Competing bilinear and biquadratic exchange couplings in spin-1 Heisenberg chains

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A spin-1 magnetic chain with bilinear and biquadratic exchange couplings is studied to determine its phase diagram. The character of the ground state and its degeneracy is determined from an analysis of the low-lying levels of finite chains and from the instability of the uniform lattice against dimerization. Evidence for a ferromagnetic phase, two antiferromagnetic phases (with doubled and tripled periods), and a singlet phase is found.

I. INTRODUCTION

In the description of the behavior of magnetic systems with localized magnetic moments, the most widely used Hamiltonian is the Heisenberg exchange Hamiltonian. It contains bilinear couplings between the moments. If the symmetry of the crystal is high enough and only two-body forces are taken into account, this exchange coupling is the most general interaction, provided the length of the localized spin is $S=\frac{1}{2}$. For higher spins more complicated couplings can appear, e.g., for $S=1$ a term with biquadratic exchange. In an isotropic model the Hamiltonian would take the form

$$H=-J\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j-K\sum_{i,j}(\mathbf{S}_i\cdot\mathbf{S}_j)^2 . \tag{1.1}$$

In particular cases, the biquadratic exchange can be comparable to the bilinear exchange. The competition between the two terms can lead to unusual orderings, e.g., to quadrupole ordering. A mean-field theory of possible ordered phases in three-dimensional systems has been given by Chen and Levy.[1] The experimental situation concerning the role of biquadratic terms has been reviewed by Nagaev.[2]

In the one-dimensional case, where mean-field theory is not applicable, interesting new features can arise. While for $S=\frac{1}{2}$ the Heisenberg model can be solved exactly by the Bethe ansatz, this is not true for higher spins. However, if the biquadratic term is taken into account, the model becomes soluble in the case $S=1$ for special values of the couplings.[3–6] For higher-spin values high-order polynomials of the exchange coupling lead to soluble models. In the soluble cases the spin-wave spectrum is identical to that of the $S=\frac{1}{2}$ isotropic antiferromagnet;[4] the dispersion relation of the elementary excitations does not depend on S.

This may not be true in the usual Heisenberg model. The model with purely bilinear exchange has been the subject of extensive studies following Haldane's conjecture,[7] according to which the $S=1$ isotropic antiferromagnet and any integer-spin model behaves differently than models with half-integer spin. It is only in the latter case that the excitation spectrum is similar to that of the $S=\frac{1}{2}$ model. For integer spins the isotropic antiferromagnet has no soft spin-wave modes, the gap is finite, and the ground state is singlet. Numerical calculations on finite chains[8–10] seem to support this conjecture, although it is *a priori* not clear how long chains have to be considered in order to see the asymptotic behavior.[11–13]

Assuming that the $S=1$ Heisenberg antiferromagnet $(J<0,K=0)$ has a singlet ground state with a finite gap, and knowing that at the exactly soluble points $K=\pm J, J<0$ the spectrum is gapless, one can ask how the two couplings compete to produce a massive or massless phase. Affleck,[14] using a mapping to the Wess-Zumino model, suggested that the $S=1$ model with both bilinear and biquadratic exchange is generically massive, and has a finite gap in that range of couplings where the mapping holds. The gap will vanish at special values of the couplings only, namely, for $K=\pm J$. Numerical studies by Kung[15] and by Oitmaa *et al.*[16] do not completely support this claim. The results of finite-size scaling studies of the model were interpreted as indicating a finite gap for $K>-J$. In the region $0<K<-J$, on the other hand, there seems to be a critical value K_c such that for $K_c\le K\le -J$, the gap remains zero. The massive phase appears for $K<K_c$ only.

This conclusion was reached by analyzing the primary gap, i.e., the gap between the ground state and the first excited state of finite chains. Since this result is not unambiguous, it seems worthwhile to make a more detailed study of this model by considering other properties as well. In this paper I will present the results of such a study. Together with the primary gap I have considered the secondary gap, too. Finite-size scaling on this quantity yields additional information about the degeneracy of the ground state in the infinite system.

Indirectly, the spin-Peierls transition can also give information about the absence or presence of a gap in the excitation spectrum. The uniform lattice is unstable against spontaneous dimerization only if the excitation spectrum is gapless and the spin-spin correlation functions decay with a power law $\langle S^x(r)S^x(0)\rangle\sim r^{-\eta}$, with $\eta>\frac{1}{2}$. I studied the problem of spin-Peierls transition in the presence of biquadratic exchange to get further indication about the possible gapless regions in the coupling space.

