in Fig. 14. One can see that above some critical \( \alpha = \alpha_{L}^{\text{var}} \simeq 0.32 \), the minimum of the excitation energy is found for a momentum \( k = q_0 \neq \pi \), and \( q_0 \) tends to \( 2\pi/3 \) as \( \alpha \) tends to \( \alpha_{L}^{\text{var}} = \frac{2}{3} \) (see Fig. 11). One may speculate this point \( \alpha_{L}^{\text{var}} \) can be identified with the Lifshitz point, though in fact there are no incommensurate correlations in the AKLT state. Note that in the numerical calculations the lowest excitation becomes doubly degenerate when \( \alpha \) crosses the Lifshitz point. This can be easily explained by the fact that the two minima of the dispersion curve at \( k = \pm q_0 \) are physically inequivalent if \( q_0 \neq 0, \pi \).

The gap does not disappear at the transition point \( (\Delta_{\text{var}}(\alpha = 0.75) \simeq 0.325) \), indicating a first-order phase transition (or absence of a phase transition). The \( \alpha \) dependencies of the gap \( \Delta_{\text{var}} \) and of the wavevector \( q_{0,\text{var}}^{\text{var}} \) with minimal excitation energy obtained from this simple calculation qualitatively agree with the numerical data (see Figs. 7 and 11).

On the other side of the transition point we take the NNN-AKLT state (Fig. 1) as a variational ground state, and the soliton dispersion in the thermodynamic limit \( L \to \infty \) (when the chains become decomposed in the NNN-AKLT picture) can be obtained from (16) by first setting \( \alpha \) to zero, replacing \( k \to 2k \), and finally scaling the whole expression by \( \alpha \); this gives for \( \alpha > 0.75 \) the gap \( E_g = 2\alpha/9 \) (similarly to \( E_g = 2/9 \) at the Heisenberg point \( \alpha = 0 \)) and \( q_0 = \pi/2 \) as wavevector with minimal excitation energy. Actually, as it follows from the numerics, \( E_g(\alpha) \to \alpha E_g(0) \) only asymptotically at \( \alpha \to \infty \), but one can also see from the numerical data that this asymptotic linear behavior above \( \alpha = 0.75 \) sets in rather quickly.
B. 4 × 4 Matrix Product Variational Ansatz

The “purely AKLT” description presented above is of course not very satisfactory: in fact, we did not even have any variational parameters and simply compared two VBS configurations being intuitively good candidates for the ground state. However, it is easy to see that those two choices are not the only possible ones: 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. One thus may try to consider some more general variational wavefunction capable of interpolating between different VBS states.

We have found that such wavefunctions can be constructed in the matrix product states formalism, at the price of going to a higher matrix dimension and considering larger clusters. One possible simplest choice for the elementary matrix is

$$\Gamma_{12} = \sum_{ij} |t_{ij}\rangle \{ A\delta_{ij} (\mathbb{1} \otimes \mathbb{1}) + iB\varepsilon_{ijk} (\sigma_k \otimes \mathbb{1}) + iC (\sigma_i \otimes \sigma_j) \} \ ,$$

where the matrix state $\Gamma_{12}$ lives on a cell consisting of two adjacent spins 1 and 2. $\sigma_i$, $i = x, y, z$ are the usual Pauli matrices (in the cartesian basis), $\mathbb{1}$ denotes the $2 \times 2$ identity matrix, and $|t_i\rangle$ denotes the triplet of spin-1 states in the cartesian basis:

- $|t_x\rangle = -(1/\sqrt{2})(|+\rangle - |-\rangle)$,
- $|t_y\rangle = (i/\sqrt{2})(|+\rangle + |-\rangle)$,
- $|t_z\rangle = |0\rangle$.

Since both the Pauli matrices and the triplet wavefunctions $|t_i\rangle$ behave as vectors under rotations, the matrix $[\text{17}]$ behaves as a scalar. Therefore, the matrix product state

$$|\Omega\rangle = \text{Tr} \left( \prod_t \Gamma_{2t-1,2t} \right) \ ,$$

constructed from such elementary matrices, obeys the rotational invariance of the problem (note that the usual AKLT matrix $[\text{14}]$ is unitary equivalent to $(1/\sqrt{3}) \sum \sigma_i |t_i\rangle$, and this
is the only possible rotationally invariant ansatz if the dimension is 2×2 and the matrix lives at one site, but in higher dimensions and for larger cluster sizes the number of choices rapidly increases).

