Haldane Gap and Hidden Order in the $S = 2$ Antiferromagnetic Quantum Spin Chain

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We have investigated Haldane’s conjecture for the $S=2$ isotropic antiferromagnetic quantum spin chain with nearest-neighbor exchange $J$. Using a density matrix renormalization group algorithm for chains up to $L=350$ spins, we find in the thermodynamic limit a finite gap of $\Delta = 0.085(5)J$ and a finite spin-spin correlation length $\xi = 49(1)$ lattice spacings. We establish the ground state energy per bond to be $E_0 = -4.761248(1)J$. We show that the ground state has a hidden topological order that is revealed in a nonlocal string correlation function. This means that the physics of the $S=2$ chain can be captured by a valence-bond solid description. We also observe effective free spin-1 states at the ends of an open $S=2$ chain.

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Since Haldane’s conjecture\cite{1} that the physical properties of (isotropic) antiferromagnetic quantum spin chains depend crucially on whether the spin is integer or half-integer, his prediction of a ground state with a finite spin-spin correlation length and a finite gap to spin excitations for integer spins has been studied in numerous papers. Numerical methods have served to establish quantitative results where analytical work had to rely on often uncontrolled approximations.

Both the existence of a finite gap between a ground state singlet and excited states and of a finite correlation length is well established for the $S=1$ isotropic antiferromagnetic quantum spin chain\cite{2}. Recent estimates of the Haldane gap are discussing the fifth digit: $\Delta = 0.41050(2)$\cite{3} from the Density Matrix Renormalization Group (DMRG) algorithm\cite{4}, and $\Delta = 0.41049(2)$\cite{5} from extrapolation of exact diagonalization results for chains up to length $L=22$. Similarly, the correlation length is $\xi = 6.03(1)$\cite{3,6}. The spin wave velocity is then found to be $c = \Delta \xi = 2.475(5)$, to be compared to the semiclassical value $c = 2S = 2$.

In this work we have established numerical values for the respective quantities for the $S=2$ isotropic antiferromagnetic spin chain with nearest-neighbor exchange using the DMRG algorithm. We show that Haldane’s conjecture is obeyed in this case: the Haldane gap also exists for $S=2$, further supporting the case that the gap exists for all integer spins. In addition our results show that a valence-bond-solid picture\cite{7} is valid for the $S=2$ spin chain.

The investigation of the $S=2$ case is hindered by the fact that one expects $\Delta_{S=2} \ll \Delta_{S=1}$ and $\xi_{S=2} \gg \xi_{S=1}$. This belief is due to the asymptotic form $\Delta_S \approx S^2 \exp(-\pi S)$\cite{1}. One may approximatively expect $\Delta_{S=2} \approx 0.07$ and $\xi_{S=2} \approx 70$. The much larger correlation length makes finite size extrapolations feasible only for much longer chains than in the $S=1$ case; furthermore, the inherent statistical or systematical imprecisions of all numerical methods become more worrisome due to the small size of the gap. At the same time, the number of states per site rises from 3 to 5, greatly reducing the length of numerically tractable chains. At the present time, there are only a few preliminary estimates\cite{8,9} in the literature.

The DMRG algorithm allows to treat very long chains while retaining good precision for the energies and expectation values by an iterative truncation of the Hilbert space down to M basis states. For a detailed discussion of the method we refer to \cite{3,4}. In the following we have investigated chains up to a length of $L=350$, which we will find to be about $7\xi$. This allows for sensible finite size extrapolations. At the same time, we have retained up to $M=210$ states, which allows for reasonable accuracy. As the DMRG is much more precise for open than for closed chains, we have considered only open chains.

To calculate the gap, we consider an open $S=2$ chain with a spin-1 at each end ($S_1 = S_L = 1$; $S_i = 2$ otherwise):

\[
H = J_{\text{end}} S_1 \cdot S_2 + J \sum_{i=2}^{L-2} S_i \cdot S_{i+1} + J_{\text{end}} S_{L-1} \cdot S_L.
\] (1)

We set $J_{\text{end}} = J$ and the results will be given in units of $J$ from now on.
Throughout this study we are guided by the so-called valence-bond-solid (VBS) wavefunctions [7]. They are exact ground states of very special spin Hamiltonians (VBS hereafter). For $S=1$ it is well established that the simplest Heisenberg Hamiltonian [10] shares a similar physics with the VBS Hamiltonian. These VBS ground states have a finite correlation length and there is a gap to spin excitations. From these VBS Hamiltonians it is known that the ground state of the open VBS-chain with integer spin $S$ is exactly $(S+1)^2$-fold degenerate [7], because the chain ends act like free $S/2$ spins. For a generic “Haldane-like” Hamiltonian we expect this manifold of states to be split due to interactions between end spins. We couple a spin-$S/2$ to each end with an antiferromagnetic coupling $J_{\text{end}}>0$ (we chose $J_{\text{end}}=1$) to select a state in this manifold.