The results known on the bilinear-biquadratic exchange model are summarized in Sec. II. The ferromagnetic part of the phase diagram is considered in Sec. III. Our finite-size scaling results on the primary and secondary gaps for the antiferromagnetic region are given in Sec. IV. The problem of spin-Peierls transition and its relationship to the problem of gap is studied in Sec. V. Finally, the results are discussed in Sec. VI and a possible phase diagram is given.

II. THE MODEL

The model with bilinear and biquadratic exchange couplings is defined by the Hamiltonian given in Eq. (1.1). The biquadratic exchange term can be expressed in terms of the six tensor operators

$$T_{\alpha\beta}=\tfrac{1}{2}(S_\alpha S_\beta+S_\beta S_\alpha)$$

using the relation

$$\sum_{\alpha,\beta=x,y,z} T_{\alpha\beta,i}T_{\alpha\beta,i+1}=\tfrac{1}{2}\mathbf{S}_i\cdot\mathbf{S}_{i+1}+(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2 , \tag{2.1}$$

or in terms of the quadrupole operators

$$\begin{aligned} &Q_0=3S_z^2-2,\quad Q_2=S_x^2-S_y^2 ,\\ &Q_{xy}=S_xS_y+S_yS_x ,\\ &Q_{yz}=S_yS_z+S_zS_y ,\\ &Q_{zx}=S_zS_x+S_xS_z ,\end{aligned} \tag{2.2}$$

taking into account that

$$\tfrac{1}{3}Q_{0,i}Q_{0,i+1}+Q_{2,i}Q_{2,i+1}+Q_{xy,i}Q_{xy,i+1}+Q_{yz,i}Q_{yz,i+1}+Q_{zx,i}Q_{zx,i+1}=\mathbf{S}_i\cdot\mathbf{S}_{i+1}+2(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2-\tfrac{2}{3}S(S+1) . \tag{2.3}$$

This form is useful to study how in a three-dimensional system the biquadratic exchange can lead to quadrupole ordering.

Alternatively, using the Schrödinger exchange operator

$$P_{ij}=(\mathbf{S}_i\cdot\mathbf{S}_j)+(\mathbf{S}_i\cdot\mathbf{S}_j)^2-1 , \tag{2.4}$$

which simply exchanges the spin states between sites i and j, the Hamiltonian can be written as

$$H=-(J-K)\sum_{i,j}\mathbf{S}_i\cdot\mathbf{S}_j-K\sum_{i,j}(P_{ij}+1) . \tag{2.5}$$

At $J=K$ the SU(3) symmetric model of Sutherland[3] is recovered, while otherwise the symmetry is SU(2) only.

Another exactly soluble case is $J=-K$, both for antiferromagnetic[4,5] and ferromagnetic couplings.[6] In order to cover easily all possible choices for the couplings, it is convenient, following Affleck,[14] to parametrize J and K as

$$J=-A\cos\theta,\quad K=-A\sin\theta . \tag{2.6}$$

A just sets the energy scale and will be taken as unity. Considering nearest-neighbor interaction in a one-dimensional chain, the Hamiltonian will have the form

$$H=\sum_i[(\cos\theta)(\mathbf{S}_i\cdot\mathbf{S}_{i+1})+(\sin\theta)(\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2] . \tag{2.7}$$

The SU(3) symmetric model of Sutherland[3] corresponds to $\theta=\pi/4$. At this point the spectrum is gapless; the soft modes appear at $k=0$ and $\pm 2\pi/3$. As shown by Takhtajan[4] and Babujian,[5] the model is soluble at $\theta=-\pi/4$, too. The spectrum is again gapless, the soft modes being at $k=0$ and π. Between these two exactly soluble points, $\theta=-\pi/4$ and $\pi/4$, lies the usual antiferromagnetic point $\theta=0$, where according to Haldane[7] the excitation gap is finite. Moreover, Affleck[14] predicted that the gap is finite everywhere between $\theta=-\pi/4$ and $\pi/4$, except for these two special points. Furthermore, according to Affleck the gap is finite for $\theta<-\pi/4$ as well, especially at $\theta=-\pi/2$, where only the biquadratic term is present.

