

## Isotropic spin-1 chain with twisted boundary condition

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The possible ground states and the phase transitions of a spin-1 chain with bilinear-biquadratic exchange are studied numerically. In order to see better the real asymptotic behavior of the infinite system and to determine the necessary degeneracies, a twisted boundary condition is used that reduces the finite-size effects. This calculation confirms that a second-order Ising-type phase transition occurs at the Takhtajan-Babujian point from the dimerized phase to the singlet Haldane phase. The transition at the Lai-Sutherland point, to a massless phase with three soft modes, is found to be of Kosterlitz-Thouless type.

### I. INTRODUCTION

Finite-size scaling is one of the most efficient methods to study the low-energy behavior of lattice models, either in field theory or in statistical physics. It can almost always be effective even for such ranges of parameters where approaches like strong or weak coupling expansions or other nonperturbative approximate methods are unsatisfactory. Finite-size scaling was originally invented in statistical physics by Fisher and Barber,<sup>1</sup> then applied to lattice field theories by Hamer and Barber<sup>2</sup> and Roomany and Wyld.<sup>3</sup> Based on the relationship between the thermodynamic quantities of classical systems in two dimensions and their quantum analogs in 1+1 dimensions, and using the scaling properties of the classical model near the transition point, one can deduce how quantities, like the ground-state energy or the mass gap should depend on the system size at the critical point. These asymptotic forms are valid for large enough systems. Thus, analyzing the scaling properties of different finite-size approximants, one can locate the transition points, obtain the phase structure of the model, and determine the critical behavior of the infinite system.

In order to carry out a finite-size scaling study the first step is to diagonalize exactly the Hamiltonian of the finite system of linear size  $N$  for different sizes. Even with modern-day computers the accessible sizes are rather limited, especially for two- or three-dimensional systems. While in some cases relatively small system sizes are sufficient to see the asymptotic behavior, there are models where strong finite-size effects mask the expected scaling behavior. They can make the reliable extrapolation impossible, or lead to false conclusions.

There is, however, a freedom, which is our main concern in this paper, in the choice of the boundary condition (BC) of the finite system. Boundary conditions should have no influence on the quantities of interest in the thermodynamic limit, nevertheless they do have an effect in finite systems. Finding the most suitable BC can help to "transform out" the most disturbing finite-size corrections, and the system can show its "real" behavior for

much smaller sizes already.

To illustrate this let us cite the example of the antiferromagnetic spin- $S$  Heisenberg chain. It was clearly demonstrated in the pioneering work by Bonner and Fisher<sup>4</sup> for the  $S = \frac{1}{2}$  chain, that the finite-size estimates of different thermodynamic quantities are very sensitive to the chain length. They used periodic boundary condition (PBC) and found that the finite-size corrections are definitely smaller for chains with even numbers of sites. Similar oscillations appear for general  $S$ , too. Although the ground state is disordered, the short-range correlations are alternating in sign. Therefore PBC proves advantageous only if the chain consists of an even number of sites. Chains of odd length should rather be studied with an antiperiodic BC. As it will be shown in this paper, in some cases the scaling properties can be further improved by using a more subtle BC, a twisted one.

Our aim in this paper is to study the phase structure of the antiferromagnetic spin-1 chain described by the Hamiltonian

$$H = \sum_i [\cos \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin \theta (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2]. \quad (1)$$

This model is expected to show a rather colorful phase structure. In the range  $-3\pi/4 < \theta < \pi/2$ , where the ground state of finite chains is a singlet, the infinite system is believed to have at least three different phases. Using an approximate field-theory mapping to the Wess-Zumino-Witten model, Affleck<sup>5</sup> argued that there is a conventional second-order phase transition of the Ising type at  $\theta_{\text{TB}} = -\pi/4$ . At this point the model is integrable, as was shown by Takhtajan<sup>6</sup> and Babujian.<sup>7</sup> The excitation spectrum has two soft modes, at  $k = 0$  and  $k = \pi$ . For  $-3\pi/4 < \theta < -\pi/4$  the model has a doubly degenerate dimerized ground state, while for  $-\pi/4 < \theta < \pi/4$  the ground state is unique. According to Affleck<sup>5</sup> a finite gap opens above the ground state on both sides of  $\theta_{\text{TB}}$ , linearly in  $|\theta - \theta_{\text{TB}}|$ . The latter region,  $-\pi/4 < \theta < \pi/4$ , includes the traditional Heisen-

berg point  $\theta = 0$ , for which Haldane<sup>8</sup> predicted a massive behavior with a nondegenerate ground state for any integral spin  $S$ . The gap vanishes again at  $\theta_{\text{LS}} = \pi/4$ . This is another integrable point in the parameter space, where the model is equivalent to the permutation model of Lai and Sutherland.<sup>9</sup> The Bethe ansatz can be used here, too, and it gives a massless spectrum with three soft modes, at  $k = 0$  and  $k = \pm 2\pi/3$ . Affleck's mapping<sup>5</sup> to the Wess-Zumino-Witten model cannot be used for  $\theta > \theta_{\text{LS}}$ , thus there is no prediction of the field-theory model for the behavior of the magnetic system in this third region.

This picture of three phases is supported by some analytic results. At  $\theta = -\pi/2$  there is an exact correspondence between the model in Eq. (1) and the 9-state Potts model or the antiferromagnetic spin- $\frac{1}{2}$  Heisenberg-Ising chain with appropriately chosen easy-axis anisotropy.<sup>10</sup> This latter model is known to have a doubly degenerate ground state. The value of the gap can be calculated from the Bethe ansatz solution and it is nonzero. On the other side of  $\theta_{\text{TB}}$ , at  $\theta_{\text{VB}} = \arctan(\frac{1}{3})$  the ground state is an exact valence-bond state.<sup>11</sup> It is unique, the two-point correlation function decays exponentially and the existence of a finite excitation gap can also be verified.

The phase diagram was intensively studied numerically, too, to see if the above scenario is true, or to find the limitations of the approximate field-theoretic mappings. Despite the great number of works, some details still remained unclear. For the transition at  $\theta_{\text{TB}}$  some authors<sup>12,13</sup> found an extended critical region around the integrable point, others<sup>14</sup> predicted non-Ising-like scaling indices, i.e., nonlinear opening of the gap. The situation around  $\theta_{\text{LS}}$  is even less understood. Nomura and Takada<sup>15</sup> argued that for  $\theta > \theta_{\text{LS}}$  the ground state will be threefold degenerate, but this trimerized phase should be massive. Our earlier calculations<sup>13,16</sup> indicate a massless behavior with three soft modes, like at the integrable  $\theta_{\text{LS}}$  point itself. The type of the phase transition from the Haldane phase to the tripled-periodic phase has not yet been analyzed, either.

In this paper we present further finite-size scaling results on the bilinear-biquadratic model. Instead of the usual PBC, however, we use a *twisted boundary condition* in the hope of improving the scaling behavior. So far the twisted BC has been used for this model in the case  $\theta = 0$  only.<sup>17</sup> Now we extend the calculations to the whole range  $-3\pi/4 < \theta < \pi/2$ . The extrapolated properties of infinite chains can then be compared to previous results.

Our results confirm the Ising-type character of the transition at  $\theta_{\text{TB}}$ . We find further arguments to support the prediction of an extended *critical* phase for  $\theta > \pi/4$ . Based on our study of the behavior of the Callan-Symanzik  $\beta$  function, the transition to this critical phase at  $\theta_{\text{LS}}$  is proposed to be of the Kosterlitz-Thouless type.

The layout of the paper is as follows. In Sec. II the twisted boundary condition is defined and its influence on the energy spectrum is reviewed. Section III contains our results for the transition at  $\theta_{\text{TB}} = -\pi/4$  and Sec. IV those for  $\theta_{\text{LS}} = \pi/4$ . Section V contains a brief summary.

