INTEGRABLE SU(2)-INVARIANT SPIN CHAINS AND THE HALDANE CONJECTURE

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ABSTRACT
We perform a systematic exact algebraic search for integrable spin-$S$ chains which are isotropic in spin space, i.e. are $su(2)$-invariant. The families of spin chains found for $S \leq 13.5$ support recent arguments in favour of the complete classification of all such integrable chains. The integrable families of spin chains are discussed in the light of the conjectured spin-dependent properties of the Heisenberg chain.

1. Introduction
We are all familiar with the great interest of Green and Hurst in exact solutions. As emphasized in their beautiful book, such solutions “have an intrinsic interest quite apart from the illumination they impart to physical problems”. Indeed, the study of exactly solved models has since evolved into one of the key areas of mathematical physics, with the original physical motivations left far behind in the wake. In this paper, we also follow the original spirit of Green and Hurst and pay attention to a particular physical phenomena. In particular, we address the question of whether or not exactly solved models have a bearing on the so-called Haldane conjecture. This involves a surprise from quantum mechanics in one dimensional systems.

Haldane argued that the properties of the Heisenberg antiferromagnet

$$\mathcal{H} = \sum_{j=1}^{N} S_j \cdot S_{j+1}$$

(1)

should differ substantially if the spin $S$ is integer or half-odd integer. For integer spin, there is a gap towards spin excitations, whereas for half-odd integer spin, the model is massless with no gap. Of course, for $S = \frac{1}{2}$ the model was solved long ago via the Bethe Ansatz, and subsequent investigations revealed that the $S = \frac{1}{2}$ model is indeed massless. Evidence for the Haldane conjecture has been obtained mainly for $S = 1$ via explicit numerical computations where the gap is of magnitude 0.41049(2) and ingenious experiments on related compounds, in particular with NENP.

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In this paper we take up the systematic search for integrable isotropic spin-$S$ chains with nearest-neighbour interaction. Here our notion of an integrable Hamiltonian is one associated with an $R$-matrix satisfying the Yang-Baxter equation. There are of course very interesting spin chains which fall outside this notion of integrability, such as the $S = 1$ Hamiltonian

$$ \mathcal{H} = \sum_{j=1}^{N} S_j \cdot S_{j+1} + \frac{1}{3} (S_j \cdot S_{j+1})^2, \quad (2) $$

which possesses an exact valence bond groundstate and a gap, thus fulfilling the Haldane scenario. On the other hand, there are three known integrable $S = 1$ chains. However, two of these chains have no gap. They are

$$ \mathcal{H} = \sum_{j=1}^{N} S_j \cdot S_{j+1} + (S_j \cdot S_{j+1})^2, \quad (3) $$
discussed first by Uimin, and

$$ \mathcal{H} = \sum_{j=1}^{N} S_j \cdot S_{j+1} - (S_j \cdot S_{j+1})^2, \quad (4) $$

which originates from the work of Kulish and Sklyanin. The remaining chain,

$$ \mathcal{H} = - \sum_{j=1}^{N} (S_j \cdot S_{j+1})^2, \quad (5) $$
does possess a gap, of magnitude $0.173178 \ldots$ This is the biquadratic chain, discussed by a number of authors.

The natural question arises, are there any other integrable $S = 1$ chains of this type? And more generally, what is known for arbitrary $S$? In a recent paper Kennedy initiated a systematic search for such integrable $su(2)$-invariant chains. A numerical search for solutions of the Yang-Baxter equation for $S \leq 6$ revealed four spin-$S$ families of integrable chains along with an additional integrable chain at $S = 3$. More recently, we identified these $su(2)$-invariant chains with known $G$-invariant $R$-matrices, where $G$ is a simple Lie algebra, and gave arguments that Kennedy’s results may well constitute the complete classification of such integrable chains. These results are briefly reviewed in the next section. In section 3 we extend Kennedy’s search to $S \leq 13.5$ by means of exact algebraic computation, thus avoiding the possibility of missing any solutions due to roundoff error. To conclude we discuss the integrable families of spin chains in the light of the Haldane conjecture.
2. List of $su(2)$-invariant $R$-matrices

Integrable spin chains follow from the “Master Key to Integrability” – the Yang-Baxter equation – which we write in the form (for reviews, see, e.g. [10, 18, 19])

$$
(\hat{R}(\lambda) \otimes 1) \left( 1 \otimes \hat{R}(\lambda + \mu) \right) \left( \hat{R}(\mu) \otimes 1 \right) = \left( 1 \otimes \hat{R}(\lambda + \mu) \right) \left( \hat{R}(\mu) \otimes 1 \right),
$$

with $\hat{R}(0) = 1$. Given a solution $\hat{R}(\lambda)$, the Hamiltonian $H$ follows via the expansion

$$
\hat{R}(\lambda) = 1 + \lambda H + \sum_{n=2}^{\infty} \lambda^n \hat{R}^{(n)}.
$$

It is thus clear that the search for $su(2)$-invariant Hamiltonians is equivalent to the search for $su(2)$-invariant $R$-matrices.

