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The spin 1/2 Heisenberg model and the Railroad Trestle geometry

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Abstract. We study the spin 1/2 Heisenberg model on the 'Railroad Trestle' geometry of two lines of close packed atoms. Our motivation is to try to establish a link between triangular geometries and the Haldane gap. The classical limit of the model involves incommensurate spiralling, but there is a collinear state nearby in energy. We believe that quantum fluctuations stabilize the symmetry associated with the collinear state. We give numerical evidence to suggest that the state stabilized has a spontaneously broken symmetry with similar short range correlations to those found in the spin 1 chain, together with a gap to excitations.

1. Introduction

The Heisenberg model is probably the simplest isotropic model of magnetism. For a long period this model was used primarily as a description for magnetically ordered materials and their low temperature behaviour. The relevant magnetic limit of the model is the high-spin classical limit. More recently the quantum limit of low spin, mainly spin 1/2, has come under closer scrutiny. Quantum fluctuations of the spins weaken the magnetic order and for some geometries the magnetic order can be completely destroyed and replaced with a strange type of paramagnetic phase. It is to achieve an understanding of this paramagnetic phase which motivates most studies including our own.

In many compounds atoms exhibit a unique valence state with a non-zero total spin: local moments. Experimentally it is observed that almost always these local atomic moments order if the temperature is lowered sufficiently. Interest is aroused when for some reason the local moments do not order. The compounds of most interest are heavy fermions [1] and perovskite superconductors [2], both of which have local moments which do not order much at low temperatures in the most interesting metallic phases, although there are reports of small ordered moments in heavy fermion systems [3]. Although the most probable physical cause of the paramagnetism is charge motion in these systems, the state stabilized at low temperatures may well have similar characteristics to those stabilized by quantum fluctuations. There are also some insulators with local moments and frustrated geometries which show no magnetic order [4]. These systems can be interpreted directly.

Although concrete experimental examples are few and far between, there are several theoretical geometries which can be solved well enough to prove the absence of long range order. So far we have:

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(i) The spin 1/2 chain with nearest neighbour interactions which has no long range order although it does have long range correlations with power law decay and excitations at infinitesimal energies [5].

(ii) The spin 1 chain with nearest neighbour interactions which has no long range order, an exponential decay of spin–spin correlations together with a gap to excitations: the Haldane gap [6].

(iii) The spin 1/2 chain with next nearest neighbour interactions precisely half the size of the nearest neighbour interactions. This system exhibits *very* short range correlations with spin–spin correlations vanishing at next nearest neighbours and beyond, combined with a gap to excitations [7].

(iv) The spin 1/2 'Sawtooth' geometry which has very similar behaviour to the previous example [8].

(v) Spin 1/2 'Diamond' geometries which also have short range spin–spin correlations and a gap to excitations [9].

In this article we will analyse the 'Railroad Trestle' geometry, depicted in figure 1, and previously studied in the context of the triangular lattice and the so-called resonating valence bond (RVB) state [10]. Our motivation is to try to suggest that the solution to the 'Railroad Trestle' geometry has more in common with the spin 1 chain, yielding further insight into the Haldane gap, than it does with the triangular lattice which has been the previous motivation [10].

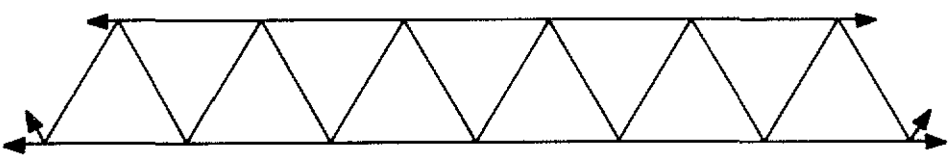


Figure 1. The Railroad Trestle geometry. We will refer to the 'zig-zag' bonds as nearest neighbour bonds in the text, although all the depicted bonds are assumed of equal strength.

The reason that such a connection might be plausible can be found from a study of figure 2. If the dotted and full lines denote primed and unprimed bonds respectively and we denote nearest neighbour, next nearest neighbour and third nearest neighbour interactions by J_1, J_2 and J_3 respectively, then the previously mentioned soluble geometries correspond to:

(i)	$J_1 = J_1' = J$	$J_2 = J_2' = J_3 = J_3' = 0$	
(ii)	$J_1 = \alpha J$	$J_1' = J_2 = J_2' = J_3 = J$	$J_3' = 0$ and $\alpha \leqslant 1.4$
(iii)	$J_1 = J_1' = J$	$J_2 = J_2' = J/2$	$J_3 = J_3' = 0$
(iv)	$J_1 = J_1' = J_2 = J$	$J_2' = J_3 = J_3' = 0$	
Railroad	$J_1 = J_1' = J_2 = J_2' = J$	$J_3 = J_3' = 0$	

It is clear that the only difference between the spin 1 chain and the Railroad Trestle geometry is the single third nearest neighbour bond, J_3. It is also clear that the only difference between the Sawtooth and the Railroad Trestle geometry is the single second nearest neighbour bond, J_2'. In order to try to make a connection between these different geometries we will study the families of systems where these bonds are allowed to vary continuously between the relevant geometries.

In section 2 we discuss the classical limit and in section 3 we look at some numerical work on the quantum spin 1/2 system. In section 4 we conclude.