The point $\theta=\pi$ corresponds to the usual Heisenberg ferromagnet. A weak biquadratic exchange will not destroy this order and a ferromagnetic ground state is expected for $3\pi/4<\theta<5\pi/4$. The magnon spectrum and the two-magnon bound state have been calculated by Papanicolaou and Psaltakis[17] for $\pi\leq\theta\leq 5\pi/4$. The other half of the ferromagnetic region $(3\pi/4\leq\theta\leq\pi)$ was not considered, except for the point $\theta=3\pi/4$ where the model is again exactly soluble.[6] The region between $\theta=\pi/2$ and $3\pi/4$ was not studied either, although it is known that at $\theta=\pi/2$ the model describes an SU(3) symmetric ferromagnet.[14]

III. FERROMAGNETIC REGION, $\pi/2\leq\theta\leq 5\pi/4$

In order to study the ground-state and low-lying excitations of the system, I have performed calculations on finite chains with up to $N=12$ sites. First of all, it is found that the ground state of the finite system is ferromagnetic if $\pi/2\leq\theta\leq 5\pi/4$. The lowest energy state corresponds to a configuration where all spins are oriented parallel to each other and the energy per site is

$$E_0=\cos\theta+\sin\theta . \tag{3.1}$$

The one-spin-flip excitations above this ground state can be obtained in the usual way leading to an excitation spectrum

$$\epsilon(k)=-2(\cos\theta)(1-\cos k) . \tag{3.2}$$

Note that in the range $\pi/2<\theta<5\pi/4$ these excitation energies are positive; the spectrum is gapless with a soft mode at $k=0$. The two-magnon excitation energies can be calculated by using the Bethe ansatz for the wave function as described by Papanicolaou and Psaltakis.[17]

For any momentum k there is a two-magnon continuum lying between the energies

$$\epsilon_{\pm}(k) = -4(\cos\theta)[1 \pm \cos(k/2)] \ . \tag{3.3}$$

In fact the excitations in the continuum can be characterized by two momenta k_1 and k_2, as usual, and the energy is just the sum of two free-magnon energies,

$$\epsilon(k_1,k_2) = -4(\cos\theta)[1 - \tfrac{1}{2}(\cos k_1 + \cos k_2)] \ , \tag{3.4}$$

or using the notation

$$k_1 = \tfrac{1}{2}k + q, \quad k_2 = \tfrac{1}{2}k - q \ , \tag{3.5}$$

we get

$$\epsilon(k,q) = -4(\cos\theta)[1 - (\cos\tfrac{1}{2}k)(\cos q)] \ . \tag{3.6}$$

In addition to this continuum there can be one or two bound states outside the continuum. Papanicolaou and Psaltakis[17] analyzed the region $\pi \le \theta \le 5\pi/4$ only and found a bound state below the continuum. This bound state is present also for $3\pi/4 < \theta < \pi$ and merges into the continuum at $\theta = 3\pi/4$, as shown in Fig. 1. For smaller values of θ an extra two-magnon state is found above the continuum, separated from it by a finite gap. This gap vanishes first at $k = \pi$ for $\theta = 3\pi/4$. As θ increases this extra state merges gradually into the continuum, disappearing finally at $k = 0$ at $\theta = 0.885\pi$. The development of the two-magnon spectrum between $\pi/2 \le \theta \le \pi$ is shown in Fig. 1.

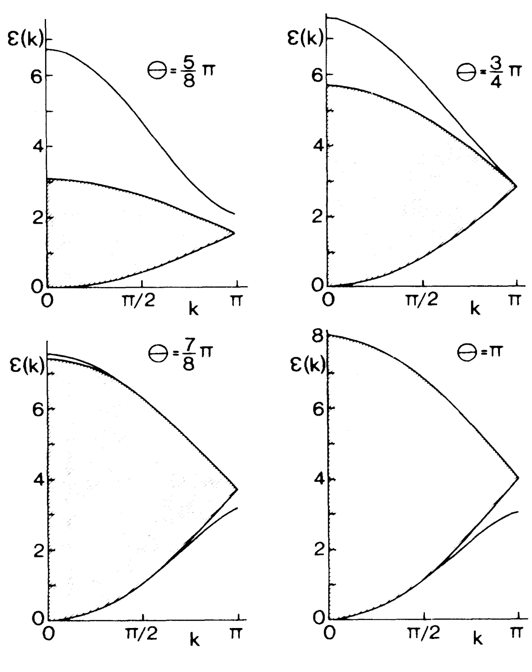

FIG. 1. Two-magnon spectrum for $\theta = 5\pi/8$, $6\pi/8$, $7\pi/8$, and $8\pi/8$ showing the development of the two extra states above and below the continuum (hatched region).

IV. ANTIFERROMAGNETIC REGION, $-3\pi/4 < \theta < \pi/2$

Outside the ferromagnetic region the ground state of a finite chain with an even number of sites is a spin singlet, $S_T^z = 0$. The first excited state is in the subspace $S_T^z = 1$. The gap between these two states was analyzed by Kung[15] in the region $-\pi/4 \le \theta \le 0$ and by Oitmaa *et al.*[16] for $-\pi/2 \le \theta \le 0$. In both cases chains up to $N = 12$ sites were considered and a periodic boundary condition was used.

