

## Spontaneous trimerization of spin-1 chains

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1993 J. Phys.: Condens. Matter 5 7489

(<http://iopscience.iop.org/0953-8984/5/40/023>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.96

The article was downloaded on 11/05/2010 at 01:58

Please note that [terms and conditions apply](#).

## Spontaneous trimerization of spin-1 chains

Y Xian

Department of Mathematics, University of Manchester Institute of Science and Technology (UMIST), PO Box 88, Manchester M60 1QD, UK

Received 27 May 1993, in final form 15 July 1993

**Abstract.** Spontaneous trimerization of the one-dimensional spin-1 Heisenberg-biquadratic model is discussed in terms of a valence-bond (VB) analysis. A spin-wave theory based on a simple trimer VB state is developed and applied to the model. Within the theory a self-consistent picture is obtained: the system is trimerized for an extended region of couplings, with a non-zero energy gap that collapses at both ends of the region. Agreement with the exact results of Lai and Sutherland is found at one end of the region.

### 1. Introduction

Low-dimensional spin-lattice systems continue to attract a great deal of attention because they possess a variety of interesting properties, some of which are quite unexpected. The critical phase of the one-dimensional (1D) spin- $\frac{1}{2}$  Heisenberg model exactly solved by Bethe's *ansatz* [1], and the Haldane conjecture of non-zero gap for the 1D spin-1 Heisenberg model [2], are two classical examples. More recently, the two-dimensional (2D) systems with various couplings and lattice structures [3], including those relevant to the high-temperature superconductors [4], have been under intensive study.

For the case of 1D spin-1 systems, the Heisenberg-biquadratic model is particularly interesting. There are some exact results available for the model at several coupling constants [5–8]. Based on these exact results, and other analytical and numerical works [9–12], it seems reasonable to assume that there are at least three phases within the antiferromagnetic region of the system: the dimerized phase with doubly degenerate ground states, the homogeneous, non-degenerate phase with a non-zero energy gap but without any conventional symmetry breaking (including the conjectured Haldane phase of the pure Heisenberg model), and the trimerized phase in which a threefold periodicity is expected. While the dimerized phase has recently been studied by Chubukov [10] using a spin-wave theory based on a simple dimer state, much attention has been devoted to the non-degenerate phase of the system since Haldane conjectured the existence of a non-zero gap for the pure Heisenberg model about ten years ago [2]. Despite the early works of Lai and Sutherland [8], and a simple valence-bond (VB) analysis [11] and a recent finite-size calculation [12], the trimerized phase, if it exists, is not well understood, particularly with regard to its long-range order and excitations.

In this article I intend to investigate these problems by the use of a spin-wave theory. I first discuss the trimerization of the spin-1 system in terms of VB configurations. As discussed in [11], it is found that in addition to the dimerization and the homogeneous, non-degenerate configurations, the spin-1 system has a strong tendency to trimerize also, producing a sequence of spin-singlet states formed from every three adjacent atoms. I then

develop a spin-wave theory based on this trimer VB state and obtain the energy spectra for the excitations. Based on these spectra, I discuss the stability of the trimerization for various values of the coupling constants. It should be stressed that this spin-wave theory is inspired by the similar technique developed in 1979 by Parkinson [13] who focused on the 1D spin- $\frac{1}{2}$  Heisenberg model. He used a simple dimer state as his model state and was able to obtain a triplet excitation, in agreement with the exact result [1].

The outline of this article is as follows. In section 2 a brief review of the exact results of the spin-1 Heisenberg-biquadratic model is given. Then the three representative VB configurations are discussed. Section 3 is devoted to the three-atom system in the spin-1 case. The spin-wave theory based on the simple trimer configuration is developed in detail in section 4. The excitation spectra are derived and a non-zero energy gap is predicted. Comparison with the exact results [8] of Lai and Sutherland at one of the critical points is made. I conclude this article with a discussion in section 5.

## 2. The model and the valence bonds

The 1D spin-1 Heisenberg-biquadratic Hamiltonian is given by

$$H = \cos \theta \sum_{i=1}^N \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sin \theta \sum_{i=1}^N (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \quad (2.1)$$

where the sums are over all lattice sites with the usual periodic boundary condition,  $\mathbf{S}_i$  are spin vectors with  $|\mathbf{S}_i| = 1$ , obeying the usual angular momentum commutation relationships, and the coupling constants are expressed through the angular parameter  $\theta$ . The antiferromagnetic region is given by  $-\frac{3}{4}\pi < \theta < \frac{1}{2}\pi$ , and the rest is ferromagnetic. The pure Heisenberg model is given by  $\theta = 0$ .

There are exact results available for the following coupling constants. At  $\theta = -\frac{1}{2}\pi$ , the exact ground state and low-lying excited states can be obtained by a partial mapping to the spin- $\frac{1}{2}$  anisotropic model which has the exact solutions by Bethe's *ansatz* [5]. There is a non-zero energy gap and the ground state is doubly degenerate, possibly with a dimer long-range order. At  $\theta = -\frac{1}{4}\pi$ , the system is integrable by Bethe's *ansatz* and has a gapless excitation [6]. At  $\tan \theta = \frac{1}{3}$ , the ground state is given by a simple non-degenerate, homogeneous VB configuration [7], details of which are given later; a finite energy gap is shown to exist at this point. Finally, at  $\theta = \frac{1}{4}\pi$ , the system is again integrable and, most interestingly for present purposes, has been shown to have a triple periodicity with a gapless excitation at the lattice momenta  $k = 0$  and  $\frac{2}{3}\pi$  [8].

An exact and complete phase diagram for the system is not known, but it seems reasonable to assume that there are at least three phases in the antiferromagnetic region, namely, the dimerized, homogeneous (non-degenerate), and trimerized phases. The phase transition from the dimerized phase to the non-degenerate phase is likely to be at  $\theta = -\frac{1}{4}\pi$  where the system becomes critical and has a gapless excitation [6]. A finite energy gap opens up away from this point in both directions. The pure Heisenberg model (with the conjectured Haldane phase) is in the non-degenerate phase region. Both dimerized and non-degenerate phases have a double periodicity. The field-theory approach [9] based on the Wess-Zumino-Witten model and the dimerized spin-wave theory [10] both seem to agree with this picture. It is interesting to note that the massive dimerized phase was conjectured [9] before the exact results [5] were available at  $\theta = -\frac{1}{2}\pi$ .

