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An exact solution to a spin-1 chain model

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Abstract. We present a new class of exactly solvable spin models. The solutions involve broken translational symmetry, in contrast to the Haldane gap, and constitute a new type of ground state for a spin-one chain. The models have ground states with precipitously short-range spin correlations and exhibit gaps to solitonic spin excitations. We construct a solvable model for *each* value of the total spin of the underlying atoms, with the solution corresponding to the natural generalization to the Majumdar–Ghosh state, of 'dimer' pairing, to larger spin magnitudes.

1. Introduction

Atoms which lose their charge degrees of freedom but retain an open shell are said to have 'local moments'. In almost all cases local moments order at low temperatures, but in rare cases no long-range order is observed down to the lowest attainable temperatures, and certainly at lower energies than the scale on which the local moments interact. Strangely, the systems without order appear to be some of the most physically interesting. High-temperature superconductors and heavy fermions both have local moments which do not order (appreciably), and systems which are theoretically predicted not to order have recently also come under intense experimental study [1].

There are two fundamental issues of theoretical interest. Firstly, which physical effects prefer spin states which lack long-range order, and secondly what is the nature of the state stabilized in the place of the ordered state. The first question would appear to have several possible answers. Geometric frustration theoretically causes difficulties, on account of the degeneracy that it introduces into the ordering options. There is some experimental evidence supporting the idea that geometry can prohibit long-range order [2]. Quantum fluctuations can also theoretically eliminate long-range order. Both theoretically and experimentally the one-dimensional chain of spin-one atoms appears to have only short-range order [3], although the three-dimensional character of the physical systems dominates eventually. The most interesting experimental systems conduct electricity and *frequent* exchange of the conduction electrons with the local moments also seems to severely curtail any magnetic order. Although the cause of the loss of order is of great importance, we cannot address this issue directly and we can only give a minor insight into the lesser problem of which types of interaction between local moments can eliminate order.

The second theoretical issue, involving the *nature* of a low-temperature state of a spin system without long-range order, is more open-ended. An understanding of the physics of a system can be developed in many parallel ways. One quite powerful idea is to find or construct an *exactly solvable* model for which the ground state and excitations can be (fairly) unambiguously deduced. Any other model which can be reached by continuously varying

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parameters without incurring a phase transition should then have the 'same' physics. It is this basic technique that we propose to use.

This idea of finding an exactly solvable model 'close by' in parameter space has been successfully applied to the spin-one chain Heisenberg model [4], in order to try to understand the Haldane gap [5] and give a physical picture for the low-lying excitations. Since the fundamental concepts used in this previous calculation are central to our analysis, we shall devote space to explaining them in the next section.

In this paper we will take a simple elementary state as our 'solution' and construct a particular Hamiltonian for which it is an eigenstate. The Hamiltonian derived will be seen to be uniquely determined by the constraints we impose. There is a class of exactly solvable models for spin-half systems, known as 'dimer' solutions, for which our solutions are the natural generalization to larger spin magnitudes.

In section 2 we introduce projection operators and interpret some of the known solutions to spin models in terms of them. In section 3 we develop our exactly solvable models and in section 4 we present some numerical verification to our assertions. We present our conclusions in section 5.

2. Projection operators

In this section we consider possible generalizations to the Heisenberg model, with larger values of spin for the underlying atoms, arguing that various possibilities are reasonable and can lead to quite different physics. There are two assumptions which we make, each leading to a refinement of the class of models to be considered. Our first assumption is the restriction to two-body interactions and our second assumption is that of isotropic spin interactions. Neither assumption is likely to be found experimentally, where a host of crystal-field, spin–orbit and similar interactions break these symmetries, but there remains a simple class of models with relatively few residual degrees of freedom and a surprising wealth of possible ground states.

With two spins, the only isotropic quantity remaining is the scalar product between the spins and so the interaction takes the form

$$H = \sum_{ij} \tilde{p}_{ij}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j) \tag{2.1}$$

where $\tilde{p}_{ij}(x)$ is a function of the real variable x. Since the total spin of each atom is assumed to be fixed, with value S say, we could equally well use the total spin of the pair of interacting spins, $(\boldsymbol{S}_i + \boldsymbol{S}_j) \cdot (\boldsymbol{S}_i + \boldsymbol{S}_j) = 2S(S+1) + 2\boldsymbol{S}_i \cdot \boldsymbol{S}_j \equiv \hat{S}_{ij}^2$, say, in terms of which

$$H = \sum_{ij} p_{ij}(\hat{S}_{ij}^2) \tag{2.2}$$

where $p_{ij}(x) = \tilde{p}_{ij}[x/2 - S(S+1)]$ is the derived function. In fact, the functions $p_{ij}(x)$ can be chosen to be polynomials of order $2S$, since the operator $\hat{S}_{ij}^2$ satisfies

$$\prod_{n=0}^{2S} [\hat{S}_{ij}^2 - n(n+1)] = 0 \tag{2.3}$$

which is a polynomial of order $2S+1$. This result is a direct consequence of the fact that the sum of two quantum-mechanical spins yields another spin which takes values for its magnitude lying between the sum and difference of the two original spin magnitudes.

For the case of spin-half, we find that

$$\hat{S}_{ij}^2(\hat{S}_{ij}^2 - 2) = 0 \tag{2.4}$$

and so the Hamiltonian reduces to

$$H = \sum_{ij} J_{ij}\hat{S}_{ij}^2 = 2\sum_{ij} J_{ij}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \tfrac{3}{4}) \tag{2.5}$$

and all that remains is the Heisenberg model with interaction strength J_{ij} (up to an irrelevant constant).

For the case of spin-one, however, we find that

$$\hat{S}_{ij}^2(\hat{S}_{ij}^2 - 2)(\hat{S}_{ij}^2 - 6) = 0 \tag{2.6}$$

and so we find the more complicated model

$$H = \sum_{ij} J_{ij}\hat{S}_{ij}^2 + \sum_{ij} K_{ij}(\hat{S}_{ij}^2)^2 = 4\sum_{ij} K_{ij}(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^2 + 2\sum_{ij}(J_{ij} + 8K_{ij})\boldsymbol{S}_i \cdot \boldsymbol{S}_j + 4\sum_{ij}\sum(J_{ij} + 4K_{ij}). \tag{2.7}$$

It is usually assumed that the spin interactions are short-range, and indeed they are often restricted to nearest neighbours. Under this assumption, combined with periodicity on a linear chain, we find the model

$$H = J\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + K\sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 \tag{2.8}$$

for spin-one atoms, which reduces to

$$H = (J - \tfrac{1}{2}K)\sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} \tag{2.9}$$

for spin-half atoms. One might anticipate that the two models have similar behaviour, but this is simply not true.