Oitmaa *et al.*[16] infer from the finite-chain calculations that the singlet-triplet gap is finite for $-\pi/2 \le \theta < -\pi/4$. For $\theta > -\pi/4$ finite-size scaling seems to indicate an extended gapless phase; the boundaries of this phase could not be determined, however.

In order to have a better picture of the ground state I have extended these calculations to the whole antiferromagnetic (or singlet) region, $-3\pi/4 < \theta < \pi/2$, in two respects. I have calculated not only the singlet-triplet gap, but also the gap between the $S_T^z = 0$ ground state and the lowest $S_T^z = 2$ excited state. Furthermore, I have considered also chains with an odd number of sites, using both periodic and antiperiodic boundary conditions. The longest chain had $N = 12$ sites.

Considering first chains with an even number of sites and using a periodic boundary condition I have determined the lowest-lying states in the sectors $S_T^z = 0$, 1, and 2. The scaled gaps $N\Delta E$ for the singlet-triplet ΔE_{01} and singlet-quintet ΔE_{02} gaps are shown in Figs. 2 and 3, respectively.

The first gap ΔE_{01} has a maximum at $\theta = -\pi/2$, and there the scaled gap increases with the chain length. This lead Oitmaa *et al.*[16] to the conclusion that at this point, and in fact in the whole range $-\pi/2 \le \theta < -\pi/4$, the gap scales to a finite value. Close to $\theta = -3\pi/4$ and for $\theta > -\pi/4$ there seems to be a region where the gap scales to zero as $1/N$. To have a better estimate of the extent of these critical regions, I considered the secondary gap in the same region of θ. Contrary to the primary gap, the secondary gap has a maximum close to $\theta = -\pi/4$. This difference in the behavior comes from the difference in the symmetries of the three levels considered. The $S_T^z = 0$ ground state is translationally invariant; its wave vector is $k = 0$ for $-3\pi/4 \le \theta \le 0$. This is true also for the lowest $S_T^z = 2$ state. In the $S_T^z = 1$ subspace a translationally invariant $k = 0$ state is the lowest one for $-3\pi/4 \le \theta \le -\pi/2$. For $-\pi/2 \le \theta \le 0$, however, the lowest-lying state is a $k = \pi$ state. The level crossing at $\theta = -\pi/2$ between these $k = 0$ and $k = \pi$ states leads to the break in ΔE_{01}.

A finite-size scaling analysis of the secondary gap could indicate a finite gap in the whole $-3\pi/4 < \theta \le 0$ range, since the scaled gap increases with the system size. This apparent increase of the scaled gap can, however, be just a finite-size effect, showing that the corrections to the $1/N$ scaling of the gap are important at the available chain lengths. As seen in Fig. 3, for finite systems ΔE_{02} has a maximum very close to $\theta = -\pi/4$. On the other hand, it is known from the exact solution of the model that at $\theta = -\pi/4$ the secondary gap vanishes in the infinite chain. Unless there is a dramatic change

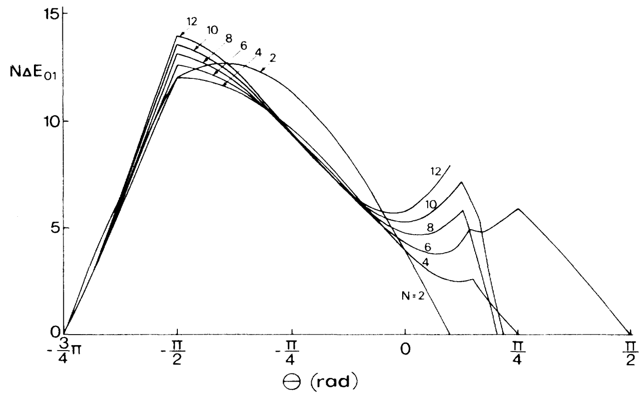

FIG. 2. Scaled gap between the lowest-lying levels of the $S_T^z=0$ and $S_T^z=1$ sectors for different chain lengths N.