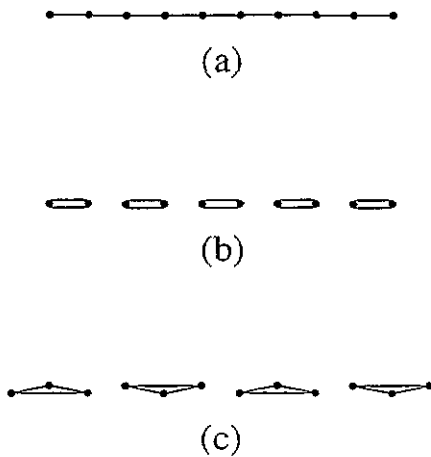


Figure 1. The three simple VB states: (a) homogeneous, (b) dimer, and (c) trimer. A bar represents a VB defined by equation (2.4).

However, the transition from the non-degenerate phase to the trimerized phase, if it even exists, is far from clear. A recent finite-size calculation [12] does confirm the existence of a finite region in which the system possesses a triple periodicity, but this work also supports the result that the system is gapless in this region. This is contrary to the conclusion of [11] whose authors believe the trimerized phase to be massive.

The possible three antiferromagnetic phases mentioned are well represented by the three simple corresponding VB configurations, i.e., homogeneous, dimer, and trimer states. In fact, the study of spin systems in terms of VB configurations has a long history [14]. It has resurged [7, 15–18] since Haldane’s conjecture [2] and the discovery of high-temperature superconductors. In [11] a discussion of trimerization in terms of VB configurations was perhaps first made. For completeness, some of the ideas are repeated here.

In any discussion of VB configurations, it is useful to express the spin operators in terms of two pairs of Schwinger boson operators as

$$S^+ = a^+b \quad S^- = ab^+ \quad S^z = \frac{1}{2}(a^+a - b^+b) \tag{2.2}$$

where  $a, a^+$  and  $b, b^+$  obey the usual boson commutation relations.

A VB is simply a spin-singlet configuration. For example, a system of two atoms each with spin  $\frac{1}{2}$  has the ground state which can be represented by a VB as

$$|\Phi_1\rangle = C_{12}^+|0\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{2.3}$$

where  $|0\rangle$  is the vacuum state of the bosons, the spin- $\frac{1}{2}$  up and down states are represented by the obvious notations, and the VB operator  $C_{ij}^+$  is defined by

$$C_{ij}^+ \equiv a_i^+b_j^+ - a_j^+b_i^+ \tag{2.4}$$

A VB configuration for a system of  $N$  atoms each with spin  $S$  is formed by connecting each atom with  $2S$  bonds. It has been shown that all VB states are in the sector of  $S_{\text{total}} = 0$ , and the ground state of the system is given by a linear combination of all independent VB configurations without bond crossing [7, 15, 17].

The three representative VB configurations shown in figure 1, where a bar represents a VB defined by equation (2.4). It is clear that the homogeneous state has correlations of arbitrary long range (exponential-decay function [7]), but the correlation lengths of dimer and trimer configurations are very short, only two and three lattices respectively. Furthermore, the homogeneous configuration is obviously non-degenerate, while dimer and trimer configurations have double and triple degeneracies respectively, and the translational symmetry is broken in both the dimer and trimer states.

In figure 1, a single double-bond configuration in fact gives the singlet ground state of the two-atom spin-1 system, i.e.

$$|\Phi_2\rangle = (C_{ij}^+)^2|0\rangle = 2(|1 - 1\rangle + |-1 1\rangle - |0 0\rangle) \quad (2.5)$$

where in the last equation, I have used the three  $S^z$  values (0,  $\pm 1$ ) to denote the single-atom states of spin 1. Also, a single three-bond configuration gives the singlet ground state of the three-atom system, i.e.

$$|\Phi_3\rangle = C_{12}^+ C_{23}^+ C_{31}^+ |0\rangle = 2(|01 - 1\rangle + |1 - 10\rangle + |-101\rangle - |0 - 11\rangle - |-110\rangle - |10 - 1\rangle). \quad (2.6)$$

As emphasized in [11], this three-bond configuration is an eigenstate of all three spin-paired operators,  $S_1 \cdot S_2$ ,  $S_2 \cdot S_3$ , and  $S_3 \cdot S_1$ .

The homogeneous, dimer, and trimer VB states in figure 1, denoted as  $|H\rangle$ ,  $|D\rangle$  and  $|T\rangle$  respectively, can be written in terms of  $C_{ij}^+$  as

$$|H\rangle = \frac{1}{\sqrt{3 + 3^N}} \prod_{i=1}^N C_{i+1}^+ |0\rangle \quad (2.7)$$

$$|D\rangle = \frac{1}{(2\sqrt{3})^{N/2}} \prod_{i=0}^{N/2} (C_{2i+1}^+)^2 |0\rangle \quad (2.8)$$

$$|T\rangle = \frac{1}{(2\sqrt{6})^{N/3}} \prod_{i=0}^{N/3} C_{3i+1}^+ C_{3i+2}^+ C_{3i+3}^+ |0\rangle. \quad (2.9)$$

Taking these three VB states as trial wave functions, it is a straightforward calculation to obtain the corresponding energy expectation values as a function of  $\theta$ . They are given by [7], [18] and [11] respectively:

$$\frac{E_0}{N} = \begin{cases} -\frac{4}{3} \cos \theta + 2 \sin \theta & \text{(homogeneous)} \\ -\cos \theta + \frac{8}{3} \sin \theta & \text{(dimer)} \\ -\frac{2}{3} \cos \theta + \frac{10}{9} \sin \theta & \text{(trimer)}. \end{cases} \quad (2.10)$$

For completeness, these values are shown in figure 2 as a function of  $\theta$ , together with the numerical results obtained by extrapolating the data of the finite-size exact calculations of Parkinson [19]. We note that the homogeneous VB state is the *exact* ground state for the Hamiltonian (2.1) at  $\tan \theta = \frac{1}{3}$  [7]. The dimer state has lower energy than that of the homogeneous state for  $\theta < \tan^{-1}(-\frac{1}{2}) \simeq -26.6^\circ$ ; for larger  $\theta$ , however, the homogeneous state has lower energy. At even larger  $\theta$ , it is interesting to see that the trimer state has the lowest energy. This occurs when  $\theta > \tan^{-1}(\frac{3}{4}) \simeq 36.9^\circ$ . As can be seen from the figure, the lower envelope of the three curves is quite close to the 'exact' results over the entire antiferromagnetic region. This crude approximation certainly seems to give a clear picture for the phase diagram of the spin-1 system, so far as the ground-state energy is concerned.