We calculated the gap for $L=60, 90, 120, 150, 210, 270$, as the difference between the total energies of the lowest energy states in the $S^z_{\text{total}}=0$ and $S^z_{\text{total}}=1$ subspaces. We have kept $M=210$ states in the DMRG. White has given a procedure [4], which allows to ameliorate iteratively the results found for the total energies of a chain of fixed length $L$. For short chains, the DMRG algorithm truncates less well than for long chains; after the chain has grown to full length $L$, the results can be used to ameliorate the truncations at the start of the algorithm. We do not apply this iteration to the ground state, but iterate once for the excited state. From test calculations we found that iterating (further) does not substantially increase the precision obtained or influence our extrapolation. We extrapolate the results first for fixed $L$ to $M=\infty$, and then these extrapolated values are used to investigate the thermodynamic limit $L=\infty$.

We have extrapolated the energies to $M=\infty$ and deduced the gap values by subtraction. We find that both for the (uniterated) ground state energy and (iterated) excitation energy the deviation from the asymptotic value is proportional to $(1-\sum \lambda_i)$, where $\lambda_i$ are the eigenvalues of the states of the density matrix that are kept at the last iteration. The proportionality coefficient is in both cases of order 10 (much larger for the uniterated excitation energy), the truncation error $1-\sum \lambda_i$ for $M=210$ between $3.7 \times 10^{-8}$ and $9.4 \times 10^{-8}$ for the ground state energy and $6.7 \times 10^{-8}$ and $5.3 \times 10^{-7}$ for the iterated excitation energy for $L$ between 60 and 210. The precision of the gap is in reality better than estimated, because both energies are overestimated due to the variational character of the DMRG, and there will be partial cancellation of the errors.

The ground state energy results allow us to calculate the ground state energy per site $E_0$. We find that for $L \approx 120$, for each $M \leq 210$ considered the ground state energy per site has converged to a precision of $10^{-6}$. These values we then extrapolate in $M$, again finding a linear dependence of the error on the truncation error. We conclude that $E_0 = -4.761248(1)$.

We can extrapolate our results for $90 \leq L \leq 270$ to $L=\infty$ by fitting an $L^{-1}$-law (figure 1) and obtain a gap estimate of $0.081(1)$ for $L=\infty$. We note that deviations from perfect linear behaviour are extremely small in the range of chain length we have considered. However it is important to note that the asymptotic behaviour
of the gap in an open chain is expected to be $1/L^2$: the massive quasiparticles have dispersion

$$E_k = \sqrt{\Delta^2_\infty + c^2(k-\pi)^2} \approx \Delta_\infty + c^2(k-\pi)^2/2\Delta_\infty$$

near the bottom of the band. On an open chain the quasiparticle cannot stay in a stationary state with $k=\pi$ but instead $k-\pi \approx \pi/L$ as a particle in a box since there is no translational invariance. This means that the lowest excited state has a gap $\Delta_\infty + c^2\pi^2/2\Delta_\infty L^2 + O(1/L^3)$. This behaviour has not yet been reached for $L=270$. Thus there must be a crossover point to parabolic behaviour of $\Delta(L)$.

As a consequence we can obtain an upper bound on the gap by assuming that the parabolic behaviour sets in immediately beyond $L=270$. We match a parabolic curve $\Delta(L) = \Delta_\infty + aL^{-2}$ to our extrapolated linear gap curve at $L=270$ such that up to the first derivative the two regimes meet continuously. This leads to $\Delta_\infty = 0.090$ (and $a \approx 620$). We have also estimated the correlation length (see below) to be $\approx 50$ and thus $c = \xi\Delta_\infty \approx 4.2$. This gives an estimate of the coefficient of the $1/L^2$ parabolic term. Using this estimate ($a_0 \approx 1024$) we now say that there is a crossover length $L_0$ at which asymptotic behaviour $\Delta(L) = \Delta_\infty + a_0/L^2$ sets in. Matching the parabolic curve to the straight line requires

$$\Delta_\infty = 0.085 \text{ and } L_0 \approx 450.$$ 

This is a perfectly consistent set of results. We thus choose as a central value for the gap $\Delta_\infty = 0.085$ the lower bound being fixed by the linear fit of our data and the upper bound being 0.09. We quote our final result as $\Delta = 0.085(5)$. A gapless state is excluded beyond any doubt.