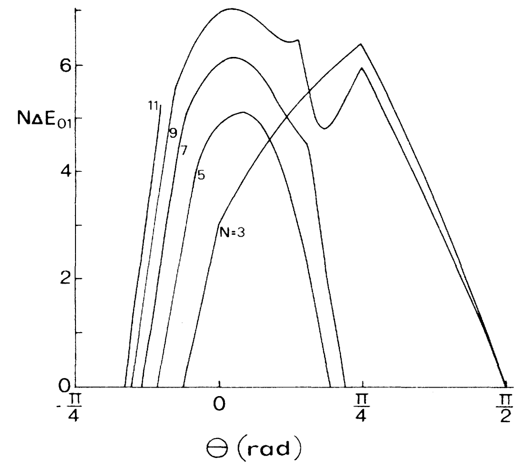

FIG. 4. Scaled primary gap for chains with an odd number of sites, using a periodic boundary condition.

in the behavior of the secondary gap for a very long chain, the numerical results indicate that the gap will vanish in an extended region around $\theta=-\pi/4$. It is tempting to conclude that in the whole range $-3\pi/4\leq\theta\leq-\pi/4$, including the point $\theta=-\pi/2$, the system is gapless. This conclusion will be further supported as other quantities are calculated.

On the other side of the $\theta=-\pi/4$ point, the conclusion is less clear. The analysis of the secondary gap does not help to determine the extent of the region where the gap scales to zero as $1/N$, and beyond which it remains finite. In this region our results coincide with those of Kung[15] and of Oitmaa *et al.*[16]

In the range $0<\theta<\pi/2$, which has not been studied before, new features appear. The primary and secondary gaps have one or two break points. This is due to the fact that the lowest-lying states in the $S_T^z=0$, 1, or 2 sectors are not necessarily translationally invariant. The wave vector of these states is either $k=0$ or $2\pi n/N$ with an integer n such that k is close to $2\pi/3$. This is not surprising since we know that at $\theta=\pi/4$ the soft modes are at $k=0$ and $k=\pm2\pi/3$. As a consequence, the ground state of the infinite system is periodic under translation with three lattice constants. Finite-size calculations should respect this periodicity. I have therefore done the calculations for chains with an odd number of sites, too, to include $N=3$ and 9. The scaled primary gap for finite odd chains using a periodic boundary condition is shown in Fig. 4. One characteristic feature is that the gap is identically zero for $-3\pi/4\leq\theta\leq-\pi/4$, confirming our earlier conclusion about this region. The gap becomes finite in the interval $(-\pi/4,0)$. It cannot be excluded that as $N\to\infty$ the gap becomes finite in this whole interval. The gap has a maximum between $0<\theta<\pi/4$ and vanishes again at $\theta=\pi/2$. When considering in this range chains with $N=3n$ sites ($N=3$ and 9 from Fig. 4 and $N=6$ from Fig. 2), it is found that for $\theta>\pi/4$ in good approximation the gap scales to zero as $1/N$. This indicates that the gapless, tripled-period phase obtained for $\theta=\pi/4$ is stable in the whole range $\pi/4\leq\theta\leq\pi/2$. In this interval of θ the soft modes are at $k=0$ and $\pm2\pi/3$. Below $\theta=\pi/4$ the gap both at $k=0$ and $k=\pm2\pi/3$ becomes finite. The spectrum changes in such a way that when at a θ_c in the interval $(-\pi/4,0)$ the gap vanishes again, the soft modes are at $k=0$ and π.

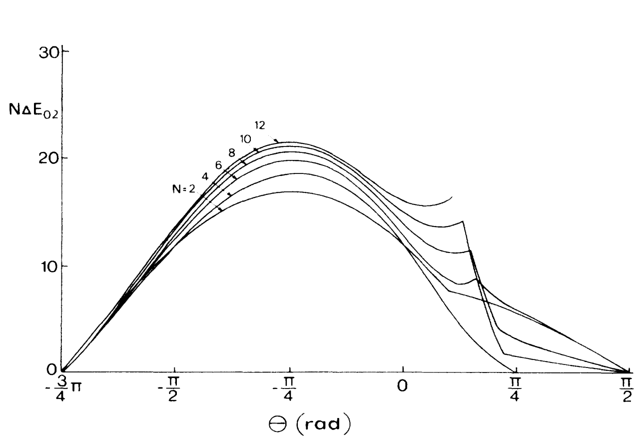

FIG. 3. Scaled gap between the lowest-lying levels of the $S_T^z=0$ and $S_T^z=2$ sectors for different chain lengths N.

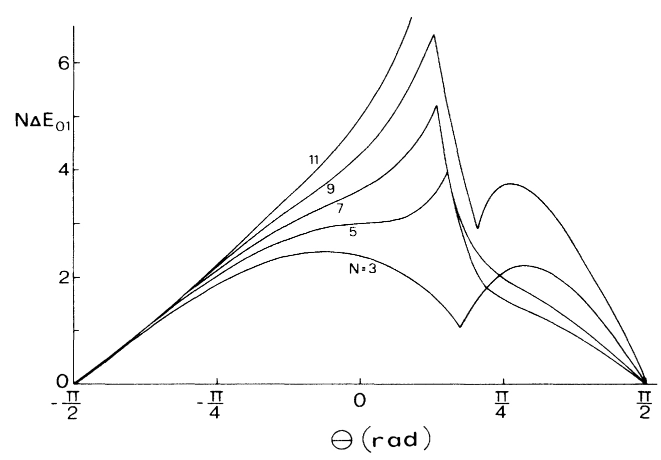

FIG. 5. Scaled primary gap for chains with an odd number of sites, using a modified boundary condition.