The spin-half model is exactly solvable, yielding pure ferromagnetism when $(J - \frac{1}{2}K) < 0$ and a one-dimensional form of antiferromagnetism [6] when $(J - \frac{1}{2}K) > 0$. Quantum fluctuations eliminate long-range order in one dimension, and so only power-law correlations remain in the antiferromagnetic case. However, power-law correlations are sufficient to enforce a divergent sublattice magnetization and to allow gapless spin-wave-like excitations, analogous to antiferromagnetism in higher dimensions.

The spin-one model has surprisingly rich behaviour, however, involving several new types of ordering. The pure Heisenberg system ($K = 0$) has been heavily studied, exhibiting pure ferromagnetism when $J < 0$, analogous to the spin-half case, but for $J > 0$ there are only short-range spin correlations and the Haldane gap to excitations [5]. This result is a surprise to most people, because it suggests that spin-one atoms might be radically different from spin-half atoms. It could also be argued, however, that using the spin-one Heisenberg

model in order to generalize the spin-half Heisenberg model is not very *natural!* Indeed, when $J = K > 0$ the spin-one chain is exactly solvable with power-law spin correlations and gapless excitations [7]. This model would appear to be a more natural generalization for the Heisenberg model to spin-one, since the properties of the *solution* are so similar. There are three other exactly solved limits of the model: $J = 3K > 0$, which is thought to be continuously connected to the Heisenberg model and constitutes a useful simple model from which the physics of the Haldane gap can be deduced; $J = -K > 0$, which yields a second gapless phase; and $J = 0$ $K < 0$, which yields a gapped phase which is probably continuously connected to the solution presented in this article. The first solution is the content of [4] which has continually been alluded to and the final solution has been solved by Bethe ansatz and other techniques [8].

One fact which should be born in mind when comparing the spin-half Heisenberg model with the exactly solvable gapless spin-one model with $J = K$, is that both models may be thought of as permutation group models. In fact, with the inclusion of an arbitrary constant, both models can be chosen to act only on pairs of states with spins in 'different directions', $|\sigma\sigma'\rangle$ say, yielding $H|\sigma\sigma'\rangle = -\frac{1}{2}(|\sigma\sigma'\rangle - |\sigma'\sigma\rangle)$, a result that is independent of which particular spin labels are chosen. For spin-half there are only two spin labels, but for spin-one there are three spin labels which are all being treated as equivalent. In the spin-one Heisenberg model, the two states $|10\rangle$ and $|\bar{1}1\rangle$ play quite different roles and this permutation symmetry is broken.

Although the present representation in terms of powers of scalar products is physically quite natural, it is not the easiest representation to work with. The action of the Hamiltonian in this representation is quite difficult to interpret. Fortunately, there is a representation with a straightforward interpretation which is technically much more useful: total-spin projectors. Instead of using powers of the scalar product between two spins, one can use operators which project the total spin of the pair onto each of its different possible values: $P^n_{i,j}$ where the total spin of the resulting pair becomes $\langle \hat{S}^2_{ij} \rangle = n(n+1)$.

The transformation which converts the original description into total-spin projectors is linear and can be constructed from the identities

$$P^n_{i,j} = \prod_{n \neq m=0}^{2S} \frac{[\hat{S}^2_{ij} - m(m+1)]}{[n(n+1) - m(m+1)]} \tag{2.10}$$

which clearly project out all other possible values of the total spin and are normalized to unity. Using the identities

$$\prod_{m=0}^{2S} [\hat{S}^2_{ij} - m(m+1)] = 0 \tag{2.11}$$

it is straightforward to show that the $P^n_{i,j}$ are orthogonal projection operators which satisfy

$$P^n_{i,j} P^{n'}_{i,j} = \delta^{nn'} P^n_{i,j} \tag{2.12}$$

and by considering the sum of projectors as a polynomial in $\hat{S}^2_{ij}$ of order $2S$, which takes the value of unity at the $2S + 1$ values of $n(n+1)$, then also

$$\sum_{m=0}^{2S} P^m_{i,j} = 1 \tag{2.13}$$

and the projectors are *complete*. The inverse transformation is more elementary to construct because of the projector characteristics:

$$(\hat{S}_{ij}^2)^a = \sum_{m=0}^{2S} [m(m+1)]^a P_{i,j}^m \tag{2.14}$$

and so the projectors may be understood as the representation which diagonalizes the total spin of a pair.

In the projector representation a general isotropic two-particle interaction may be written as

$$H = \sum_{ij} \sum_{m=0}^{2S} J_{ij}^m P_{i,j}^m \tag{2.15}$$

where the completeness relation means that one of the projectors can be eliminated in favour of the others if desired.

The previous description of the linear chain with nearest-neighbour coupling is slightly simplified in the projector representation:

$$H = -\sum_i (J - \tfrac{1}{2}K) P_{i,i+1}^0 \tag{2.16}$$

is the usual choice for spin-half, and

$$H = -\sum_i [3(J-K) P_{i,i+1}^0 + 2J P_{i,i+1}^1] \tag{2.17}$$

is natural for spin-one. The exact solutions to the spin-one case correspond to particular projectors: the gapless solution ($J = K$) is just the spin-one projector with a negative matrix element, the Haldane-like solution ($3K = J$) is just the spin-two projector with a positive matrix element, and the solution akin to the present article ($J = 0$) is just the spin-zero projector with a negative matrix element.

The final concept that is worth explaining, although it will be of little help in the present analysis, is that of a 'valence bond'. Any spin can be represented in terms of a sum of constituent spin-half particles which are all parallel. States can then be constructed for which the constituent spins in one atom are made into spin singlets or valence bonds with constituent spins on other atoms. The constraint that the constituent spins on any one atom are all parallel then 'shares' the valence bond equally between all constituent spin-halves but does not annihilate it. The power of the construction is that the states constructed have restricted values of total spin. For example, a pair of atoms which incorporate a valence bond between them can never be totally parallel. If it is possible to lay down a valence bond between *all* relevant pairs, then a state can be constructed for which the maximal spin-projector vanishes on all such pairs. This argument allows the P^2 model for the spin-one chain to be solved [4], since the unique state with a valence bond between each nearest-neighbour ensures that the positive definite Hamiltonian attains its minimum value of zero. As was pointed out in the previous work, there are several interesting generalizations, including the solution of the spin-two chain with an interaction of the form $J_1 P^3 + J_2 P^4$ with $J_1 > 0$ and $J_2 > 0$ which is exactly solved by placing *two* valence bonds between neighbouring atoms.