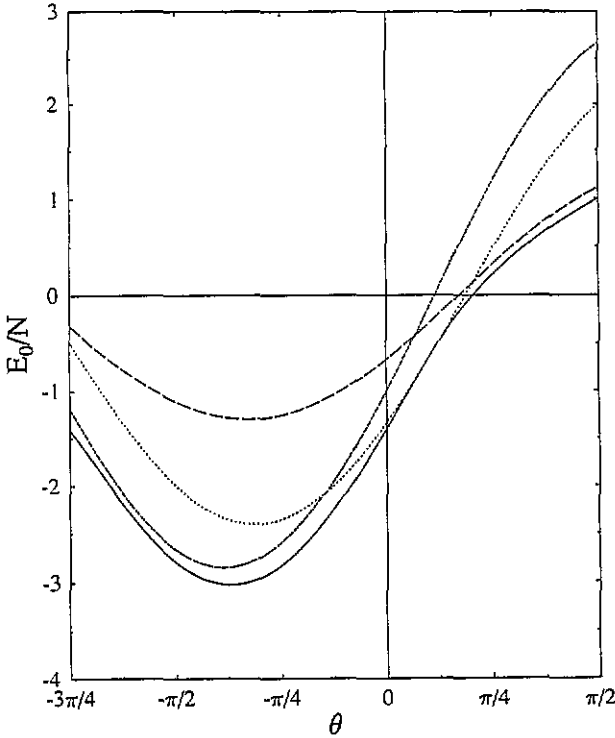


Figure 2. The expectation values  $E_0$  of the 1D spin-1 Heisenberg-biquadratic Hamiltonian with respect to the three simple VB states, i.e., homogeneous (dotted curve), dimer (short-dashed curve), and trimer (long-dashed curve), shown as functions of the coupling parameter  $\theta$  in the antiferromagnetic region. Also shown are the 'exact' results of [19] (full curve).

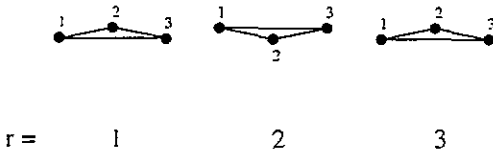


Figure 3. Trimer index labellings for equation (4.1).

Of course, the precise locations of the critical points given here are not to be trusted because of the gross simplification.

I should also point out that the trimer VB state has a feature which is not shared by the other two: it contains no Néel state configurations, as can be seen from equation (2.6). In terms of the three single-atom states, a Néel state of spin-1 chain is simply given by  $|1 - 1 1 - 1 \dots\rangle$ , without any  $S^z = 0$  state. Furthermore, every term in the trimer VB state has an equal number of  $S^z = 0, \pm 1$  states. This feature certainly reminds us of the exact solution of Lai and Sutherland [8] at  $\theta = \frac{1}{4}\pi$ , where the ground state is given by all possible permutations of the three single-atom states, and hence the Néel state is not present. One also notices that the spin- $\frac{1}{2}$  and other half-odd-integer-spin systems do not favour this trimer configuration because they cannot form a singlet-spin state with three atoms.

From the above analysis, it is clear that for the extended spin-1 chain the trimer VB state is a good model state for study of possible trimerization; any additional correlations in the system can then be built upon this trimer model state. This is exactly analogous to the case for the dimerized system where the dimer VB state should be used [10].

### 3. Three-atom system

Since an atom of spin 1 has three states with  $S^z = 0$  and  $\pm 1$  respectively, a three-atom system has  $3^3 (= 27)$  states. With  $S_{\text{total}}$  ( $S_{\text{total}} \equiv S_1 + S_2 + S_3$ ) and  $S_{\text{total}}^z$  as good quantum numbers, these 27 states can be obtained in terms of the three single-atom states by a simple diagonalization procedure. It is found that each state with  $S_{\text{total}} = 1$  has a triplet 'accidental' degeneracy, and each state with  $S_{\text{total}} = 2$  has a doublet 'accidental' degeneracy. Corresponding to  $S_{\text{total}} = 0, 1, 2,$  and  $3$ , the eigenvalues of the three-atom Hamiltonian,  $S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_1$ , are  $-3, -2, 0,$  and  $3$  respectively.

The following is a list of those 27 states,  $|n\rangle$  with  $n = 1, 2, \dots, 27$ , with the prime and double primes indicating the degenerate states, all normalized and orthogonal to one another:

