Absence of gap for infinite half–integer spin ladders with an odd number of legs

A. G. Rojo

Department of Physics, The University of Michigan, Ann Arbor, MI 48109-1120

Abstract

A proof is presented for the absence of gap for spin 1/2 ladders with an odd number of legs, in the infinite leg length limit. This result is relevant to the current discussion of coupled one–dimensional spin systems, a physical realization of which are vanadyl pyrophosphate, (VO)$_2$P$_2$O$_7$, and stoichiometric Sr$_{n-1}$Cu$_{n+1}$O$_{2n}$ (with $n = 3, 5, 7, 9, \ldots$).

The magnetic properties of low dimensional systems have been the subject of intense theoretical and experimental research in recent years. Haldane’s conjecture, which states that one–dimensional chains of integer spin should have a gap in the excitation spectrum, whereas the half integer spin chains should be gapless, was confirmed by a number of experiments in quasi one–dimensional systems. The recent interest on the spin 1/2 Heisenberg model in two dimensions (2D) is largely due to the fact that the undoped parent compounds of the high-Tc superconductors are accepted to be described by this model. Although an exact solution is lacking in 2D, numerical results indicate long range order in the ground state, and gapless excitations. Most of these calculations involve scaling the results obtained for an $M \times M$ square lattice to the limit $M \to \infty$.

More recently, the crossover from one to two dimensions has been studied in ladder type geometries of $N_x \times N_y$ sites, by taking the limit of $N_x \to \infty$ first. Remarkably, these results show that the scaling as a function of $N_y$ is not smooth: ladders of even $N_y$ have a finite gap, while those of odd $N_y$ have zero gap. This interesting property turns
out to be more than an academic curiosity, since, as pointed out in Ref. 8, real compounds like stoichiometric \( \text{Sr}_{n-1}\text{Cu}_{n+1}\text{O}_{2n} \) (with \( n = 3, 5, 7, 9, \ldots \)) can be described by Heisenberg spin ladders with \( N_y = \frac{1}{2}(n + 1) \). Also, \((\text{VO})_2\text{P}_2\text{O}_7\) (vandyl pyrophosphate), has a ladder \((N_y = 2)\) configuration of spin 1/2, \( \text{V}^{+4} \) ions.

A qualitative explanation of the difference between even and odd \( N_y \) ressorts to the strong coupling limit \( J'/J \gg 1 \), with \( J' \) being the exchange integral in the direction of the rungs of the ladder. In the limit \( J \to 0 \) the system decouples into open chains of \( N_y \) sites. Chains with odd \( N_y \) are gapless due to Kramers degeneracy, whereas those of even \( N_y \) have a gap; for example, for \( N_y = 2 \), the spin gap \( E_g = J' \). For odd \( N_y \) and \( J'/J \gg 1 \), the Kramers doublets in different chains can be coupled perturbatively, the resulting effective Hamiltonian being a one–dimensional infinite chain of spin 1/2 that has zero gap. Since for both the opposite extremes of \( J'/J \gg 1 \) and \( J' = 0 \) the system is gapless for odd \( N_y \), one expects a gapless spectrum for intermediate values of \( J' \). An alternative explanation is offered in Ref. 11 using arguments similar to those of Haldane for one dimensional chains: for odd \( N_y \) chains, the topological term governing the long-wavelength dynamic of the lattice does not vanish for odd \( N_y \) and the system is gapless. For even \( N_y \) a gap remains that scales as \( E_g(N_y) \sim \exp(-N_y) \). In this paper, I show that the absence of a gap for odd \( N_y \) is a rigorous result. This I do by reanalyzing the Lieb, Shultz and Mattis (LSM) theorem — which is valid for one dimensional spin-1/2 chains—for ladder geometries with \( N_y = 2P + 1 \) sites in the \( y \)–direction, and \( N \) sites in the \( x \)–direction, in the limit \( N \to \infty \). The proof is valid if \( N \) is even. For odd \( N \) the total number of sites is odd, the ground state has total spin projection \( S^z_{\text{tot}} = \pm 1/2 \), and is therefore doubly degenerate.