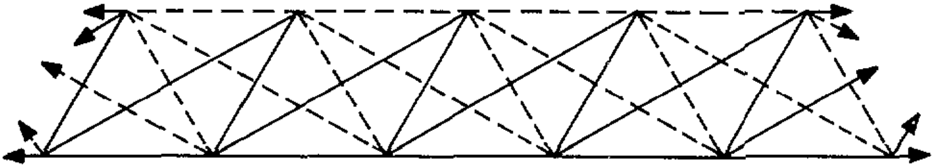


Figure 2. A generalized geometry which simultaneously describes: the Sawtooth, the Railroad and both the spin 1 and spin 1/2 chains. The shortest 'zig-zag' bonds are called first nearest neighbour, the edge bonds are called second nearest neighbour and the long bonds are called third nearest neighbour in the text.

The behaviour of the classical Heisenberg model is relatively straightforward: spins order antiferromagnetically. The ground state usually has long range magnetic order and fluctuations in this order constitute excitations. Our aim is to try to understand how quantum mechanics might modify this simple picture. For bipartite lattices we believe that quantum effects are minor and yield a small reduction in the ordered moment; the basic physical picture remains unchanged. A little more interest is aroused in topologically frustrated geometries. For this case two new types of states are sometimes found at the classical level: spiralling solutions, which use two spin dimensions, and non-trivially degenerate solutions. The role of quantum mechanics seems more interesting for these situations.

Quantum fluctuations prefer neighbouring spins to be in relative spin singlets: spins fluctuate in absolute orientation, but not in relative orientation. This desire to break up into independent singlets can have two major effects. Firstly, spiralling solutions can become unfavourable and collinear states can be stabilized. Secondly, the spins can break up into independent regions with the absolute orientation of the order in a region fluctuating, but the spins locally being collinear in a region. This second effect is associated with a loss of long range magnetic order. The present geometry is a concrete manifestation of these general ideas at work.

2. The classical limit

The first task in any quantum mechanical analysis of the Heisenberg model is to solve the corresponding classical limit in order to establish the types of long range coherence to be expected. The resulting long range ordered solutions act as useful interpretational aids when the quantum analogue is studied. It is quite usual to find the same basic symmetry of solution together with short range remnants of the classical solution in the quantum ground state. It is situations where the ground state is completely different which are the interesting cases.

Since we are trying to connect the different types of geometry, we will analyse two one parameter families of models. Firstly, when comparing the spin 1 chain with the Railroad, there is only one missing bond, namely J_3, and so the natural parameter is the ratio of this bond to the other bonds, $\lambda = J_3/J$, which is allowed to vary between unity, corresponding to the spin 1 chain, and zero, corresponding to the Railroad. Secondly, when comparing the Sawtooth with the Railroad, once again there is a single missing bond, this time J_2', and so the natural parameter is the ratio of this bond to the other bonds, $\kappa = J_2'/J$, which is allowed to vary between zero, corresponding to the Sawtooth, and unity, corresponding to the Railroad.

2.1. The Railroad versus the spin 1 chain

The spin 1 chain has two atoms per unit cell, and so we must solve the family of models allowing two independent spin degrees of freedom. This type of problem is by no means trivial in general, but for the present case we find that only one wavevector and its reciprocal are ever excited in the ground state and therefore this particular problem is easily soluble. The solution is obtained by transforming to reciprocal space, where the Hamiltonian becomes:

$$H = JN \sum_k [\, S^*_{k0} \quad S^*_{k1} \,] \begin{bmatrix} 2c^2 - 1 & c + \frac{\lambda}{2}x^3 \\ c + \frac{\lambda}{2}x^{*3} & 2c^2 - 1 \end{bmatrix} \begin{bmatrix} S_{k0} \\ S_{k1} \end{bmatrix}$$

in terms of the fourier spin components:

$$S_{j\alpha} = \sum_k S_{k\alpha} e^{i(jk + k\alpha/2)} = \sum_k S_{k\alpha} x^{(\alpha+2j)}$$

where $x = e^{i(k/2)}$ and $c = (x + x^*)/2 = \cos(k/2)$. The real space constraints that the spins are of fixed length become $\sum_k S^*_{k\alpha} \cdot S_{k\alpha} = S^2$ for the normalization, together with $S_{k\alpha} \cdot S_{k\alpha} = 0$ for the orthogonalization.

The solution for $\lambda \epsilon (\frac{1}{5}, 1)$ corresponds to the quantum solution to the spin 1 chain: all the spins pair up in real space with both atoms of each pair being parallel. Each neighbouring pair of pairs point in opposite directions. The energy of this spin configuration is $E = JNS^2(-1 - \lambda/2)$, and the spin arrangement is depicted in figure 3.

Only in the interval $\lambda \epsilon (0, \frac{1}{5})$ do we find a more sophisticated solution. For this small interval in the vicinity of the Railroad geometry we find an incommensurate spiralling solution. The wavevector of the spiral is defined by $C = \cos k = 2c^2 - 1 = (\Delta - 1 - \lambda)/(4\lambda)$ in terms of $\Delta^2 = (1 - \lambda)(1 - 4\lambda)$. The state stabilized involves *two* degrees of freedom: the spiralling wavevector and the coupling between the two atoms which were originally parallel and paired. The physical picture is that of a large relative rotation of the two sublattices, which were originally parallel and paired, combined with a slow spiralling of the spins along each sublattice. The angle between the two sublattices satisfies $\cos\phi = [(1 - \lambda)^2 - \Delta(1 + \lambda)]/(2\lambda\Delta)$ and very quickly increases from zero to approximately a right angle. The energy of the corresponding state is $E = JNS^2(\Delta - 1 - \lambda - \lambda\Delta)/(4\lambda)$. An example of this type of spin configuration is also depicted in figure 3.