## II. TWISTED BOUNDARY CONDITION

In the numerical study of the energy spectrum of the model in Eq. (1), the Hamiltonian of a finite chain is diagonalized, fixing somehow a BC. The most commonly used BC is the periodic one. It preserves the translational invariance and the isotropy of the Hamiltonian, thus allowing to classify the energy levels according to the momentum  $k$  and the total spin quantum number  $S_T$ , and to block diagonalize the problem. The numerical diagonalization is done independently in the different blocks. The Hamiltonian with PBC will be denoted by  $H_p$ . It can be written in the form

$$H_p = \sum_{j=1}^N [\cos \theta h_{j,j+1}^{(p)} + \sin \theta (h_{j,j+1}^{(p)})^2], \quad (2)$$

with

$$h_{j,j+1}^{(p)} = \frac{1}{2} (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+) + S_j^z S_{j+1}^z, \quad (3)$$

where the PBC requires

$$\mathbf{S}_{N+1} \equiv \mathbf{S}_1. \quad (4)$$

As mentioned before, in most of this paper we will treat the model in Eq. (1) with a twisted BC. If the two ends of the chain are attached with a twist of angle  $\Phi$  around the  $z$  axis, the BC is

$$\begin{aligned} S_{N+1}^x &= S_1^x \cos \Phi - S_1^y \sin \Phi, \\ S_{N+1}^y &= S_1^x \sin \Phi + S_1^y \cos \Phi, \\ S_{N+1}^z &= S_1^z. \end{aligned} \quad (5)$$

Using raising and lowering operators,

$$\begin{aligned} S_{N+1}^+ &= S_1^+ e^{i\Phi}, \\ S_{N+1}^- &= S_1^- e^{-i\Phi}, \\ S_{N+1}^z &= S_1^z. \end{aligned} \quad (6)$$

The Hamiltonian  $H_t(\Phi)$  of this twisted model has the same form as  $H_p$  defined in Eqs. (2) and (3), except that the BC in Eq. (4) is replaced by Eq. (6). Thus the Hamiltonian takes the form

$$\begin{aligned} H_t(\Phi) &= \sum_{j=1}^{N-1} [\cos \theta h_{j,j+1}^{(p)} + \sin \theta (h_{j,j+1}^{(p)})^2] \\ &\quad + \cos \theta h_{N,1} + \sin \theta (h_{N,1})^2, \end{aligned} \quad (7)$$

where  $h_{N,1}$  is obtained from  $h_{N,N+1}^{(p)}$  by using Eq. (6) for  $\mathbf{S}_{N+1}$ ,

$$h_{N,1} = \frac{1}{2} (S_N^+ S_1^- e^{-i\Phi} + S_N^- S_1^+ e^{i\Phi}) + S_N^z S_1^z. \quad (8)$$

Due to this boundary term,  $H_t(\Phi)$  is neither translational invariant nor isotropic. The translational invariance can be restored, still maintaining the total twist  $\Phi$ , by twisting all neighboring bonds in the chain by an angle  $\Phi/N$ , i.e., analogously to Eq. (8), each bond  $h_{j,j+1}^{(p)}$  is replaced by

$$h_{j,j+1}^{(t)} = \frac{1}{2} \left( S_j^+ S_{j+1}^- e^{-i\Phi/N} + S_j^- S_{j+1}^+ e^{i\Phi/N} \right) + S_j^z S_{j+1}^z. \quad (9)$$

This yields a translationally invariant twisted Hamiltonian,

$$\tilde{H}_t(\Phi) = \sum_{j=1}^N [\cos \theta h_{j,j+1}^{(t)} + \sin \theta (h_{j,j+1}^{(t)})^2], \quad (10)$$

which is now subject to a PBC,  $\mathbf{S}_{N+1} \equiv \mathbf{S}_1$ .

It can be checked easily that the Hamiltonians  $H_t(\Phi)$  and  $\tilde{H}_t(\Phi)$  are connected by a unitary transformation,

$$\tilde{H}_t(\Phi) = U_\Phi^\dagger H_t(\Phi) U_\Phi, \quad (11)$$

where

$$U_\Phi = e^{A_\Phi}, \quad A_\Phi = \frac{i\Phi}{N} \sum_{j=1}^N j S_j^z. \quad (12)$$

In the bulk of the paper both  $H_p$  and  $\tilde{H}_t(\Phi)$  will be used simultaneously. Although our aim is to draw conclusions on  $H_p$ , the study of  $\tilde{H}_t(\Phi)$  turns out to be useful to reach these conclusions.

Being connected by a unitary transformation, the energy eigenvalues of  $H_t(\Phi)$  and  $\tilde{H}_t(\Phi)$  are identical. Moreover, as it can be seen directly from the definition in Eqs. (7) and (8), the spectrum of  $H_t(\Phi)$  and hence  $\tilde{H}_t(\Phi)$  should be identical to that of  $H_p$  at  $\Phi = \Phi_l \equiv 2\pi l$  for any integer  $l$ . For such values of  $\Phi$ ,  $H_p$  and  $\tilde{H}_t(\Phi)$  are connected by the transformation

$$\tilde{H}_t(\Phi_l) = U_{\Phi_l}^\dagger H_p U_{\Phi_l}. \quad (13)$$

Let  $\psi_p(k_p)$  be an eigenstate of  $H_p$  with energy  $E$  and momentum  $k_p$ . According to Eq. (13) there should exist an eigenstate  $\psi_t(k_t)$  of  $\tilde{H}_t(\Phi_l)$  with the same energy  $E$ . The momentum of this state is  $k_t$ . First we show, following Kolb,<sup>17</sup> that  $k_p$  and  $k_t$  satisfy the relation

$$k_p = k_t - \Phi_l S + \frac{\Phi_l}{N} S_T^z, \quad (14)$$

where  $S$  is the length of the spin (for our spin-1 chain  $S = 1$ ) and  $S_T^z$  is the  $z$  component of the total spin, which is a good quantum number even in the twisted case.

We prove this relationship for nondegenerate eigenstates. Generalization to degenerate eigenstates is quite straightforward. According to Eq. (13),  $\psi_p(k_p)$  and  $\psi_t(k_t)$  can be related by

$$\psi_p(k_p) = U_{\Phi_l} \psi_t(k_t). \quad (15)$$

The  $k_t$  dependence of  $\psi_t$  can be written explicitly as

$$\psi_t(k_t) = \sum_{\mathbf{n}} a_{\mathbf{n}} \sum_{m=1}^N e^{ik_t m} S_{n_1+m}^- \cdots S_{n_r+m}^- |0\rangle, \quad (16)$$

where  $|0\rangle$  is the fully aligned ferromagnetic state with  $S_T^z = NS$ , and  $\mathbf{n} = (n_1, \dots, n_r)$  denotes the possible configurations of misaligned spins in a given sector  $S_T^z = NS - r$ . Since an  $S^-$  operator decreases the  $z$  component

by 1, for  $S > \frac{1}{2}$  the same lattice site can appear more than once in the configuration  $\mathbf{n}$ . Only such configurations should be considered that cannot be obtained from each other by translation. The indices  $n_j + m$  of the translated sites are understood modulo  $N$ , i.e., they are transformed back to the interval  $1, \dots, N$ . The coefficients  $a_{\mathbf{n}}$  should be determined from the Schrödinger equation, but their explicit form will not be needed now.

It can be shown easily that

$$U_\Phi S_j^- = e^{-i\frac{\Phi}{N}j} S_j^- U_\Phi, \quad (17)$$

thus

$$U_\Phi \psi_t(k_t) = \sum_{\mathbf{n}} a_{\mathbf{n}} \sum_{m=1}^N e^{ik_t m} e^{-i\frac{\Phi}{N}[(n_1+\dots+n_r)+rm-l_mN]} \times S_{n_1+m}^- \cdots S_{n_r+m}^- U_\Phi |0\rangle, \quad (18)$$

where  $l_m$  is an integer that depends on  $m$ , and comes from the index transformation mentioned above. For  $\Phi_l = 2\pi l$  ( $l$  integer),  $e^{-i\frac{\Phi_l}{N}l_m N} \equiv 1$ , thus it cancels from Eq. (18). Using the explicit form of  $U_\Phi$  in Eq. (12), we find  $U|0\rangle = e^{iS\Phi_l/N} \sum_j |j\rangle$ . Inserting this into Eq. (18), gathering the  $m$  dependent factors,  $\psi_p(k_p)$  of Eq. (15) takes the form

$$\psi_p = e^{iS\frac{\Phi_l}{N} \sum_j} \sum_{\mathbf{n}} a_{\mathbf{n}} e^{-i\frac{\Phi_l}{N}(n_1+\dots+n_r)} \times \sum_{m=1}^N e^{im[k_t - \frac{\Phi_l}{N}r]} S_{n_1+m}^- \cdots S_{n_r+m}^- |0\rangle, \quad (19)$$

from which the wave vector of the state is

$$k_p = k_t - \frac{\Phi_l}{N} r. \quad (20)$$

Substituting the expression  $r = NS - S_T^z$  into Eq. (20), the statement (14) follows.

