Exact ground state and kink-like excitations of a two dimensional Heisenberg antiferromagnet

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A rare example of a two dimensional Heisenberg model with an exact dimerized ground state is presented. This model, which can be regarded as a variation on the kagomé lattice, has several features of interest: it has a highly (but not macroscopically) degenerate ground state; it is closely related to spin chains studied by earlier authors; in particular, it exhibits domain-wall-like “kink” excitations normally associated only with one-dimensional systems. In some limits it decouples into non-interacting chains, purely dynamically and not because of weakening of interchain couplings: indeed, paradoxically, this happens in the limit of strong coupling of the chains.

Exact many-body solutions are rare in physics. “Integrable systems”, systems which have as many integrals of motion as degrees of freedom and can in principle be solved exactly, are much sought after and nearly all the interesting examples are one dimensional. Even the more modest goal of obtaining an exact ground state for a non-trivial many body problem is not easy. The value of an exact ground state is obvious in studying the low temperature physics. Nevertheless, in the spin half Heisenberg model of magnetism, for instance, very few exact ground states (other than Bethe’s famous solution of the nearest-neighbour chain) are known in the antiferromagnetic case: notable examples are mostly quasi-one-dimensional, such as the Majumdar-Ghosh chain and the sawtooth lattice (fig. 1). These have doubly degenerate, dimerized ground states, and consequently, localized domain-wall-like excitations. In two dimensions, this author knows of only two exact solutions. One is by Shastry and Sutherland of a square lattice with alternating diagonal bonds; an experimental realization has recently been found and the model extended to three dimensions. The other appears in a paper whose main thrust is something else (chiral terms and three-spin interactions). Both models have non-degenerate ground states and excitations consist of breaking of singlet pairs; unlike in the 1D systems, there are no propagating domain walls.

Here I present what is, as far as I know, only the third example of a two dimensional spin half Heisenberg antiferromagnet with an exact ground state, one which is quite different from the two above. The lattice is shown in figure 2; it bears some visual similarity to the much studied kagomé lattice, to which it reduces if we collapse the diamond-shaped plaquettes (for instance by introducing a strong ferromagnetic interaction between the extreme corners). But its interest arises from the facts that (a) it has exact, dimerized ground states like the Majumdar-Ghosh and sawtooth chains, (b) the ground state is highly degenerate (though not macroscopically so), and (c) the low energy excitations are domain-wall-like, connecting different ground states. This is thus the first genuinely two dimensional spin system to display these properties. These happen because it is highly anisotropic, and decouples in some limits into essentially non-interacting sawtooth-like chains; this arises from energy considerations and not from weakening of inter-chain couplings.

All the models mentioned above (except the nearest-neighbour chain) have dimerized ground states, consisting of pairs of spins in the singlet (zero-spin) state. Moreover, they all have the property that the Hamiltonian is a sum of smaller Hamiltonians each of which has an exact dimerized solution, and the full solution is constructed of these. The general idea of constructing exact solutions piecewise is not new but given the direct importance it has in our problem it is worth showing explicitly for these examples. Consider the Heisenberg antiferromagnet Hamiltonian

$$H = \sum_{i,j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$$

(1)

where $J_{ij}$ are positive constants. The Hamiltonian can be written in terms of the Pauli matrices as

$$H = \sum_{i,j} \frac{J_{ij}}{4} \left[ 2 \left( \sigma_i^+ \sigma_j^- + \sigma_j^+ \sigma_i^- \right) + \sigma_i^z \sigma_j^z \right]$$

(2)

where $\sigma^\pm = (\sigma^x \pm \sigma^y)/2$ and $\mathbf{S} = \frac{1}{2} (\sigma^x, \sigma^y, \sigma^z)$. It is easily verified that (a) the ground state of the two atom chain is a singlet (spin zero), (b) the (four-fold degenerate) ground state of the three atom ring is a singlet pair and a “free” spin.

The sawtooth chain is a chain of such triangles, joined at the corner. Thus in the ground state, each triangle has one side whose spins form a singlet, and the “free spin” of each triangle is part of a singlet pair on the next triangle (fig. 1). In all the figures, a double line joining two sites indicates a singlet pairing of those spins.

