Is the purely biquadratic spin 1 chain always massive?

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It is shown that the $sl(2)_q$-invariant open antiferromagnetic XXZ spin chain with a boundary field has a gapless sector in the thermodynamic limit when its length is odd. Owing to a Temperley-Lieb equivalence of the spectra, the same conclusion is drawn for the purely biquadratic spin 1 chain with open boundaries and odd length.

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The bilinear-biquadratic spin 1 quantum chain

\[ H = \sum_{n=1}^{L} \cos \theta S_n \cdot S_{n+1} + \sin \theta (S_n \cdot S_{n+1})^2 \]  

has been the object of very intense investigation in the last twenty years. One of the goals has been to determine the properties of the ground state and the nature of the low-lying excitations in the thermodynamic limit. In particular, whether they form a continuum with the ground state (critical chain) or whether they are separated by a finite gap (massive chain). Haldane’s prediction \[1\] that the Heisenberg antiferromagnet (\(\theta = 0\)) should be massive for integer spin has been thoroughly verified by a variety of numerical methods \[2\]. The AKLT chain (\(\tan \theta = \frac{1}{3}\)) has been rigorously proven to have a valence bond ground state and a nonzero gap \[3\]. Other cases of (1) have been analyzed in depth due to their integrability. They are the critical \(SU(3)\)-invariant Sutherland spin chain (\(\theta = \pi/4\)), solved by nested Bethe-ansatz \[4\]; the Babujian-Takhtajan chain (\(\theta = -\pi/4\)), also solvable by Bethe-ansatz and also gapless \[5,6\]. The third case is the purely biquadratic spin chain (\(\theta = -\pi/2\)), which, after some controversy, has been found to have a gap \(\Delta \simeq 0.1731788\) \[7\]; an identical gap has been revealed in the same chain, but this time with free boundary conditions

\[ H_{bQ} = -\sum_{n=1}^{L-1} (S_n \cdot S_{n+1})^2 \]  

and \(L\) even \[8\].

Now, at least for free boundary conditions, it can be shown that (2) has a band of gapless excitations when \(L\) is odd and, of course, \(L \to \infty\). This points to the fact that antiferromagnetic quantum spin chains can in principle have very different properties according to the parity of their length.

To prove this statement, one observes that the spectrum of (2) can be mapped \[8\] into the spectrum of the \(sl(2)_q\)-invariant open antiferromagnetic \(XXZ\) chain with a boundary field

\[ H_{XXZ} = -\sum_{n=1}^{L-1} \left( \sigma^x_n \sigma^x_{n+1} + \sigma^y_n \sigma^y_{n+1} - \cosh \gamma \sigma^z_n \sigma^z_{n+1} + \frac{\sinh \gamma}{2} (\sigma^z_1 - \sigma^z_L) \right) \]  

The equivalence holds when \(\cosh \gamma = \frac{3}{4}\), \(\sinh \gamma = \frac{\sqrt{5}}{2}\). At this point both (2) and (3) can be written as sums over the generators \(\{e_n\}_{n=1}^{L-1}\) of the Temperley-Lieb algebra \[8\]

\[ e_n^2 = 3e_n \quad e_n e_{n+1} e_n = e_n \quad [e_n, e_{n'}] = 0 \quad |n - n'| \geq 2 \]  

\[ H_{bQ} = H_{XXZ} - \frac{7}{4} (L - 1) \]  

Eq. (5) must be understood as a statement about the spectra. The two representations of (4), appearing in (2) and (3), are of course different since the two Hamiltonians live in Hilbert spaces of different dimensions, but their spectra should differ only in their multiplicities \[8\] (further comments on this point will be given at the end). Similar mappings, via Temperley-Lieb algebra,
have shown to be very fruitful in studying statistical mechanics models and related quantum spin chains, one notable example being the Potts model [10,11].

The spin chain (3) has been solved by means of the coordinate Bethe-ansatz (BA) [12]. In fact, it was relying on the Temperley-Lieb mapping and the numerical as well as analytical solution of the relevant BA equations that the ground state energy and the gap of (3) were computed in [8].