Before exploiting the interesting consequences of Eq. (14), we mention another theorem. Let us consider the adiabatic variation of the energy levels of  $\tilde{H}_t(\Phi)$  as  $\Phi$  is varied from zero to  $\Phi_l$  ( $l$  fixed). In general the spectrum of  $\tilde{H}_t(\Phi)$  differs from that of  $H_p$ . It follows from Eq. (13), however, that at  $\Phi = \Phi_l$  the spectrum of  $H_p$  should be recovered, i.e., the spectrum as a whole is periodic with period  $2\pi$ . Nevertheless, if we restrict ourselves to a subspace  $\mathcal{H}(S_T^z, k)$  with fixed momentum  $k$  and  $z$  component of the total spin  $S_T^z$ , which are good quantum numbers of the twisted chain, the same periodicity does not necessarily hold. Looking at the state that has the lowest energy in a given subspace at  $\Phi = 0$ , its energy  $E_0(\Phi)$  is in general not periodic with period  $2\pi$ . The energy  $E_0(0)$  can be produced at  $\Phi = \Phi_l$  by a state with a different wave number. It can be proven, however, that the twist is a small perturbation in the sense that the energy levels of  $\tilde{H}_t(\Phi)$  remain close to that of  $H_p$ . The energy difference  $E_0(\Phi_l) - E_0(0)$  can be at most of  $\mathcal{O}(1/N)$ .

Let  $\psi_p$  denote the lowest state of  $\tilde{H}_t(0) \equiv H_p$  in  $\mathcal{H}(S_T^z, k)$ , i.e.,

$$\tilde{H}_t(0) \psi_p = E_0(0) \psi_p, \quad (21)$$

and use this as a variational state for  $\tilde{H}_t(\Phi_l)$  to get an upper bound for the variation of the energy,

$$\begin{aligned} \delta E &\equiv E_0(\Phi_l) - E_0(0) \leq \langle \psi_p | \tilde{H}_t(\Phi_l) | \psi_p \rangle - \langle \psi_p | H_p | \psi_p \rangle \\ &= \langle \psi_p | U_{\Phi_l}^\dagger H_p U_{\Phi_l} - H_p | \psi_p \rangle, \end{aligned} \quad (22)$$

where we used Eq. (13). Now following the explicit calculations in Ref. 18 it is quite straightforward (but a bit lengthy) to show that the right-hand side of Eq. (22) is at most of order  $1/N$ , thus

$$\delta E \leq \mathcal{O}(1/N), \quad (23)$$

and the statement follows. This result can be understood very simply. The increase in the energy due to the twist should be an even function of  $\Phi$ . Since every bond is twisted by an angle  $\Phi/N$ , the energy increase is of order  $(\Phi/N)^2$  from each bond. The total energy change is then of order  $\Phi^2/N$ .

Following the lowest state of a subspace as a function of  $\Phi$ , level crossings may occur. Since we used variational arguments, the statement always refers to the lowest state  $E_0(\Phi)$ , and does not give us any definite information on the analytic continuation of  $E_0(\Phi)$  after such a crossing. (Note that we have a finite system in which all levels should be analytic.)

As in Ref. 18, we can express these two theorems in the language of Hamiltonian  $H_p$  only. Using Eq. (15) the statements say that in any subspace  $\mathcal{H}(S_T^z, k)$  the state  $U_{\Phi_l} \psi_p$ , which is obtained from the lowest energy state  $\psi_p$  of that sector, has momentum  $k' = k - \Phi_l S + \frac{\Phi_l}{N} S_T^z$ , and its energy differs from the ground-state energy of that sector by  $\mathcal{O}(1/N)$ . In Ref. 18 these theorems were used to show that at least for a certain range of  $\theta$  around the Heisenberg point  $\theta = 0$ , chains with integral and half-integral  $S$  may have drastically different spectra. For any  $S$  the ground state  $\psi_{GS}$  is in the  $\mathcal{H}(S_T^z = 0, k = 0)$  sector, and thus the state  $U_{2\pi} \psi_{GS}$  has momentum  $k' = 2\pi S$ . For half-integral  $S$  these two states are orthogonal to each other. Since their energy should be close to each other, of order  $1/N$ , in the thermodynamic limit the ground state is either doubly degenerate with a finite gap or the gap vanishes and soft modes appear at  $k = 0$  and  $k = \pi$ . By similar arguments it was also shown<sup>17</sup> that in the half-integer  $S$  case the dispersion relation should be symmetric not only with respect to  $k = m\pi$  ( $m$  integer) but to  $k = m\pi + \pi/2$ , too. For integral  $S$ , however,  $k' = 0$ , so no necessary degeneracies can be proven and the spectrum is symmetric with respect to  $k = m\pi$  only.

It is possible to generalize slightly these statements to show that the low-lying states of subspaces with  $S_T > 0$  necessarily form a continuum, hence a massive spectrum is possible only if the degenerate or nondegenerate ground state is in the singlet,  $S_T = 0$  sector. The argument is quite simple. Any level with  $S_T > 0$  is  $2S_T + 1$ -times degenerate. Let  $\psi_p$  denote the lowest state with momentum  $k$  for which  $S_T^z = 1$ . Let us consider now the state  $U_{2\pi} \psi_p$ . According to Eq. (14) its momentum is

$$\begin{aligned} k' &= k - 2\pi S + 2\pi/N \\ &= \begin{cases} k - \pi + \frac{2\pi}{N} & \text{if } S \text{ half-integral,} \\ k + \frac{2\pi}{N} & \text{if } S \text{ integral,} \end{cases} \end{aligned} \quad (24)$$

i.e., it is shifted by  $2\pi/N$ , which is the smallest possible step in the  $k$  space for chain length  $N$ . The  $-\pi$  for half-integral spin appears since the spectrum is periodic with  $\pi$ . The energy of this state differs from the energy of  $\psi_p$  of  $\mathcal{O}(1/N)$ , and thus it is seen that the existence of a whole continuous branch of excitations can be verified in this way.

### III. PHASE TRANSITION AT $\theta_{TB} = -\pi/4$

Before applying these general theorems to our  $S = 1$  model in Eq. (1), let us recall first the expected behavior and some of the earlier finite-size scaling results obtained by using PBC ( $\Phi = 0$ ).

The ground state of finite chains is a  $k = 0$ ,  $S_T = 0$  state in the whole  $-3\pi/4 < \theta < \pi/4$  region, except for a small  $N$ -dependent range close to  $\pi/4$ . The lowest-lying excited states differ in their quantum numbers in the different regions. The field-theoretical mapping suggests that an Ising-type phase transition from a dimerized phase to the singlet Haldane phase takes place at  $\theta_{TB} = -\pi/4$ . For  $\theta < \theta_{TB}$ , a singlet  $k = \pi$  state should be asymptotically degenerate with the singlet  $k = 0$  ground state, their energy difference vanishing exponentially for large enough systems. All other states are separated from the ground state by a finite gap. In the dimerized phase the translational invariance is broken spontaneously. This symmetry breaking leads to a doubling of the unit cell in the infinite system, hence the dispersion relation of the excitations is expected to become symmetric with respect to  $k = m\pi/2$  ( $m$  integer). The lowest (massive) excitations are expected to appear symmetrically near  $k = 0$  and  $k = \pi$ . In the region  $\theta > \theta_{TB}$  the ground state is expected to be unique, and there are indications<sup>19</sup> that the above symmetry of the spectrum does not hold anymore. The spectrum remains symmetric with respect to  $k = m\pi$  ( $m$  integer) only. The lowest (massive) excitations seem to appear near  $k = \pi$ .