Having briefly reviewed some of the features of the spin-one chain system, we are now in a position to explain our motivation. In a comparison between the spin-half and spin-one chains, there are several similarities and several differences. Both systems have a gapless phase with power-law correlations and both systems have a phase with short-range correlations and a gap to excitations. The previously mentioned P^2 Hamiltonian yields the gap for the spin-one chain, while for the spin-half chain some next-nearest-neighbour interactions can be employed to stabilize the gapped Majumdar–Ghosh [9] phase which has a fixed configuration of valence bonds. At first sight the analogy between the two systems appears strong, but upon closer inspection a difference emerges: the spin-one state is isotropic whereas the spin-half state involves a spontaneously broken symmetry. Although it is quite easy to find spin-half systems with two atoms per unit cell which are isotropic, the possibility of finding a spin-one system with a broken symmetry is a natural goal. The present article is the results from the attempt to find an elementary spin-one model with an isotropic Hamiltonian but a spontaneously broken symmetry. The recently discovered solution to the spin-zero projector Hamiltonian probably has this broken symmetry, and our solution definitely has this broken symmetry and looks numerically to be continuously connected to it.

A brief investigation of the problem should convince the reader that a solution with broken symmetry should exist. The state with all the atoms paired up into total-spin singlets ought to be stabilizable for an appropriate choice of Hamiltonian. Equivalently, in valence bond language, the state with alternating *pairs* of valence bonds between the spin-half components ought to be stabilizable. The natural choice of Hamiltonian which might stabilize this symmetry broken phase is the P^0 projector with negative matrix element. As motivation, two randomly oriented spin-one atoms are only found in a singlet one ninth of the time. Classical ordering improves this probability to one third and quantum fluctuations will further enhance it. However, it seems unlikely that quantum fluctuations in this spin-one system will do better than in the equivalent spin-half system, which would be required in order to dominate the estimate of five ninths which is found (on average) in the state with all atoms paired up into nearest-neighbour singlets. It is probable that the ground state to the chain of nearest-neighbour spin-one atoms with total-spin-zero projection interaction yields a pair of broken symmetry ground states with essentially equivalent physics to the state where spins pair up into nearest-neighbour total-spin singlets. In the next section we will present a minor modification to the Hamiltonian which exactly stabilizes the total-spin-zero 'dimer'-paired state as the ground state, together with some numerical evidence to analyse the spin zero projector conjecture in the subsequent section.

3. Exactly solvable models

In this section we use spin projectors to construct some isotropic models which have ground states involving all the atoms being paired up into nearest-neighbour total-spin singlets. Our construction includes the Majumdar–Ghosh [9] Hamiltonian as a special case, generalizing it to all possible spin magnitudes.

There are a couple of technical facts which are frequently used and could cause confusion. Firstly, spin projectors commute with any total-spin operator for a cluster of atoms which contains the two spins being projected. So, for example, if three spins are in a total-spin singlet, then if any pair are spin projected the only permissible result will find the pair with the same total spin as the third spin and in a total-spin singlet with it. More importantly for us, if four spins are in a total spin singlet, then a spin projector applied to

one pair will *automatically* spin project the other pair onto the same value of total spin. The proof of this result is elementary since the projectors are polynomial combinations of the total spin of the relevant pair $\hat{S}_{ij}^2$, and this total spin certainly commutes with any function of $S_i + S_j$ including $(S_i + S_j + \sum_\beta S_\beta)^2$. Secondly, the parity under exchange of a pair of spins in an eigenstate of total spin is $(-1)^{2S-n}$ in terms of their total spin n. This result allows us to connect permutations of spins with projection operators. A proof of this second result is less obvious and one can use valence bonds to prove it. A pair of atoms with a fixed total spin can be represented as symmetrized composites of spin-half objects for which there are a certain number, m say, of valence bonds connecting the two atoms, with all the remaining spin-half particles parallel. The parity under exchange is clearly $(-1)^m$ for this representation and also $m = 2S - n$ where n is the total spin of the pair.

We will construct the Hamiltonian in the next subsection and then derive an approximation for the low-energy excitations in the following subsection.

3.1. The ground state

We build the model as a minor extension to the nearest-neighbour total spin-zero projector Hamiltonian:

$$H_0 = -J \sum_i P_{i,i+1}^0 = -\frac{J}{2} \sum_i \left(P_{i-1,i}^0 + P_{i,i+1}^0\right) \tag{3.1}$$

where we have centred our projectors on a particular atom in the second representation. We will reexamine this Hamiltonian in subsection 3.3.

We will construct a model for which nearest-neighbour atoms pair up into independent total-spin singlets. The two possible ground states will be denoted by $|+\rangle$ and $|-\rangle$. Our first task is to apply the Hamiltonian to these states. We find

$$H_0|\pm\rangle = -\frac{N}{2} J|\pm\rangle - \frac{J}{2(2S+1)} \sum_i \hat{\Sigma}_{i-1,i+1}|\pm\rangle \tag{3.2}$$

where $\hat{\Sigma}_{i,j}$ is an operator which permutes the two spins at i and j. The first term comes from the spin projectors which act directly on the total-spin singlets, while the second summation comes from individual spin projectors applied to the uncorrelated bond neighbouring the relevant central atom i. The form that it takes requires some understanding. If we consider the three atoms at sites $i-1$, i and $i+1$, then the total spin of all three is equal to the spin of the atom which is not paired up inside the triple. When the uncorrelated bond is projected, conservation of the total spin of the triple ensures that the third atom ends up with this total spin and the spin configuration on the two edge atoms has been exchanged. The matrix element must be $1/(2S+1)$, because the probability of finding two uncorrelated spins in a total-spin singlet is $1/(2S+1)^2$, and the phase can be deduced easily from a particular representation.

We now use spin projectors to describe the permutation

$$\hat{\Sigma}_{i-1,i+1}|\pm\rangle = \sum_{n=0}^{2S} \hat{\Sigma}_{i-1,i+1} P_{i-1,i+1}^n |\pm\rangle = \sum_{n=0}^{2S} (-1)^{2S-n} P_{i-1,i+1}^n |\pm\rangle \tag{3.3}$$

where this result follows from the parity of a pair of spins in an eigenstate of total spin.

We are now in a position to construct our model, since if we use

$$H_1 = -\frac{J}{(2S+1)} \sum_{in} \tfrac{1}{2}[1-(-1)^{2S-n}] P^n_{i-1,i+1} \tag{3.4}$$

where only the anti-symmetric projectors are employed, then we find that

$$(H_0 + H_1)|\pm\rangle = -\frac{(S+1)}{(2S+1)} NJ|\pm\rangle \tag{3.5}$$

and therefore that $|\pm\rangle$ are eigenstates of the combined Hamiltonian.