For the Railroad geometry itself, the angle between the two paired spins becomes precisely half of the spiralling wavevector, $\phi = k/2$ and with $c = -1/4$ and $C = -7/8$. The state reduces to a uniform spiral with each atom being equivalent. This spiralling solution is depicted in figure 3. The state has energy $E = JNS^2(-9/8)$ which is quite similar to the energy of the collinear phase which is stable for larger values of λ. The orientations of the spins are very different however, with nearest neighbours being all parallel in one case and almost all orthogonal in the other.

The broken symmetry state, with alternate high and low spin for each bond, is very close in energy to the ground state, which leads to interesting quantum behaviour. Quantum mechanics prefers parallel spins in the ground state, and we believe that quantum fluctuations for the spin 1/2 system extends the range of stability of the state corresponding to the spin 1 chain as far as the Railroad geometry.

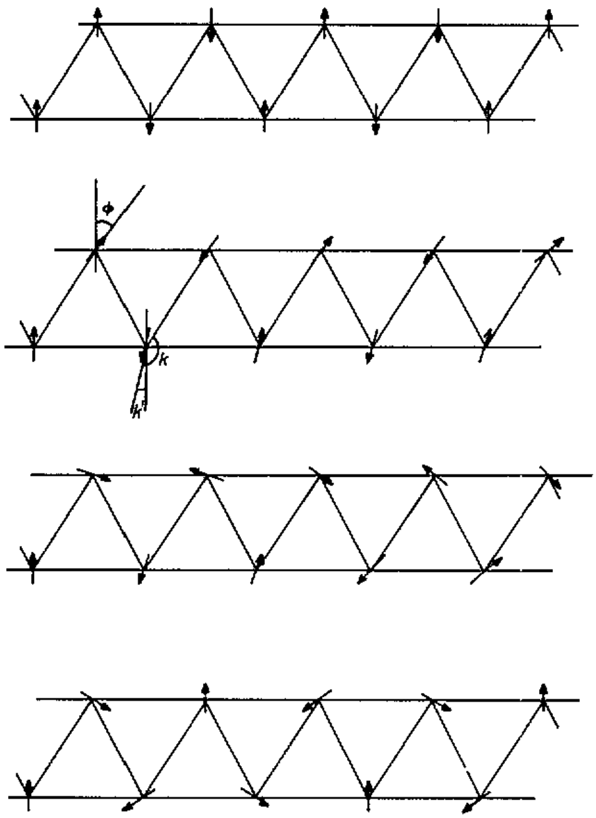


Figure 3. Examples of the classical ground states found for the families of systems described in the text. First we picture the state corresponding to the spin 1 chain ground state. Second we plot the spiralling solution which takes over from the spin 1 chain ground state. The top row and bottom row form two sublattices which gain a slow spiral of pitch k', and ϕ denotes the relative angle between the two sublattices. Third we picture the uniform spiral ground state to the Railroad and lastly we picture the 120° degree ground state to the Sawtooth.

2.2. The Railroad versus the Sawtooth

The corresponding calculation for this one parameter family of models is very similar to the previous case, there being two independent spin degrees of freedom. The system is still soluble, although the Sawtooth geometry itself has extra degeneracy and a wealth of possible classical ground states. The reciprocal space Hamiltonian is:

$$H = JN\sum_k [\, S^*_{k0} \quad S^*_{k1}\,] \begin{bmatrix} 2c^2-1 & c \\ c & \kappa(2c^2-1) \end{bmatrix} \begin{bmatrix} \mathrm{S}_{k0} \\ S_{k1} \end{bmatrix}$$

which is readily minimized by a similar uniform spiralling solution to that found for the Railroad geometry. The wavevector of the spiral satisfies $C = 2c^2 - 1 = -1/(2+2\kappa)$ and the energy of the corresponding solution is $E = JNS^2(-2(1+\kappa)^2 - 1)/(4+4\kappa)$.

The pitch of this spiral is more dramatic reaching 120° for the Sawtooth geometry which has a similar classical ground state to that of the triangular lattice. This state is also depicted in figure 3.

For both classes of system we find classical long range antiferromagnetic order as expected. The classical excitations are the spin waves which are slowly precessing fluctuations, perpendicular to the original spin directions, together with spin spirals which correspond to a change in pitch for the classical order.

The competition to be expected at the quantum level is between slow spirals with non-collinear spins and the broken symmetry state with alternating high and low spin nearest neighbour bonds. In the next section we will try to show that the spiralling solutions are never stable for the case of quantum spins and that a state analagous to the collinear high-spin low-spin bond alternation remains stable.

3. The quantum limit of spin 1/2

Of the three fundamental geometries, the Sawtooth, the Railroad and the spin 1 chain, only the quantum mechanical version of the Sawtooth is exactly soluble. For periodic boundary conditions we find two degenerate ground states, which can be chosen to be the two states for which either all the J_1 bonds are singlet, or all the J_1' bonds are singlet, with all the other bonds necessarily being uncorrelated. This solution has *none* of the properties of the classical solution. There is a broken symmetry in the ground state which is completely analagous to the bond alternation found in the spin 1 chain. For the Sawtooth we find singlet alternating with uncorrelated bonds, while for the spin 1 chain we find triplet alternating with dominantly singlet bonds. A purely quantum guess would then suggest that this broken symmetry might remain over the whole parameter range of our investigation, and this is precisely what we are suggesting. There is recent discussion of these broken symmetries in the literature [11]. The broken symmetry low-spin ground states go under the generic name of 'dimer' solutions.

