Exact Results of Dimerization Order Parameter in
$SU(n)$ Antiferromagnetic Chains

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Abstract: After a proper definition of the dimerization order parameter for a spin-$S$ system, I show that this order parameter in the $SU(n)$ ($n = 2S + 1$) antiferromagnetic chains (or equivalently the $SU(2)$ spin-$S$ chains with Hamiltonians which project out singlet states) is, in the thermodynamic limit, directly proportional to the staggered-magnetization in the corresponding spin-$\frac{1}{2}$ $XXZ$ chains which had already been mapped onto the $SU(n)$ chains.

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The spin-1 antiferromagnetic chain with the pure biquadratic exchange has the Hamiltonian
\[
H = - \sum_i (S_i \cdot S_{i+1})^2,
\] (1)
where the summation over \(i\) runs over all spins with either free ends or the usual periodic boundary condition. Parkinson [1] first discussed the possibility of a mapping of Eq. (1) onto the spin-\(\frac{1}{2}\) XXZ chain with the anisotropy \(\Delta = \frac{3}{2}\), which is in general, apart from a constant, described by the Hamiltonian
\[
H = - \sum_i H_{i,i+1}^{xxz}, \quad H_{i,i+1}^{xxz} \equiv \frac{1}{2}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + \frac{1}{2}\Delta(1 - \sigma_i^z \sigma_{i+1}^z),
\] (2)
where \(\sigma^\alpha (\alpha = x, y, z)\) are Pauli matrices and \(\Delta\) is the anisotropy parameter. Barber and Batchelor [2] later have shown that the Hamiltonian of Eq. (1) with free ends is indeed exactly equivalent to the 9-state quantum Potts chain. They then obtained the ground-state energy and the excitation gap by the mapping of the Potts chain onto the spin-\(\frac{1}{2}\) chains of Eq. (2) with \(\Delta = \frac{3}{2}\), and with fields \(\pm \frac{1}{4}\sqrt{5}\) applied to the two ends respectively. Klümper [3] obtained independently these exact results, and he also presented results for the correlation length.

Based on these exact results, Klümper [3] and Affleck [4] showed that the ground state and low-lying excited states of a series of \(SU(n)\) (with \(n = 2S + 1\)) antiferromagnetic chains can all be similarly obtained. In particular, Affleck [4] showed that the \(SU(n)\) chains with free ends can be mapped, in a similar fashion, onto the corresponding spin-\(\frac{1}{2}\) XXZ chains of Eq. (2). The generic Hamiltonian of these \(SU(n)\) chains with free ends are given by
\[
H = - \sum_{i=1}^{N-1} P_{i,i+1}^0(S),
\] (3)
where \(N\) is the number of spins in the chain, and \(P_{i,j}^J(S)\) is the projection operator which projects out the state with total spin \(J\) of the pair \(S_i\) and \(S_j\) with \((S_i + S_j)^2 = J(J+1)\). For \(S = \frac{1}{2}\), Eq. (3) reduces to the usual Heisenberg model plus a constant, whereas for
$S = 1$, Eq. (3) is equivalent to the pure biquadratic chain given by Eq. (1) with free ends because $P_{i,i+1}^0 = [(S_i \cdot S_{i+1})^2 - 1]/3$. For $S = \frac{3}{2}$, Eq. (3) becomes,

$$H = \frac{1}{1152} \sum_{i=1}^{N-1} [60(S_i \cdot S_{i+1})^3 + 80(S_i \cdot S_{i+1})^2 - 372S_i \cdot S_{i+1} - 297].$$

(4)

We note that this form of the Hamiltonian is quite similar to that of the spin-$\frac{3}{2}$ chain proposed by Babujian [5], which is fully integrable by Bethe’s ansatz. The mapping of Eq. (3) for a general $n = 2S + 1$ onto the spin-$\frac{1}{2}$ chains of Eq. (2) is given by the relation, $n = 2\Delta$. In this paper, I shall use the free-end boundary condition as in Ref. [2] and [4], and with even total number of spins $N$ in the $N \to \infty$ limit. The final results are independent of the boundary condition in the thermodynamic limit.

Although the exact values of the ground-state energy and excitation gap have been obtained for the Hamiltonians of Eqs. (1) and (3) for a general $n$ by the mapping onto the spin-$\frac{1}{2}$ $XXZ$ chains of Eq. (2) which was exactly solved by Bethe’s ansatz, and although people are convinced [2,4] that the systems described by Eq. (3) are dimerized for any $n > 2$, it does not seem possible to calculate directly the dimerization order parameter [6] which is usually defined in the thermodynamic limit, by

$$D \equiv \langle (S_{i-1} \cdot S_i - S_i \cdot S_{i+1}) \rangle,$$

(5)

where the angular brackets denote a ground-state expectation. We note that the absolute value of $D$ is independent of $i$ in the thermodynamic limit (but $i$ should be far away from boundaries since the free-end boundary condition is used here).