The wavefunction \(|\Psi\rangle\) has the remarkable property that it interpolates smoothly between the AKLT state \((A = B = 1/3, C = 0)\), the completely dimerized state \((A = 1/\sqrt{3}, B = C = 0)\), and the NNN-AKLT state \((A = B = 0, C = 1/3)\).

The quantum averages can be calculated in the usual way; however, the complexity of solving the analytic eigenvalue problem for the 16×16 transfer matrix \(G = \Gamma_{12}^\dagger\Gamma_{12}\) forced us to restrict ourselves to the case of real coefficients \(A, B, C\). Then, setting the largest eigenvalue of \(G\) to 1, one obtains the normalization condition

\[
3(A^2 + 2B^2 + 3C^2) = 1 \tag{19}
\]

which leaves us with two independent real variational parameters. The variational expression for the ground state energy per spin

\[
E_{\text{var}} = -4\alpha/3 + 4B^2(4\alpha - 3) - 3(A^2 - B^2) \tag{20}
\]

\[
+ 2(A - B)\left\{2A^3 + 10A^2B + AB^2 - 2A/3 \right. \\
+ 5B^3 - 10B/3 + \alpha[-10A^3 - 10A^2B \\
- 2AB^2 + 16(A + B)/3 - 2B^3]\right\}
\]

can be minimized numerically; the resulting dependence of the ground state energy on \(\alpha\) is presented in Fig. 10. The main feature is that though the discontinuity at the transition is less distinct than in the “naive” picture, and the transition point shifted towards larger \(\alpha \simeq 0.81\), the transition still is found to be first order. At the Heisenberg point \(\alpha = 0\) the variational result for the ground state energy is \(E_{\text{var}}^{\text{min}} = -1.364\), being slightly better than the AKLT value \(-\frac{4}{3}\). However, the disadvantage of the ansatz (18) is that it explicitly breaks the translational invariance, and thus the ground state has a built-in dimerization which is always nonzero.
The lowest excitations above this variational ground state can be calculated using the single-mode approximation in the spirit of Arovas et al.\textsuperscript{42} Since we have now two spins involved in the elementary matrix (17), it is natural to write down the wavefunction of the excited state in the form $|\tilde{C}^\mu(k)\rangle = \sum_n e^{i k n} |\tilde{C}^\mu_n\rangle$, where

$$|\tilde{C}^\mu_n\rangle = \text{Tr}(\prod_{l=1}^{n-1} \Gamma_{2l-1,2l} \cdot \Gamma^\mu_C \cdot \prod_{l=n+1}^{N} \Gamma_{2l-1,2l})\cdot \Gamma^\mu_C = (\tilde{S}_l^\mu + \lambda(k) \cdot \tilde{S}_l^\mu) \Gamma_{2n-1,2n}.$$  

Here $\tilde{S}_l^\mu$ denote the components of the spin-1 operator at the $l$-th site, $\lambda$ is an additional (complex) variational parameter whose value has to be determined numerically for each value of the wavevector $k$, and $k$ now varies from 0 to $\pi/2$ since the elementary cell is doubled. The resulting gap dependence on $\alpha$ is shown in Fig. 7. One can see that there is a local minimum around $\alpha = 0.75$, but the gap in the transition region is considerably overestimated, even comparing to the naive approach described in the previous subsection; we attribute this fact to the built-in breaking of the translational invariance in the ansatz (18) as explained above.

V. NUMERICAL RESULTS: DENSITY MATRIX RENORMALIZATION GROUP CALCULATIONS

A. General Remarks

Using the Density Matrix Renormalization Group (DMRG), we have calculated for this problem (i) the gap between the ground state and the lowest excitation, (ii) the magnetization for the lowest excited state, (iii) the string order parameter $\mathcal{O}$ and the string correlator $\mathcal{G}$ and (iv) the spin-spin correlation function. For details on the DMRG we refer to the literature.\textsuperscript{5,21} The DMRG is particularly suited for the problem under study as it is not limited to small systems like exact diagonalization and as it is not plagued by the negative sign problem which Quantum Monte Carlo typically encounters in frustrated systems at very low temperatures.
For our calculations, we have studied chains of a length up to \( L = 380 \) and typically kept \( M = 250 \) block states in each iteration. To reduce both memory usage and improve program execution speed, we have used the following DMRG features:

- We have used both the total magnetization and left-right parity as good quantum numbers. This reduces storage, but also thins out the Hilbert space, giving faster convergence of the implemented exact diagonalization, and allows for fast classification of the spectrum.