$$\begin{aligned}
 |1\rangle &\equiv |00\rangle = (1/\sqrt{6})(|0-11\rangle + |-110\rangle + |10-1\rangle - |01-1\rangle - |1-10\rangle - |-101\rangle) \\
 |2\rangle &\equiv |1-1\rangle = (1/\sqrt{15})(|-100\rangle + |0-10\rangle + |00-1\rangle - 2|-1-11\rangle - 2|-11-1\rangle - 2|1-1-1\rangle) \\
 |3\rangle &\equiv |1-1'\rangle = (1/2\sqrt{3})(|-100\rangle + |0-10\rangle - 2|00-1\rangle - 2|-1-11\rangle + |-11-1\rangle + |1-1-1\rangle) \\
 |4\rangle &\equiv |1-1''\rangle = \frac{1}{2}(|-100\rangle - |0-10\rangle - |-11-1\rangle + |1-1-1\rangle) \\
 |5\rangle &\equiv |10\rangle = (1/\sqrt{15})(3|000\rangle - |1-10\rangle - |-101\rangle - |01-1\rangle - |-110\rangle - |10-1\rangle - |0-11\rangle) \\
 |6\rangle &\equiv |10'\rangle = (1/2\sqrt{3})(2|1-10\rangle + 2|-110\rangle - |10-1\rangle - |0-11\rangle - |01-1\rangle - |-101\rangle) \\
 |7\rangle &\equiv |10''\rangle = \frac{1}{2}(|10-1\rangle + |-101\rangle - |01-1\rangle - |0-11\rangle) \\
 |8\rangle &\equiv |11\rangle = (1/\sqrt{15})(|100\rangle + |010\rangle + |001\rangle - 2|11-1\rangle - 2|1-11\rangle - 2|-111\rangle) \\
 |9\rangle &\equiv |11'\rangle = (1/2\sqrt{3})(|100\rangle + |010\rangle - 2|001\rangle - 2|11-1\rangle + |1-11\rangle + |-111\rangle) \\
 |10\rangle &\equiv |11''\rangle = \frac{1}{2}(|100\rangle - |010\rangle - |1-11\rangle + |-111\rangle) \\
 |11\rangle &\equiv |2-2\rangle = (1/\sqrt{6})(|-10-1\rangle + |0-1-1\rangle - 2|-1-10\rangle) \\
 |12\rangle &\equiv |2-2'\rangle = (1/\sqrt{2})(|0-1-1\rangle - |-10-1\rangle) \\
 |13\rangle &\equiv |2-1\rangle = (1/2\sqrt{3})(2|00-1\rangle - |0-10\rangle - |-100\rangle - 2|-1-11\rangle + |-11-1\rangle + |1-1-1\rangle) \\
 |14\rangle &\equiv |2-1'\rangle = \frac{1}{2}(|0-10\rangle - |-100\rangle - |-11-1\rangle + |1-1-1\rangle) \\
 |15\rangle &\equiv |20\rangle = \frac{1}{2}(|01-1\rangle + |10-1\rangle - |-101\rangle - |0-11\rangle) \\
 |16\rangle &\equiv |20'\rangle = (1/2\sqrt{3})(2|1-10\rangle - 2|-110\rangle + |10-1\rangle - |-101\rangle + |0-11\rangle - |01-1\rangle) \\
 |17\rangle &\equiv |21\rangle = (1/2\sqrt{3})(|010\rangle + |100\rangle - 2|001\rangle + 2|11-1\rangle - |1-11\rangle - |-111\rangle) \\
 |18\rangle &\equiv |21'\rangle = \frac{1}{2}(|100\rangle - |010\rangle + |1-11\rangle - |-111\rangle) \\
 |19\rangle &\equiv |22\rangle = (1/\sqrt{6})(2|110\rangle - |101\rangle - |011\rangle) \\
 |20\rangle &\equiv |22'\rangle = (1/\sqrt{2})(|101\rangle - |011\rangle) \\
 |21\rangle &\equiv |3-3\rangle = |-1-1-1\rangle \\
 |22\rangle &\equiv |3-2\rangle = (1/\sqrt{3})(|0-1-1\rangle + |-10-1\rangle + |-1-10\rangle) \\
 |23\rangle &\equiv |3-1\rangle = (1/\sqrt{15})(2|00-1\rangle + 2|0-10\rangle + 2|-100\rangle + |1-1-1\rangle + |-1-11\rangle + |-11-1\rangle) \\
 |24\rangle &\equiv |30\rangle = (1/\sqrt{10})(2|000\rangle + |-101\rangle + |01-1\rangle + |1-10\rangle + |10-1\rangle + |0-11\rangle + |-110\rangle) \\
 |25\rangle &\equiv |31\rangle = (1/\sqrt{15})(2|001\rangle + 2|010\rangle + 2|100\rangle + |-111\rangle + |11-1\rangle + |1-11\rangle) \\
 |26\rangle &\equiv |32\rangle = (1/\sqrt{3})(|011\rangle + |101\rangle + |110\rangle) \\
 |27\rangle &\equiv |33\rangle = |111\rangle
 \end{aligned}$$

where in each equation the two arguments in the second Dirac notations are the values of  $S_{\text{total}}$  and  $S_{\text{total}}^z$  respectively, and the Dirac notations with three arguments represent a three-atom state with the corresponding three  $S_i^z$  values.

In a matrix representation, these 27 states can be represented by a column matrix with a single non-zero element, and any single-atom spin operator can therefore be written as a  $27 \times 27$  matrix. There are nine such operators, i.e.,  $S_i^z, S_i^\pm$  with  $i = 1, 2, 3$ . Following Parkinson [13], I decompose these spin operators by introducing a new set of  $27 \times 27$  matrices,  $A_{n,m}$ , which have a single non-zero element (unity) on the  $n$ th row and  $m$ th column, i.e.,  $\langle n' | A_{n,m} | m' \rangle = \delta_{n,n'} \delta_{m,m'}$ . The physical meaning of an  $A_{n,m}$  operator is obvious: it transforms state  $|m\rangle$  into state  $|n\rangle$ , i.e.,  $A_{n,m} |m\rangle = |n\rangle$ . For example,  $A_{n,m}$  with  $n, m = 1, 5, 6, 7, 15, 16, 24$  are operators which leave  $S_{\text{total}}^z$  unchanged; and  $A_{1,n}$  with  $n = 2, 3, 4, 13, 14, 23$  and  $A_{n,1}$  with  $n = 8, 9, 10, 17, 18, 25$  are operators which increase  $S_{\text{total}}^z$  by a unit, etc. One can see also that the diagonal operators,  $A_{n,n}$ , are the usual projection operators.

The single-atom spin operators can then be written by linear combinations of  $A_{n,m}$  operator. For example,  $S_3^z$  is given by,

$$\begin{aligned} S_3^z = & -\sqrt{2/3}A_{1,7} - \frac{1}{3}A_{2,2} + \frac{1}{3}\sqrt{5}A_{2,3} + (1/\sqrt{5})A_{2,13} + \frac{1}{3}\sqrt{5}A_{3,2} - \frac{1}{6}A_{3,3} + \frac{1}{2}A_{3,13} - \frac{1}{2}A_{4,4} \\ & - \frac{1}{2}A_{4,14} + \frac{2}{15}A_{5,15} + (1/\sqrt{3})A_{6,15} - (2/\sqrt{6})A_{7,1} - (1/\sqrt{3})A_{7,16} + \frac{1}{3}A_{8,8} \\ & - \frac{1}{3}\sqrt{5}A_{8,9} + (1/\sqrt{5})A_{8,17} - \frac{1}{3}\sqrt{5}A_{9,8} + \frac{1}{6}A_{9,9} + \frac{1}{2}A_{9,17} + \frac{1}{2}A_{10,10} \\ & - \frac{1}{2}A_{10,18} - \frac{1}{3}A_{11,11} - \frac{1}{3}\sqrt{2}A_{11,22} - A_{12,12} + (1/\sqrt{5})A_{13,2} \\ & + \frac{1}{2}A_{13,3} - \frac{1}{6}A_{13,13} - (4/3\sqrt{5})A_{13,23} - \frac{1}{2}A_{14,4} - \frac{1}{2}A_{14,14} + (2/\sqrt{15})A_{15,5} \\ & + (1/\sqrt{3})A_{15,6} - \sqrt{2/5}A_{15,24} - (1/\sqrt{3})A_{16,7} + (1/\sqrt{5})A_{17,8} + \frac{1}{2}A_{17,9} + \frac{1}{6}A_{17,17} \\ & - (4/3\sqrt{5})A_{17,25} - \frac{1}{2}A_{18,10} + \frac{1}{2}A_{18,18} + \frac{1}{3}A_{19,19} - \frac{1}{3}\sqrt{2}A_{19,26} \\ & + A_{20,20} - A_{21,21} - \frac{1}{3}\sqrt{2}A_{22,11} - \frac{2}{3}A_{22,22} - (4/3\sqrt{5})A_{23,13} \\ & - \frac{1}{3}A_{23,23} - \sqrt{2/5}A_{24,15} - (4/3\sqrt{5})A_{25,17} + \frac{1}{3}A_{25,25} - \frac{1}{3}\sqrt{2}A_{26,19} \\ & + \frac{2}{3}A_{26,26} + A_{27,27}. \end{aligned} \quad (3.1)$$

Similar formulae are easily derived for all other single-spin operators.