We show in Fig. 1 the energy of the singlet  $k = \pi$

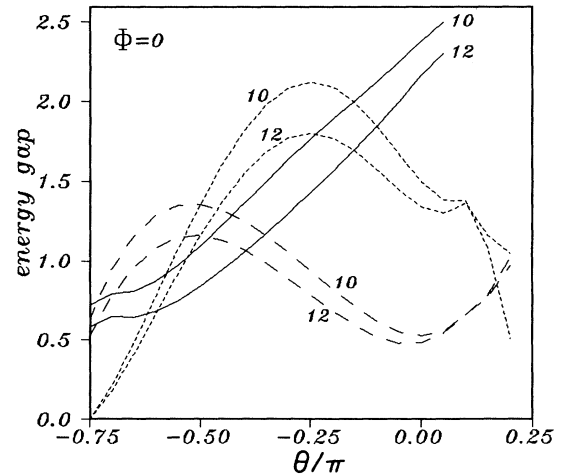


FIG. 1. The energies of the lowest-lying  $S_T = 0$ ,  $k = \pi$  (solid line),  $S_T = 1$ ,  $k = \pi$  (dashed line), and  $S_T = 2$ ,  $k = 0$  (dotted line) states relative to the ground state vs  $\theta$  for chain lengths  $N = 10$  and  $12$ .

level, relative to the ground state, as a function of  $\theta$  for two different chain lengths. Chang *et al.*<sup>20</sup> analyzed this singlet-singlet gap around  $\theta_{\text{TB}}$  and found definite support for the predictions. Using the standard methods to locate the phase transition point from the scaled gap, they concluded that it is certainly  $\theta_{\text{TB}}$ . For  $\theta < \theta_{\text{TB}}$  the gap converges to zero more rapidly than  $1/N$ , while nonzero values can be extrapolated for  $\theta > \theta_{\text{TB}}$ .

In finite systems, close to  $\theta_{\text{TB}}$ , a triplet  $k = \pi$  level may, however, have lower energy than the singlet  $k = \pi$  state. These levels are also shown in Fig. 1. A level crossing occurs between these low-lying  $k = \pi$  states. For  $\theta < \theta_c$  the singlet state lies lower, while for  $\theta > \theta_c$  the order of the two levels is reversed. The position of the crossing,  $\theta_c(N)$  depends on  $N$  in such a way that  $\theta_c(N) < \theta_c(N+2) < \theta_{\text{TB}}$ . We plot in Fig. 2 the position of the crossing point  $\theta_c(N)$  versus  $1/N$ . Extrapolation to  $N \rightarrow \infty$  indicates that  $\theta_c$  converges to  $\theta_{\text{TB}}$ , in agreement with the expectation that in the infinite system, for  $\theta < \theta_{\text{TB}}$ , the triplet state should have higher energy than the two singlet states. In fact, it should be separated by a *finite* gap from the doubly degenerate ground state.

The singlet-triplet gaps, obtained with periodic BC, are smooth functions of  $\theta$  near  $\theta_{\text{TB}}$ , as seen in Fig. 1. They decrease monotonically until about  $\theta \sim 0$  where they start to increase and reach an almost size-independent value at  $\theta_{\text{VB}}$ . The analysis<sup>12,13</sup> of the scaled gap of chains with  $N \leq 12$ , indicated an extended critical region above  $\theta_{\text{TB}}$ . Although the gap of finite systems continues to decrease for  $\theta > \theta_{\text{TB}}$ , from these same curves Blöte and Capel<sup>14</sup> inferred that above  $\theta_{\text{TB}}$  the gap opens approximately as  $(\theta - \theta_{\text{TB}})^{1.8}$ . The curves, however, show very strong finite-size effects close to  $\theta_{\text{TB}}$ , which make it almost impossible to draw any reliable quantitative conclusion. This may also be the reason, why the obtained behavior is different from the expected Ising-like expression.

Furthermore the next level in the  $k = 0$  subspace (also shown in Fig. 1) will be of interest, too. It is a quintuplet  $S_T = 2$  state, which, on both sides of  $\theta_{\text{TB}}$ , is expected to be separated by a finite energy gap from the ground state as  $N \rightarrow \infty$ , except at the transition point itself.

The numerical results allow to draw even less clear conclusions on the behavior of this singlet-quintuplet gap.

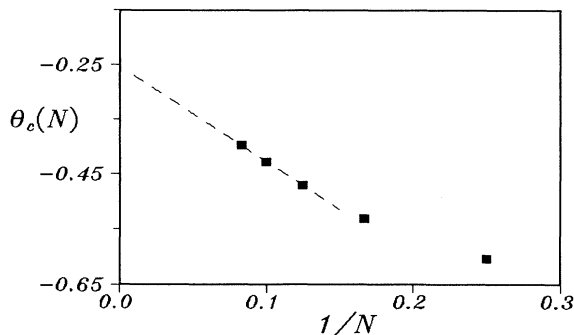


FIG. 2. The crossing points  $\theta_c(N)$  between the lowest singlet and triplet states in the  $k = \pi$  sector plotted against  $1/N$ . The dashed line shows the extrapolation to  $N \rightarrow \infty$ .

As seen in Fig. 1, at least for the available chain lengths, this gap has a maximum around  $\theta_{\text{TB}}$ . Since it is known that this gap vanishes exactly at the integrable point  $\theta_{\text{TB}}$  in infinitely long chains, one was tempted to conclude<sup>13</sup> that this gap vanishes in an extended range  $-3\pi/4 < \theta < 0$ . The results of the field-theoretical predictions could be reconciled with the numerical data only if a cross-over to the massive behavior occurs in much longer chains.

In this paper these four levels are going to be studied to understand the transition around  $\theta_{\text{TB}}$ . Since the numerical results with PBC show rather strong finite-size effects, in this paper we study these low-lying levels with a twisted BC in the hope that the finite-size effects will be reduced and the asymptotic behavior can be better observed. Using the Lanczos method we computed the energies of a few lowest levels in each possible sector of given  $S_T^z$  and  $k$  in the whole range  $-3\pi/4 < \theta < \pi/2$ . Chain lengths up to  $N = 15$  were considered. Around the Takhtajan-Babujian point,  $\theta_{\text{TB}} = -\pi/4$  we studied chains with  $N$  even, while for the transition at the Lai-Sutherland point,  $\theta_{\text{LS}} = \pi/4$  chains with  $N \equiv 0 \pmod{3}$  were taken. The Lanczos algorithm was continued until a precision better than  $10^{-6}$  was reached in all the lowest levels we were interested in, generally the lowest two. It was found that approximately 50–60 Lanczos steps were sufficient even for  $N = 15$ .

In all what follows, the level that is obtained from the  $k = 0$ ,  $S_T = 0$  state as  $\Phi$  is varied adiabatically, will be denoted by  $a$ . It will be referred to as the ground-state level even though it may not be the lowest one of the finite system for general  $\Phi$ . Similarly, the  $k = \pi$  singlet level will be denoted by  $b$ . The energy of the  $k = \pi$ ,  $S_T = 1$  state will be split due to the twist. The spin-flip symmetry assures that the energy depends on  $|S_T^z|$ . The levels with  $S_T^z = 0$  and  $\pm 1$  will be denoted by  $c_0$  and  $c_1$ , respectively, while the three levels with  $S_T^z = 0$ ,  $\pm 1$  and  $\pm 2$  which split off the  $k = 0$  quintuplet state will be denoted by  $d_0$ ,  $d_1$  and  $d_2$ . Figures 3(a)–3(d) show these levels as a function of  $\Phi$  for four different  $\theta$  values.

