Edge states in Open Antiferromagnetic Heisenberg Chains

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The antiferromagnetic Heisenberg spin chains has been a subject of immense interest in the last decade since Haldane conjectured that the low energy physics of integer and half integer spin chains are fundamentally different. It is now generally believed that half-integer Heisenberg spin chains have gapless excitation spectrum, whereas gaps exist in integer spin chains (Haldane gap). More recently, there has been increasing interests in studies of spin chains with defects. In particular, the properties of broken $S = 1$ quantum spin chains have received much attention because of the experimental observation of $S = 1/2$ excitations localized at the ends of broken $S = 1$ spin chains. More generally, one may address the question of whether edge states are genuine properties of finite quantum spin chains as in Fractional Quantum Hall Effect. Recently, a theory of edge states based on the Non-linear-sigma model ($NLσM$) plus topological $\theta$-term has been developed by one of us where it was conjectured that edge states are genuine properties of antiferromagnetic quantum spin chains with spin value $S > 1/2$. In this letter, we study the question for both integer and half integer spin chains numerically using the recently developed density matrix renormalization group (DMRG) method. We shall present results for open spin chains with spin values $S = 1/2, 1, 3/2, 2$ up to chain length of 100 sites.

The DMRG method has proved to be tremendously successful in studying $S = 1$ and $S = 1/2$ antiferromagnetic Heisenberg spin chains. The method was found to be particularly suitable for studying spin chains with open boundary condition and is thus well suited for our purpose of studying edge states. We use the infinite chain algorithm in our study. Two new sites are added to the spin chain in each optimal step of the calculation from length $L = 4$ to $L = 100$. That is, open spin chains with even number of sites are studied. The number of the kept optimized states in our calculation is $m = 120$. The largest truncation errors for $S = 1/2, 1, 3/2, 2$ and 2 chains are found to be smaller than $10^{-10}$, $10^{-8}$, $3 \times 10^{-6}$ and $10^{-5}$ respectively when the chain length reaches $L = 100$ in the final step. Properties of the ground state and a few lowest excited states are obtained by looking at the lowest energy state with fixed total z-component of spin angular momentum $S^z$. In particular, the ground state corresponds to the lowest energy state in the sector $S^z = 0$. We shall look at the excitation energies of various states with different $S^z$ and the corresponding average z-component of angular momentum on each site $i = < S^z_i >$. The dimmerization parameter $q(i) = < S^z_i, S^z_{i+1} - S^z_{i-1}, S^z_i >$ for the ground state will also be examined.

We start with the excitation energies for integer spin chains. Fig.1 shows the excitation energies $E_n - E_0$ for $n = 1$ to 3 as a function of chain length $L$ for the $S = 1$ spin chain. $E_n$ is the energy of the lowest energy state in the sector $S^z = n$. Energy is measured in units of Heisenberg coupling $J$. According to the valence bond picture, for $S = 1$ spin chain, two $S = 1/2$ spins are left at two ends of the spin chain, and are coupled with effective coupling $J_{eff} \sim J e^{-L/\xi}$, where $\xi$ is the correlation length. For even spin chains, the coupling is antiferromagnetic and the resulting ground state is a spin singlet ($S^z = 0$). The lowest energy state with $S^z = 1$ can be constructed by exciting the singlet formed by the two edge spins into a triplet, and the excitation energy is of order $J_{eff}$, which goes to zero exponentially as length of spin chain increases. Excited states with larger $S^z$ cannot be constructed by exciting only the edge spins any more and bulk excitations must be involved in constructing states with $S^z > 1$, implying that the excitation energy will be of order $E_n - E_0 \sim (n-1) \times E_H$ as $L \to \infty$.
where $E_H$ is the Haldane gap. This predicted behavior is clearly confirmed by our numerical result presented in Fig.1. The Haldane gap $E_H$ and correlation length $\xi$ are estimated to be $E_H = 0.41 J$ and $\xi = 6.0$ from $E_2 - E_0 \rightarrow 0.41 J$ and $E_3 - E_0 \sim 0.7 e^{-L/6.0}$ for large $L$, respectively, in agreement with result obtained by White [9]. Fig.2 shows similar results for $S = 2$ spin chain. Notice that in this case, the $S^z_{tot} = 2$ state also has excitation energy going to zero as $L \rightarrow \infty$, whereas higher $S^z_{tot}$ states have finite energy gap. This behavior is consistent with valence bond picture which predicts that for $S = 2$ spin chain, the edge state spin magnitude is $S/2 = 1$, and the two edge spins are coupled again by $J_{eff} \sim J e^{-L/\xi}$, where $\xi$ is now the correlation length for $S = 2$ spin chain. In this case both $S^z_{tot} = 1$ and $S^z_{tot} = 2$ states can be constructed by exciting edge spins only, and have excitation energy $\sim 0$ as $L \rightarrow \infty$, which is exactly the behavior obtained in our numerical calculation. The Haldane gap and the correlation length are estimated to be $E_H \sim 0.02$ and $\xi \sim 33$ from $E_3 - E_0 \rightarrow 0.02 J$, $E_1 - E_0 \sim 0.1 e^{-L/33}$, and $E_2 - E_0 \sim 0.4 e^{-L/33}$ for large $L$, respectively from our numerical results. However, the accuracy of these estimated numbers are much worse than the $1$ case because of the much larger truncation error found in our calculation for the $S = 2$ spin chain.