The first few examples are as follows. For spin-half:

$$H = -J \sum_i P^0_{i,i+1} - \frac{J}{2} \sum_i P^0_{i-1,i+1}. \tag{3.5}$$

For spin-one:

$$H = -J \sum_i P^0_{i,i+1} - \frac{J}{3} \sum_i P^1_{i-1,i+1}. \tag{3.6}$$

For spin-$\frac{3}{2}$:

$$H = -J \sum_i P^0_{i,i+1} - \frac{J}{4} \sum_i (P^0_{i-1,i+1} + P^2_{i-1,i+1}). \tag{3.7}$$

3.2. Excitations

Although we have only managed to show that the states $|\pm\rangle$ are eigenstates of our constructed Hamiltonian, in fact they are ground states. A 'dirty' but rigorous proof, is to decompose our Hamiltonian into 'centred' pieces, $H = \sum_i H_i$ with $H_i = -(J/2)(P^0_{i-1,i} + P^0_{i,i+1}) + [J/(2(2S+1)](\hat{\Sigma}_{i-1,i+1} - 1)$, and then to exactly solve H_i on the three relevant atoms. This provides a lower bound to the ground-state energy for the chain problem which agrees with the energy of our solution. The next natural question to address is the nature of the excitations in this type of system. It is not possible for us to perform an exact analysis of the excitations, but using the ideas already presented, we can produce a surprisingly accurate analytic description for them. The states used are equivalent to those generated in previous work on the Majumdar–Ghosh model [9], although our technical generalization follows a rather different route.

The states we employ are denoted by $|i\rangle$, where the atom at position i has a fixed spin, decorrelated from the rest, and all the other spins are paired off into nearest-neighbour spin singlets. These states are locally eigenstates of the Hamiltonian with the exception of the bonds surrounding the special atoms i. Applying the Hamiltonian yields

$$H|i\rangle = -\frac{(S+1)}{(2S+1)} NJ|i\rangle + \frac{(S+1)}{(2S+1)} J|i\rangle - \tfrac{1}{2}(P^0_{i-1,i} + P^0_{i,i+1})|i\rangle$$
$$- \frac{1}{(2S+1)} \sum_{n=0}^{2S} \tfrac{1}{2}[1-(-1)^{2S-n}] P^n_{i-1,i+1}|i\rangle. \tag{3.8}$$

The first term is just the ground-state energy. The second term is the energy loss from the terms centred on atom i. The third term comes from the nearest-neighbour projectors and the fourth comes from the next-nearest-neighbour projectors. The third term can be seen to involve the projection of an uncorrelated pair of spins in a triple which contains a pair in a total-spin singlet. Total spin conservation for the triple means that the uncorrelated spin is permuted with a spin which is two atoms away. Since a singlet is reflected in the process there is a natural phase picked up. The third term yields

$$+\frac{J(-1)^{2S+1}}{2(2S+1)}(|i-2\rangle+|i+2\rangle) \tag{3.9}$$

where the relative phase of the states is chosen by constructing all states by uniform translations. The fourth term yields the original state combined with the state where the two spins surrounding the decorrelated atom are permuted, $|\hat{i}\rangle$ say. Thus

$$H|i\rangle = E_0|i\rangle + \tfrac{1}{2}J|i\rangle + \frac{J(-1)^{2S+1}}{2(2S+1)}(|i-2\rangle+|i+2\rangle) + \frac{J}{2(2S+1)}|\hat{i}\rangle \tag{3.10}$$

The final step in the argument involves the *four* spins surrounding the decorrelated spin, which are in a total-spin singlet. This fact means that if we use either the pair to the left *or* to the right to effect a projection decomposition, then *both* are simultaneously projected onto the same total spin:

$$|\hat{i}\rangle = \sum_{n=0}^{2S} P^n_{i+1,i+2}|\hat{i}\rangle = \sum_{n=0}^{2S} P^n_{i-2,i-1}P^n_{i+1,i+2}|\hat{i}\rangle = \frac{1}{2S+1}|i\rangle + \sum_{n=1}^{2S} P^n_{i-2,i-1}P^n_{i+1,i+2}|\hat{i}\rangle \tag{3.11}$$

and so finally

$$\begin{aligned} H|i\rangle = E_0|i\rangle &+ \frac{J}{2}\left(1+\frac{1}{(2S+1)^2}\right)|i\rangle + \frac{J(-1)^{2S+1}}{2(2S+1)}(|i-2\rangle+|i+2\rangle) \\ &+ \frac{J}{2(2S+1)}\sum_{n=1}^{2S} P^n_{i-2,i-1}P^n_{i+1,i+2}|\hat{i}\rangle. \end{aligned} \tag{3.12}$$

This result enables us to find the dispersion of our additional uncorrelated spin approximately. The initial difficulty is that the states $|i\rangle$ are *non–orthogonal*. This difficulty is usually prohibitive, but for the present case we have a saviour. All the terms appearing in the final contribution are individually orthogonal to each and every state $|i\rangle$. This is easy to see because either one of the two spin projectors gives no overlap with one of the total-spin singlets contained in $|i\rangle$, or there are an infinite number of mismatched singlets. Finding the dispersion in the restricted subspace generated by $|i\rangle$ yields

$$\epsilon_k = \frac{J}{2}\left(1+\frac{2\cos[2k+(2S+1)\pi]}{(2S+1)}+\frac{1}{(2S+1)^2}\right). \tag{3.13}$$

There is a gap of $G = \frac{1}{2}J\left[2S/(2S+1)\right]^2$ to a cosine band of halfwidth $W = J/(2S+1)$ predicted.

Using similar types of argument, it is possible to include the wavefunction

$$|\bar{i}\rangle = \sum_{n=1}^{2S} P^n_{i-2,i-1}P^n_{i+1,i+2}|\hat{i}\rangle \tag{3.14}$$

into our variational calculation. Without direct proof, which is complicated, we quote the next variational estimate to the dispersion:

$$\epsilon_k = \frac{J}{2}\left[3 + \frac{c}{S'} - \frac{1}{S'^2} - \left(4 - \frac{7}{S'^2} + \frac{5}{S'^4} - \frac{4c}{S'} + \frac{6c}{S'^3} + \frac{c^2}{S'^2}\right)^{1/2}\right] \tag{3.15}$$

where $S' = 2S + 1$ and $c = \cos[2k + (2S + 1)\pi]$. This result will be tested in the next section.

3.3. The total-spin-zero projector Hamiltonian H_0

The nearest-neighbour total-spin-zero projector Hamiltonian

$$H_0 = -J \sum_i P^0_{i,i+1} \tag{3.16}$$

has additional symmetries which facilitate interpretation and comparison between models with different total-spin S. The symmetries are controlled by the previously mentioned *local* conservation laws of total spin under projection. Perhaps the clearest explanation uses a non-orthogonal sometimes incomplete and sometimes overcomplete 'basis' based upon grouping spins into pairs. The states we consider find all the spins paired up into *parallel* eigenstates of total spin. The reason for this choice is that such a pairing is 'conserved' by a term-by-term application of our Hamiltonian. The P^0 projector acting on such a pair gives unity if the pair is in a singlet and vanishes otherwise. When two spins are projected from distinct pairs, however, the local conservation laws ensure that the pair projected becomes a singlet and the remaining pair receives the sum of the total spins of the original pairs.