As in all BA solvable systems, the spectrum of (3) is expressed in terms of rapidities \(\{\alpha_1, \ldots, \alpha_n\}\) that solve a set of coupled equations. In the case at hand, they are

\[
\frac{1}{\pi} \Theta(\alpha_j; \gamma/2) - \frac{1}{2\pi L} \sum_{k=1, k\neq j}^{n} \left( \Theta(\alpha_j - \alpha_k; \gamma) + \Theta(\alpha_j + \alpha_k; \gamma) \right) = \frac{I_j}{L}, \quad j = 1 \ldots n
\]

\[
\Theta(\alpha; x) \equiv -i \ln \frac{\sinh(x + \frac{\gamma}{2})}{\sinh(x - \frac{\gamma}{2})} = 2 \arctan(\frac{\alpha}{2} \coth x)
\]

Solutions are labelled by the set of positive integers \(\{I_j\}_{j=1}^n\). The branch cut in (7) is chosen to make \(\Theta(\alpha; x)\) a differentiable, increasing function for \(\alpha\) real, with \(\Theta(-\alpha; x) = -\Theta(\alpha; x)\) and \(\Theta(\alpha + 2\pi; x) = \Theta(\alpha; x) + 2\pi\). Only positive real rapidities in the \((0, \pi)\) interval need to be considered here. Given a solution of (3), the corresponding energy and spin \(S_{\text{tot}}^z = \frac{1}{2} \sum_{j=1}^{L} \sigma_j^z\) are [12]

\[
E = \frac{1}{2} (L - 1) \cosh \gamma - 2 \sinh \gamma \sum_{j=1}^{n} \Theta'(\alpha_j; \gamma/2), \quad S_{\text{tot}}^z = \frac{L}{2} - n
\]

It’s now crucial to determine the range of allowed vacancies for the set \(\{I_j\}_{j=1}^n\). This is done by rewriting (3) in terms of the counting function [13], defined as

\[
Z_L(\alpha) \equiv \frac{1}{\pi} \Theta(\alpha; \gamma/2) + \frac{1}{2\pi L} \left[ \Theta(\alpha; \gamma) + \Theta(2\alpha; \gamma) \right] - \frac{1}{2\pi L} \sum_{k=-n}^{n} \Theta(\alpha - \alpha_k; \gamma)
\]

\[
Z_L(\alpha_j) = \frac{I_j}{L}, \quad j = -n, -n+1, \ldots, n-1, n
\]

Rapidities have been doubled by reflection through \(\alpha = 0\) [12]: \(\{\alpha_1, \ldots, \alpha_n \mid \alpha_j > 0\} \rightarrow \{\alpha_{-n}, \ldots, \alpha_{-1}, 0, \alpha_1, \ldots, \alpha_n \mid \alpha_{-j} = -\alpha_j\}\), so that (8) is completely equivalent to (3). Since the rapidity range is \((0, \pi)\), or \((-\pi, \pi)\) after reflection, and the counting function is monotonically increasing, the largest allowed \(I_j\) is read from \(LZ_L(\pi)\), or, conceptually more correctly but with equal numerical result

\[
\lim_{\alpha_j \to \pi} LZ_L(\alpha_j) = L - n + 1
\]

The limit does not depend on the numerical value of the remaining \(\alpha_k, k \neq j\). Eq. (4) would suggest \(I_{\text{max}} = L - n + 1\). Actually this value is forbidden because the wave-function vanishes when one rapidity is \(\pi\) (\(\alpha\) is related to the variable \(k\) of [12] by \(e^{ik} = (e^{i\alpha} - e^{-\gamma})/(1 - e^{i\alpha - \gamma})\)). Hence the largest possible integer is