Consider, next, a four-spin system made by combining two of these triangles: the Hamiltonian of this system is the sum of two triangle Hamiltonians, which is equal to a square with sides of strength $J$ and a diagonal exchange
of strength $2J$. A possible ground state of this system is a dimer along this diagonal. Another ground state is a pair of dimers along opposite sides. For a diagonal exchange $J'$ different from $2J$ the former remains an eigenstate, and in fact it is the ground state for $J'$ is more than roughly $1.41J$. The total spin of the diagonally-connected pair is conserved: labelling these as $S_1$ and $S_2$, and the other two as $S_3$ and $S_4$, the Hamiltonian is $J'S_1 \cdot S_2 + J(S_1 + S_2) \cdot (S_3 + S_4)$ which commutes with $(S_1 + S_2)$.

The Majumdar-Ghosh chain can be regarded as a chain of such side-sharing triangles (fig. 3). Again, the Hamiltonian is a sum of triangle-like Hamiltonians, and the dimerized states are ground states for each of these individual Hamiltonians—hence for the whole system.

To extend this sort of model to two dimensions is another matter. The only published examples this author knows of are the two mentioned earlier, the square lattice with alternating diagonal interactions and the model of Sen and Chitra, both of which can again be built up of these elementary pieces. By analogy with the sawtooth chain of corner-sharing triangles, the Kagome lattice may seem to be a candidate, but such “dimerization” is not possible on it, nor on any two dimensional lattice of corner sharing triangles. To see this, note (fig. 2) that any two-dimensional dimerized network of corner-sharing triangles must contain two infinite chains of triangles (or closed loops for a periodic lattice), containing one triangle in common; but if one chain is fully dimerized, it is impossible to fully dimerize the other. In particular one cannot “deplete” a Kagome lattice to obtain an exact dimerized ground state, while retaining its 2D character. One can, of course, deplete the Kagome lattice in such a way as to destroy its two-dimensional character, and then a dimerized ground state is possible.

With this background, consider the lattice in figure 4. This lattice is superficially similar in appearance to the Kagome lattice, which can be viewed as a set of connected sawtooth chains: but by introducing the additional rhombuses between the chains, with interactions $J'$ along the sides and $J''$ along the short diagonals, where $J'' > 1.41J'$ roughly, we obtain a system with an exact ground state. This is a state where the sawtooth-like chains are dimerized as usual, while the connecting rhombuses are dimerized along their short diagonals. $J'$ must be sufficiently small compared to $J''$ for the dimerization of the rhombus to be its ground state, but is otherwise arbitrary, and $J$ is arbitrary compared to both of these. The ground state of such a system with periodic boundary conditions has a degeneracy $2^L$, where $L$ is the number of sawtooth-like chains, each such chain being doubly degenerate.

In the limit $J \gg J'$, $J''$, of course, the system decouples into noninteracting sawtooth chains; but the interesting thing is that the same thing happens, effectively, even when $J'' \gg J' \gg J$, which would appear to be a strong coupling limit between the chains. For in this case it is expensive to break the diagonal singlet pairs in the rhombuses, so they tend to remain in their ground states, and the spin dynamics becomes confined within each chain. In both these limits, there is little to add in the treat-
ment of this lattice to the discussion of the sawtooth chain. To recapitulate the discussion in [3], there are two kinds of domain-wall excitations, which can be dubbed “kinks” and “antikinks”, of which the “kinks” are exact eigenstates with zero energy, while the “antikinks” are not exact eigenstates and have a non-trivial dispersion with a gap. If we write a momentum eigenstate using antikinks as follows:

$$|k⟩ = \frac{1}{N} \sum_{n=1}^{N} e^{ikn} |n⟩ \quad (3)$$

where $|n⟩$ is the state with an antikink on the $n$th triangle, we can estimate the energy of such a state by calculating the expectation $⟨k|H|k⟩/⟨k|k⟩$. This yields a dispersion

$$E = (5/4 + \cos k)J \quad (4)$$

derived by Sen et al. [3]. To get a better estimate they consider more states, and show that the correction isn’t very large. In particular, the system has a gap of around 0.25J. In a periodic system the kinks and antikinks must exist in pairs. So the system as a whole has a gap, and at low temperatures, travelling kink-antikink excitations. In our two-dimensional system, if $J'' > 1.41J' > J$, the system will consist of effectively non-interacting sawtooth chains with horizontal kink-antikink excitations but, at low temperatures, no excitations travelling in the “vertical” direction.