To calculate the correlation length, we partially lift the ground state degeneracy of the open chain by adding a spin-1 on one end of the $S=2$ chain ($S_L = 1$; $S_i = 2$ otherwise):

$$H = J \sum_{i=1}^{L-2} S_i \cdot S_{i+1} + J_{\text{end}} S_{L-1} \cdot S_L. \tag{2}$$

The ground state will then be a spin-1 triplet; at the spin-2 end of the chain (position 1) one expects an effective free spin-1. If we consider the ground state with $S_{\text{total}}^z = 1$, it is expected that $\langle S_i^z \rangle$ decays purely exponentially from a value around $\pm 1$: $\langle S_i^z \rangle \propto (-1)^{i-1}\exp(-(i-1)/\xi)$. From this equation the correlation length $\xi$ can be obtained much more precisely than from $\langle S_i \cdot S_j \rangle$, as it is derived from a one-point correlation, where the systematic errors of the DMRG tend to cancel partially, whereas they build up for the two-point correlations, as correlated states in each half-chain are systematically neglected at the same time, underestimating $\xi$.

Because of the slow increase of precision with $M$ for $S=2$, we have to perform an extrapolation of $\xi$ with respect to $M$. At the same time we consider chains of length $L=270$ and repeat some calculations for $L=350$, to study possible finite size effects. We find that those are minor, as are effects of the choice of $J_{\text{end}}$, and concentrate on the extrapolation in $M$. In figure 2, we give $\ln|\langle S_i^z \rangle|$ vs. $i$. The generic behaviour is the same for all $M$: After the expected decay of $S^z$,
there is a small increase towards the other end of the chain (greatly exaggerated by the logarithmic scale). With increasing M, the minimum shifts to the right, the spin expectation value at the right end of the chain is greatly reduced, the decay becomes more exponential and approaches a limiting curve which we take to be the M=\infty result. To derive ξ, we give in figure 3 the local decay length $2/(\ln |S_i| - \ln |S_{i+2}|)$ (averaged over two neighbouring sites to reduce odd-even site oscillations). One sees that at the spin-2 end of the chain, the correlation length is first rather short, but saturates to its bulk value (the shoulder). For M=180, the convergence of ξ for M→∞ can be well established, and we find a correlation length ξ = 49(1) in a system which has thus length $L \approx 5.5\xi$, which is consistent with minor finite size effects. At the same time, we find that $\langle S_i^z \rangle$ converges towards 1.13(1), supporting the picture of an effective free spin-1 at the end of the chain.

Furthermore, we have measured the following nonlocal string correlation:

$$G(n, m) = \langle S_n^z \exp\left(\frac{i\pi}{2} \sum_{i=n+1}^{m-1} S_i^x\right) S_m^z \rangle. \quad (3)$$

For the S=2 VBS-chain G(n, m) → −1 for |n − m| → ∞, revealing a hidden topological order. Investigating isotropic Heisenberg S=2 chains up to L=270 and keeping up to M=150 states, we find that G(n, m) saturates to −0.726(2) for |n − m| → ∞ indicative of hidden topological long-range order in the Heisenberg S=2 chain[11]. These results imply that the physics of the Heisenberg S=2 chain can be captured by a VBS description.

For the isotropic AFM quantum spin-2 chain we find from $\Delta = 0.085(5)$ and ξ = 49(1) a spin wave velocity $c = 4.2(3)$. This result indicates that, as expected, S=2 is more classical than S=1. We have also shown that the S=2 spin chain has hidden long-range order as in the VBS model. There is excellent evidence that the S=1 Haldane gap is realized in the compound NENP[12]. It is an open and interesting question to find an experimental system with S=2 spins to check our findings.

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1 Figure Captions

**Figure 1**: Gap vs. $L^{-1}$ for L=90, L=120, L=150, L=210 and L=270 for different M, the number of kept states. Full squares: extrapolated values for M→∞. Solid line: extrapolation of the gap values to L→∞, yielding a lower bound. The dashed line is an upper bound on gap behaviour which is obtained by assuming that the asymptotic form $\Delta(L) = \Delta_\infty + a/L^2$ starts at L=270. Since we have no evidence for such a behaviour, the dashed curve should be a strict upper bound on the gap.
Figure 2: \( \ln |\langle S_z^i \rangle| \) vs. site \( i \) for an open \( S=2 \) chain with a spin-1 attached at the right end \( (J_{\text{end}} = 1) \). Note that for increased chain length the straight-line fit for the slope is possible for larger \( i \), while the slope itself remains virtually unchanged. The expectation values for the right end of the chain have obviously not converged yet, whereas the asymptotic \( M \to \infty \) slope value can be determined.

Figure 3: Two-site average of the local correlation length \( 2/(\ln |\langle S_z^i \rangle| - \ln |\langle S_z^{i+2} \rangle|) \) vs. site \( i \) for \( i < 125 \) for the same chain as in Figure 2. The deviations from the shoulder in the center of the diagram are finite size and finite precision effects (for the right end).

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Figure 2: Schollwoeck & Jolicoeur

$\ln |\langle S_i^z \rangle|$