\[
I_{\text{max}} = L - n
\]
If $L$ is even, $n = \frac{L}{2}$ for the ground state (sector $S^x_{tot} = 0$) and there’s exactly $\frac{L}{2}$ vacancies for $\frac{L}{2}$ positive integers. But if $L$ is odd, the lowest energy states have $n = \frac{L-1}{2}$ (sector $S^x_{tot} = 1/2$) and there are $\frac{L+1}{2}$ vacancies for $\frac{L-1}{2}$ integers, hence one hole. Altogether a band of $\frac{L+1}{2}$ configurations, specified by a sequence of closely packed integers with one hole $I^{(h)}$, $1 \leq I^{(h)} \leq \frac{L+1}{2}$. The ground state for finite $L$ has $I^{(h)} = \frac{L+1}{2}$, that is at the edge of the band, as it will be proven shortly.

Denote by $\{\alpha_j\}_{j=1}^n$ the rapidities of the state with $I^{(h)} = \frac{L+1}{2}$, by $\{\alpha'_j\}_{j=1}^n$ the rapidities of any other state in the band ($1 \leq I^{(h)} \leq \frac{L-1}{2}$) and by $Z^{(0)}_L(\alpha)$ and $Z^{(1)}_L(\alpha)$ the relevant counting functions. One defines a hole rapidity $\alpha^{(h)}$ by

$$Z^{(1)}_L(\alpha^{(h)}) = \frac{I^{(h)}}{L}$$

This number does not belong to the set $\{\alpha'_j\}_{j=1}^n$, but it is convenient to include it, adding and subtracting its contribution to the counting function, which reads after reflection

$$Z^{(1)}_L(\alpha) = \frac{1}{\pi} \Theta(\alpha; \gamma) + \frac{1}{2\pi L} \left[ \Theta(\alpha; \gamma) + \Theta(2\alpha; \gamma) \right] - \frac{1}{2\pi L} \sum_{k=-n-1}^{n+1} \Theta(\alpha - \alpha'_k; \gamma) + \frac{1}{2\pi L} \left( \Theta(\alpha - \alpha^{(h)}; \gamma) + \Theta(\alpha + \alpha^{(h)}; \gamma) \right)$$

so that

$$Z^{(0)}_L(\alpha_k) - Z^{(1)}_L(\alpha'_k) = 0 \quad -\frac{L+1}{2} \leq k \leq \frac{L-1}{2} \quad (11)$$

For these values of $k$, define $\delta \alpha_k = \alpha'_k - \alpha_k = O(1/L)$. The two (after reflection) unpaired edge rapidities are handled separately. Since $\{\alpha_j\}_{j=-n}^n$ fill the interval $(-\pi, \pi)$ in the thermodynamic limit [10], one can set $\alpha'_0 = \pi + o(1)$ and $\alpha'_{-1} = -\pi + o(1)$ as $L \to \infty$. The next steps follow a well-established method for handling the BA equations [14,15]. Defining $\Delta \alpha_k = \alpha_{k+1} - \alpha_k = O(1/L)$ and the backflow $\delta(\alpha) = \lim_{L \to \infty} \frac{\delta \alpha}{\Delta \alpha_k} = O(1)$, it is found that the terms $O(1)$ in (11) cancel and the terms $O(1/L)$ yield

$$\delta(\alpha) + \frac{1}{2\pi} \int_{-\pi}^{\pi} d\beta \Delta(\alpha - \beta; \gamma) \delta(\beta) = \frac{1}{2\pi} \left[ \Theta(\alpha - \pi; \gamma) + \Theta(\alpha + \pi; \gamma) \right]$$

$$\Delta E(\alpha^{(h)}) = \lim_{L \to \infty} \left( E^{(1)}(\alpha^{(h)}) - E^{(0)} \right) = -\sinh \gamma \int_{-\pi}^{\pi} d\alpha \Theta''(\alpha; \gamma/2) \delta(\alpha)$$

$$+ 2 \sinh \gamma \left( \Theta'(\alpha^{(h)}; \gamma/2) - \Theta'(\pi; \gamma/2) \right) \quad (13)$$