- We have implemented a prediction algorithm which gives a guess for the eigenstates of a DMRG step based on the eigenstates of the preceding DMRG step. This algorithm, similar in spirit to the one introduced recently by White, allows for a substantial reduction of the number of iterations needed in the exact diagonalization, truncating it by a factor of up to 10. It should however be mentioned that the speed-up due to the prediction algorithm is biggest when the studied system has a rather short correlation length; so its use is somewhat limited there where most performance would be needed. A further problem is that it does not cut the time needed for the calculation of expectation values, a dominant feature of our calculations.

It is important to realize that (unlike in exact diagonalization studies) it is not sufficient to extrapolate results to the thermodynamic limit in \( L \) only. The performance of the DMRG depends crucially on the number \( M \) of block states kept; as a rule of thumb, the number of states \( M \) to be kept increases dramatically close to critical points or phase transitions, which reflects the increasing number of low-energy fluctuations or competing states. The precision of the DMRG is indicated by the truncation error, which allows for extrapolations to the exact \( M = \infty \) result. Let us remark that good agreement between DMRG and exact diagonalization results for a given \( M \) is not necessarily an indicator of good DMRG precision: exactly diagonalizable systems are notoriously small, and our results indicate that DMRG errors build up severely with system length.

We found that close to the disorder and Lifshitz points (a region where the ground state
should have a relatively simple valence bond structure) $M = 80$ is sufficient to give highly precise results; near the phase transition, convergence up to $M = 200$ was poor, forcing us to go up to $M = 250$ states. It was not possible to go to the limit of very high $\alpha$: in this case, the chain essentially decouples into two subchains, leading to a ground state which can be understood as a product state of the ground states of two unfrustrated chains. The description of such a product state implies a dramatic increase in $M$, as already observed in other works.

The numerical investigation of the phase transition was further complicated by the fact that the DMRG works best for open boundary conditions. At the transition point it was therefore not possible to use periodic boundary conditions, as the precision obtained for open ones was already only moderate. Open boundary conditions may however introduce additional edge states into the spectrum which suggest often radically different physical properties. A good example is provided by the unfrustrated open integer spin chain with spin $S$, where there are two effectively free $S/2$ spins at each chain end. For the $S = 1$ chain these free spins introduce the well-known Kennedy triplet, which degenerates with the ground state. One therefore has the fifth state as the first bulk excitation. In the frustrated chain, the situation will be shown to be not always as clear. To identify the lowest bulk excitation, it is therefore necessary to calculate $\langle S^z_i \rangle$ for all low-lying states. Edge excitations due to the open chain ends can be identified by very small $\langle S^z_i \rangle$ in the chain center and big $\langle S^z_i \rangle$ at the chain ends and thus excluded.

B. Calculation of Correlations

For $\alpha < \alpha_D$ spin-spin correlation lengths can be obtained by a fit of the spin-spin correlations to a law $(-1)^x \exp(-x/\xi)/\sqrt{x}$, which is in all cases extremely well obeyed, except exactly at the disorder point. Note that all DMRG correlation lengths are underestimations of the true correlation length. For the longest correlation length in that region (at $\alpha = 0$), we obtain $\xi \approx 5.8$, underestimating the true result by about 3 percent. As the
correlation length decreases as well as the truncation error with $\alpha$ (it is essentially 0 at the disorder point), the error diminishes. The correlation length at the disorder point we estimate to be precise to the order of 1 percent or better. All other correlation lengths lie in between. For $\alpha > \alpha_D$, correlation lengths are obtained by a least square fit of the data to a law $\cos qx \exp(-x/\xi)/\sqrt{x}$, with $q$ and $\xi$ to be determined. Extremely good such fits could be obtained. Alternatively, one may simply plot $|\langle S_i S_j \rangle|/\sqrt{|i-j|}$ logarithmically. As the logarithm is not very sensitive close to correlation function maxima, simply drawing an upper straight-line envelope gives a very simple estimate which is hardly worse despite the incommensurate correlations. Again, the correlations obtained in that way are underestimated. Considering the results for various $M$ we claim that we underestimate at worst by about 20 percent around the transition; at the transition itself, the data is inconclusive on the NNN-AKLT side. Just below the transition, edge effects become strong, and have to be excluded from the calculation of the correlation length. In short chains, the bulk behaviour may not be visible. Edge effects can be identified by calculating longer chains: the region of bulk behavior extends with $L$.