There are many conceptual difficulties in dealing with this type of basis, so we will make the discussion specific to start with. Let us consider the total-spin-zero subspace, where all pairs are in spin-singlets. This subspace contains the ground state to our problem. The first clear difficulty is that the number of such states is astronomically large in comparison to the *actual* number of independent total-spin singlets. This basis is of little use unless the number of *relevant* pair configurations can be severely curtailed. It is the action of the Hamiltonian, and which particular configurations it creates, which can be used to restrict the state space. For a bipartite connectivity, the bonds only occur *between* the two natural sublattices, and so we can restrict attention to pairings that pair spins one from each sublattice. This is a huge reduction, but still not sufficient to make the basis useful. It is only when one applies the nearest-neighbour Hamiltonian to the linear chain that the true and useful restriction becomes apparent: we may restrict attention to pairings for which no two singlets are 'interleaved', i.e. either both or neither of any particular paired pair of spins are found between any other paired pair. This result has been used before [10], and significantly reduces the size of the relevant basis for a nearest-neighbour spin Hamiltonian. There are precisely as many such configurations as there are total-spin-zero states for the spin-half model, and we give a quick counting proof in the appendix. For the spin-half model this 'basis' is complete although non–orthogonal. For the spin-one model this 'basis' is incomplete and describes only a fraction of the total number of states. The action of the Hamiltonian is closed on this subspace and the problem has been 'block' diagonalized in a sense. Some of the additional states may be constructed from the inclusion of total-spin-zero triples, which are also preserved by the Hamiltonian. When we move away from total-spin-zero, the basis remains useful, leading to the lowest-lying excitation for example, but the completeness result is lost. In the total-spin triplet subspace the 'basis' is overcomplete for spin-half and undercomplete for spin-one.

We now arrive at the interpretational value to this representation. We can compare the action of our Hamiltonian on systems with different underlying values of spin, S. Our chosen basis is pictorially identical for all values of spin, S, and the action of the Hamiltonian has only minor modification. For our basis, any nearest-neighbour spin-singlet pair yields an energy $-J$, and so there is a diagonal contribution counting the number of nearest-neighbour singlet-pairs. Obviously this contribution strongly favours our states $|\pm\rangle$. When acting on two spins in different pairs, we obtain the state where these two spins are paired into a singlet leaving the other two also in a singlet. If one sublattice always precedes the other in our singlet definitions, then the matrix element is always $-J/(2S+1)$ for this process. The Hamiltonian matrix is positive definite, as is the orthogonality matrix, and so the ground-state wavefunction is positive definite in this representation. The only difference between the different values of spin, S, is that the longer-range spin correlations are reduced for large spin because the matrix elements connecting them are smaller, whilst their cost remains invariant. An interesting question is: for which value of total spin (if any) does the system achieve a broken symmetry? As $S \mapsto \infty$, the ground state appears to become $|\pm\rangle$, and so it seems natural that a critical spin, S_c say, ought to exist. On the other hand, we are attempting to exchange the limits $N \mapsto \infty$ and $S \mapsto \infty$ with this argument and there are no guarantees.

We have employed our basis to construct analytic solutions to H_0 for up to 14 spins analytically, obtaining the correct answers for both spin-half and spin-one, which can be calculated independently using exact diagonalization methods on a complete basis. Using these admittedly rather small systems we have finite-size scaled the gap to the *second* lowest-lying spin-zero excitation, for increasing values of spin S. Obviously, the first total-spin-zero excitation becomes the second ground-state in a symmetry-broken system. It is numerically quite clear that there is a gap to this second excitation for spin-two moments, and the gap appears incontrovertible for spins as large as ten. We have observed the expected exponential decay of the first total-spin-zero excitation as expected, and feel fairly safe in concluding that the symmetry-breaking does become fact for a finite fairly small value of S. Unfortunately, the spin-1 and spin-$\frac{3}{2}$ systems are simply too small to predict the existence or not of a gap, and so we have been unable to successfully predict the particular value of S at which the transition occurs. Using a numerical representation for the non-interleaved basis we extended the length of the numerical chain to 32 spins, but still the system is ambiguous for spin-1. Given the exact results for these systems [8], it is not surprising that the numerical analysis is ambiguous. The correlation length of around 21 means that either huge systems, or investigations into parameter dependence are required. A more accurate investigation is attempted in the next section, where we attempt to verify that there is no change of phase between our exact solution and the spin-zero projector Hamiltonian.

4. Numerical results

Since the theory is supposed to be exact, one can ask why numerical work was actually embarked upon. There were several reasons. Firstly, although we believe in the arguments presented, there are several areas of mathematical 'woolliness' in which numerical confirmation can increase confidence. Secondly, although we have shown that our exact solutions are eigenstates, we have no trivial mathematical evidence that they are ground states. The numerical calculations provide evidence that the solutions are indeed ground states. Thirdly, although the ground states are exact eigenstates, the predicted excitations are *not* eigenstates and involve an approximation. We can determine the spectrum of the lowest-lying topological excitation numerically and compare it to the analytic solution. Finally, we

can use the computer to vary parameters in the model and hence to test the extent of stability of our proposed type of ground state. In particular, we can try to determine whether the sum of nearest-neighbour spin-zero projectors also has this symmetry-broken ground state.

For both the spin-half chain and the spin-one chain our solution does indeed provide the numerical ground state for up to 24 and 16 spin-loops respectively. It should be noted in passing that the solution can rigorously be proved to be the ground state for the spin-half chain, using a different method of proof [9].