Let $\mathcal{G}$ be a simple Lie algebra of rank $n$ with fundamental weights denoted by $\Lambda_1, \ldots, \Lambda_n$. Furthermore, let $\pi_\Lambda$ be an irreducible representation (irrep) of $\mathcal{G}$ with highest weight $\Lambda$ on the vector space $V_\Lambda$. Then the $R$-matrix $\hat{R}^{\Lambda,\Lambda}(u) \in \text{End}(V_\Lambda \otimes V_\Lambda)$ is said to be $\mathcal{G}$-invariant if

$$
[ \hat{R}^{\Lambda,\Lambda}(u), \pi_\Lambda(\mathcal{G}) \otimes 1 + 1 \otimes \pi_\Lambda(\mathcal{G}) ] = 0.
$$

For a given pair $(\mathcal{G}, \Lambda)$ the imposition of such a condition sometimes (but not always) allows the Yang-Baxter equation for $\hat{R}^{\Lambda,\Lambda}(u)$ to be solved. In particular, for any $\mathcal{G}$ (except $E_8$) and $\Lambda$ corresponding to the lowest dimensional irreps the solutions are known explicitly.

Such a $\mathcal{G}$-invariant $R$-matrix turns out also to be $su(2)$-invariant with spin $S$ if the space $V_\Lambda$ can be identified with a space $V_{2S\Lambda_1}$ on which $su(2)$ is represented irreducibly. We were unable to give a complete classification of all pairs $(\mathcal{G}, \Lambda)$ such that this condition holds. However, an examination of the tables of branching rules for simple Lie algebras revealed only the solutions:

(i) $(A_n = su(n+1), \Lambda_1)$ for $n \geq 1$,

(ii) $(B_n = so(2n+1), \Lambda_1)$ for $n \geq 3$,

(iii) $(C_n = sp(2n), \Lambda_1)$ for $n \geq 2$, and

(iv) $(G_2, \Lambda_2, \Lambda_2)$.

In particular, we note that the $R$-matrices associated with the fundamental representations of $D_n$, $E_6$, $E_7$ and $F_4$ are not $su(2)$-invariant.

We will now list the known $su(2)$-invariant $R$-matrices. In addition to the spin $S$, we need extra labels $\{I, IIa, IIb, III, IV\}$ to distinguish between different families. In spectral form ($P^{(i)}$ are projection operators onto $su(2)$-irreps in $V_{2S\Lambda_1} \otimes V_{2S\Lambda_1}$), they are given by

$$
\hat{R}^{2S\Lambda_1,2S\Lambda_1}_I(u) = (1-u) \sum_{i \text{ even}} P^{(i)} + (1+u) \sum_{i \text{ odd}} P^{(i)}.
$$

(9)
In order to lend further weight to the above list of integrable systems, we follow Kennedy and hence integrable solutions of the Yang-Baxter equation. Our interest lies in quantum chains with Hamiltonians of the form

\[ H = \sum_{j=1}^{N} H_{j,j+1} \]  

where

\[ \tilde{R}_{IIa}^{2S\Lambda_1,2S\Lambda_1}(u) = \left( 1 - u \right) \left( 1 - \left( S - \frac{1}{2} \right) u \right) P^{(0)} + \left( 1 + u \right) \left( 1 - \left( S + \frac{1}{2} \right) u \right) \sum_{i \text{ odd}} P^{(i)} + \left( 1 + u \right) \left( 1 + \left( S - \frac{1}{2} \right) u \right) \sum_{i \text{ even} \neq 0} P^{(i)} \quad (S \text{ integer}) \] 

and

\[ \tilde{R}_{IIb}^{2S\Lambda_1,2S\Lambda_1}(u) = \left( 1 - u \right) \left( 1 + \left( S + \frac{1}{2} \right) u \right) P^{(0)} + \left( 1 + u \right) \left( 1 + \left( S + \frac{1}{2} \right) u \right) \sum_{i \text{ odd}} P^{(i)} + \left( 1 + u \right) \left( 1 - \left( S + \frac{1}{2} \right) u \right) \sum_{i \text{ even} \neq 0} P^{(i)} \quad (S \text{ half odd integer}) \] 