Next we turn to the excitation energies for half-integer spin chains. Fig.3 shows the excitation energies $E_n - E_0$ for $n = 1$ to $3$ as a function of inverse chain length $L^{-1}$ for $S = 1/2$ spin chain. According to (abelian) bosonization theory [13] the excitation energy is given by $E_n - E_0 = (S^z_{tot})^2 \times (\pi/L)$. The bosonization prediction is also drawn on Fig.3 (dash line). Notice that bosonization theory is correct only in the asymptotic limit $L \rightarrow \infty$, whereas higher $S^z_{tot}$ terms of order $(\ln L)^{-1}$ are neglected [13]. It is thus not surprising that our numerical results and bosonization theory predictions show only qualitative agreement with each other. Notice also that bosonization theory for finite $S = 1/2$ spin chain predicts no edge states in this case. Fig.4 shows similar results for $S = 3/2$ spin chain where the excitation energies are shown up to state with $S^z_{tot} = 4$. It is apparent that $E_n - E_0 \sim 1/L$ in all four cases. Notice however, that edge state with spin magnitude $S = 1/2$ is predicted to exist in this case, according to the conjecture by Ng [8]. However it does not seem to show up clearly as for integer spin chains in the energy curve.

To understand this behavior we examine the edge state in $S = 3/2$ spin chain in more detail. According to Ng [8], the low energy physics of open $S = 3/2$ spin chain can be described by an effective $S = 1/2$ spin chain coupled antiferromagnetically to two impurity spins with magnitude $S_{imp} = 1$ at two ends of the spin chain. The impurity spin will be partially screened by a Kondo type effect at low energy [13], leaving "free" spins of magnitude $S_{edge} = 1/2$ at the ends, coupling ferromagnetically to the bulk $S = 1/2$ spin chain. Again, the coupling of the "impurity" spin to the bulk $S = 1/2$ spin chain can be analyzed using renormalization group technique.