Things are less simple when $J$, $J'$, $J''$ are comparable. Then excitations can propagate in the “vertical” direction too. Particularly interesting is the choice $J' = J$, $J'' = 2J$: in this case the Hamiltonian can be written as a sum of triangles, with the exchange interaction $J$ along each “side”. It is clear that excitations with energy of at least order $J$ should exist, and this is not too far away from the sawtooth-chain gap of 0.25J. We improve on this below.

While the “horizontal” chains are disjoint in that they have no common sites, and can be treated individually, this is not true of the “vertical” chains, which crisscross and intersect heavily. In other words, it would not be reliable to treat the vertical excitations as excitations of vertical chains. We instead present a very rough calculation (which can be treated as a liberal upper bound only) of the dispersion of an excitation in one such vertical chain.

We write the Hamiltonian as a sum of triangle terms,

$$H = \sum_{i} H_i \quad (5)$$

where each individual triangle Hamiltonian is a sum of spin-spin interactions over each side of a triangle

$$H_i = J (S_{1i} \cdot S_{2i} + S_{2i} \cdot S_{3i} + S_{3i} \cdot S_{4i} + \frac{3}{4} J_i) \quad (6)$$

FIG. 5. Propagation of excitation along vertical chain: Four basis states used in variational estimate of energy

The constant piece $3J/4$ changes the energy of a dimerized triangle (therefore also the ground state energy) to zero. The subscript $l$ denotes the $l$-th triangle. The propagation of the excitation along a chain may be regarded as occurring as shown in figure 5. A single non-dimerized triangle travels through the chain via rearrangements of singlet bonds. (Incidentally, the chain itself is another example of a spin chain with an exact dimerized ground state. Since each pair of corner-sharing triangles can exist in one of two states independently of the rest of the chain, from which it is separated by a rhombus, the ground state is macroscopically degenerate.) Thus excitations we consider are not domain-wall excitations. Since the corner-sharing triangles here are part of the sawtooth chains in the full lattice, it would be expensive for a propagating domain wall to disturb them, so we assume that they remain unchanged except at the sites of the excitation, which is macroscopically degenerate. We use a variational calculation with a momentum eigenstate formed from the four basis wavefunctions shown in figure 5.

$$|k⟩ = \sum_{n=1}^{N} e^{ikn} (|nα⟩ + |nβ⟩ + |nγ⟩ + |nδ⟩) \quad (7)$$

where the sum is over units of the sort shown in fig. 5, and there are $N$ such units, for each of which we assume one of the four basis states in fig. 5. $|nα⟩$ means the $n$th unit has configuration $|α⟩$, and so on. The wavefunction is orthogonal to the ground state in the $N \to ∞$ limit. There are, of course, many more possible basis states, but the calculation grows tedious and our purpose, which is to demonstrate that low-energy excitations along such chains can exist, will be served with this wavefunction.

The above basis states can be written

$$|α⟩ = (↑↓ - ↓↑) (↑↓ - ↓↑) (↑↓ - ↓↑) \quad (8)$$
$$|β⟩ = (↑↓ - ↓↑) (↑↓ - ↓↑) (↑↓ - ↓↑) \quad (9)$$
$$|γ⟩ = (↑↑ - ↓↓) (↑↑ - ↓↓) (↑↑ - ↓↓) \quad (10)$$
$$|δ⟩ = (↑↑ - ↓↓) (↑↑ - ↓↓) (↑↑ - ↓↓) \quad (11)$$