Further, we have

\[ \tilde{R}_{III}^{2S\Lambda_1,2S\Lambda_1}(u) = \sum_{k=0}^{2S} \left( \prod_{j=1}^{k} (j-u) \prod_{j=k+1}^{2S} (j+u) \right) \]  

\[ \tilde{R}_{IV}^{2S\Lambda_1,2S\Lambda_1}(u) = 1 + \frac{a - ae^{u}}{e^{u} - a^{2}} (2S + 1) P^{(0)}; \quad a + \frac{1}{a} = 2S + 1 \quad (S \geq 1). \] 

The results are found to be

\[ \tilde{R}_{IIa}^{2S\Lambda_1,2S\Lambda_1} [su(2)] = \tilde{R}_{IIa}^{2S\Lambda_1,2S\Lambda_1} [su(2S + 1)] \quad (S \text{ half integer}), \]

\[ \tilde{R}_{IIb}^{2S\Lambda_1,2S\Lambda_1} [su(2)] = \tilde{R}_{IIb}^{2S\Lambda_1,2S\Lambda_1} [so(2S + 1)] \quad (S \text{ integer}), \]

\[ \tilde{R}_{III}^{2S\Lambda_1,2S\Lambda_1} [su(2)] = \tilde{R}_{III}^{2S\Lambda_1,2S\Lambda_1} [sp(2S + 1)] \quad (S \text{ half odd integer}), \]

\[ \tilde{R}_{IV}^{2S\Lambda_1,2S\Lambda_1} [su(2)] = \tilde{R}_{IV}^{2S\Lambda_1,2S\Lambda_1} [G_{2}] \quad (S = 3). \]

The above R-matrices \( \tilde{R}_{IIa}^{2S\Lambda_1,2S\Lambda_1} [su(2)] \) correspond to the trivial embedding of \( A_{1} \) in itself and are thus already in the “proper” Lie algebraic setting. The remaining solution, \( \tilde{R}_{IV}^{2S\Lambda_1,2S\Lambda_1} [su(2)] \), is not rational in \( u \), unlike the others under consideration, and is in a class of its own – being related to the Temperley-Lieb algebra.

### 3. Systematic Exact Search

In order to lend further weight to the above list of \( su(2) \)-invariant R-matrices and hence integrable \( su(2) \)-invariant spin chains being complete, we turn now to an exact systematic search of solutions of the Yang-Baxter equation following Kennedy. Our interest lies in quantum chains with Hamiltonians

\[ H = \sum_{j=1}^{N} H_{j,j+1} \]
such that $H_{j,j+1}$ is a copy of $H$ acting on sites $j$ and $j+1$, which in turn is $su(2)$-invariant. As in the above, we restrict our attention to models for which the spin $S$ at each site is the same.

The condition of $su(2)$-invariance implies that $H$ can be written as a linear combination of the $su(2)$-projectors $P^{(j)}$ for $j = 0, \ldots, 2S$. As we are interested in the Hamiltonian only up to constants (and since $1 = \sum_{j=0}^{2S} P^{(j)}$ is the resolution of the identity), it is sufficient to set

$$H = \sum_{j=0}^{2S-1} c_j P^{(j)},$$

where the coefficients $c_j$ are to be determined. The projectors can be explicitly constructed from the matrix representatives of the Casimir operator. For large $S$, it is more efficient to construct them from Clebsch-Gordan coefficients.

Given the expansion (16), a necessary condition for $\tilde{R}(\lambda)$ to satisfy the Yang-Baxter equation (6) is Reshetikhin’s condition

$$[H \otimes 1 + 1 \otimes H, [H \otimes 1, 1 \otimes H]] = 1 \otimes X - X \otimes 1,$$

for some operator $X$. Following Kennedy, we can simplify this condition further for $su(2)$-invariant chains by taking the matrix elements $\langle S, j, k | \cdot \cdot \cdot | j + k - S, S, S \rangle$ ($k < S$ and $j + k \geq 0$), which results in the right hand side vanishing and hence $X$ drops out of consideration. We note that this simplified Reshetikhin condition is necessary but not sufficient for the Reshetikhin condition to hold, which itself is necessary but (possibly) not sufficient for the YBE to hold.

When the simplified Reshetikhin condition is expanded out, we obtain

$$\langle S, j, k | (1 \otimes H)(H^2 \otimes 1) - 2(H \otimes 1)(1 \otimes H)(H \otimes 1) - \cdots | j + k - S, S, S \rangle = 0,$$

for $k < S$ and $j + k \geq 0$. This can be evaluated in terms of the matrix elements of $H$ which in turn are given by the known projector matrix elements and the unknown constants $c_j$. Reshetikhin’s condition (simplified) then reduces to a system of homogeneous cubic equations in the $c_k$’s, which can be solved recursively. At each step of the recursion only a quadratic equation needs to be solved.

We have solved this system of equations algebraically using Mathematica for $S \leq 13.5$, which is a significant extension of the numerical calculations performed for $S \leq 6$. We have confirmed that no new solutions appear. The only integrable $su(2)$-invariant spin chains we see for $S \leq 13.5$ are those following from the $R$-matrices listed in (9)-(14).