Odd chains ($N=3$ and 9) are useful for studying the period tripling near $\theta=\pi/4$. Their use with a periodic boundary condition is less clear for $\theta<0$, where period doubling is expected. It is probably more reasonable to use an antiperiodic boundary condition. In Fig. 5, I show the results obtained with a modified boundary condition. At the boundary the sign of the couplings are changed for the x and y components of the spin, but not for the z components, i.e., the two end spins are coupled as

$$(\cos\theta)(-S_N^xS_1^x-S_N^yS_1^y+S_N^zS_1^z)+(\sin\theta)(-S_N^xS_1^x-S_N^yS_1^y+S_N^zS_1^z)^2 . \tag{4.1}$$

As seen in Fig. 5, the primary gap vanishes identically at $\theta=-\pi/2$. Between $\theta=-\pi/2$ and $\theta=0$ the gap increases monotonously. Knowing that at $\theta=-\pi/4$ the gap has to vanish, we find again that the gap will vanish everywhere between $\theta=-\pi/2$ and $\theta=-\pi/4$. Below $\theta=-\pi/2$ the ground state of finite chains is not in the $S_T^z=0$ subspace; the lowest $S_T^z=1$ state lies lower. However, the energy difference scales to zero as $1/N$, indicating that here as well the gap vanishes.

V. SPIN-PEIERLS TRANSITION

It is well known that the spin-$\frac{1}{2}$ isotropic Heisenberg antiferromagnet is unstable against lattice distortions.[18] In a uniform lattice the excitation spectrum is gapless; the quantum zero-point fluctuations are important. On the other hand, in a dimerized lattice a gap opens in the excitation spectrum, the fluctuations become less important, and the ground-state energy is lowered. If this energy lowering is larger than the increase in the elastic energy, a spontaneous deformation takes place.

Suppose that in the distorted lattice the spins are at the positions

$$r_i=ia[1+(-1)^i\delta] , \tag{5.1}$$

where a is the original lattice constant and δ is the dimerization. The lowering of the ground-state energy is proportional to $\delta^{2\nu}$ and the gap to δ^{ν}. According to Cross and Fisher,[19] $\nu\simeq\frac{2}{3}$ for the $S=\frac{1}{2}$ isotropic antiferromagnet. Therefore, for small δ the energy gain is always larger than the elastic energy of the deformed lattice,

$$E_{\text{elastic}}=NK\delta^2 , \tag{5.2}$$

for any value of the elastic constant K. The minimum of the total energy is at a finite value of δ; the lattice is necessarily dimerized.

In the anisotropic $S=\frac{1}{2}$ Heisenberg model the lattice distortion will necessarily occur in the planar phase where the excitation spectrum is gapless and the correlation function

$$\langle S^x(r)S^x(0)\rangle \simeq r^{-\eta}$$

decays with an exponent $\eta>\frac{1}{2}$, i.e., for $J_z<0$. In the case of Ising-type anisotropy, where the gap is finite, the lattice distortion will appear only if K is smaller than a critical K_c. This is also the case in the planar region for $J_z>0$. Although the excitation spectrum is gapless, the magnetic energy gain due to the dimerization is not sufficient to overcome the elastic energy if K is large. In the ground state the chain remains undistorted.

The spin-Peierls transition seems to be related to the absence of a gap in the excitation spectrum. A gapless spectrum is a necessary but not sufficient condition for the lattice instability. For this reason I have studied the possibility of lattice distortion in the model with bilinear and biquadratic exchange interactions. For simplicity the effect of deformation on the two couplings is assumed to be identical, i.e., I have considered the Hamiltonian

$$H=\sum_i \{(\cos\theta)[1+(-1)^i\delta](\mathbf{S}_i\cdot\mathbf{S}_{i+1}) +(\sin\theta)[1+(-1)^i\delta](\mathbf{S}_i\cdot\mathbf{S}_{i+1})^2\} . \tag{5.3}$$

The total energy will of course contain the elastic part, too, given in Eq. (5.2).