The string order parameter is a quantity particularly suited for treatment by the DMRG: It reaches its thermodynamical limit very fast; the decay to the thermodynamical limit is on a scale of the order of half the bulk spin-spin correlation length, as was already observed for unfrustrated spin chains. Its convergence to its exact value in $M$ is also very fast, unlike the convergence of the correlation length.

C. Gap Calculations: The Spectrum of Open Chains

The calculation of the bulk excitation gap was the most difficult calculation performed, because of the already mentioned problem of edge excitations inherent to open chains as used by the DMRG. Ground state and lowest excited state energies were first extrapolated in $M$ for fixed $L$ (using the roughly linear dependence of the error in energies on the DMRG truncation error) and then extrapolated in $L$ using quadratic convergence laws, which are
very well verified. This allows us to obtain gaps with a precision up to $10^{-3}$, at least 0.02 at the transition. The essential difficulty arises from the correct identification of the lowest bulk excitation. For most values of frustration, this can be nicely done by calculating the $\langle S^z_i \rangle$ distribution along the chain for $S^z_{\text{total}} = S_{\text{total}}$ (see Fig. 12). Typically, it is very easy to distinguish true bulk excitations from edge excitations. To devise a more stringent criterion, it is useful to study the rather rich behavior of the low-energy excitation spectrum of open frustrated chains, as the DMRG deals best with open systems. In fact, though the open chain spectrum is more complicated, the mechanism of the phase transition is better revealed here, as the associated symmetry breaking is obvious in the presence or absence of effectively free end spins. We find the following scenario (all statements for chains of even length; example spectra are given in Fig. 13; the arrow indicates the gap energy):

- $\alpha < \alpha_D$: The ground state is given by the lowest 0+ state: there is an odd number of singlet bonds in the bulk, the two effectively free end spins are linked by an extremely weak singlet bond, giving a total even number of singlet bonds. Exciting this weak singlet bond gives a 1− triplet excitation, degenerating with the ground state (the Kennedy triplet). The first bulk excitation is given by the 2+ quintuplet excitation, combining a bulk and an edge excitation. The 2− quintuplet is not degenerate with the 2+ quintuplet, and can be identified as an edge excitation.

- $\alpha_D < \alpha < \alpha_L$: The open boundary conditions introduce a further parasitic edge excitation 1+: this edge excitation we identify from its evolution with $\alpha$ as a precursor of the phase transition and the NNN-AKLT phase. Even parity coupling of edge spins is energetically disfavored in the AKLT phase, 1+ lies much higher than 1−.

- $\alpha_L < \alpha < \alpha_T$: As already described for the closed chain, the bulk excitations degenerate in pairs of odd and even parity excitations with identical total spin. The ground state is still the same 0+ state, there is a degenerate Kennedy triplet 1−. The lowest bulk excitations are now given by the degenerate 2± quintuplet excitation, combining a 1± bulk excitation with a 1− edge excitation (see Fig. 12). The 1+ edge excitation
lowers its energy with $\alpha$, degenerating with the ground state at $\alpha_T$. For numerical calculations it is important to realize that there may be two $S = 1$ excitations below the true bulk excitation. Following the gap calculation procedure described by Pati et al.,\textsuperscript{16} we can explain the difference between their and our gap curve for $\alpha \approx 0.5$ arguing that they have measured the energy difference between the two edge excitations. The numbers we obtain that way agree perfectly with theirs. As the 1+ edge excitation degenerates with the 1− excitation at the transition, a vanishing gap is suggested, as reported in their work. This is however not the true bulk excitation.

• $\alpha = \alpha_T$: For the behavior of the spectrum at the transition, we refer to Section III D.

• $\alpha > \alpha_T$: Beyond the transition, the ground state 0+ is unique, as the Kennedy triplet disappears. The situation is basically not very complicated for the lowest bulk excitation: there is a doubly degenerate 1± bulk excitation as below the transition. The actual location of this state in the complete spectrum of the open chain however varies: just above the transition, there are low-lying 1± edge excitations. The bulk excitation is hidden in the lowest 2± state. For intermediate and strong frustration, the chain decouples effectively into two subchains which are only weakly interacting: The nearest-neighbor singlet bonds at the chain ends become increasingly easy to excite for increasing $\alpha$, giving four free spins-$1\over 2$. These couple into 16 states degenerating for $\alpha \rightarrow \infty$, coupling into one 0+, two 1−, one 1+ and one 2+ state. The bulk gap, on the other hand, scales with $\alpha$. As soon as edge excitation energies drop below the bulk gap energy, the bulk excitation will only be present in higher spin states, which have to be identified by the magnetisation. Numerically, one can keep the bulk excitation in the 1± state by increasing the interaction strengths at the chain ends, to disfavor edge excitations.