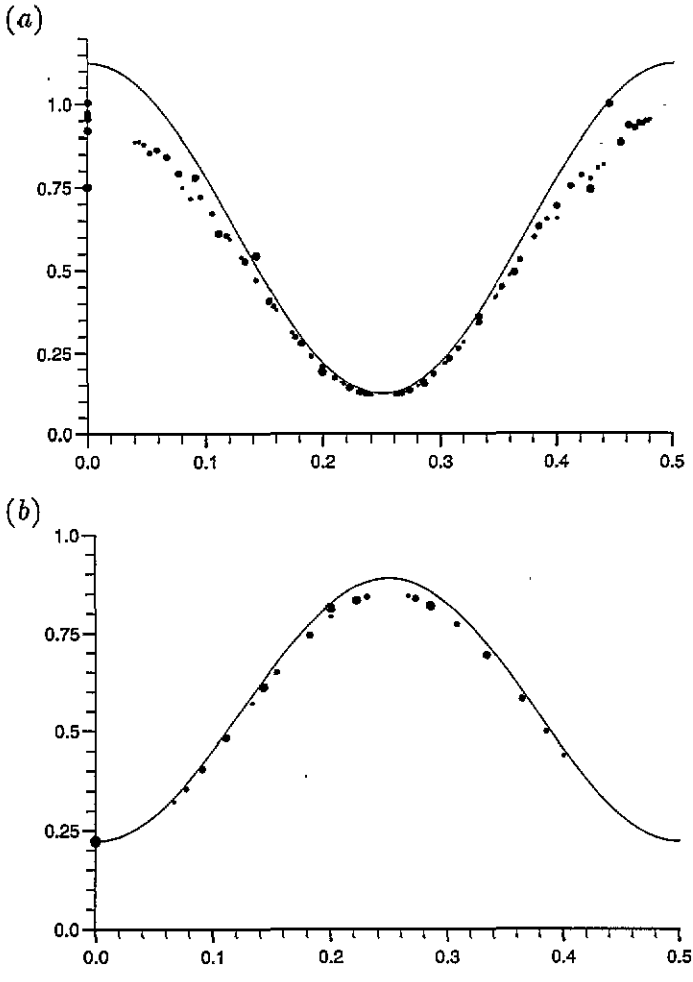


Figure 1. A finite-size scaling calculation of the dispersions of the lowest-lying solitonic excitation for (*a*) the spin-half case and (*b*) the spin-one case. The excess ground-state energies (in units of J) of odd-membered chains of increasing length are plotted as a function of Bloch momentum, k (in units of 2π), over and above the even-membered chain energy. The longer the chain the smaller the point plotted. The bold curve is the analytical estimate described in the text and the dotted curve is the variational analytical correction quoted in the text.

A numerical study of our low-lying excitations is much simplified by the observation that they are topological excitations and can only be created and destroyed in pairs. A judicious choice of boundary conditions then ensures that only one such excitation exists and can be studied in isolation. For the present problem, odd-membered chains with periodic boundary conditions is the natural choice. In figure 1 the excitation energy as a function of Bloch momentum is plotted and overlayed for a sequence of chains of increasing length. For the spin-half case there is a slow convergence whereas for the spin-one chain there is a much faster convergence. The analytic predictions are seen to be excellent, indicating that our proposal is indeed probably the lowest-lying topological excitation. The form of the

dispersion is also exactly as expected, having two periods and being translated for the spin-half case. The only major difference occurs at high energies, where the calculated dispersion is lower than our approximate prediction. The states omitted in our approximation explain this small disagreement, and inclusion of the state omitted in the spin-half case is analytically tractable, yielding the dotted curve in figure 1(*a*).

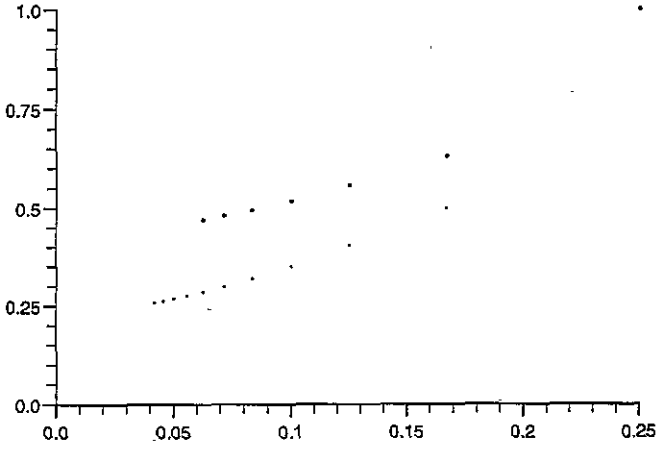


Figure 2. The energy gap (in units of J) to the lowest-lying excitations of the even-membered chains, plotted as a function of the inverse length of the chain, $1/N$. The small points are spin-half and the large points are spin-one.

In many systems, although a single soliton is the lowest-lying excitation, two such solitons *bind* [11]. In order to test this hypothesis numerically, we have finite-size scaled the energy gap to excitations for the even-membered rings in figure 2. As anticipated, the gap scales towards twice the gap for the soliton and the slope of the convergence indicates that the two solitons repel each other.

Our final calculations are devoted to a problem that we have not tackled analytically: the range of parameters over which our solution is stable. Our conjecture is that for the spin-one chain the symmetry-broken state remains the ground state for the nearest-neighbour spin-zero projector Hamiltonian. This result is certainly not true for the spin-half variant, where it is known by exact solution that the ground state is isotropic and gapless.

The technique that we use in order to look for a broken symmetry has been explained and tested in a previous publication [12]. We use a two-stage process in which the initial analysis involves total-energy calculations. The existence of the broken symmetry shows up as a twofold spin-zero degeneracy, which is exponentially observed in a finite-size scaling analysis, combined with a gap to the lowest-lying total-spin-triplet excitation. These calculations are plotted in figure 3 and with the use of polynomial extrapolation it is easy to believe that there is an exponentially decaying gap to the singlet excitation but that any gap to triplet excitations becomes too small to measure. The secondary analysis involves spin–spin correlation functions. The symmetry broken combinations of the two states which become degenerate in the long-chain limit are determined and the correlation functions associated with the order parameter are finite-size scaled. These calculations are also plotted in figure 3, and with further polynomial extrapolation it seems most natural to believe that there is a residual broken symmetry.

Due to the difficulties in picking up the gap to triplet excitations, we made a further attempt to find a gap to solitonic excitations. Employing the odd-membered rings with periodic boundary conditions, and using an even-membered ring with either one more or one less spin in order to estimate the ground-state energy per bond, we finite-size scaled an