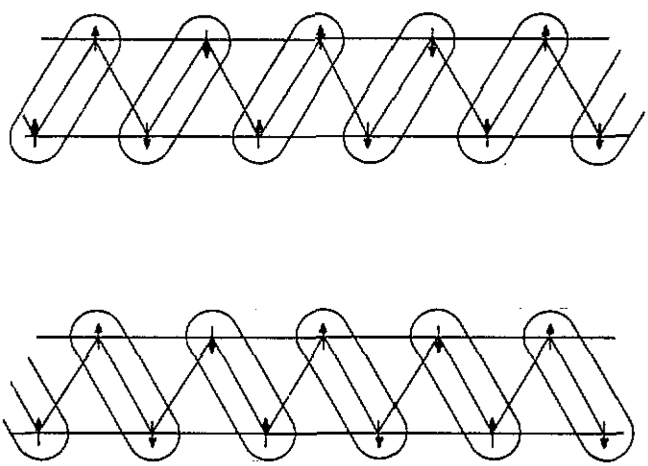


Figure 4. The two ways of combining nearest neighbours which maintains local collinear behaviour. The top picture is stable for the spin 1 chain, and the lower picture corresponds to the Sawtooth ground state.

The fundamental physical principle is that quantum fluctuations tend to stabilize states with locally antiparallel spins [12]. In figure 4 we depict the collinear ground state found near the classical limit of the spin 1 chain. The two local possibilities for maintaining collinear spins are shown; either the parallel pairs can stay approximately parallel with spin fluctuations occuring between neighbouring pairs, or the pairs can split up with the spins in a pair becoming decorrelated and the nearest neighbours between pairs becoming locally parallel. The first case is clearly valid near the spin 1 chain, and the second case exactly describes the Sawtooth ground state. We are suggesting that there is a smooth transition between these two states, with none of the spiralling solution found in the classical limit.

It is not possible to exactly solve these spin 1/2 Heisenberg models and so we must resort to numerical simulations of small finite systems in order to try to deduce the behaviour of the infinite system. Our first problem is to try to deduce whether or not there is a broken spatial symmetry in the ground state.

3.1. Spontaneous broken spatial symmetry

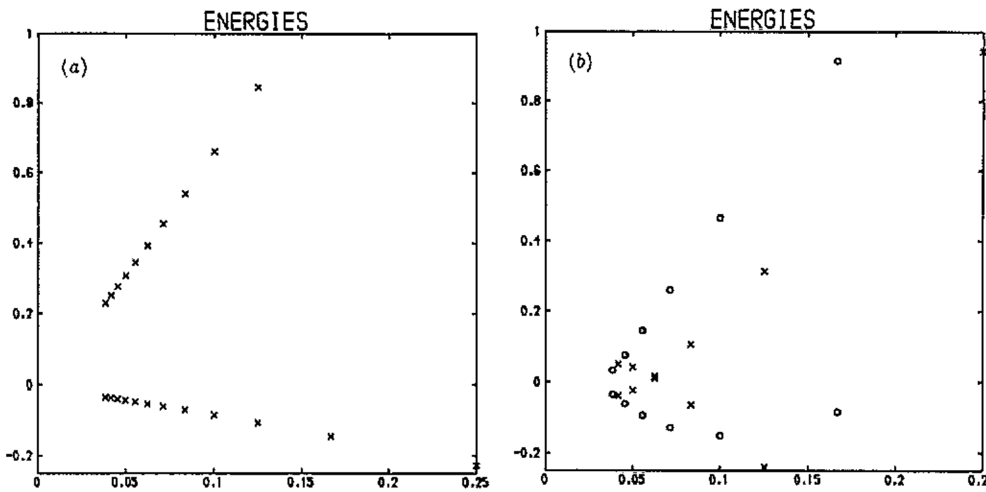
There is an important physical difference between the spin 1 chain and the Railroad geometries. The spin 1 chain has two atoms per unit cell whereas the Railroad only has one. The high-spin low-spin bond alternation is perfectly natural for the spin 1 chain, but constitutes a *spontaneously* broken symmetry if true for the Railroad. For the Sawtooth geometry there is indeed a spontaneously broken symmetry. The reader is directed to an interesting discussion of the relationship between states with only short-range correlations and the existence or not of a broken symmetry [13].

How might we numerically observe such a broken symmetry? For the Railroad, the symmetry breaking would be associated with a degeneracy between the zone centre and zone boundary ground states, with the two *symmetry broken* ground states being formed from the sum and difference of the two Bloch states. The symmetry breaking itself should then be manifested in the spin correlations of the derived states. There are therefore *two* elements to any such calculation: a total energy analysis of the lowest two energy states, and a bond alternation analysis of their sums and differences.

The total energy analysis for the two relevant states is depicted in figure 5 and a finite-size scaling analysis of the bond alternation spin correlations is presented in figure 6. The manner in which such an analysis might *fail* is not immediately obvious, and so we have performed the same analysis for the spin chain with nearest neighbour interactions. This system has been exactly solved [5], and the behaviour of its spin correlations and excitations is well understood: the ground state has full periodicity and the lowest lying singlet excitation is at infinitesimal energy.