One interesting feature of these figures is that level  $a$ , that is the ground state of the model with PBC, does not remain necessarily the lowest-lying state. Near  $\Phi = \pi$  either  $b$  or  $c_0$  has lower energy than state  $a$  at least in a certain range of  $\theta$ . If this behavior survives in the thermodynamic limit, then according to the argument in Sec. II, for such values of  $\theta$  the energies of the ground state and the lowest  $k = \pi$  state may differ at most by  $1/N$ , i.e., they should become degenerate in the  $N \rightarrow \infty$  limit.

The other important observation from Fig. 3(c) is the exact degeneracy of levels  $a$  and  $d_0$  at  $\Phi = \pi$  and  $\theta = \theta_{\text{TB}}$  for any chain length  $N$ .

While both below and above  $\theta_{\text{TB}}$  curves  $a$  and  $d_0$  are quadratic in  $\Phi$  near  $\Phi = \pi$ , a *cusp* develops as  $\theta \rightarrow \theta_{\text{TB}}$ . At the integrable point levels  $a$  and  $d_0$  change place at any  $\Phi = \pi + 2\pi l$  ( $l$  integer). As a consequence, the ground-state level  $a$  as a function of  $\Phi$  has a periodicity  $2\pi$  everywhere for  $\theta \neq \theta_{\text{TB}}$ , and the periodicity changes to  $4\pi$  at  $\theta_{\text{TB}}$ , similarly to what happens in the spin- $\frac{1}{2}$  twisted Heisenberg chain.<sup>21</sup>

One important difference is that while in the spin- $\frac{1}{2}$

chain the two levels that cross at  $\Phi = \pi$  are a  $k = 0$  and a  $k = \pi$  level, in our case both levels have momentum  $k = 0$ . This difference can be understood by considering the Bethe ansatz solutions for the models. In the ground state of the integrable spin- $S$  model the rapidities form  $2S$ -strings with  $S$ -independent distribution for the real parts. A twist  $\Phi$  in the BC is equivalent to shifting all pseudomenta by  $\Phi/N$ . The total momentum is changed by  $M\Phi/N$ , where  $M$  is the number of pseudomenta, or the number of spin flips. For the spin- $\frac{1}{2}$  chain in the ground state  $M = N/2$ , so a twist  $\Phi = 2\pi$  leads to a state with  $k = \pi$ . A twist of  $4\pi$  is needed to recover the  $k = 0$  ground state.

For integer spin  $S = 1$ , however,  $M = N$  in the ground state, so a twist with  $\Phi = 2\pi$  generates a state with  $k = 0$ . Unlike the spin- $\frac{1}{2}$  chain, there is no general argument why the ground state should be periodic with period  $4\pi$ . Nevertheless, the sharp cusp at  $\theta = \theta_{\text{TB}}$  can

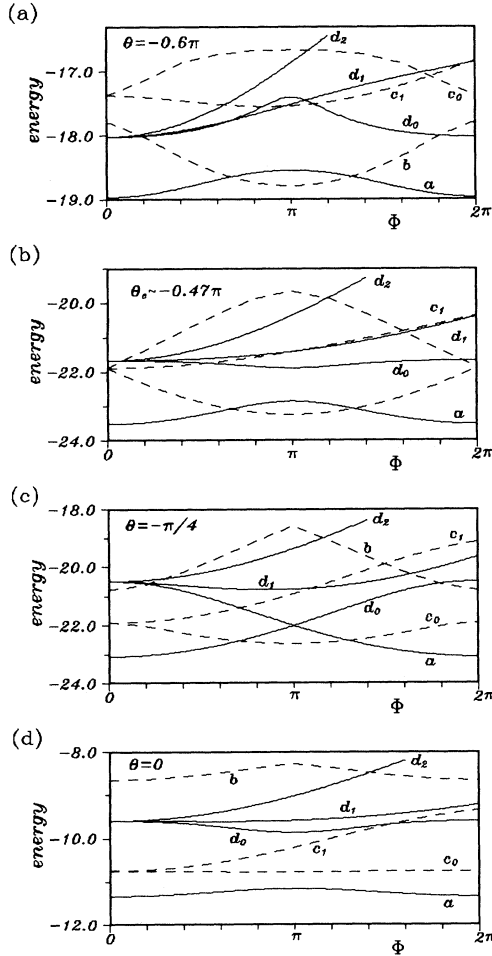


FIG. 3. Adiabatic variation of the relevant energy levels of a chain with  $N = 8$  as a function of the twist angle  $\Phi$ , for (a)  $\theta = -0.6\pi$ , (b)  $\theta_c \approx 0.47\pi$ , (c)  $\theta_{\text{TB}} = -\pi/4$ , and (d)  $\theta = 0$ . Solid curves refer to momentum  $k_t = 0$ , dashed curves to momentum  $k_t = \pi$ . The labeling of the curves is explained in the text.

be interpreted as the crossing of two levels. However, since both have  $k = 0$  and  $S_T^z = 0$ , any perturbation that takes the system away from the integrable point, will lift the degeneracy and introduce a periodicity with period  $2\pi$ .

Since curve  $a$  lies lower than curve  $d_0$  on both sides of  $\theta_{\text{TB}}$  [Figs. 3(b) and 3(d)], one might think that the difference  $E_{d_0}(\Phi = \pi) - E_a(\Phi = \pi)$  should be quadratic around  $\theta_{\text{TB}}$ . We plot schematically in Fig. 4 the behavior of these levels as a function of  $\theta$ . A behavior that resembles a level crossing is found. The energies  $E_a(\Phi = \pi)$  on the left-hand side of  $\theta_{\text{TB}}$  are analytically continued in the energies  $E_{d_0}(\Phi = \pi)$  on the right of  $\theta_{\text{TB}}$ , and vice versa.

The fact of finding a break in the  $\theta$  dependence of the ground-state energy at  $\theta_{\text{TB}}$  for finite systems does not necessarily mean that the same type of nonanalyticity survives in the limit of infinite system, too. It is worth emphasizing that this extraordinary, i.e., not smooth behavior of the ground-state energy at  $\theta_{\text{TB}}$  in *finite* systems is the consequence of our modified BC ( $\Phi = \pi$ ). If we study finite chains with PBC ( $\Phi = 0$ ), as it has been done in most of the earlier works, all quantities are found to be smooth in  $\theta$ . To see the type of the phase transition at  $\theta_{\text{TB}}$  in the thermodynamic limit, we plot in the inset of Fig. 4 the left and right derivatives of the ground-state energy for different values of  $N$ . Extrapolation to  $N \rightarrow \infty$  seems to indicate a common slope on both sides of  $\theta_{\text{TB}}$ , and thus it strengthens the prediction that the transition is of second order.

As for the levels in the  $k = \pi$  sector, another unex-

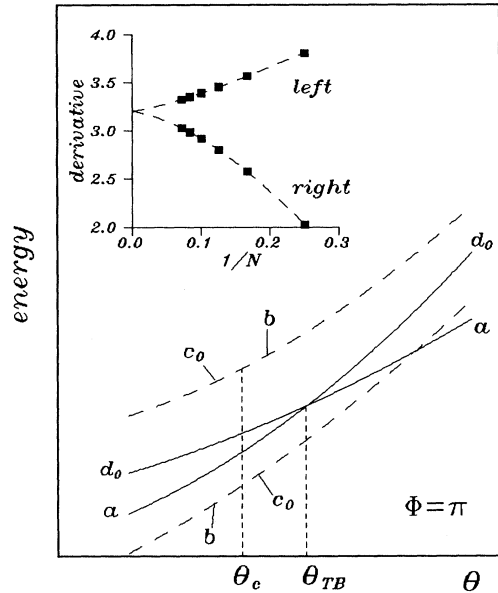


FIG. 4. Schematic illustration of the most important levels for a twist  $\Phi = \pi$  in the vicinity of  $\theta_{\text{TB}}$ . The special behaviors at  $\theta_{\text{TB}}$  and  $\theta_c$  are detailed in the text. The inset shows the left and right derivatives of the ground-state energy at  $\theta_{\text{TB}}$  vs  $1/N$ . The dashed curve is an extrapolation to  $N \rightarrow \infty$ .