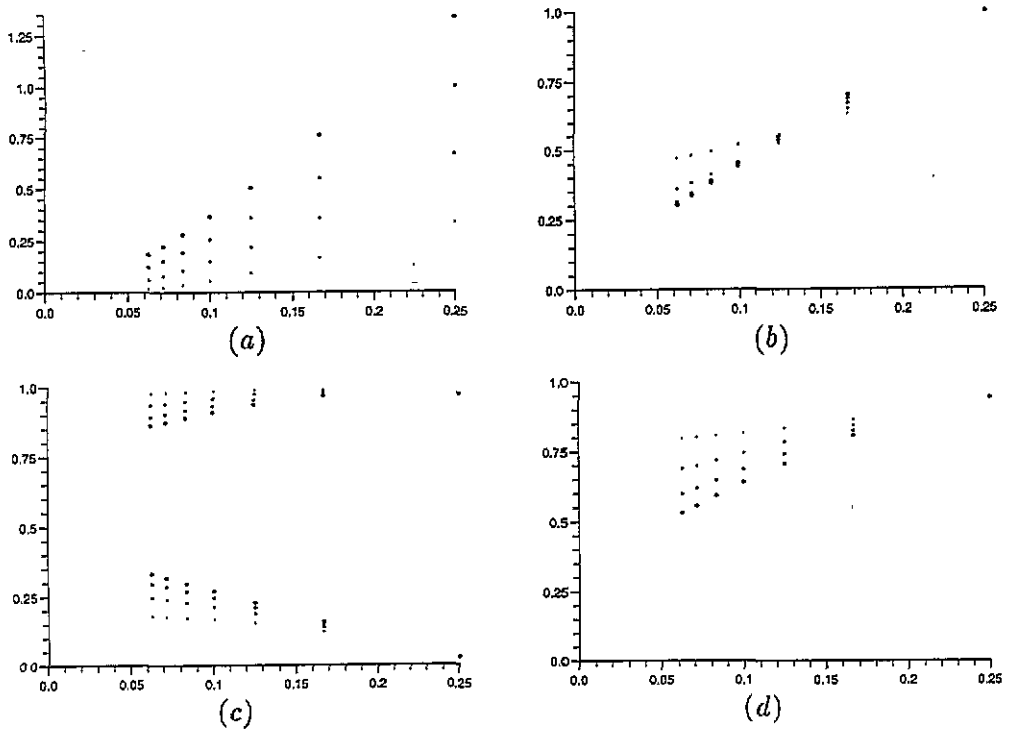


Figure 3. In this and subsequent figures we finite-size scale the results of a sequence of models which can be parametrized by $H_0 + \lambda H_1$ with $\lambda = 0$, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$ and 1. The smaller the parameter λ, the larger the points plotted. We plot (*a*) the gap to spin-singlet excitations ($\lambda = 1$ is omitted because it vanishes), (*b*) the gap to spin-triplet excitations, (*c*) the two nearest-neighbour correlation functions $\langle P^0_{i-1,i}\rangle$, $\langle P^0_{i,i+1}\rangle$ for a symmetry-broken combination of the two total-spin singlet ground-states ($\lambda = 1$ omitted) and (*d*) the symmetry-breaking order-parameter $\langle P^0_{i-1,i} - P^0_{i,i+1}\rangle$ ($\lambda = 1$ omitted), all as a function of the inverse length of the chain, $1/N$.

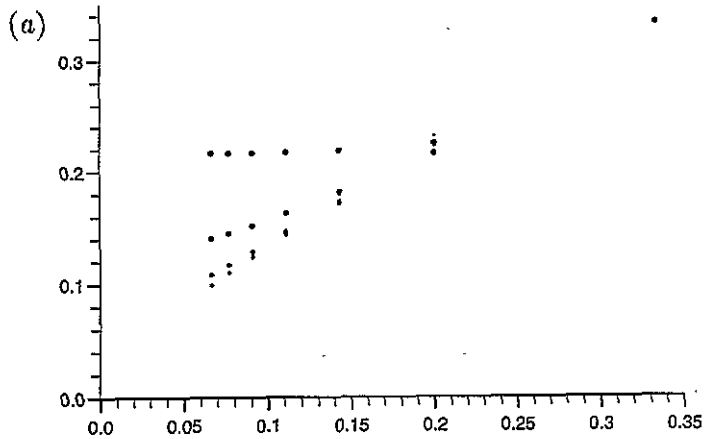
estimate for the energy to the lowest-lying solitonic excitation in figure 4. The results are much less size-dependent than those for the triplet excitations although the predictions are surprisingly similar. Extrapolation suggests that the gap vanishes just before we reach the pure projector Hamiltonian. The smaller scatter can be interpreted easily in the solitonic picture: for the even membered chains there are two solitons which repel, whereas for the odd-membered chain there is only one. Since the *effective* room for each soliton is half for the even-membered chains they converge correspondingly slower.

Our results suggest an unexpected picture of a ground state for the chain with nearest-neighbour spin-zero projectors. We predict a broken symmetry but no gap to excitations. It seems natural to believe that one of these two results must be wrong. Indeed, the exact solution to the spin-zero projector Hamiltonian provides a gap of $0.0577J$ [8], which is difficult although possible to believe from our results.

In order to clarify further what the system is actually doing, we have also finite-size scaled the extensive sublattice magnetization fractions in figure 5:

$$M = \sum_{i\neq 0}^{N} \langle S_0 \cdot S_i \rangle \tag{4.1}$$

where N is the number of atoms on one sublattice and the sum is restricted to one sublattice. Extrapolation suggests that this magnetization remains finite for all cases. If this result is



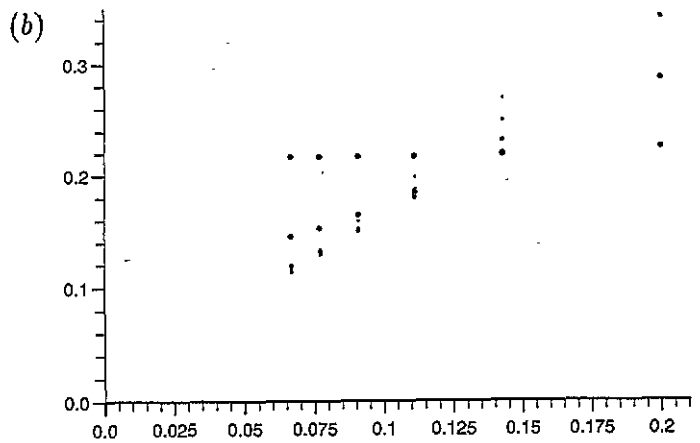


Figure 4. A finite-size scaling calculation of our estimate for the energy gap to solitonic excitations. We take the odd-membered chain ground-state energy and subtract off an estimate for the even-membered ground-state energy based on (*a*) the next-largest even-membered chain and (*b*) the next-smallest even-membered chain and then plot this 'gap' as a function of the inverse chain length, $1/N$. The smaller values of λ correspond to the smaller points for this case, in order to simplify the picture.

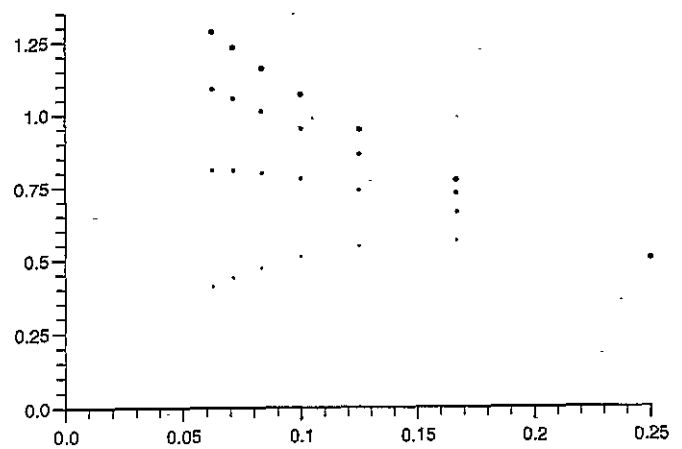


Figure 5. A finite-size scaling calculation of the magnetization, M, as a function of the inverse chain length, $1/N$. The value $\lambda = 1$ is omitted and smaller values of λ are plotted with larger points.

believed, it does not mean that there is no order, because we may have selected the wrong order parameter. It would be surprising, however, if there was no relationship between the order generated and this magnetization. We have also calculated the corresponding

sublattice magnetization for the Heisenberg model, and even without long-range order, the Heisenberg model correlations dominate those for our projector Hamiltonian.