If we try to compare the total energy calculations for even membered rings of the chain, figure 5(a), and the Railroad, figure 5(b), we find little similarity. The chain shows very smooth behaviour, with both the ground state and first excited total spin singlet state clearly converging to the analytic result. The Railroad on the other hand shows quite complicated behaviour. Firstly, the loops with odd and even membered *pairs* of atoms show very different behaviour. Secondly, there is a sort of 'periodicity', with the two states alternating between the two roles of ground state and first excited state. Thirdly, the basic linear behaviour found for the chain does not seem natural, and an exponential decay appears a better first guess.

This rather complicated behaviour can be attributed to the frustration and can be partially interpreted in terms of the classical solution. The structure factor has a minimum when, $\cos k_s = -1/4$, which leads to the classical incommensurate spiralling ground state. This special wavevector, k_s, also introduces a natural length scale into the problem, viz $\lambda_s = (2\pi)/k_s \sim 3.446$, which is the pitch of the spiral. Obviously this length has nothing to do with the oscillations, but if we extract out the *difference* in wavevector from the collinear solution, $k_d = \cos^{-1}(-1/4) - \pi/2$, then the associated



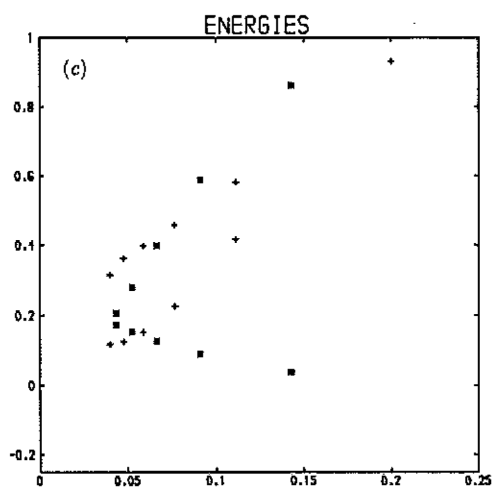


Figure 5. (*a*) A finite-size scaling calculation of the spin 1/2 chain ground state energy and the lowest lying spin 0 excitation energy. In fact there is a spin 1 excitation between the two. The infinite chain limit of $(\frac{1}{4} - \ln 2)N$ has been extracted and both curves are seen to converge to the new zero. (*b*) A finite-size scaling calculation of the lowest two states of the Railroad geometry for even membered chains. Both states are total spin singlet. One state is at the zone centre and the other is at the zone boundary. An approximate infinite chain limit of $-0.486N$ has been extracted and the curves all appear to converge to the new zero. (*c*) The corresponding analysis to (*b*) for the odd membered chains. The limit no longer appears to be zero, although it does appear to be below $0.2J$.

length, $\lambda_{\rm d} = (2\pi)/k_{\rm d} \sim 24.866$, is the right order of magnitude. We suggest that these oscillations are the residual effects of the finite loop length interfering with the length scale, $\lambda_{\rm d}$.

We believe that the fact that loops with odd and even membered pairs behave in significantly different ways is probably the best evidence that the system has broken spatial symmetry. The only way for us to interpret this fact is in terms of the solution to the spin 1 chain. If the symmetry is broken and nearest neighbour bonds become alternately high-spin and low-spin, then the resulting chain of approximately antiparallel *pairs*, is frustrated when there is an odd number of pairs and 'bipartite' when there is an even number.

If we return to the broken symmetry, then it seems clear that the two relevant states will become degenerate for the infinite chain, satisfying the first requirement. Now let us address the question of the spin correlations and whether they exhibit an order parameter.

The nearest neighbour spin correlations for the *symmetry broken* state, which is not an eigenstate except in the infinite chain limit, are finite-size scaled in figure 6. The limiting behaviour of the chain is analytically known and included for emphasis.

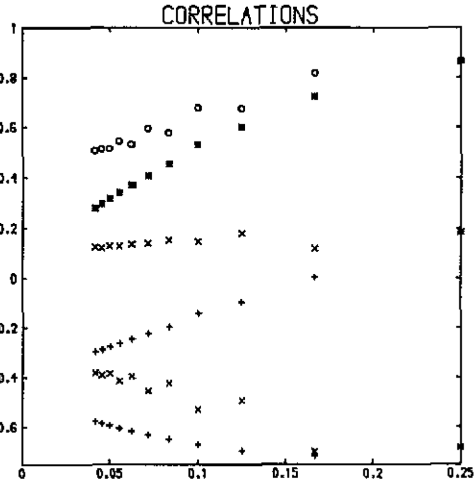


Figure 6. A finite-size scaling of the nearest neighbour spin–spin correlations for the symmetry broken ground states of both the spin 1/2 chain, plusses and stars, and the Railroad, crosses and circles. The crosses and plusses denote the two values of the correlations and the stars and circles denote the difference. The infinite limit of the spin 1/2 chain has been included. The two systems appear to behave in significantly different ways.

Although it is plausible that the points plotted are consistent with the analytic limits, the finite-size scaling analysis would not be compelling on its own. We should point out that the chain is probably a very stringent test for the analysis, because the decay properties of the spin correlations show power law behaviour which is likely to show smooth changes on *all* length scales.

The behaviour of the same correlations on the Railroad geometry show completely different characteristics. The two spin correlations on neighbouring bonds appear to converge to different limits. Although the chain suggests that the scaling might be ambiguous, a careful study of the *curvature* of the relevant plots suggests that the limits are distinct, *unless* there is a dramatic change of behaviour on an as yet undiscovered length scale. One bond appears to converge to a dominantly triplet configuration, $\sim 85\%$, and the other bond to a dominantly singlet configuration, $\sim 60\%$.