where the ordering of the spins is as shown in figure 5, and one should also include a normalizing factor of $1/√2$.
for each “singlet pair”. Our dispersion with this state will be
\[
E(k) = \langle k | H | k \rangle / \langle k | k \rangle \tag{12}
\]
where
\[
\langle k | k \rangle = \frac{1}{N} \sum_{m=1}^{N} \sum_{n=1}^{N} e^{i k (n - m)} \left( \langle m a | + \beta^* \langle m b | + \gamma^* \langle m \gamma | + \delta^* \langle m \delta | \right)
\]
\[
+ \delta \langle m \delta | \times ||n \alpha | + \beta |n \beta | + \gamma |n \gamma | + \delta |n \delta | \right). \tag{13}
\]
We need to know several matrix elements between the basis states to work this out, but the calculation is not hard. The result, for large \(N\), is
\[
\langle k | k \rangle = \frac{3}{4} + \left( \frac{15}{16} - \frac{1}{4 \sqrt{2}} \right) |\beta|^2 + \left( \frac{1}{2} - \frac{1}{4 \sqrt{2}} \right) |\gamma|^2
\]
\[
+ \frac{1}{2} |\delta|^2 - \frac{3}{4} \text{Re} \beta + \frac{1}{4 \sqrt{2}} \beta - \gamma |^2 \tag{14}
\]
To evaluate \(\langle k | H | k \rangle\), we write \(H = \sum H_l\) and note that \(\langle n, \phi | H_l | m, \psi \rangle\) (where \(\phi, \psi = \alpha, \beta, \gamma, \delta\)) is zero unless \(l = m = n\) (since \(H_l\) acting on a dimerized triangle is zero) and even for \(l = m = n\) the matrix elements will exist only for \(\phi = \psi\); \(\phi = \beta, \psi = \gamma\); or \(\phi = \gamma, \psi = \beta\). This gives
\[
\langle k | H | k \rangle = \frac{J}{4} \left[ 3 + 3 |\beta|^2 + 2 |\gamma|^2 + 2 |\delta|^2 \right]
\]
\[
- \frac{1}{\sqrt{2}} (\beta^* \gamma + \gamma^* \beta)
\]
\[
= \frac{J}{4} \left[ 3 + \left( 3 - \frac{1}{\sqrt{2}} \right) |\beta|^2 + \left( 2 - \frac{1}{\sqrt{2}} \right) |\gamma|^2
\]
\[
+ 2 |\delta|^2 + \frac{1}{\sqrt{2}} (\beta - \gamma |^2 \right) \tag{15}
\]
Now we need to minimize \(\langle k | H | k \rangle / \langle k | k \rangle\). We have five real parameters to vary, since there are three complex parameters but \(\delta\) appears only as an absolute square, and minimizing on a computer gives
\[
\beta = -1.3522, \tag{16}
\]
\[
\gamma = -0.4781, \tag{17}
\]
\[
\delta = 0, \tag{18}
\]
\[
E(k) = 0.59 J. \tag{19}
\]
This is a dispersionless excitation, but that may change with a more careful treatment. It is also interesting that \(|\delta|\) does not appear in the minimum energy wavefunction, but that too may change if we include more basis states. The important point is that the energy is not too far from the gap of the sawtooth chain (0.25J) and this estimate will certainly reduce further if we include more basis states and account for the crossings among these “vertical chains” (which intersect, unlike the horizontal sawtooth chains). So for \(J'' = 2J, J' = J\), we can expect such excitations to be present at low temperatures together with the sawtooth-chain excitations.

A final interesting point is that the system has an infinite (but not complete) set of conserved quantities, namely the total spins \(S_D = S_b + S_a\) along the short diagonals of the rhombuses where \(S_a\) and \(S_b\) are the spins on the sites connected by these short diagonals. All eigenstates of the system, and of the vertical chain discussed above, can be chosen to be eigenstates of these \(S_D\); but these will not be momentum eigenstates (since the \(S_D\) do not commute with the translation operator).

To summarize, the spin half Heisenberg model on the two dimensional lattice described here has several interesting features such as an exact dimerized ground state; a large ground state degeneracy (exponential in the square root of the system size); a decoupling into effectively noninteracting spin chains, which is dynamic and not because of weakening of inter-chain coupling; and domain-wall excitations of the kind normally found only in one-dimensional spin chains. The system is, paradoxically, most one-dimensional at high inter-chain couplings \(J'' > 1.4 J' \gg J\), and at these values it is clear that the system is gapped, because the horizontal sawtooth-chain excitations are known to be gapped. At the other extreme, \(J \gg J', J''\), the excitations are confined to the diamond-shaped plaquettes and cannot propagate, so again the system is gapped (the gap being of order \(J''\)). At intermediate values there are both horizontal (intra-chain) and vertical (inter-chain) excitations and it is not certain whether the vertical ones are gapless. Several related systems—sawtooth chains, kagome lattices, even the Shastry-Sutherland square lattice—have experimental realizations, and it would be interesting to look for experimental examples of this system too.

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