pected behavior is found around  $\theta_c(N)$ . As mentioned before, at this point there is a level crossing in the untwisted chain ( $\Phi = 0$ ) between the lowest-lying  $k = \pi$  levels of the  $S_T = 0$  and  $S_T = 1$  sectors. This level crossing has interesting consequences for the behavior of these levels when the chain is twisted. For any  $\theta \neq \theta_c$ , curves  $b$  and  $c_0$  are quadratic in  $\Phi$  near  $\Phi = 0$ , but they become linear at  $\theta = \theta_c$ . It is only  $c_1$  that remains quadratic. While for  $\theta < \theta_c$  curve  $c_0$  (i.e., the  $S_T^z = 0$  state evolving from the  $S_T = 1$  state at  $\Phi = 0$ ) lies higher than curve  $b$ , the order of the levels is reversed for  $\theta > \theta_c$ . However, there is no level crossing between these levels at any finite  $\Phi \neq 0$ . The level that is denoted by  $b$  above  $\theta_c$ , is a continuation of level  $c_0$  below  $\theta_c$  and vice versa, in much the same way as was found for levels  $a$  and  $d_0$  around  $\theta_{TB}$ . This situation is also illustrated in Fig. 4.

Now we turn to analyzing the scaling properties of the different gaps using our twisted BC with  $\Phi = \pi$ . Figure 5 shows our results for the energy difference  $\Delta_0(\theta)$  between the lowest state in the  $k = \pi$ ,  $S_T^z = 0$  sector (level  $c_0$  for  $\theta > \theta_c$  and level  $b$  for  $\theta < \theta_c$ ) and the "ground-state" level  $a$  calculated with  $\Phi = \pi$  as a function of  $\theta$ . Taking into account that  $\theta_c(N) \rightarrow \theta_{TB}$  as  $N \rightarrow \infty$ , it should scale to zero for  $\theta < \theta_{TB}$ , and to the real excitation gap for  $\theta > \theta_{TB}$ . Using the twisted BC there is a sharp break in the curves at  $\theta_{TB}$ . This break is the consequence of the unusual behavior of the ground-state energy at  $\theta_{TB}$ . For  $\theta < \theta_{TB}$  the gaps are negative, and the scaling to zero is faster than  $1/N$ . As  $\theta \rightarrow \theta_{TB}$  this tendency seems to slow down to a quasi- $1/N$  rate. This is in agreement with the asymptotic degeneracy of the two singlet levels, and with the criticality at  $\theta_{TB}$ .

On the other side of  $\theta_{TB}$ , extrapolations give positive

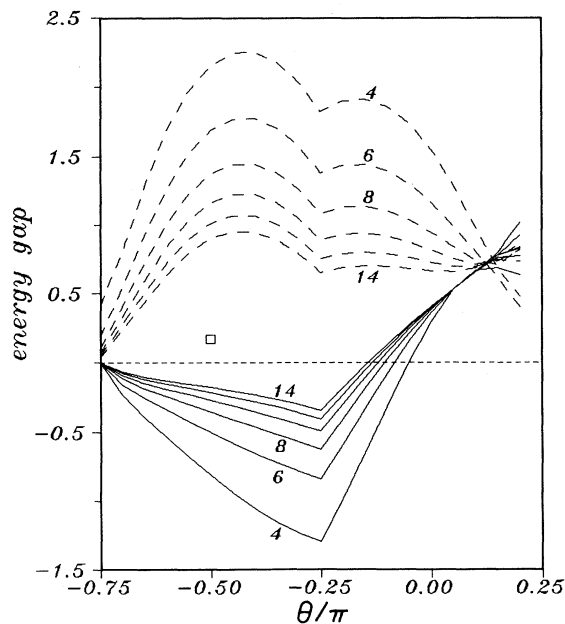


FIG. 5. The energy differences  $\Delta_0 = \min\{E_b, E_{c_0}\} - E_a$  (solid lines) and  $\Delta_1 = E_{c_1} - E_a$  (dashed lines) at  $\Phi = \pi$  plotted vs  $\theta$  for different  $N$ . The exact limiting value for  $\Delta_1$  at  $\theta = -\pi/2$  is denoted by  $\square$ .

limiting values for the gap. For any  $N$  the curves starts linearly with a very slight upward curvature (almost unobservable in the figure). In the range  $0 < \theta < 0.2\pi$ , i.e., in the neighborhood of the valence-bond state the convergence is extremely good. If the gap in this region goes continuously to zero at  $\theta_{TB}$ , it seems that the gap function should have an upward curvature. The question is whether at  $\theta_{TB}$  the gap opens linearly or with zero slope. Figure 6 shows this derivative of  $\Delta_0$  as a function of  $1/N$ . The points lie on a curve with downward curvature. Although the possibility cannot be excluded that for  $N \rightarrow \infty$  the slope goes to zero, any standard extrapolation method gives a finite intercept with approximately  $\Delta'_0 \sim 1.5$  as  $N \rightarrow \infty$ . Using again the argument that the energies at  $\Phi = \pi$  may differ from the energies at  $\Phi = 0$  by order  $1/N$ , we conclude that even with PBC ( $\Phi = 0$ ) the gap opens linearly with  $\theta - \theta_{TB}$ .

The gap  $\Delta_1(\theta)$ , using now the  $S_T^z = 1$  component  $c_1$  of the "triplet" state is also shown in Fig. 5. Since the curve  $c_1$  evolves from the  $S_T = 1$  state at  $\Phi = 0$ , this gap is expected to converge to the real excitation gap on both sides of  $\theta_{TB}$ . There is again a break in the curves at  $\theta_{TB}$ . For  $\theta < \theta_{TB}$  the gaps have definite downward curvature. The situation is different for  $\theta > \theta_{TB}$  because of the appearance of an inflection point. Computing the slope at  $\theta_{TB}$  has any relevance only if the region where the curvature is downward does not shrink to zero as  $N \rightarrow \infty$ . With this proviso, the left and right derivatives are plotted in Fig. 6 versus  $1/N$ . Extrapolation from the left derivatives  $\Delta'_{1-}$  is again uncertain because the points lie on a curve with downward curvature. For the right derivatives  $\Delta'_{1+}$ , however, this curvature is slightly upward, and thus a more reliable extrapolation is possible. The intercept  $\Delta'_{1+}(N \rightarrow \infty) \sim 0.6$  is clearly finite, indicating the linear opening of the gap in the thermodynamic limit.

As a generalization of the singlet-quintuplet gap of the model with PBC, the gap  $\Delta_2(\theta)$  between levels  $a$  and  $d_0$  is plotted in Fig. 7 as a function of  $\theta$  for different

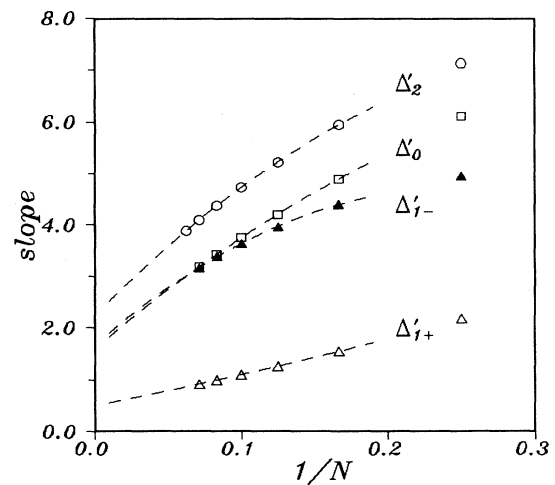


FIG. 6. Slopes of the energy gaps to various excited states at  $\theta_{TB}$  as a function of  $1/N$ . Dashed lines denote the suggested scaling behavior with finite intercept for large  $N$ .