It is our belief that the convergence properties of the Railroad are *exponential* and therefore that the finite-size scaling calculations are to be believed. The reason for our belief in a finite correlation length comes from our related belief in a gap to excitations. We will examine the numerical evidence for a gap in the next subsection, but one piece of evidence is presented in figure 5(*c*), where we find that ground states of the odd length loops appear to converge to a different limiting energy than for the even length chains.

We would like to point out that we have in this paper an example of a system which exhibits a rather unusual form of long-range order. The presence of the broken symmetry and the corresponding order parameter indicates the existence of long range order, but *not* necessarily long range magnetic order. There can be long range order in this system in the absence of long range spin–spin correlations. Although the atoms separate into dominantly parallel pairs, there is no requirement for order amongst the resulting triplets. Indeed, the spin 1 chain suggests that any such long range magnetic coherence is unlikely.

3.2. A gap to excitations?

There is a fairly widespread belief, that a magnetic order parameter leads to excitations at low energies and further that a lack of magnetic order leads to a gap in the low energy spectrum. The first result is fairly easy to motivate, in terms of 'Goldstone Modes' and small fluctuations in the order parameter, but the second is more mysterious. For magnetic systems the low energy excitations are 'Spin Waves' and 'Spin Spirals'. One of the easiest quantities to numerically analyse is the existence of a low energy gap to excitations and we now perform such an investigation. A non-zero gap indicates to us a *lack* of long range order.

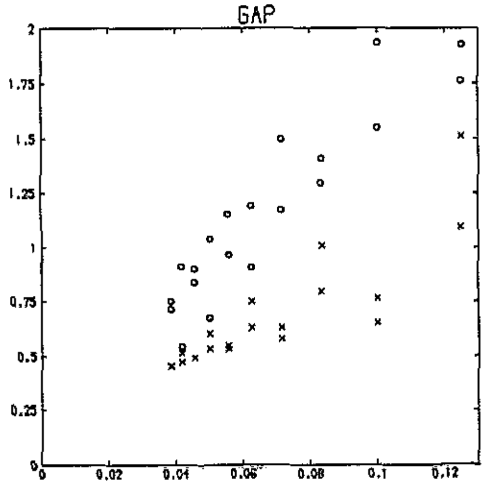


Figure 7. The 'gap' to the lowest lying spin 1, crosses, and spin 0, circles, excitations. We have plotted the 'gaps' for both zone centre and zone boundary states. There is no clear limit, but it seems natural to expect a limit of above $0.2J$.

In figure 7 we finite-size scale the lowest lying spin 1 excitations, which would naively be interpreted as Spin Waves, together with the lowest lying spin 0 excitations, which would naively be interpreted as Spin Spirals [14]. A brief study of the spin–spin correlations suggests that this interpretation is acceptable for the spin 1 excitations, which have similar correlations to the ground state, but the spin 0 excitations also have similar correlations to the ground state. The fact that there are *two* low energy 'ground states' leads to a problem in defining the 'gap' to excitations for finite systems. We have elected to calculate the gap to excitations at *fixed* Bloch momentum. This choice ensures a *smooth* variation as a function of size, but prohibits any 'absoluteness' since half of the states have the gap *between* the two ground states omitted.

The quantities calculated show a similar type of oscillation to the ground state energies. There is no *clear* evidence for a gap, but it is easiest to believe that the curves are tending to a limit which is larger than $\sim 0.2J$.

The second piece of evidence for a gap to excitations comes from the odd loop total-energy calculations depicted in figure 5(c). These total energies have had the same infinite chain limit subtraction which made the even membered loops tend towards zero energy. It seems likely that the odd loops possess an extra energy of approximately $0.2J$. An odd loop necessarily has a half integral total spin. The ground state has total spin $1/2$, and this extra spin $1/2$ can be interpreted as an excitation. The odd membered loop calculation then suggests that there is a gap of $\sim 0.2J$ to this excitation. If we assume that the pairing into nearest neighbour triplets still occurs for odd loops, then the extra or 'free' spin, which remains unpaired, acts both as a domain wall between two regions which pair out of phase, and simultaneously is the spin 1/2 excitation. This is a very natural interpretation for the excitation, as a domain wall carrying spin 1/2, an explanation which is certainly true for the Sawtooth geometry [15].

Our inability to make a clean finite-size scaling of the proposed energy gap is probably due to the fact that the system is topologically frustrated. This allows subtle variations in behaviour to compensate for minor changes in boundary conditions, and hence slow convergence in behaviour which is controlled by rather small energies. Due to the difficulties encountered in making sense of this scaling, it has not proved useful to extend our investigation of excitations to the one parameter families of systems. However we have made a brief comparison of the ground state to the one parameter families of systems.

3.3. Quantum comparisons for the Railroad

In trying to compare the three fundamental geometries, we have two major options. The natural comparison involves using the family of systems defined by the parameters λ and κ, but we can also compare the states directly. The basic problem is that numerical work involves finite-size scaling. A direct comparison involves a pure scaling analysis, but an investigation of a one-parameter family entails the study of a finite-size scaled quantity. For the present frustrated systems, scaling is *neither* straightforward *nor* accurate, and the variation in the *way* the system scales makes any such calculation suspect. We will attempt to scale the symmetry breaking spin correlations for the family of systems, but first we will make a direct comparison of the finite system ground states.