It is straightforward to solve (12) by Fourier transform. It is actually better to reduce it to an equation for $\delta'(\alpha)$ by differentiating and then using $\delta(\pi) = \delta(-\pi)$ which follows from (12) itself. $\delta'(\alpha)$ is substituted after (13) has been integrated by parts. The result is

$$\Delta E(\alpha^{(h)}) = \epsilon(\alpha^{(h)}) - \epsilon(\pi) \quad 0 < \alpha^{(h)} < \pi \quad (14)$$
\[ \epsilon(\alpha) = 2 \sinh \gamma \sum_{n=-\infty}^{\infty} \frac{e^{-in\alpha}}{2 \cosh \gamma n} = 2 \sinh \gamma \frac{K(k)}{\pi} \text{dn} \left( \frac{K(k)\alpha}{\pi}; k \right) \]

\[ \frac{K'(k)}{K(k)} = \frac{\gamma}{\pi} \]

where \( K(K') \) is the real (imaginary) quarter period and \( k \) the modulus of the elliptic \( \text{dn} \) function \[7\). This shows that \( \Delta E(\alpha^{(h)}) > 0 \) and it goes to 0 when \( \alpha^{(h)} \to \pi \), as claimed. Moreover, the whole band found for \( L \) odd in \( S_{\text{tot}}^z = 1/2 \) is degenerate with a twin band in the sector \( S_{\text{tot}}^z = -1/2 \). In fact, despite the boundary field, spectra in the sectors \( S_{\text{tot}}^z = S \) and \( S_{\text{tot}}^z = -S \) coincide because of the symmetry implemented by the unitary operator \( I \prod_{n=1}^{L} \sigma_n^x \), where \( I \sigma_n I = \sigma_{L+1-n} \).

Excitations of the XXZ chain are sometimes called spinons. When \( L \) is even they appear in even number \[13,19\], hence they are assigned a spin \( S_{\text{tot}}^z = 1/2 \). Eq.(14) shows that, when \( L \) is odd, the ground state sector must contain one spinon which can be in a whole band of dynamical states with varying energy. Such states cannot be labelled by a linear momentum because \[8\] is not translationally invariant.

The case \( L \) even is known. In the sector \( S_{\text{tot}}^z = 1 \) there are \( \frac{L}{2} \) - 1 rapidities; this, from \[10\], implies \( \frac{L}{2} + 1 \) vacancies for \( \frac{L}{2} - 1 \) integers, hence two holes leading to

\[ \Delta E(\alpha^{(h,1)}, \alpha^{(h,2)}) = \epsilon(\alpha^{(h,1)}) + \epsilon(\alpha^{(h,2)}) \quad 0 < \alpha^{(h,1)} < \alpha^{(h,2)} < \pi \]

This coincides with the well know result for the periodic XXZ chain, the only difference being that now hole rapidities lie in the restricted range \((0, \pi)\). At \( \cosh \gamma = \frac{3}{2} \) the gap is of course \( 2\epsilon(\pi) \simeq 0.1731788 \[8\].

Other quantities have a different limit for \( L \) odd or even, one example being the surface energy \( e^{(s)} \), defined by

\[ E^{(0)}(L) = e_0 L + e^{(s)} + o(1) \quad L \to \infty \]

For \( L \) even it has been calculated in \[18\] through an analysis of finite size corrections. Since the XXZ periodic chain has the same

\[ e_0 = \frac{\cosh \gamma}{2} - \sinh \gamma (1 + 4 \sum_{n=1}^{+\infty} \frac{1}{1 + e^{2n\gamma}}) \]

but no surface energy, \( e^{(s)} \) can also be found from

\[ 2E^{(0)}(L) - E^{(0,p)}(2L) = 2e^{(s)} + o(1) \quad L \to \infty \]

where the label “p” stands for periodic boundary conditions. This is an order 1 calculation which bypasses the intricacies of finite size calculations. For the periodic chain of length \( 2L \), the ground state has \( n = L \) \[14,19\]

\[ Z_{2L}^{(0,p)}(\alpha) = \frac{1}{\pi} \Theta(\alpha; \gamma) - \frac{1}{2\pi L} \sum_{k=1}^{L} \Theta(\alpha - \alpha_k; \gamma) \]

\[ Z_{2L}^{(0,p)}(\alpha_j) = \frac{I_j}{L} \]