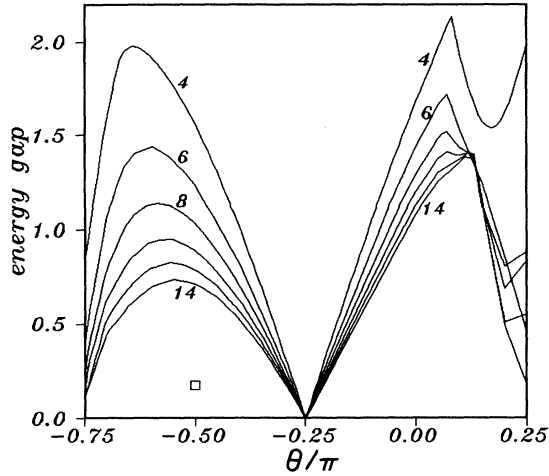


FIG. 7. Gap inside the sector  $k = 0$ . The energy difference  $\Delta_2 = E_{d_0}(\Phi = \pi) - E_a(\Phi = \pi)$  is plotted for different chain lengths  $N$ . The exact limiting value at  $\theta = -\pi/2$  is denoted by  $\square$ .

chain lengths. Although there is a very slight upward curvature on the right-hand side close to  $\theta_{TB}$ , it is almost unobservable in the figure, and up to  $N = 14$  the opening of the gap is linear in  $|\theta - \theta_{TB}|$ . In order to see that the gap is in fact finite on both sides, we show in Fig. 6 the slope of the gap  $\Delta'_2$  at  $\theta_{TB}$ . The left and right derivatives are equal for any finite  $N$  because of the level crossing. Similarly as for some of the other curves of the figure, extrapolation to  $N \rightarrow \infty$  is not easy because of the downward curvature, but again any reasonable fit gives a finite intercept and hence a finite slope for the opening of the gap.

#### IV. PHASE TRANSITION AT $\theta_{LS} = \pi/4$

In Ref. 16 we gave a detailed analysis of the model in the vicinity of the Lai-Sutherland point,  $\theta_{LS} \equiv \pi/4$  and in the region  $\pi/4 < \theta < \pi/2$ , using PBC. We have found that the exact solution<sup>9</sup> at  $\theta_{LS}$ , with three soft modes, remains stable in the whole antiferromagnetic region above  $\theta_{LS}$ , i.e., there is an extended critical phase with central charge  $c = 2$ , which replaces the massive Haldane phase if the biquadratic exchange dominates. Using chain lengths  $N \equiv 0 \pmod{3}$  the ground state is always found to be in the  $S_T = 0$ ,  $k = 0$  sector, while the first excited state has momentum  $k = \pm 2\pi/3$ . It is an  $S_T = 1$  or  $S_T = 2$  state for  $\theta < \theta_{LS}$  and  $\theta > \theta_{LS}$ , respectively.

The tripled-periodic state was also reported independently by Nomura and Takada,<sup>15</sup> although they argued that it is a trimerized massive phase. This does not seem to agree with our finding. Even for relatively short chains,  $N \leq 15$ , the gap to the quintuplet  $k = \pm 2\pi/3$  state scales to zero as  $1/N$  in the whole  $\theta_{LS} \leq \theta < \pi/2$  regime. Provided we see the real asymptotic behavior, i.e., the quintuplet states are really degenerate with the ground state in that range, our arguments in Sec. II exclude the possibility of a massive spectrum. There must

exist a low-lying *continuous* branch of  $S_T > 1$  excitations which involves the quintuplet  $k = \pm 2\pi/3$  states, as well.

Some of the main questions that remained open in Ref. 16 concern the location and the type of the phase transition. Using PBC we found a local minimum in the gap below  $\theta_{LS}$ , which seemed to indicate a transition point  $\theta_c < \theta_{LS}$ . Reliable extrapolation was, however, not possible due to strong finite-size effects. The same effect made impossible to determine the type of transition at  $\theta_{LS}$ . On the other hand, as we have found a whole line of critical points, our first guess could be an unconventional Kosterlitz-Thouless-type phase transition.<sup>22</sup> In the rest of this section we try to study these problems using our modified BC.

Since the model is integrable at  $\theta_{LS}$ , it could be expected that the adiabatic variation of the energy levels shows special behavior at this point, too. We show in Fig. 8 the energies of the two lowest levels as a function of the twist angle for a chain with  $N = 9$  sites. One evolves from the singlet  $k = 0$  state, while the other from the  $S_T^z = 0$  component of the triplet (for  $\theta < \theta_{LS}$ ) or from the quintuplet (for  $\theta > \theta_{LS}$ )  $k = \pm 2\pi/3$  state. It is found for  $\theta = \theta_{LS}$  [see Fig. 8(b)] that the two levels become exactly degenerate for any finite  $N$  at  $\Phi = \pm 2\pi/3 + 2\pi m$  ( $m$  integer). Thus, using a twisted BC with  $\Phi = 2\pi/3$ , there are no finite-size corrections to the gap, it vanishes

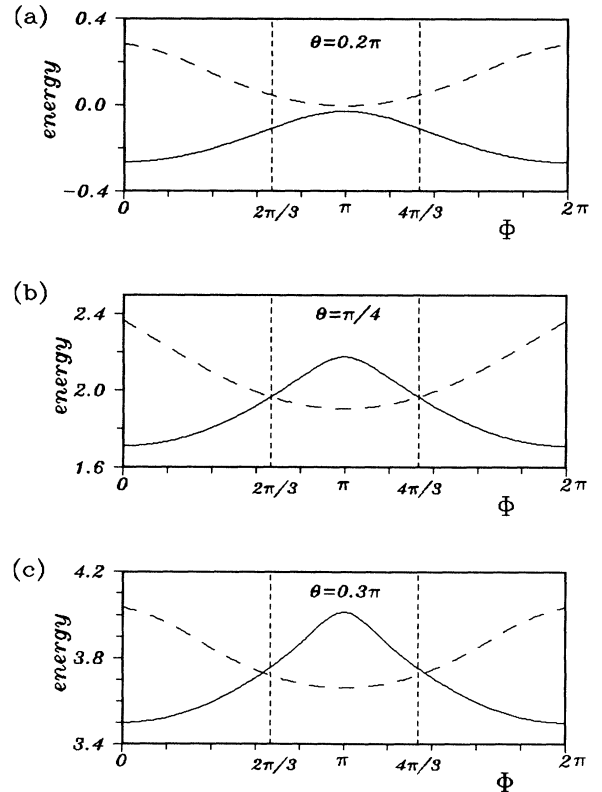


FIG. 8. Adiabatic variation of the  $S_T^z = 0$  components of the lowest energy levels with momentum  $k = 0$  (solid line) and  $k = 2\pi/3$  (dashed line) of a chain with  $N = 9$  as a function of the twist  $\Phi$  for (a)  $\theta = 0.2\pi$ , (b)  $\theta_{LS} = \pi/4$ , (c)  $\theta = 0.3\pi$ .



identically for all  $N$ . Looking first at the range  $\theta > \theta_{LS}$ , it is seen in Fig. 8(c) that the crossing points move toward  $\Phi = 0$  and  $2\pi$  as  $\theta$  increases. In the whole interval  $[2\pi/3, 4\pi/3]$  the order of the levels is reversed, compared to the situation at  $\Phi = 0$ . Using again that the variation of the energy is of order  $1/N$ , we conclude that at  $\Phi = 0$  the energies of the  $k = 0$  singlet and the  $k = \pm 2\pi/3$  quintuplet states should be close of order  $1/N$ , and therefore the phase must be gapless. Further confirmation is obtained if we plot in Fig. 9 the energy difference of the  $k = 0$  and  $k = \pm 2\pi/3$  levels at  $\Phi = 2\pi/3$ . In the region  $\theta_{LS} < \theta < \pi/2$  the gap seems to scale somewhat faster than  $1/N$ . Nevertheless extrapolations show that the scaled gap tends to finite values here, i.e., the scaling rate is still  $1/N$  for long enough chains. This is in full accordance with our previous results in Ref. 16.