In figure 8 we plot a finite-size scaling of the square of the overlap between the Railroad ground state and the other two ground states. As well as the probability that the Railroad ground state *is* the ground state to the other Hamiltonians, we plot some correlation functions for comparison. The point to the extra correlations plotted is that the spin 1 chain ground state, $|H\rangle$, and the symmetry broken Sawtooth ground state, $|S\rangle$, satisfy:

$$|H\rangle = \prod_{\{ii'\}} \left[\frac{3}{4} + \boldsymbol{S}_i \cdot \boldsymbol{S}_{i'}\right] |H\rangle$$

$$|S\rangle = \prod_{\{ii'\}} \left[\frac{1}{4} - \boldsymbol{S}_i \cdot \boldsymbol{S}_{i'}\right] |S\rangle$$

where the pairs $\{ii'\}$ are *any* combination of the bonds which are triplet, for the spin 1 case, and singlet for the Sawtooth case. All of these pair operators are projection operators and so the overlaps presented could equally have been calculated with the *projected* Railroad ground state. The calculations plotted correspond to the sequence of probabilities that an increasing number of consecutive pairs have a fixed total spin. For the spin 1 chain it is the probability of finding consecutive spin triplets while for the Sawtooth it is the probability of finding consecutive spin singlets. These calculations demonstrate that the likelihood of finding neighbouring pairs with different

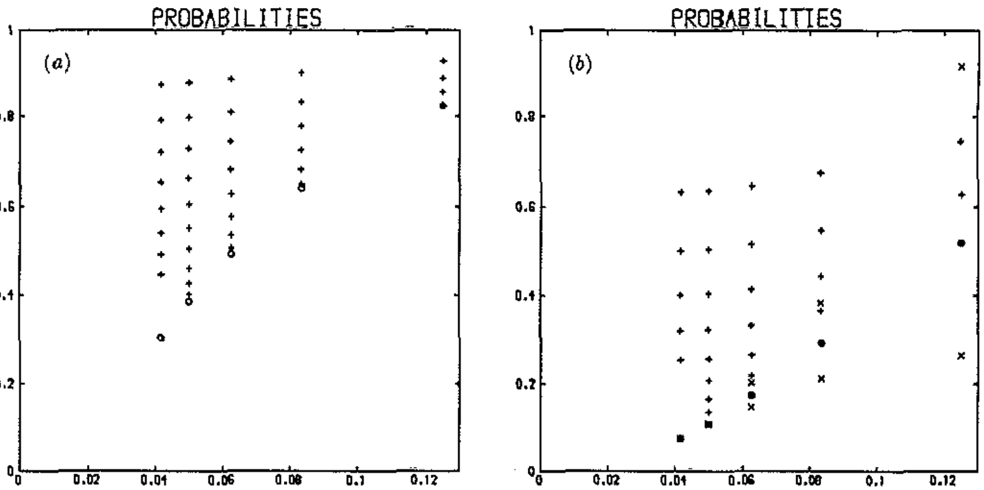


Figure 8. A finite-size scaling of the square of the overlaps between the symmetry broken ground state of the Railroad geometry and: (a) the spin 1 chain ground state; (b) the Sawtooth ground state. The circles denote the squares of the overlaps and the plusses denote the sequence of probabilitities that a row of consecutive pairs each have the same total spin. For the Sawtooth, if all bar one pair are singlet, then the final pair is necessarily singlet. Also for the Sawtooth, if all the pairs are singlet, then we find a Sawtooth ground state. We have also plotted the squares of the overlaps between the Bloch eigenstates of the Railroad with the corresponding symmetric eigenstates of the Sawtooth, denoted by crosses.

total spins is fairly random in the Railroad ground state. It also shows that the dominant differences between the relevant states are the local spin correlations and not the longer range correlations.

The ground state to the spin 1 chain is very similar to the symmetry broken solutions to the Railroad for these small systems. There are two possible sources of difference; firstly when pairs cease to be in local triplet configurations and secondly if the triplets were to show different local spin correlations. It seems likely that the dominant effect is the loss of the local triplet configurations at this small cluster size.

The ground state to the Sawtooth is also similar to the Railroad, but not as similar as the spin 1 chain ground state. Once again there are two possible differences, with the dominant effect being the loss of local singlet correlations. For this comparison the loss of singlet correlations is large.

It is important not to try to carry this comparison too far. Although for these small clusters the dominant difference is the short range correlation associated with the symmetry breaking order parameter, the correlation length of the antiferromagnetic correlations is quite different for the three systems. For the spin 1 chain there is a correlation length of $\sim$ 5–7 pairs of atoms [6] while for the Sawtooth the correlation length is only one pair of atoms. For the Railroad, the correlation length is somewhere between these two values, although we have been unable to calculate this length accurately. For the longer chains these correlation lengths will play a role in any comparison.

Our final calculation is of the symmetry breaking order parameter across our single parameter families of systems. For the family connecting the spin 1 chain to the Railroad, the high-spin low-spin bond alternation is natural and occurs in the unique ground state. For the family connecting the Sawtooth to the Railroad, the bond alternation only emerges in the symmetry broken combination of the *two* ground states. The finite-size scaling analysis of the Railroad convinced us that the spin correlations were fairly well converged at small chain lengths, and so the basic picture can be deduced from a fixed chain length. In figure 9 we depict the relevant spin–spin correlations for the family of chains with sixteen atoms. The changeover of roles between the symmetry broken states and the unique ground state is observed near the Railroad geometry. We view this as a finite-size phenomenon of no interest to the infinite chain limit. The bond alternation is clearly large over both families of systems, and finite-size scaling suggests that the infinite chain limit is not dissimilar from this example.