In the course of studying spin-lattice dimerization and trimerization problems [7], I have come to realize that there is another effective, perhaps more proper, definition of the dimerization order parameter for a general spin-$S$ system. This new order parameter, which was given by the ground-state expectation of a square matrix with dimension given by the number of states for a two-atom spin-$S$ system [7], can in fact be equivalently expressed as the ground-state expectation of the projection operator $P_{i,j}^0$ of Eq. (3) as,

$$D(n) \equiv \langle (P_{i-1,i}^0(S) - P_{i,i+1}^0(S)) \rangle, \quad n = 2S + 1.$$

(6)
For $S = \frac{1}{2}$, this definition of order parameter is identical to the usual definition of Eq. (5), but it is certainly different from Eq. (5) for any $S > \frac{1}{2}$, though it is obvious that both definitions can effectively measure the order of dimerization. It is clear that the key difference between the definitions of Eqs. (5) and (6) lies in the fact that operator $S_i \cdot S_{i+1}$ of Eq. (5) has in principle a projection of all states with a $J$ value of the paired spins with $(S_i + S_{i+1})^2 = J(J+1)$, unlike $P_{ii+1}^0$ of Eq. (6), which projects out only the singlet state of the pair.

Both Eqs. (5) and (6) for the definition of dimerization order parameter are still meaningful for systems with the periodic boundary condition. However, some care should be taken since a dimerized system has two degenerate ground states and the expectation with respect to an equal admixture of them will yield zero result in Eqs. (5) and (6). With the free-end boundary condition, one has the advantage of a non-degenerate ground state.

To see how one comes to the definition of Eq. (6), we consider the case of perfect dimerization for a spin-$S$ chain. It is convenient to discuss dimerized states in the valence-bond basis. Spin operators can be usefully written in terms of two pairs of Schwinger bosons as,

$$S^+ = a^+ b, \quad S^- = ab^+, \quad S^z = \frac{1}{2}(a^+ a - b^+ b),$$

(7)

where $a, a^+$ and $b, b^+$ obey the usual boson commutation relations. In this representation, a spin-$S$ state with $S^z = m$ ($-S \leq m \leq S$) is written as

$$|m\rangle = \frac{(a^+)^{S+m}}{\sqrt{(S+m)!}} \frac{(b^+)^{S-m}}{\sqrt{(S-m)!}} |0\rangle,$$

(8)

where $|0\rangle$ is the vacuum state of the bosons. A valence bond is simply a spin-singlet configuration, which can be written by the so called valence bond operator $C^+_{ij}$, defined by

$$C^+_{ij} \equiv a^+_i b^+_j - a^+_j b^+_i.$$

(9)
For example, the singlet state of two-atom spin-$\frac{1}{2}$ system is given by a single valence-bond configuration,

$$|\Phi_1\rangle = C_{ij}^+|0\rangle = |\frac{1}{2},-\frac{1}{2}\rangle - |\frac{1}{2},\frac{1}{2}\rangle;$$  \hspace{1cm} (10)

for $S = 1$, this singlet state is given by a two-bond configuration,

$$|\Phi_2\rangle = (C_{ij}^+)^2|0\rangle = 2(|1,-1\rangle + |−1,1\rangle − |0,0\rangle).$$  \hspace{1cm} (11)

Generally, the singlet ground state of a two-atom system, each with spin $S$, is given by a $2S$-bond configuration as

$$|\Phi_{2S}\rangle = (C_{ij}^+)^{2S}|0\rangle.$$  \hspace{1cm} (12)

The perfect dimerization state, $|D\rangle$, of the spin-$S$ chain can then be written as

$$|D\rangle = \left(\frac{1}{n((n−1)!)^2}\right)^{N/2} \prod_{i=1}^{N/2} (C_{2i-1,2i}^+)^{n-1}|0\rangle, \hspace{1cm} n = 2S + 1,$$

where I have included the normalization factor. It is clear that if the periodic boundary condition is used, the dimerization state of Eq. (13) will be doubly degenerate, as mentioned earlier. But as we are using the free-end boundary condition here, $|D\rangle$ of Eq. (13) is the only choice for the perfect dimer state. The basic algebras in the $SU(n)$ chain of Eq. (3) are given by the following two operations,

$$P_{ij}^0(S) (C_{ij}^+)^{2S}|0\rangle = (C_{ij}^+)^{2S}|0\rangle;$$  \hspace{1cm} (14)

and

$$P_{ij}^0(S) (C_{k,l}^+)^{2S} (C_{j,l}^+)^{2S}|0\rangle = \frac{1}{n} (C_{ij}^+)^{2S} (C_{ik}^+)^{2S}|0\rangle,$$

where the four indices $k, i, j, l$ are all different from one another and, as before, $n = 2S + 1$. From these two equations, one can in fact prove that the operator, $n \cdot P_{i_{i+1}}^0(S)$, obeys the Temperley-Lieb algebra [8], which is the key to the mapping of Eq. (3) onto the spin-$\frac{1}{2}$ $XXZ$ chain of Eq. (2) with the free-end boundary condition [2,4], by considering all possible valence-bond configurations of the type of Eq. (12) involving
four consecutive atoms. Affleck [4] has provided another more elegant proof by using
the fermion representation.