We have calculated the lowest energy-states in the following sectors of the Hilbert space: 0+, 1+, 1−, 2+ and 2−, to verify the above scenario by considering the bulk magnetiza-
tion. For sufficiently long chains, it was always possible to clearly separate bulk from edge excitations as in the above scenario.

VI. CONCLUSION

The numerical results presented above together with the variational calculations allow to devise a clear and coherent picture of the behavior of a frustrated $S = 1$ isotropic Heisenberg spin chain. Its behavior is fundamentally governed by the underlying classical model, which is characterized by a phase transition from an antiferromagnetic to a spiral ordered phase. On the other hand, pure quantum effects are prominent. As predicted from the non-linear sigma model, the system is gapped for all values of frustration. However, there are two clearly separated phases present. The first one for small frustrations can be well understood in terms of the Affleck-Kennedy-Lieb-Tasaki model and is characterized by a non-vanishing conventional string order parameter. The classical phase transition is reflected by the presence of a so-called disorder point, where the spin-spin correlations become incommensurate. The classical phase transition is thus not linked to the first order phase transition found for larger frustration. The disorder point is clearly related to the disorder point in a bilinear-biquadratic quantum spin chain, which is exactly the AKLT model. The phase transition found at $\alpha = 0.7444(6)$ is purely quantal in character. It is first order, characterized by a non-vanishing gap and a finite correlation length on the AKLT side. We observe a non-continuous change both in the string order parameter and in the correlation length. The $Z_2 \times Z_2$ symmetry broken in the AKLT phase is thus restored. A string correlator which considers only every second spin characterizes this phase. We also suggest that if one includes the alternation of $[1 + (-1)^i\delta]$ type in the nearest-neighbor interaction in the Hamiltonian $[I]$, there will be a first-order transition line in the $(\alpha \delta)$ plane. Assuming that the transition line is characterized by vanishing string order, we suggest that it should be identified with the $(BC)$ line in Fig. 3 of Ref. [3] separating the region with fourfold degenerate ground state from the region where the ground state is unique. Since
for $\alpha \to 0$ and large $\delta$ the latter region coincides with the well-studied dimerized phase. The question arises whether our NNN-AKLT phase transforms smoothly into the dimerized phase or there is one more transition line separating the dimerized and the NNN-AKLT phases.

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FIGURES

FIG. 1. Schematic representation of the AKLT model and its next-nearest neighbor generalization. Circles are spin-1 sites, dots represent a spin $\frac{1}{2}$, and fat links are singlet bonds between spins. Note the presence of a free spin $\frac{1}{2}$ at each end of the open AKLT chain. In the NNN-AKLT model, the dashed line represents the underlying chain.

FIG. 2. Spin-spin correlations for various frustration values just below and above the disorder point. We show the logarithm of $|\langle S_i S_j \rangle|$ times the square root of the spin-spin distance. Purely antiferromagnetic correlations can thus be most easily distinguished from incommensurate ones, which show prominent peaks.

FIG. 3. Spin-spin correlation length $\xi(\alpha)$ in the vicinity of the disorder and Lifshitz points. Note that these correlation lengths are systematically underestimated by the DMRG. From the known $\alpha = 0$ result and the dependence of the error on the DMRG truncation error we estimate the error to be 3 percent in the worst case, typically 1 percent or better close to the disorder point.

FIG. 4. Correlation wave numbers $q(\alpha)$ in the vicinity of the disorder point obtained by fits of the correlation function to an expected Ornstein-Zernike behavior of the correlations.

FIG. 5. Structure function $S(q)$ for various values of frustration $\alpha$. The values of $\alpha$ are, ordered by decreasing $S(\pi)$, 0.3, 0.32, 0.34, 0.36, 0.37, 0.375, 0.38, 0.4, 0.5, 0.6, 0.7, and 1.5. Note the developing double peak structure for $0.37 < \alpha < 0.375$. The double peak shifts to $q = \pm \pi/4$, due to the doubling of the lattice spacing in the decoupled chains in the $\alpha \to \infty$ limit.

FIG. 6. String order parameter $\lim_{|i-j| \to \infty} O(i,j)$. The full squares show the string order parameter for the 0+ ground state; there is a discontinuous drop of 0.085 at $\alpha_T$. 
FIG. 7. Bulk excitation gap $\Delta(\alpha)$. The precision of the gap values is between 0.001 and 0.02 (close to the transition). Within the error bars, shown values were chosen to be a lower bound to the exact gap. For large $\alpha$, the gap approaches the asymptotic value $\Delta(\alpha) = \alpha \Delta(0)$. The solid and pointed lines are the analytical results for the $2\times2$ and the $4\times4$ matrix product ansatz, respectively.