There are two ways to study the spin-Peierls transition from numerical calculations on finite systems. The first is to consider the magnetic part of the Hamiltonian, Eq. (5.3), and to analyze the δ dependence of the ground-state energy and of the gap.[20–22] I show in Fig. 6 the δ dependence of the ground-state energy for $\theta=-\pi/2$.

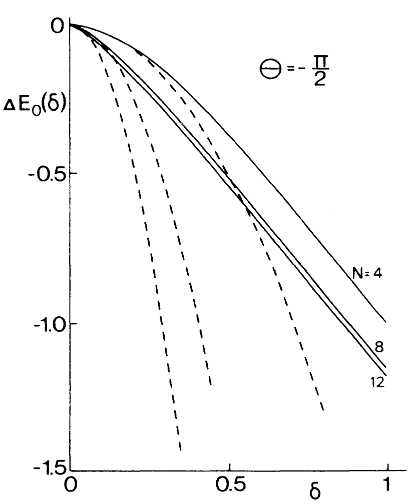

FIG. 6. Lowering of the ground-state energy as a function of the dimerization δ for different chain lengths N for $\theta=-\pi/2$. The dashed lines show the parabolic fit to the small δ region.

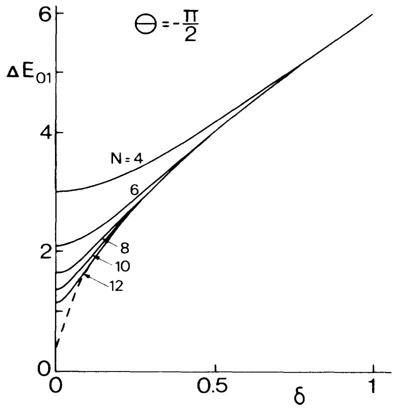

FIG. 7. Primary gap of the dimerized model for $\theta=-\pi/2$. The dashed curve is $A\delta^{\nu}$ with $\nu=0.55$.

For small δ the energy lowering is proportional to δ^2. As the chain length increases, this parabolic behavior is valid in a very narrow range, ultimately shrinking to zero as $N\rightarrow\infty$. Beyond the parabolic part, $\Delta E\sim\delta^{2\nu}$ with $\nu\sim0.5$ at $\theta=-\pi/2$. At $\theta=-\pi/4$ similar behavior is found with $\nu\sim0.7$.

The primary gaps as a function of δ are shown in Figs. 7 and 8 for $\theta=-\pi/2$ and $-\pi/4$, respectively. As the chain length increases, the gap approaches a curve that can be described as $A\delta^{\nu}$ with $\nu=0.55\pm0.02$ for $\theta=-\pi/2$ and $\nu=0.70\pm0.02$ for $\theta=-\pi/4$. These values are in good agreement with the ν determined from the lowering of the ground-state energy, where the error in the determination of ν is much larger. Since for both cases $\nu<1$, a spin-Peierls transition should take place. Furthermore, the existence of the spin-Peierls transition implies that even at $\theta=-\pi/2$ the spectrum is gapless.

For the analysis of the extent of the region where the spin-Peierls transition will take place I used another method proposed earlier[23] in the study of spin-Peierls transition for $S>\frac{1}{2}$ Heisenberg chains. When the elastic energy, Eq. (5.2), is taken into account, for a finite system there always exists a critical value, K_c of the elastic constant, such that for $K>K_c$ the ground state is uniform and the minimum of the total energy is at $\delta=0$, while for $K<K_c$ the minimum is at a finite δ and the system is dimerized. If K_c diverges as $N\rightarrow\infty$, a spontaneous deformation of the lattice is always favorable and a spin-Peierls transition takes place. Figure 9 shows the value of K_c determined for different chain lengths. Close to $\theta=-3\pi/4$ and to $\theta=0$ the dimerization appears at K_c discontinuously as K is varied; otherwise the transition is continuous. The critical value of θ beyond which the dimerization transition is discontinuous decreases as the chain length increases, as shown in the inset of Fig. 9. As $N\rightarrow\infty$, θ_c may approach $\theta=-\pi/4$, although at this point K_c will have to diverge. In the neighborhood of $\theta=-\pi/2$ K_c increases linearly with the chain length and diverges as $N\rightarrow\infty$. Therefore K_c will diverge for $-\pi/2\leq\theta\leq-\pi/4$, and the infinite chain is always dimerized, indicating a gapless spectrum in agreement with the other approach.