One can also define a normalized version of Eq. (6) as

\[ D'(n) \equiv \frac{1}{D_0} \langle (P^0_{i-1,i}(S) - P^0_{i,i+1}(S)) \rangle, \quad n = 2S + 1, \tag{16} \]

where \( D_0 \) is the expectation value of \((P^0_{i-1,i}(S) - P^0_{i,i+1}(S))\) with respect to the perfect
dimerized state \( |D\rangle \) of Eq. (13). Using Eqs. (13)-(15), it is a straightforward calculation
to obtain this expectation value as \( D_0 = 1 - 1/n^2 \).

Since operator \( n \ast P^0_{i,i+1}(S) \) obeys the Temperley-Lieb algebra [2,4], one can write

\[ P^0_{i,i+1} \to \frac{1}{n} [H^{xxz}_{i,i+1} + \frac{1}{2} \sinh \theta (\sigma^z_{i+1} - \sigma^z_i)], \tag{17} \]

where \( \sigma^\alpha (\alpha = x, y, z) \) are Pauli matrices and \( H^{xxz}_{i,i+1} \) is given by Eq. (2) with \( \Delta = \cosh \theta = \frac{n}{2} \). Using this transformation, one can straightforwardly calculate the order
parameter \( D'(n) \) of Eq. (16) by using the mappings of the exact ground-state of Eq. (3)
o nto that of the corresponding spin-\( \frac{1}{2} \) chains of Eq. (2). One thus obtains

\[ D'(n) = \frac{n}{n^2 - 1} \sqrt{n^2 - 4 \langle \sigma^z_i \rangle}, \tag{18} \]

where the expectation is with respect to the ground-state of the spin-\( \frac{1}{2} \) XXZ chain
of Eq. (2) with the anisotropy \( \Delta = n/2 \), and where I have used the fact that, in the
thermodynamic limit, one has

\[ \langle H^{xxz}_{i-1,i} \rangle = \langle H^{xxz}_{i,i+1} \rangle, \quad \text{and} \quad \langle \sigma^z_{i-1} \rangle = \langle \sigma^z_{i+1} \rangle = -\langle \sigma^z_i \rangle, \tag{19} \]

in the same expectation. Eq. (19) simply reflects the well-known fact that the infinite
spin-\( \frac{1}{2} \) XXZ chain has no dimerization long-range order but a staggered magnetization
order. Fortunately, this staggered magnetization had already been exactly calculated
by Baxter [9] twenty years ago as a function of the anisotropy,

\[ \sqrt{\langle \sigma^z_i \rangle} = 1 + 2 \sum_{n=1}^{\infty} (-1)^n \exp(-2n^2\theta) \]

\[ = \sqrt{\frac{2\pi}{\theta}} \sum_{n=1}^{\infty} \exp[\frac{-(n - 1/2)^2 \pi^2}{2\theta}], \tag{20} \]
where two expressions are equivalent, the first being rapidly convergent at large $\theta$ while the second at small $\theta$. For $S = 1$ and $\frac{3}{2}$, $\langle \sigma_i^z \rangle \approx 0.5028$ and $0.7335$ respectively to the accuracy of four significant figures. Therefore, one has $D'(3) \approx 0.4216$ and $D'(4) \approx 0.6776$ to the same accuracy of four significant figures for the corresponding $SU(3)$ and $SU(4)$ chains of Eq. (3) respectively. One sees also that in the limit of $S \to \infty$, $\langle \sigma_i^z \rangle = 1$ and hence $D'(\infty) = 1$ as expected.

Based on the definition of the order parameter in Eq. (6), one can define a corresponding ‘four-spin’ correlation function as $\langle (P_0^{i+1} P_0^{j+1}) \rangle$, in similar fashion to the usual definition of the four-spin correlation function, $\langle (S_i \cdot S_{i+1}) (S_j \cdot S_{j+1}) \rangle$, for the order parameter of Eq. (5). Likewise, by taking the long-range limit (i.e., $|j - i| \to \infty$) in $\langle (P_0^{i+1} P_0^{j+1}) \rangle$, one should be able to obtain the value of order parameter $D(n)$ (or $D'(n)$). This is useful if one is to carry out finite-size calculations with periodic boundary conditions.

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