Conversely, each  $A_{n,m}$  can be expressed in terms of the single spin operators, in terms of which they are obviously nonlinear. For example, one can express  $A_{1,1}$  for this trimer spin-1 system as

$$A_{1,1} = \frac{1}{18}S_{123}(6 + S_{123} - S_{123}^2) \quad (3.2)$$

with  $S_{123}$  defined by  $S_{123} \equiv S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_1$ . It is in this sense that I refer to these  $A_{n,m}$  matrices as *composite operators*. These composite operators have simple commutation relations

$$[A_{n,m}, A_{k,l}] = A_{n,l} \delta_{m,k} - A_{k,m} \delta_{n,l}. \quad (3.3)$$

The spin-wave theory of trimerization is developed in the following section, using these  $A_{n,m}$  matrices, and their commutation relations, equation (3.3).



#### 4. Spin-wave theory

In the previous section, the single spin operators are expressed in terms of  $27 \times 27$  matrices and then decomposed into linear combinations of the so-called composite operators,  $A_{n,m}$ . The original Hamiltonian, equation (2.1), can accordingly be expressed exactly in terms of these composite operators. It is in this form that the approximation of the spin-wave theory is made.

Firstly, I introduce the trimer index as shown in figure 3. Equation (2.1) is then written as

$$H = \sum_{r=1}^{N/3} (H_r + H_{r,r+1})$$

$$H_r \equiv \cos \theta [(S_1 \cdot S_2)(r) + (S_2 \cdot S_3)(r)] + \sin \theta [(S_1 \cdot S_2)^2(r) + (S_2 \cdot S_3)^2(r)] \quad (4.1)$$

$$H_{r,r+1} \equiv \cos \theta S_3(r) \cdot S_1(r+1) + \sin \theta [S_3(r) \cdot S_1(r+1)]^2.$$

where all the single-spin operators should be expressed in terms of  $A_{n,m}$  operators, and I have used the notation  $(S_i \cdot S_j)(r) \equiv S_i(r) \cdot S_j(r)$  for simplicity. After this is done, equation (4.1) is obviously a very long expression. I therefore will not list it explicitly.

##### 4.1. Equations of motion

Following Parkinson [13], I derive the equations of motion for all composite operators. Consider first those operators which leave  $S_{\text{total}}^z$  unchanged, i.e.,  $A_{1,n}$ ,  $A_{n,1}$  and  $A_{n,m}$  with  $n, m = 5, 6, 7, 15, 16, 24$ .

Since the equations are still very involved, I adopt a truncation scheme to simplify the procedure of the spin-wave approximation. This is to disregard those trimer states in the final expression of equation (4.1), which have  $S_{\text{total}} > 1$  (i.e., states  $|11\rangle$ – $|27\rangle$ ); hence all matrices involved are reduced to  $10 \times 10$ . This means that in equation (4.1) only those  $A_{n,m}$  with  $n, m \leq 10$  are retained. Within this truncation approximation, those operators which leave  $S_{\text{total}}^z$  unchanged are  $A_{n,1}$ ,  $A_{1,n}$  and  $A_{n,m}$  with  $n, m = 5, 6, 7$ . The justification for this truncation scheme lies in the fact that for a three-spin system as discussed in section 3, the energy difference between the singlet state and those states with  $S_{\text{total}} = 1$  is one unit, whereas the energy difference between the singlet state and those states with  $S_{\text{total}} = 2$  or 3 is three or six units respectively.

Using equation (3.3), I derive the following equation of motion for  $A_{5,1}$  with the eigenvalue denoted by  $\omega$ , after disregarding any  $A_{n,m}$  with  $n > 10$  or  $m > 10$ :

$$\omega A_{5,1}^r = [H, A_{5,1}^r] = [H_r, A_{5,1}^r] + [H_{r-1,r}, A_{5,1}^r] + [H_{r,r+1}, A_{5,1}^r] \quad (4.2)$$

where

$$[H_r, A_{5,1}^r] = \cos \theta \left( \frac{2}{3} A_{5,1}^r + \frac{1}{3} \sqrt{5} A_{6,1}^r - \sqrt{5/3} A_{7,1}^r \right) + \sin \theta \left( \frac{10}{3} A_{5,1}^r - \frac{1}{3} \sqrt{5} A_{6,1}^r + \sqrt{5/3} A_{7,1}^r \right) \quad (4.3)$$

and

$$[H_{r-1,r}, A_{5,1}^r] = -\cos \theta \{ S_3^z(r-1) [-(1/\sqrt{2}) A_{5,6}^r + (1/\sqrt{6}) A_{5,7}^r] \\ + \frac{1}{2} S_3^+(r-1) [A_{5,9}^r - (1/\sqrt{3}) A_{5,10}^r - \frac{1}{3} \sqrt{2} A_{2,1}^r - \frac{1}{3} \sqrt{5/2} A_{3,1}^r - \sqrt{5/6} A_{4,1}^r] \}$$

$$\begin{aligned}
& + \frac{1}{2}S_3^-(r-1)[-A_{5,3}^r + (1/\sqrt{3})A_{5,4}^r - \frac{1}{3}\sqrt{2}A_{8,1}^r - \frac{1}{3}\sqrt{5/2}A_{9,1}^r - \sqrt{5/6}A_{10,1}^r] \\
& - \sin\theta\{[S_3^z(r-1)]^2[\frac{2}{3}A_{5,1}^r + (1/3\sqrt{5})A_{6,1}^r + (1/\sqrt{15})A_{7,1}^r] \\
& + \frac{1}{2}(S_3^z S_3^+)(r-1) \\
& \times [-\frac{1}{2}A_{5,9}^r + (1/2\sqrt{3})A_{5,10}^r + \frac{7}{15}\sqrt{2}A_{2,1}^r + \frac{2}{3}\sqrt{2/5}A_{3,1}^r + (1/2\sqrt{3})A_{4,1}^r] \\
& + \frac{1}{2}(S_3^+ S_3^z)(r-1) \\
& \times [\frac{1}{2}A_{5,9}^r - (1/2\sqrt{3})A_{5,10}^r + \frac{2}{15}\sqrt{2}A_{2,1}^r - (1/3\sqrt{10})A_{3,1}^r - (1/\sqrt{30})A_{4,1}^r] \\
& + \frac{1}{2}(S_3^z S_3^-)(r-1) \\
& \times [-\frac{1}{2}A_{5,3}^r + (1/2\sqrt{3})A_{5,4}^r - \frac{7}{15}\sqrt{2}A_{8,1}^r - \frac{2}{3}\sqrt{2/5}A_{9,1}^r - 2\sqrt{2/5}A_{10,1}^r] \\
& + \frac{1}{2}(S_3^- S_3^z)(r-1) \\
& \times [\frac{1}{2}A_{5,3}^r - (1/2\sqrt{3})A_{5,4}^r - \frac{2}{15}\sqrt{2}A_{8,1}^r + (1/3\sqrt{10})A_{9,1}^r + (1/\sqrt{30})A_{10,1}^r] \\
& + \frac{1}{4}(S_3^+ S_3^-)(r-1) \\
& \times [-\frac{2}{3}A_{5,1}^r + (1/\sqrt{2})A_{5,6}^r - (1/\sqrt{6})A_{5,7}^r - (1/3\sqrt{5})A_{6,1}^r - (1/\sqrt{15})A_{7,1}^r] \\
& + \frac{1}{4}(S_3^- S_3^+)(r-1) \\
& \times [-\frac{2}{3}A_{5,1}^r - (1/\sqrt{2})A_{5,6}^r + (1/\sqrt{6})A_{5,7}^r - (1/3\sqrt{5})A_{6,1}^r - (1/\sqrt{15})A_{7,1}^r]
\end{aligned} \tag{4.4}$$