5. Conclusions

Perhaps the most interesting conclusion is that the spin-physics of the isotropic nearest-neighbour pairwise interacting spin-one chain is richer than the corresponding spin-half chain. As well as the isotropic gapped ground states to the Heisenberg model and P^2 projector, which are directly analogous to the spin-half 'dimer' phases, there may also be the symmetry-broken ground state to the $-P^0$ projector. In between these two phases is a gapless phase affecting the transition. The three types of states can all be described by the representation $-P^0 - \lambda P^1$, with $\lambda = 0$ possibly being symmetry broken, $\lambda = 1/3$ being the gapless intermediate and with $\lambda = 2/3$ or 1 being the Heisenberg model and P^2 projector respectively. As well as this sequence of phases there are also transitions similar to that found in the spin-half model, namely out of the gapless $-P^1$ permutation state into the $-P^1 - 3P^2$ Heisenberg ferromagnet for example.

In order to try to demonstrate the existence of the symmetry breaking for the $-P^0$ projector, we have included a second contribution into the Hamiltonian in order to make it solvable. In physical terms, it would be quantum fluctuations alone that cause the symmetry breaking for the $-P^0$ model, whereas for our exact solution we have included some geometric frustration to further destabilize the ordered phase. An ordered Neel-like state finds next-nearest neighbours parallel, and the inclusion of the next-nearest $-P^1/3$ projector enhances the probability of finding them in other spin configurations, eventually decorrelating them. This interpretation is born out by an analysis of the numerical spin-spin correlation functions.

There exists a second framework in which to interpret our results: 'dimer' states. Dimers are pairs of spins which are in a total-spin singlet state. As such, they are correlated only with each other and not with any other spins. Quantum fluctuations prefer dimers which allow spins to locally explore all orientations in contrast to classical ordering for which each spin has a most probable orientation. The first such dimer state was found for spin-half [9] and our exact solutions are the natural generalization to larger spin magnitudes. In order to stabilize the pure state it is necessary to weaken the classical ordering energy allowing the quantum fluctuations to dominate. This is achieved by introducing geometric frustration into the system, penalizing the longer-range consequences of the classical order.

Our initial model, including only total-spin-zero projectors, is strongly quantum mechanical in contrast to the Heisenberg model. Only if spins fluctuate in direction does the system gain energy. This fact leads to several counter-intuitive consequences. Firstly, the symmetry breaking, which should be viewed as a quantum effect, is stronger in the *classical* limit, where trying to correlate the motion of more than two spins is impractical: if we consider three spins in a line, then the two relevant states find the central spin in a total-spin singlet with each of the two edge spins. The overlap of these two states is $1/(2S+1)$ which scales to zero for large spins enforcing the symmetry breaking. Secondly, the low-lying excitations are solitonic carrying spin S, so for the classical limit the excitations carry a huge spin in contrast to spin waves. This result is a consequence of the dominant role of a dimer, the breaking of which *requires* the formation of uncorrelated spins which have spin S. Clearly a *pair* of such excitations can have any total spin ranging from zero to $2S$. Thirdly, the excitation solutions themselves involve more classical spin correlations in the *quantum* limit, since the stronger matrix elements allow some of the lost quantum-fluctuation energy

to be recouped as classical ordering energy around the soliton. This final result explains why the spin-one soliton is so much better predicted by the analytic calculation.

Another consequence of the additional stability for the spontaneous symmetry breaking in the classical limit, is the increase in the magnitude of the spin gap. The analytic prediction is $\frac{1}{2}(1 + 1/2S)^{-2}$ which tends to 1/2 from the initial sequence of 1/8, 2/9, 9/32, 8/25, ... This additional stability leads to the natural conjecture that the geometric frustration contribution between next-nearest neighbours will become irrelevant for higher spins. For spin-half the geometric frustration is crucial, since the linear chain is known to have an isotropic gapless ground-state [6]. It is our belief that the broken-symmetry ground state remains for the spin-one chain and higher spins. The only evidence we have is numerical, and as can be seen from the previous section this evidence is not conclusive. It is however known that there is a gap to excitations for the spin-one projector [8], although the existence of symmetry-breaking appears to remain a conjecture.

The final important issue is that of physical relevance. Unfortunately, the dominant interaction for the more itinerant systems is the Heisenberg interaction. The usual kinetic exchange argument acts on the constituent electrons making up a spin, depending dominantly on the probability that any two on different atoms are in a total-spin singlet and this probability is directly related to the Heisenberg interaction since all electrons are equivalent when all are parallel. Only the more localized systems, dominated by spin–orbit and Coulombic forces rather than kinetic exchange, are candidates for our solution and it appears that the assumption of isotropy is poor for these systems being strongly broken by spin–orbit interactions combined with crystal-field interactions. Physical realizations of our model are unlikely.

Appendix

In this appendix we verify that the number of non-interleaved singlet states composed of singlet pairs connecting one sublattice to another is the same size as the total-spin singlet subspace for a spin-half problem. If we denote this number of non-interleaved states as S_n, for n *pairs* of atoms, then this result is

$$S_n = \frac{(2n)!}{n!(n+1)!}. \tag{A1}$$

We prove this result by considering free boundary conditions and an atom at one end of the chain. This atom must be paired with another atom, and the non-interleaved hypothesis means that this second atom must cut the chain into two unconnected pieces. Adding up over all possible intermediate second atoms, we find

$$S_{n+1} = \sum_{m=0}^{n} S_m S_{n-m} \tag{A2}$$

where $S_0 = 1$. Transforming via

$$S(x) = \sum_{m=0}^{\infty} S_m x^m \tag{A3}$$

yields

$$S(x) = 1 + xS(x)S(x) \tag{A4}$$

which can be immediately solved to give

$$S(x) = \frac{1 - \sqrt{1 - 4x}}{2x}. \tag{A5}$$

It is elementary to expand this square root in a power series to deduce that

$$S(x) = \sum_{n=0}^{\infty} \frac{(2n)!}{n!(n+1)!} x^n \tag{A6}$$

as required.

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