### 4. List of $su(2)$-invariant Spin Chains

The families of integrable spin chains under discussion are all of the form (15), (16). The first family has two-body interactions

$$H_1 = \mathcal{P},$$

and

$$H_2 = \mathcal{P},$$

where $\mathcal{P}$ is a projector.
where $\mathcal{P} = (-)^{2S} \sum_{i=0}^{2S} P^{(i)}$ is the permutation or exchange operator. The second family can be written in the combined form

$$H_{\text{II}} = \left[ S + \frac{1}{2} - (-)^{2S} \right] \mathcal{P} - (-)^{2S} (2S + 1) P^{(0)}.$$  

(20)

For the third family,

$$H_{\text{III}} = \sum_{k=0}^{2S} \left( \sum_{j=1}^{k} \frac{1}{j} \right) P^{(k)}.$$  

(21)

The Temperley-Lieb family is simply

$$H_{\text{IV}} = P^{(0)}.$$  

(22)

The $S = 3$ $G_2$ chain has Hamiltonian

$$H_{\text{V}} = 11 P^{(0)} + 7 P^{(1)} - 17 P^{(2)} - 11 P^{(3)} - 17 P^{(4)} + 7 P^{(5)} - 17 P^{(6)}.$$  

(23)

All of the above expressions follow from the $su(2)$-invariant $R$-matrices of the preceding section up to overall multiplicative and additive factors. They can all be alternatively written, subject to the same caveat, in terms of the more familiar spin operators $X_j = S_j \cdot S_{j+1}$ via

$$P^{(i)} = \prod_{k=0}^{2S} \frac{X_j - x_k}{x_i - x_k},$$  

(24)

where $x_k = \frac{1}{2} k(k + 1) - S(S + 1)$. In this way we see, for example, for $S = 1$, $H_{\text{I}}$ reduces to the Hamiltonian (3), while $H_{\text{II}}$ and $H_{\text{III}}$ reduce to (4) and $H_{\text{IV}}$ reduces to (5).

5. Concluding Remarks

We first remark that there are no other integrable $su(2)$-invariant $S = 1$ chains beyond the three mentioned in the Introduction. Apart from the fifth solution at $S = 3$, there are four integrable spin chains for each value of $S$ when $S > 1$. We believe that this latter statement holds for arbitrary $S$.

Among the integrable $su(2)$-invariant spin chains we do not see the Heisenberg chain (1). One may harbour a faint hope that it may appear for some high value of $S$ by some miraculous vanishing of coefficients in one of the integrable families. However, we have not seen this to be the case for $S$ up to 100. Thus it appears most unlikely that, apart from the $S = \frac{1}{2}$ case, an integrable spin chain can yield either an exact confirmation or counterexample to the Haldane conjecture. Nevertheless, it is still of interest to investigate the properties of the integrable chains in light of the conjectured properties of the Heisenberg chain.

Among the integrable families of spin chains, the Temperley-Lieb chains appear to be the only ones with a gap. This gap is known exactly and opens up with
Integrable $su(2)$-invariant spin chains

Increasing $S \geq 1$. However, the gap exists for all $S \geq 1$. So in this case we see no dramatically different behaviour depending on whether $S$ is integer or half-odd integer. The remaining families of spin chains all appear to be critical for all $S$, with no gap. Nevertheless, there does appear to be an integer vs half-odd integer distinction in the Hamiltonian (20) arising from family II. Recall that this chain is associated with $so(2S + 1)$ for $S$ integer, and with $sp(2S + 1)$ for $S$ half-odd integer. For critical models, it is now both rather well understood and confirmed for a number of cases that the central charge defining the underlying universality class is given by

$$c = \frac{mD}{m + h}, \quad (25)$$

where $D = \dim \mathcal{G}$, $h$ is the Coxeter number and $m$ is the level of the representation. Thus for $\mathcal{G} = B_n = so(2n + 1)$, where $D = n(2n + 1)$, $h = 2n - 1$, $m = 1$ and $n = S$, we expect the value $c = S + \frac{1}{2}$. On the other hand, for $\mathcal{G} = C_n = sp(2n + 1)$, where $D = n(2n + 1)$, $h = n + 1$, $m = 1$ and $2n = 2S + 1$, we expect the value $c = (2S + 1)(2S + 2)/(2S + 5)$. Work to confirm these values is currently in progress. In particular, for the $so(2S+1)$ family, the Bethe Ansatz roots defining the groundstate form a sea of 2-strings in the complex plane for all $S \geq 1$, thus allowing a direct application of a recently developed method for deriving the central charge for such cases via the dominant finite-size correction to the groundstate energy.

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