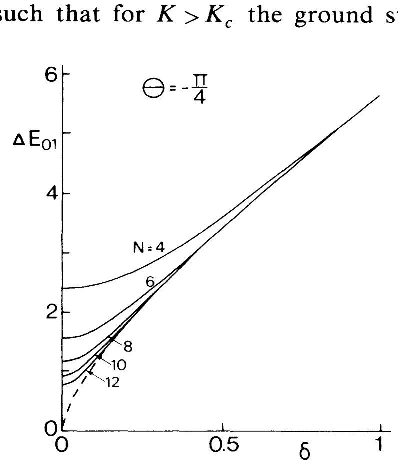

FIG. 8. Primary gap of the dimerized model for $\theta=-\pi/4$. The dashed curve is $A\delta^{\nu}$ with $\nu=0.7$.

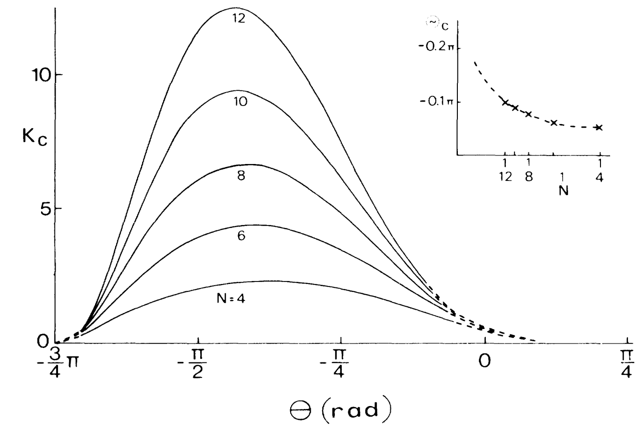

FIG. 9. The critical elastic constant K_c separating the uniform and dimerized phases for finite chains. The dashed curves show the region where the transition is discontinuous. The inset shows the critical values of θ vs $1/N$, where the transition becomes discontinuous.

It is interesting to note that there is a special value $\theta=0.1024\pi$, which is the solution of the equation $\cos\theta=3\sin\theta$, where $K_c=0$ for any chain length; i.e., the chain will never be dimerized. This may be related to the fact that for larger θ values the ground state has a tripled period. Instead of forming dimers the chains may prefer to form trimers.

VI. DISCUSSION

In the present paper the possible ground states of a spin-1 magnetic chain with bilinear and biquadratic exchange couplings have been considered. Using the parametrization (2.6) for the couplings, it was expected[14] that the ferromagnetic phase is stable for $3\pi/4\leq\theta\leq5\pi/4$. I have shown that the ground state is ferromagnetic in a wider range, namely for $\pi/2\leq\theta\leq5\pi/4$, and I have determined the spin-wave spectrum as well as the two-spin deviation states. In addition to the two-magnon continuum, there are two extra states, one below the continuum for $3\pi/4\leq\theta\leq5\pi/4$ and one above it for $\pi/2 \le \theta \le 0.885\pi$.

Outside the ferromagnetic regime the ground state is an $S_T^z=0$ state. I have used finite chain calculations up to $N=12$ sites to study the possible degeneracies in the infinite system. Extending the earlier finite-size scaling analysis of Kung[15] and Oitmaa *et al.*,[16] I have calculated not only the primary, but also the secondary gap in the $-3\pi/4 < \theta < \pi/2$ region. Near $\theta=\pi/4$, where a tripled-period ground state is expected, further information can be obtained from the results on chains with an odd number of sites. Furthermore, since the existence of a spin-Peierls transition is closely related to the absence of a gap in the excitation spectrum, I have also studied the possibility of spin-Peierls distortion.

All these considerations lead us to the conclusion that in the range $-3\pi/4 \le \theta \le \pi/2$ the phase diagram consists of three different phases. For $-3\pi/4 \le \theta \le \theta_c$, where $-\pi/4 \le \theta_c \le 0$, the ground state has the same character as at the exactly soluble point $\theta=-\pi/4$, i.e., the excitation spectrum is gapless; the soft modes are at $k=0$ and π. On the other hand, in the region $\pi/4 \le \theta \le \pi/2$ the ground state has the same character as at the other exactly soluble point, $\theta=\pi/4$. The excitation spectrum is again gapless; the soft modes are, however, at $k=0$ and $\pm 2\pi/3$. While in the first case the ground state is periodic under translation by $2a$, here it is periodic under translation by $3a$. Between these two phases with different symmetries there is a region, where the ground state is a nondegenerate singlet, and the spectrum has a finite gap. The present calculation cannot give a precise location for θ_c and therefore is not decisive in the controversy around Haldane's claim[7] of a massive spectrum at $\theta=0$. It seems to be, however, in contradiction to Affleck's claim[14] of massive behavior around $\theta=-\pi/2$. I believe that the results presented above give strong evidence that mappings to continuum field-theory models have to be performed with extreme care.

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