where for simplicity I still keep the notations for those single spin operators  $S_i(r-1)$  with  $i = 1, 2, 3$ . The equation for  $[H_{r,r+1}, A_{5,1}^r]$  is derived in similar fashion.

I have also derived the equations of motion for  $A_{6,1}$ ,  $A_{7,1}$  and  $A_{n,m}$  with  $n, m = 5, 6, 7$  respectively. Again, I do not list them here.

## 4.2. Spin-wave theory

Now I apply the approximation of the spin-wave theory to all these equations. This spin-wave theory, referred to as the decoupling approximation by Parkinson [13], consists of replacing each operator in any product  $A_{i,j}^r A_{k,l}^{r\pm 1}$ , in turn, by its expectation value in the simple trimer VB model state,  $|T\rangle$ , given by equation (2.9). Obviously, the only non-zero expectation value is  $\langle T|A_{1,1}^r|T\rangle = 1$ . After expressing the corresponding operators in terms of these  $A_{n,m}$  operators, one has  $\langle T|(S_i^z)^2|T\rangle = \frac{2}{3}$ , and  $\langle T|S_i^+ S_i^-|T\rangle = \langle T|S_i^- S_i^+|T\rangle = \frac{4}{3}$ , with  $i = 1, 2, 3$ . In this spin-wave theory equation (4.2) and the similar equations for  $A_{6,1}$  and  $A_{7,1}$  are then reduced to,

$$\begin{aligned}
\omega A_{5,1}^r & \simeq \frac{2}{3}a A_{5,1}^r + \frac{1}{3}\sqrt{5}b A_{6,1}^r - \sqrt{5/3}b A_{7,1}^r \\
\omega A_{6,1}^r & \simeq \frac{1}{3}\sqrt{5}b A_{5,1}^r + \frac{5}{3}c A_{6,1}^r + (1/\sqrt{3})c A_{7,1}^r + (1/\sqrt{3})d(A_{1,7}^{r-1} + A_{7,1}^{r-1}) \\
\omega A_{7,1}^r & \simeq -\sqrt{5/3}b A_{5,1}^r + (1/\sqrt{3})c A_{6,1}^r + c A_{7,1}^r + (1/\sqrt{3})d(A_{1,6}^{r+1} + A_{6,1}^{r+1}) \\
& \quad - \frac{1}{3}d[(A_{1,7}^{r-1} + A_{7,1}^{r-1}) + (A_{1,7}^{r+1} + A_{7,1}^{r+1})]
\end{aligned} \tag{4.5}$$

where the four constants  $a$ ,  $b$ ,  $c$  and  $d$  are defined by

$$\begin{aligned} a &\equiv \cos \theta + 5 \sin \theta & b &\equiv \cos \theta - \sin \theta \\ c &\equiv \frac{1}{2} \cos \theta + \sin \theta & d &\equiv \cos \theta - \frac{1}{2} \sin \theta \end{aligned} \quad (4.6)$$

and where I have also used the fact that the equations of motion for all other operators, i.e.,  $A_{n,m}$  with  $n, m = 5, 6, 7$ , give zero within the spin-wave approximation. For example, the equations of motion for  $A_{5,6}$  and  $A_{5,7}$  read, respectively

$$\omega A_{5,6} \simeq 0 \quad \omega A_{5,7} \simeq 0. \quad (4.7)$$

The equations of motion for the corresponding conjugate operators,  $A_{1,5}$ ,  $A_{1,6}$  and  $A_{1,7}$ , are derived simply by the fact that  $[H, A_{1,n}^r] = -[H, A_{n,1}^r]^\dagger$ , with  $n = 5, 6, 7$ . One therefore has a set of six coupled equations.

Before I solve this set of six equations for the eigenvalue  $\omega$ , it is worthwhile discussing the physical implications of the spin-wave approximation given above. According to the definitions in section 3, when  $A_{n,1}$  acts on the trimer state  $|1\rangle$ , it transforms  $|1\rangle$  into state  $|n\rangle$ . Therefore, within the spin-wave theory in which the trimer VB state  $|T\rangle$  is taken as the model state, operators  $A_{5,1}$ ,  $A_{6,1}$ ,  $A_{7,1}$  can be considered as the 'raising' operators: they increase  $S_{\text{total}}$  by one unit. Similarly, their conjugates,  $A_{1,5}$ ,  $A_{1,6}$ ,  $A_{1,7}$ , correspond to the 'lowering' operators. Any other operators that also leave  $S_{\text{total}}^z$  unchanged are considered as higher-order operators. For example, one can always write  $A_{5,6}$  as  $A_{5,6} = A_{5,1}A_{1,6}$ , hence it is quadratic. Therefore, it is quite natural that the equations of motion for  $A_{5,6}$  and other higher-order operators give zero value, as given by equation (4.7). One can certainly draw an analogy here with the traditional spin-wave theory of Anderson [20], where the model state is the classical Néel state and the spin-raising (lowering) operators increase (decrease)  $S_{\text{total}}^z$  respectively.