FIG. 8. Spin-spin correlation lengths. Correlations lengths are systematically underestimated due to the DMRG. Around the transition the error is maximal, but will generously estimated not exceed 20 percent.

FIG. 9. Decay behavior of the generalized string correlator for various frustration values in the nnn-AKLT phase.

FIG. 10. In this figure variational and numerical ground state energies are shown. The dashed and solid lines correspond to the $2 \times 2$ and $4 \times 4$ variational ansatz respectively, the solid squares are numerical results. Numerical errors are smaller than $10^{-5}$.

FIG. 11. Dependence of the peak wavevector in the structure factor on the next-nearest neighbor coupling constant $\alpha$ is shown. Solid squares are DMRG data, the solid line is the variational result for the wavevector with the minimal excitation energy, according to (16).

FIG. 12. Magnetization of various lowest excitations for $\alpha = 0.5$. The $1^+$ and $1^-$ states are edge excitations; the $1^-$ state is the Kennedy triplet. The $2\pm$ states are a combination of the $1^-$ edge excitation and a true bulk excitation.

FIG. 13. Evolution of the excitation spectrum in the AKLT phase. E stands for pure edge excitation. Note the double degeneracy of the first excitation beyond the Lifshitz point and the appearance of a low-lying edge state beyond the disorder point. The arrow indicates the states to be compared for gap calculations.
FIG. 14. Typical dispersion curves of a soliton (“crackion”) excitation above the AKLT (solid lines) and NNN-AKLT (dashed lines) states, for different values of the next-nearest neighbor coupling $\alpha$. 
Figure 1

AKLT

| 1 | 2 | 3 | 4 | 5 | 6 |

NNN-AKLT

1 2 3 4 5 6
Figure 2

\[ \ln \left( \frac{\langle S_i S_j \rangle}{\sqrt{|i-j|}} \right) \]

\( \alpha = 0.280 \)

\[ \ln \left( \frac{\langle S_i S_j \rangle}{\sqrt{|i-j|}} \right) \]

\( \alpha = 0.285 \)

\[ \ln \left( \frac{\langle S_i S_j \rangle}{\sqrt{|i-j|}} \right) \]

\( \alpha = 0.300 \)

\[ \ln \left( \frac{\langle S_i S_j \rangle}{\sqrt{|i-j|}} \right) \]

\( \alpha = 0.400 \)
Figure 3

spin–spin correlation length

α

disorder pt  Lifshitz pt
Figure 4

wave number $q/\pi$

\begin{align*}
\text{disorder pt} & \quad \text{Lifshitz pt} \\
\alpha & \quad 0.3 \\
0.2 & \quad 0.4
\end{align*}
Figure 5

Structure function $S(q)$ versus wave number $q/\pi$. 

The graph shows multiple curves labeled with values 0.3, 0.5, 0.7, and 1.5. Each curve represents a different value of $q/\pi$. The curves peak at specific wave numbers, indicating the variation of the structure function with wave number.
Figure 6

The graph shows the string order parameter as a function of the parameter \( \alpha \). The graph includes points indicating disorder, Lifshitz, and transition points. The axes are labeled as follows:

- Y-axis: String order parameter
- X-axis: \( \alpha \)

Key features:
- Disorder point
- Lifshitz point
- Transition point
Figure 7

bulk excitation gap

transition

disord. pt  Lifshitz pt

\( \alpha \)
Figure 8

spin–spin correlation length

disorder pt

transition

$\alpha$
Figure 10

plot showing the ground state energy / spin against $\alpha$.
Figure 11
Figure 12

\[ \langle S_i^z \rangle \]

2−

\[ \langle S_i^z \rangle \]

2+

\[ \langle S_i^z \rangle \]

1−

\[ \langle S_i^z \rangle \]

1+
Figure 13

\[
\begin{align*}
\text{E} & \quad 0+ , 1- \\
\alpha = 0.28 & \\
\text{E} & \quad 0+ , 1- \\
\alpha = 0.32 & \\
\text{E} & \quad 0+ , 1- \\
\alpha = 0.4 & \\
\text{E} & \quad 0+ , 1- \\
\alpha = 0.5 & \\
\end{align*}
\]
Figure 14