We consider the celebrated Heisenberg model, which is described by the Hamiltonian

\[
H = J \sum_{\langle ij \rangle} S(i) \cdot S(j),
\]

where \( i \) and \( j \) are vectors of the lattice, \( S(i) \) denotes spin–1/2 operators, and the symbol \( \langle i,j \rangle \) stands for near neighbors. The boundary conditions are periodic, and the lattice constant equals to 1, in such a way that \( i = (n_x, n_y) \), with \( n_x \) and \( n_y \) integers.
Let |Ψ₀⟩ be the ground state of H with energy E₀. Define a state |Ψₓ(k)⟩ which is obtained from |Ψ₀⟩ by applying a twist of wave vector k in the x–direction:

|Ψₓ(k)⟩ = exp[i\k \sum_i n_x S^z(i)]|Ψ₀⟩ ≡ Uₓ(k)|Ψ₀⟩. \hspace{1cm} (2)

Note that spins with the same nₓ coordinate are subject to the same twist.

The proof of existence of gapless excitations for \( N \to \infty \) can be divided in two steps. In step one, the orthogonality of |Ψₓ(k)⟩ with |Ψ₀⟩ is established. It is precisely in this step where the distinction between even and odd widths becomes apparent: for even widths, the twisted state |Ψₓ(k)⟩ will not be orthogonal to the ground state. In step two, the expectation value of H in the twisted wave function is proven to be equal to E₀ in the limit \( N \to \infty \).

**Step 1.** Consider the operator \( Tₓ \), which translates the system by a lattice constant in the x–direction:

\[ TₓS(nₓ, n_y)Tₓ^{-1} = S(nₓ + 1, n_y), \]
\[ TₓS(N, n_y)Tₓ^{-1} = S(1, n_y). \]

Since \( Tₓ \) commutes with H, and we have \( Tₓ |Ψ₀⟩ = e^{iδ} |Ψ₀⟩ \), with δ some constant phase. Here we are using the assumption of uniqueness of the ground state, which can actually be proven for finite \( N \) (see below). This allows us to write

\[ \langle Ψ₀|Ψₓ(k)⟩ = \langle Ψ₀|Tₓ \exp[i\k \sum_i n_x S^z(i)]Tₓ^{-1}|Ψ₀⟩. \hspace{1cm} (3) \]

The evaluation of \( Tₓ \exp[i\k \sum_i n_x S^z(i)]Tₓ^{-1} \) is straightforward, giving

\[ TₓUₓ(k)Tₓ^{-1} = Uₓ(k) \exp[-i\k \sum_i S^z(i)] \exp[iNk \sum_{n_y=1}^{N_y} S^z(1, n_y)]. \hspace{1cm} (4) \]

Since, by Marshall’s theorem, the ground state is in the subspace of \( S^z_{\text{Tot}} = 0 \), we have

\[ \exp[-i\k \sum_i S^z(i)]|Ψ₀⟩ = |Ψ₀⟩. \hspace{1cm} (5) \]

We now prove that, if one chooses \( k = 2\pi m/N \), with m an odd integer, then

\[ \exp[iNk \sum_{n_y=1}^{N_y} S^z(1, n_y)]|Ψ₀⟩ = -|Ψ₀⟩. \hspace{1cm} (6) \]
Let
\[ |\Psi_0\rangle = \sum_\Gamma c(\Gamma)|\Gamma\rangle, \]
where the sum runs over all the spin configurations \( \Gamma \) with \( S_{\text{Tot}}^z = 0 \). Then
\[
\exp[iNk \sum_{n_y=1}^{N_y} S_z^z(1, n_y)]|\Psi_0\rangle = \sum_\Gamma \exp[i2\pi m Q_\Gamma]c(\Gamma)|\Gamma\rangle,
\]
with \( Q_\Gamma = \frac{1}{2}(N_{\uparrow,\Gamma} - N_{\downarrow,\Gamma}) \), and \( N_{\uparrow,\Gamma} \) ( \( N_{\downarrow,\Gamma} \) ) the number of up (down) spins in row 1 in configuration \( \Gamma \). If \( N_y(\equiv N_{\uparrow,\Gamma} + N_{\downarrow,\Gamma}) \) is odd, then \( Q_\Gamma \) is half integer, and \( \exp[i2\pi m Q_\Gamma] = -1 \).
This implies that
\[
\langle \Psi_0|\Psi_x(k)\rangle = -\langle \Psi_0|\Psi_x(k)\rangle = 0,
\]
and the states are in fact orthogonal. We stress that the proof in this step is valid only for odd widths. For even widths \( Q_\Gamma \) is integer and \( \exp[i2\pi m Q_\Gamma] = 1 \). We could have chosen \( k = \pi m/N \) in this case, but still the sign of \( \exp[i2\pi m Q_\Gamma] \) will depend on \( \Gamma \) through \( N_{\downarrow,\Gamma} \), and cannot be taken out of the summation in (7). The failure of the present proof for even widths has certainly the same formal origin than the case of strictly one dimensional chains of integer spin.