For  $\theta < \theta_{LS}$  the behavior is different. As seen in Fig. 8(a), the  $\theta$  values where the levels cross, approach each other, and eventually the level crossing will disappear, indicating that a finite gap might open here. Figure 9 shows that for  $\theta < \theta_{LS}$  the gap converges rapidly to a finite value. The scaled gap  $N\Delta$  increases rapidly with  $N$ , except for the immediate vicinity of  $\theta_{LS}$ . This allows to define a renormalization transformation and to study the critical behavior of the model. In the spirit of finite-size scaling it is required that the model of  $N$  sites with coupling  $\theta$  should have the same behavior as another system of  $N'$  sites with coupling  $\theta'$ . Since the scaled gap should be independent of the system size, a renormalization-group transformation from  $(N, \theta)$  to  $(N', \theta')$  can be generated by requiring, that

$$N\Delta(\theta, N) = N'\Delta(\theta', N'). \quad (25)$$

The Callan-Symanzik  $\beta$  function, defined by

$$\beta(\theta) \equiv -N \left. \frac{\partial \theta}{\partial N} \right|_{N\Delta = \text{const}}, \quad (26)$$

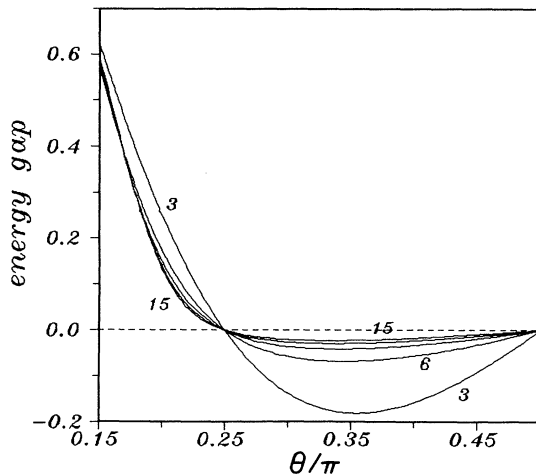


FIG. 9. Excitation gap  $E_0(k = 2\pi/3) - E_0(k = 0)$  between the lowest state with momentum  $k = \pm 2\pi/3$  and the  $k = 0$  ground state vs  $\theta$  at a twist angle  $\Phi = 2\pi/3$  for different chain lengths  $N$ .

contains all the relevant information on the transition. From the scale invariance of the scaled gap we get

$$\frac{\partial(N\Delta)}{\partial\theta} d\theta + \frac{\partial(N\Delta)}{\partial N} dN = 0, \quad (27)$$

and thus

$$\beta(\theta) = \frac{N\partial(N\Delta)/\partial N}{\partial(N\Delta)/\partial\theta} = \frac{\partial \ln(N\Delta)/\partial \ln N}{\partial \ln(N\Delta)/\partial \theta}. \quad (28)$$

In a second-order phase transition the gap opens with a power law. Near the transition point  $\theta_c$

$$\Delta(\theta) \propto (\theta_c - \theta)^\nu, \quad (29)$$

and in that region of  $\theta$  the  $\beta$  function is linear,

$$\beta(\theta) = (\theta_c - \theta)/\nu. \quad (30)$$

In the case of a Kosterlitz-Thouless-type phase transition, however, the gap opens as

$$\Delta(\theta) = \begin{cases} \text{const} \cdot \exp[-c(\theta_c - \theta)^{-\sigma}] & \text{for } \theta < \theta_c, \\ 0 & \text{for } \theta > \theta_c, \end{cases} \quad (31)$$

and

$$\beta(\theta) = \begin{cases} -\frac{1}{c\sigma}(\theta_c - \theta)^{1+\sigma} & \text{for } \theta < \theta_c, \\ 0 & \text{for } \theta > \theta_c. \end{cases} \quad (32)$$

Roomany and Wyld<sup>3</sup> have shown that for discrete lattices, where the chain length can be varied by multiples of the lattice constant only, the expression for the  $\beta$  function in Eq. (28) should be approximated by

$$\beta(\theta) = \frac{\ln[N'\Delta(\theta, N')/N\Delta(\theta, N)]}{\ln(N'/N) \frac{1}{2} \frac{\partial}{\partial \theta} \ln[\Delta(\theta, N)\Delta(\theta, N')]} \quad (33)$$

These  $\beta$  functions computed for  $(N = 6, N' = 9)$ ,  $(N = 9, N' = 12)$ , and  $(N = 12, N' = 15)$  are plotted in Fig. 10. They show only minute-size dependence for  $\theta < \theta_{LS}$ . As they behave definitely nonlinearly below  $\theta_{LS}$  we fitted

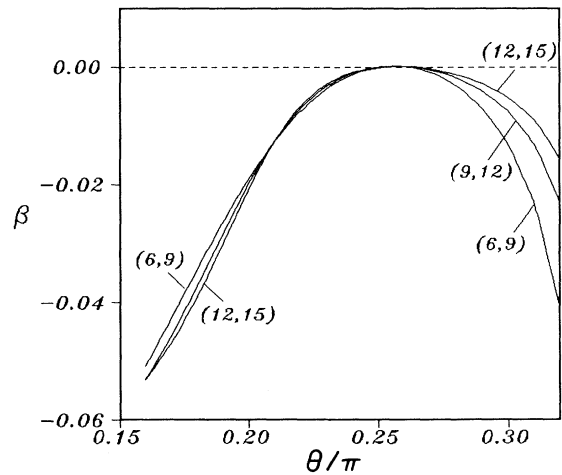


FIG. 10. The Callan-Symanzik  $\beta$  function calculated for different pairs of chain length  $(N, N')$ .

them by the form in Eq. (32) assuming  $\theta_c = \theta_{LS}$ . The best fit for the parameters  $c$  and  $\sigma$  gives

$$c = 1.1 \pm 0.3, \quad \sigma = 0.8 \pm 0.2. \quad (34)$$

From this we conclude that the transition is of the Kosterlitz-Thouless type. For  $\theta > \theta_{LS}$  the finite-size effects are quite strong in the  $\beta$  functions. Since the gap vanishes identically at  $\theta = \theta_{LS}$  and  $\theta = \pi/2$ , there is always a value between them where its derivative is zero. As this derivative appears in the denominator of Eq. (28), this leads to a necessary divergence in the  $\beta$  function. Otherwise, as the chain lengths are increased, the curves seem to converge to the expected  $\beta \equiv 0$  value on both sides of the discontinuity.

## V. CONCLUSIONS

In this paper we studied numerically the phase transitions in the bilinear-biquadratic isotropic spin-1 chain. The strong finite-size corrections that generally hinder the observation of the true asymptotic behavior for small system sizes were reduced by appropriately modifying the boundary condition. It was found that at both integrable points,  $\theta_{TB}$  and  $\theta_{LS}$ , a suitably chosen twisted BC gives identically vanishing gap for arbitrary chain lengths. Although, it was not possible to totally get rid of the size dependence *inside* the various phases, the finite-size effects proved to be much easier to handle.

The transition at  $\theta_{TB} = -\pi/4$  was studied using a twist  $\Phi = \pi$ . We analyzed the behavior of several energy levels and gaps, and concluded that for  $\theta < \theta_{TB}$  the energies of the singlet  $k = 0$  and  $k = \pi$  levels become degenerate and these two levels form the ground state. For  $\theta > \theta_{TB}$  the ground state is a nondegenerate singlet  $k = 0$  state. The gap was found to open linearly on both sides of  $\theta_{TB}$ . These results are in agreement with the predictions by Affleck<sup>5</sup> who argued, using an approximate field-theory mapping, that this transition belongs to the same universality class as the (1+1)-dimensional Ising model.

In the next part of the paper the vicinity of the other integrable point,  $\theta_{LS} = \pi/4$  was studied. Both numerical and analytical arguments were given to support our previous finding that in the region  $\pi/4 \leq \theta < \pi/2$  the model is massless. The analysis of the Callan-Symanzik  $\beta$  function indicates that the transition from the Haldane phase to this critical phase with three soft modes is of the Kosterlitz-Thouless type. The characteristic parameters of this transition were also estimated.

## ACKNOWLEDGMENTS

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