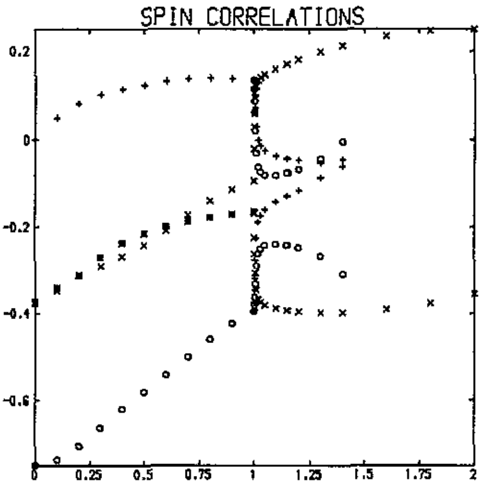


Figure 9. A calculation of the nearest neighbour spin–spin correlations across our two families of systems for a sixteen atom loop. The left half is as a function of κ, taking us from the Sawtooth to the Railroad. The right half is as a function of $1+\lambda$ taking us from the Railroad to the spin 1 chain. The circles and plusses denote the symmetry broken ground states and the crosses and stars denote the symmetric ground states. For all systems there is clearly a large difference between the two possible spin correlations.

4. Conclusions

It is our belief that there is a natural progression of ground states from the spin 1 chain through the Railroad geometry to the Sawtooth geometry. We believe that there is a symmetry breaking with nearest neighbour bonds alternating between high and low spin throughout the sequence. Between the Railroad and Sawtooth, this constitutes *spontaneous* symmetry breaking. We believe further that *all* the systems have a gap to excitations with the value of the gap varying between $\sim 0.4J$ for the spin 1 chain to $\sim 0.2J$ for the Sawtooth. Connected to the existence of a gap, we believe that all the systems have a finite magnetic correlation length, which varies from about $5 \sim 7$ pairs of atoms for the spin 1 chain down to less than one pair for the Sawtooth. The best measure for the change in ground state as we move smoothly between systems seems to be the nearest neighbour spin correlation which varies between parallel for the spin 1 chain to uncorrelated for the Sawtooth.

On a more general level, we believe that for spin 1/2 systems, any incommensurate or non-collinear phase predicted by the classical limit is unlikely to be the quantum ground state, although the actual nature of the ground state remains a mystery to us.

Our numerical evidence for the picture just presented is *very* patchy. The strongest evidence is for the spontaneous symmetry breaking. The difference between the spin correlations on neighbouring bonds appears to converge to a well defined non-zero limit for both families of systems studied, although the spin 1/2 chain, which we know is translationally invariant in the infinite loop limit, does not *clearly* limit to zero. The *actual* behaviour of the spin 1/2 chain remains unresolved by our numerical work but the convergence is clearly compatable with the analytic solution. Our results are suggestive but prove nothing.

The similarity between the spin 1 chain ground state and the Railroad ground state is quite surprising. For example, with 24 atoms, the probability that the symmetry broken Railroad ground state actually *is* the spin 1 chain ground state is above 1/4. The low lying excitations are *not* particularly similar however.

The Sawtooth geometry is soluble [8] and has the same spatial broken symmetry that we are proposing for the Railroad. The existence of *two* degenerate ground states allows the possibility of a domain wall excitation. Domain walls, although admittedly of two distinct varieties, constitute the gapped low energy spectrum of the Sawtooth [15]. The short range character of the spin correlations does not seem to allow 'Spin Wave' like solutions.

For the Railroad geometry, the two degenerate ground states remain, also permitting domain wall excitations. The odd loop calculations are best interpreted in this way and these domain walls are probably gapped, although the numerical work is inconclusive. The spin–spin correlation length for this system is larger, and this allows the possibility of 'Spin Wave' like excitations. For the analytically solved spin 1/2 chain, domain walls form the lowest lying excitations, but two domain walls *bind* to form a 'local' spin 1 'Spin Wave' excitation [14]. This interpretation appears to successfully apply to the Railroad, where the spin–spin correlations remain virtually unaffected for the lowest lying spin 1 excitation, indicating that it is 'local'. Strangely, however, even the lowest lying spin 0 excitations behave in this way, suggesting a similar rather implausible interpretation for them. It is probable that our clusters are simply too small to isolate the true nature of the excitations.

The possibilities for the spin 1 chain are rather different. There is no longer a ground state degeneracy and therefore no possibility of spin 1/2 domain walls. Indeed, this result can be rigorously proven. Only the 'Spin Wave' like excitations remain, although Spin Spirals for the triplet pairs become a possibility. The character of the excitations must change somewhere between the spin 1 chain and the Sawtooth, even though the ground states are remarkably similar.

Using the classical limit as motivation, we have suggested that the spin 1 chain and Railroad geometries behave in a similar way. An understanding of this behaviour may prove useful. The fundamental understanding that we seek is that of the role of quantum fluctuations in systems with spin 1/2 atoms. For both perovskite superconductors and heavy fermions, a single electron often carries the whole spin of an atom, and exchange is therefore a quantum effect. The way quantum fluctuations break down the magnetic order, replacing it with short range singlets, may be an interpretational aid for these more physical systems.

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