**Step 2.** We now need to evaluate \( U_x(k)^{-1}HU_x(k) \). The “\( S^z S^z \)” component of \( H \) remains unchanged since \( U_x(k) \) commutes with \( S^z(i) \). The transformation of the \( xy \) component is easy to obtain by noting that
\[
e^{-i\alpha S^z(i)}S^\pm(i)e^{i\alpha S^z(i)} = e^{\mp i\alpha}S^\pm(i),
\]
for \( \alpha \) an arbitrary constant. This implies that the \( xy \) component of \( H \) corresponding to the rungs of the ladder is also unchanged. For the transformed Hamiltonian we have
\[
U_x(k)^{-1}HU_x(k) = H + \frac{i}{2}J[\cos(k) - 1] \sum_{n_x=1}^{N_x} \sum_{n_y=1}^{N_y} [S^+(n_x, n_y)S^-((n_x + 1, n_y) + h.c] + \\
\frac{i}{2}J \sum_{n_x=1}^{N_x} \sum_{n_y=1}^{N_y} [S^+(n_x, n_y)S^-((n_x + 1, n_y) - h.c].
\]
Since the coefficients \( c(\Gamma) \) are real,
\[
\langle \Psi_0|[S^+(n_x, n_y)S^-((n_x + 1, n_y) - h.c]|\Psi_0\rangle = 0.
\]
Now we expand the cosine for small $k$, in particular we will take $m = 1$ ($k = 2\pi/N$): 
$$
\cos(k) - 1 \approx \frac{2\pi^2}{N^2}.
$$
Also, we make use of the inequality
$$
\frac{1}{2}\langle \Psi_0| [S^+(n_x, n_y)S^-(n_x + 1, n_y) + h.c]|\Psi_0 \rangle \leq S^2,
$$
to write a bound for the energy of the twisted state:
$$
\langle \Psi_x(k)|H|\Psi_x(k) \rangle = \langle \Psi_0|U_x(k)^{-1}HU_x(k)|\Psi_0 \rangle \leq E_0 + \frac{2\pi^2 JS^2 N_y}{N} + O(N_y/N^3).
$$
It is clear that if the limit $N \to \infty$ is taken for fixed $N_y$, the twisted state is degenerate with the ground state, and the proof is complete for the existence of gapless excitations for infinite ladders with an odd number of legs. Note that the proof can be extended immediately to the following cases: (a) coupling constants that are different in the vertical and horizontal directions, as long as translational invariance in the $x$–direction is preserved, (b) half integer spins higher than $\frac{1}{2}$, (c) quasi one dimensional “wires” of a two dimensional cross section with an odd number of spins.

The question of the uniqueness of the ground state was addressed for the case of chains by Affleck and Lieb\[15\] (AL), whose considerations apply also to ladders. In particular, one can prove that the ground state is unique for finite $N$. The proof is as follows. For $N$ even we can define two sublattices $A$ (for which $n_x + n_y$ is even) and $B$ (for which $n_x + n_y$ is odd), and rotate all the spins in the $A$ sublattice in such a way that $S^z(i) \to S^z(i)$, and $S^\pm(i) \to -S^\pm(i)$. This canonical transformation has the effect of changing the sign of the “$S^+S^-$” term in (1). After this transformation, all the off diagonal elements between configurations $\Gamma$ and $\Gamma'$ which are connected by the $S^+S^-$ term are negative. Therefore, in the minimum energy state, all the weights $c(\Gamma)$ will have the same sign. If we call $E(\Gamma)$ the diagonal energy of configuration $\Gamma$, and $\Gamma'$ a configuration obtained by applying the $S^+S^-$ term to $\Gamma$, we have that $c(\Gamma)$ obeys the equation of motion\[14\] $[E(\Gamma) - E_0] c(\Gamma) = J/2 \sum_{\Gamma'} c(\Gamma')$. Since all $C(\Gamma)$ have the same sign, this implies that all $c(\Gamma) \neq 0$. Therefore the ground state is non–degenerate. However, it could happen that, as $N \to \infty$, some weights $c(\Gamma)$ become exponentially small and the ground state splits up into two broken symmetry states. Possibilities are an
antiferromagnetically ordered state, which will have gapless spin-wave excitations, and a spontaneously dimerized one, which will have a gap. We have therefore proven that in the limit \( N \to \infty \) either there are degenerate ground states or vanishing gap.

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