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Consider, when $L$ is odd, the lowest-lying state in the previously discussed band of the open spin chain. Its \((L - 1)/2\) rapidities, which become exactly $L$ after reflection, will now be denoted \(\{\alpha'_j\}_{j=-(L-1)/2}^{(L-1)/2}\), whereas \(\{\alpha_j\}_{j=-(L-1)/2}^{(L-1)/2}\) will be the $L$ symmetrically distributed ground state rapidities of the periodic chain of length $2L$. Hence

\[
Z_L^{(0)}(\alpha'_j) = Z_{2L}^{(0,p)}(\alpha_j) = \frac{j}{L}, \quad -\frac{L-1}{2} \leq j \leq \frac{L-1}{2}
\]

The relevant equations in the thermodynamic limit are now

\[
\delta(\alpha) + \frac{1}{2\pi} \int_{-\pi}^{\pi} d\beta \Theta'(\alpha - \beta; \gamma)\delta(\beta) = -\frac{1}{2\pi} \left[ \Theta(\alpha; \gamma) + \Theta(2\alpha; \gamma) \right]
\]

\[
2e^{(s)} = -\cosh \gamma + 2 \sinh \gamma \Theta'(0; \gamma/2) - 2 \sinh \gamma \int_{-\pi}^{\pi} d\alpha \Theta''(\alpha; \gamma/2)\delta(\alpha)
\]

for the backflow $\delta(\alpha) = \lim_{L \to \infty} \frac{\delta \alpha_j}{\Delta \alpha_j}$ (as before $\delta \alpha_j = \alpha'_j - \alpha_j$, $\Delta \alpha_j = \alpha_{j+1} - \alpha_j$). The upshot is

\[
e^{(s, odd)} = -\frac{\cosh \gamma}{2} + \sinh \gamma \left( 1 + 2 \sum_{k=1}^{+\infty} \frac{2 - e^{-2k\gamma}}{\cosh 2k\gamma} - \sum_{k=0}^{-\infty} \frac{2}{\cosh(2k + 1)\gamma} \right)
\]

For $L$ even, the calculation is slightly more involved, because now the numbers $I_j$ are half-odd for the periodic chain of length $2L$, yet it can be carried out along the same lines, leading to

\[
e^{(s, even)} = -\frac{\cosh \gamma}{2} + \sinh \gamma \sum_{k=1}^{+\infty} \frac{1 - e^{-2k\gamma}}{\cosh 2k\gamma}
\]

A similar method was used in [21] for general boundary fields but, again, for $L$ even only. When $\cosh \gamma = 3/2$, the biquadratic chain surface energy is, from [3], $e^{(s)}_{bQ} = e^{(s)} + 7/4$, or

\[
e^{(s, odd)}_{bQ} \simeq 1.7415986 \quad e^{(s, even)}_{bQ} \simeq 1.6550092
\]

The second value coincides with that in [18].

I have checked numerically, for small chains of odd length, that: 1. eq. (6) admit a solution for any value of $I^{(h)}$ within the allowed range; 2. the corresponding energies show up in the spectrum of (3), as found by direct diagonalization, and $I^{(h)} = \frac{L+1}{2}$ yields the ground state energy; 3. the same eigenvalues show up in the spectrum of (2), also obtained by direct diagonalization. The last check was carried out in [3] too (perhaps only for $L$ even).

Actually, the eigenvalue problem of (2) has a direct BA solution that does not rely on the mapping (4,5) [20], but the relevant BA equations do not seem to have been studied in detail. This would provide a further check. Finally, it should be pointed out that, very recently, peculiarities of $L$ odd have been noticed also for the periodic $XXZ$ chain in the critical regime [22].
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