### 4.3. Energy spectra

After introducing the new variables,

$$X^\pm(r) \equiv A_{5,1}^r \pm A_{1,5}^r \quad Y^\pm(r) \equiv A_{6,1}^r \pm A_{1,6}^r \quad Z^\pm(r) \equiv A_{7,1}^r \pm A_{1,7}^r \quad (4.8)$$

and their Fourier transformations

$$X^+(r) = \sqrt{\frac{3}{N}} \sum_k \exp(3ikr) X^+(k)$$

etc, where one has used the fact that the spacing for the trimer VB configuration is three with the lattice constant chosen as unity, one can reduce the six equations (i.e., equations (4.5) and their corresponding Hermitian conjugates) into three equations. The corresponding eigenequation is therefore third order in  $\omega^2$ .

After some considerable algebra, this eigenequation can be derived as

$$36\varepsilon^3 + 36a_2\varepsilon^2 + a_1\varepsilon + 2a_0 = 0 \quad (4.9)$$

where  $\varepsilon \equiv \omega^2$  and the coefficients are defined by

$$a_2 \equiv 7 \cos 2\theta - 13$$

$$a_1 \equiv (192 \cos 4\theta - 156 \sin 4\theta + 240 \cos 2\theta + 360 \sin 2\theta - 240) \cos 3k \\ + 73 \cos 4\theta - 264 \sin 4\theta - 990 \cos 2\theta + 360 \sin 2\theta + 1225$$

$$a_0 \equiv (51 \cos 6\theta - 93 \sin 6\theta - 168 \cos 4\theta + 174 \sin 4\theta \\ - 99 \cos 2\theta - 279 \sin 2\theta + 120) \cos 3k \\ - 151 \cos 6\theta + 18 \sin 6\theta + 118 \cos 4\theta - 24 \sin 4\theta \\ + 99 \cos 2\theta + 54 \sin 2\theta - 170.$$

The solutions of equation (4.9) as functions of the coupling parameter  $\theta$  are discussed below.

(i)  $\theta = \frac{1}{4}\pi$ . This is the Lai-Sutherland [8] model where the exact solution is available. In this case, equation (4.9) becomes

$$(\varepsilon - 8)[\varepsilon^2 - 5\varepsilon + 2(1 - \cos 3k)] = 0. \quad (4.10)$$

One obvious solution to the above equation is the constant,  $\varepsilon = 8$ . The other two are given by

$$\varepsilon_{\pm}(k) = \frac{1}{2}(5 \pm \sqrt{17 + 8 \cos 3k}) \quad (4.11)$$

which depend on the wave vector  $k$ . Recalling that  $\omega^2 = \varepsilon$ , after discarding the unphysical negative solution,  $\omega = -\sqrt{\varepsilon}$ , one obtains the low-lying spectrum,  $\omega_k = \sqrt{\varepsilon_{-}(k)}$ , which is gapless at  $k = 0$  and  $\frac{2}{3}\pi$ , and has a spin-wave velocity of  $3/\sqrt{5} \simeq 1.342$ . This spectrum compares well with the exact result [8] which has a spin-wave velocity of  $\frac{1}{3}\sqrt{2}\pi \simeq 1.481$ . However, the other gapless spectrum with a periodicity of  $\frac{4}{3}\pi$  from the exact result [8] is not present in this simple spin-wave theory.

(ii)  $\theta = \frac{1}{2}\pi$ . This is the phase transition point, beyond which, i.e., for  $\theta > \frac{1}{2}\pi$ , the system is ferromagnetic. Equation (4.9) then reduces to

$$\varepsilon(9\varepsilon^2 - 180\varepsilon - 72 \cos 3k + 572) = 0. \quad (4.12)$$

One sees immediately that there is a constant zero spectrum,  $\omega_k = 0$ , as expected for the corresponding ferromagnetic phase transition, but with two other spectra which are massive.

(iii)  $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$ . In this region, the low-lying spectrum obtained from equation (4.9) always has a non-zero gap with identical minima at  $k = 0$  and  $\frac{2}{3}\pi$ . For example, at  $\theta = \frac{1}{3}\pi$ , equation (4.9) becomes

$$\varepsilon^3 - \frac{33}{2}\varepsilon^2 + \frac{1}{72}[(516\sqrt{3} - 912) \cos 3k + 624\sqrt{3} + 3367]\varepsilon \\ - \frac{1}{36}[(267\sqrt{3} - 609) \cos 3k - 42\sqrt{3} + 859] = 0. \quad (4.13)$$

The minimum gap is given by  $k = 0$  (or  $\frac{2}{3}\pi$ ) with the value  $\varepsilon_0 \simeq 0.315$ .

(iv) Other regions. For other couplings immediately beyond the region  $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$ , i.e., for  $\theta < \frac{1}{4}\pi$  or  $\theta > \frac{1}{2}\pi$ , the low-lying spectrum obtained from equation (4.9) becomes imaginary, clearly indicating the instability of the trimerized state. Therefore, one expects a phase change at both  $\theta = \frac{1}{4}\pi$  and  $\frac{1}{2}\pi$ .

From the above results, a clear picture within the spin-wave theory emerges: the spin-1 system is trimerized in the region given by  $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$  and becomes critical at both ends of the region. While at  $\theta = \frac{1}{2}\pi$  this picture agrees with the well known fact that the system becomes ferromagnetic, it also indicates that the transition from the trimerized phase to any other antiferromagnetic phase, possibly the non-degenerate phase, is at  $\theta = \frac{1}{4}\pi$ .

I should also point out that there are some other points and regions of  $\theta$  where the low-lying spectrum obtained from equation (4.9) remains real. These include  $\theta = -\frac{1}{4}\pi$  (or  $\frac{3}{4}\pi$ ). However, as  $\theta$  either increases or decreases, the low-lying spectrum becomes imaginary. One expects that for higher-order approximations beyond the simple spin-wave theory employed here, this singular point may become unstable. After all, the exact solution [6] at  $\theta = -\frac{1}{4}\pi$  clearly shows that the system has a double periodicity. Also, in the region of  $-\frac{3}{4}\pi < \theta < -\frac{1}{2}\pi$ , the spectra are identical to those in the region of  $\frac{1}{4}\pi < \theta < \frac{1}{2}\pi$ . This is simply due to the fact that the Hamiltonian has a symmetry  $H \rightarrow -H$  when  $\theta \rightarrow \theta + \pi$ .

#### 4.4. Equations of motion for other operators

Finally, I consider the equations of motion for those operators that change  $S_{\text{total}}^z$  by  $-1$ , i.e.,  $A_{n,1}$  with  $n = 2, 3, 4$ ,  $A_{1,n}$  with  $n = 8, 9, 10$ , and many other higher-order operators, e.g.,  $A_{2,5}$ ,  $A_{2,6}$ ,  $A_{2,7}$ , etc. The conjugates of these operators correspond to those which increase  $S_{\text{total}}^z$  by one.

Within the similar spin-wave approximation, the energy spectra obtained from these operators are in fact identical to those obtained above, i.e., equation (4.9). In other words, the spectra given by equation (4.9) are in fact triplet excitations. This is not surprising since the model state of the spin-wave approximation developed here,  $|T\rangle$ , is in the sector of  $S_{\text{total}} = 0$ , and one expects the low-lying excitation to be triplet with  $S_{\text{total}} = 1$ . This is similar to the cases for the spin- $\frac{1}{2}$  Heisenberg model studied by Parkinson [13], and for the dimerized spin-wave theory of Chubukov [10], but contrasts with the traditional spin-wave theory [20] where the model state is the Néel state and the excitation is definitely doublet.

### 5. Discussion and conclusions

In this article I have discussed the possibility of trimerization of the spin-1 system in terms of VBs. I introduced the so-called composite operators,  $A_{n,m}$ , which are the proper operators for dealing with problems of spin-1 trimerization. A spin-wave theory based on these composite operators has been developed, taking the simple trimer VB state as the model state.

The application of this spin-wave theory under a truncation scheme to the 1D spin-1 Heisenberg-biquadratic model confirms the existence of the trimerized phase over an extended region of couplings. In this trimerized region, a non-zero energy gap for the triplet excitation is predicted within the spin-wave theory. This agrees with the conclusions of [11] but contradicts those of the finite-size calculation of [12], which claims that the trimerized region is gapless. Agreement with the exact results of Lai and Sutherland [8] is also found at one end of the region.

It is possible to extend and reformulate the current spin-wave theory so that the ground-state energy, order parameter, and other ground-state properties are also obtained. This can be achieved by the method of bosonization for those composite operators. For the problem of the dimerized phase for the 1D spin- $\frac{1}{2}$  system, it has already been done [21]. Chubukov [10] has also provided another technique for the dimerization problem by employing a

beautiful boson transformation similar to the well known Holstein–Primakoff transformation. However, this is beyond the scope of this paper for the trimerization problem. In any case, it is perhaps more interesting to generalize the current spin-wave theory to higher dimensionalities, particularly the 2D spin-1 systems with various couplings and/or lattice structures.

In order to provide a more convincing argument for the existence of the extended region where the spin-1 system is trimerized and has a non-zero energy gap, it is necessary to include those excitations with  $S_{\text{total}} > 1$  and, more importantly, to go beyond the simple spin-wave approximation made in this paper. In fact, a microscopic analysis based on these composite operators can be formulated, particularly by applying a powerful many-body technique, namely the coupled-cluster method, which has already been very successfully applied to various spin models with an anticipated Néel order [22].

### Acknowledgments

I thank R F Bishop, J B Parkinson, and C E Campbell for many useful discussions. I am grateful to J B Parkinson for drawing my attention to [12] which stimulated my interest in this work, and to R F Bishop for a critical reading of the manuscript. Part of this work was done in the Department of Physics at the University of Minnesota, USA, where C E Campbell was my thesis advisor.

### References

- [1] Bethe H A 1931 *Z. Phys.* **71** 205  
des Cloiseaux J and Pearson J J 1962 *Phys. Rev.* **128** 2131  
Faddeev L D and Takhtajan L A 1981 *Phys. Lett.* **85A** 375  
Bogoliubov N M, Izergin A G and Korepin V E 1986 *Nucl. Phys. B* **275** 687
- [2] Haldane F D M 1983 *Phys. Lett.* **93A** 464; 1983 *Phys. Rev. Lett.* **50** 1153  
Affleck I and Haldane F D M 1987 *Phys. Rev. B* **36** 5291
- [3] For a review of numerical calculations of the 2D Heisenberg model, see Trivedi N and Ceperley D M 1990 *Phys. Rev. B* **41** 4552; for the 2D  $J_1 - J_2$  (frustrated) square lattice model, see Chubukov A V and Jolicoeur Th 1991 *Phys. Rev. B* **44** 12 050; for a review of 2D Heisenberg triangle and *Kagomé* lattices, see Sachdev S 1992 *Phys. Rev. B* **45** 12 377
- [4] Chakravarty S, Halperin B I and Nelson D R 1987 *Phys. Rev. Lett.* **60** 1057
- [5] Parkinson J B 1988 *J. Phys. C: Solid State Phys.* **21** 3793  
Barber M N and Batchelor M T 1989 *Phys. Rev. B* **40** 4621  
Klümper A 1990 *J. Phys. A: Math. Gen.* **23** 809
- [6] Takhtajan L A 1982 *Phys. Lett.* **87A** 479  
Babujian H M 1982 *Phys. Lett.* **90A** 479; 1983 *Nucl. Phys. B* **215** 317
- [7] Affleck I, Kennedy T, Lieb E and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799; 1988 *Commun. Math. Phys.* **115** 477
- [8] Lai C K 1974 *J. Math. Phys.* **15** 1675  
Sutherland B 1975 *Phys. Rev. B* **12** 3795
- [9] Affleck I 1986 *Nucl. Phys. B* **265** 409  
Affleck I and Haldane F D M 1987 *Phys. Rev. B* **36** 5291
- [10] Chubukov A V 1991 *Phys. Rev. B* **43** 3337
- [11] Nomura K and Takada S 1991 *J. Phys. Soc. Japan* **60** 389
- [12] FÁth G and Sólyom J 1991 *Phys. Rev. B* **44** 11 836
- [13] Parkinson J B 1979 *J. Phys. C: Solid State Phys.* **12** 2873
- [14] Hulthén L 1938 *Ark. Mat. Astron. Fys. A* **26** 1  
Anderson P W 1973 *Mater. Res. Bull.* **8** 153
- [15] Arovas D P, Auerbach A and Haldane F D M 1988 *Phys. Rev. Lett.* **60** 531

- [16] Anderson P W 1987 *Science* **235** 1196
- [17] Xian Y 1989 *PhD Thesis* University of Minnesota
- [18] Chang K, Affleck I, Hayden G W and Soos Z G 1989 *J. Phys. C: Solid State Phys.* **1** 153
- [19] Courtesy of J B Parkinson
- [20] Anderson P W 1952 *Phys. Rev.* **86** 694
- Oguchi T 1960 *Phys. Rev.* **117** 117
- [21] Xian Y 1993 *Preprint* UMIST Manchester
- [22] Bishop R F, Parkinson J B and Xian Y 1991 *Phys. Rev. B* **43** 13 782; 1991 *Phys. Rev. B* **44** 9425; 1992 *Phys. Rev. B* **46** 880; 1992 *J. Phys.: Condens. Matter* **4** 5783