For ferromagnetic coupling, the corresponding operator is marginally irrelevant, implying that a free $S_{edge} = 1/2$ is left at each end of the spin chain as $L \rightarrow \infty$. For a finite spin chain, an RKKY type coupling between the two edge spins will be found, and the resulting ground state is a spin-singlet for even chains, as is in the case of integer spin chains. The RKKY coupling $J_{R}$ between the two edge spins comes from exchange of spinwaves, and has a length dependence $J_{R} \sim g/L$, where $g$ is some effective coupling constant. Thus we expect that the excitation energy for the edge spins $E_{ed}$ is proportional to $g/L$. Notice that at large distance $L$, the coupling constant $g$ will be renormalized with $g \rightarrow g/(1 + g \ln(L))$ (ferromagnetic Kondo effect) and corresponding correction to energy $E_{ed}$ will be found. In particular, at large $L$, $E_{ed} \sim 1/(\ln(L))$. Assuming that the low energy bulk excitations are described by bosonization theory as an effective $S = 1/2$ spin chain, we conclude that the lowest $(S^z_{tot} = 1)$ excited state for $S = 3/2$ open spin chain is an edge excitation as in integer spin chains, since the bulk excitation energies scale as $1/L$, and will be always higher in energy then $E_{ed}$ as $L \rightarrow \infty$. More detailed analysis of the energy spectrum supports our edge state energy analysis which we shall discuss in a later paper. In the following, we shall present a more direct numerical evidence supporting our edge states picture for Heisenberg spin chains. Fig.5 shows the expectation value $<S^z_i>$ for the $S^z_{tot} = 1$ state for all four spin chains $S = 1/2, 1, 3/2, 2$ with 100 sites, i.e. $i = 1, 100$. The four cases are arranged from top to bottom in increasing order of spin magnitude, i.e. the top one is for $S = 1/2$, and bottom one for $S = 2$, etc. For spin singlet ground states, $<S^z_i>$ will be zero for all sites $i$. Thus $<S^z_i>$ for the $S^z_{tot} = 1$ state gives information about the wavefunction of the first excited state in the spin system. Notice that for all four spin values, Fig.5 shows that the excited states all carry staggered magnetization because of the underlying antiferromagnetic interaction. For $S = 1/2$ spin chain, Fig.5 suggests clearly that the first excited state can be thought of as a standing spin wave. The same qualitative result is also obtained from bosonization theory of finite $S = 1/2$ spin chain. In fact the feature can be understood in the much simpler $S = 1/2$ XY-model with $J_z = 0$. The $S = 1/2$ XY-model can be mapped onto a non-interacting spinless fermion model. It is easy to show that similar feature exists in this case. The introduction of nonzero $J_z$ term just modified the feature quantitatively. It is clear from Fig.5 that the wavefunction of the first excited states in the $S > 1/2$ spin chains are qualitatively different from that of the $S = 1/2$ spin chain. In fact, in all three cases we considered, $<S^z_i>$ suggests clearly that the first excited states are all consist of spin excitations which are localized around edges of spin chains, i.e. they are edge excitations. It is also clear from the figure that the correlation length of the edge state in $S = 2$ spin chain is much larger than the corresponding correlation length of the $S = 1$ spin chain,
in agreement with general expectation and with results obtained from excitation energy analysis. One can also study \(< S_i^z > \) for the \( S_i^{tot} = 2 \) states and looks at the difference in \(< S_i^z > \) between the \( S_i^{tot} = 2 \) and \( S_i^{tot} = 1 \) states. For the \( S = 3/2 \) spin chain, the difference is found to have a spinwave like feature similar to \(< S_i^z > \) for \( S = 1/2 \) spin chain with \( S_i^{tot} = 1 \), suggesting clearly that the spin magnitude of the edge state is \( S_{edge} = 1/2 \), and excitations with \( S_i^{tot} > 1 \) involves bulk excitations, in agreement with previous conjecture by Ng [8].

We have also examined the dimmerization parameter \( q(i) = < S_i . S_{i+1} - S_i . S_{i-1} > \) for the ground states of the four spin chains we considered. For integer spin chains, \( q(i) \)'s are found to be nonzero around ends of spin chains and decay exponentially as one move into the interior, in agreement with prediction by Ng [8]. For half-integer spin chains, \( q(i) \)'s are found to be large at the ends and decay with power law into the interior of spin chain. Similar results were also obtained by White [9] for \( S = 1 \) and \( S = 1/2 \) chains. For \( S = 1/2 \) chain, the dimmerization parameter \( q(i) \) can again be examined using bosonization techniques where it can be shown that \( q(L/2) \sim (1/L)^2 \), where \( \beta = 1/2 \) in bosonization theory. Similar behavior is observed in our numerical results for both \( S = 1/2 \) and \( S = 3/2 \) chains, with \( \beta \sim 1/2 \) for \( S = 1/2 \) chain and \( \beta \sim 0.6 \) for \( S = 3/2 \) chain. The huge difference in behavior of \( q(i) \) between integer and half-integer open spin chains reflects the fact that half-integer spin chains are more susceptible to spin-Peierls instability and furnish another interesting parameter distinguishing between integer and half-integer spin chains.

Lastly, we want to list our calculated ground state energies (per site) \( \epsilon_0 \) for the four spin chains. We obtain \( \epsilon_0 = -0.443147 \) for \( S = 1/2 \) chain and \( \epsilon_0 = -1.401484 \) for \( S = 1 \) chain, in good agreement with exact Bethe ansatz solution and the result obtained by S. White et al [11]. We have also computed the ground state energies for \( S = 3/2 \) and \( S = 2 \) chains with good precision, with \( \epsilon_0 = -2.8283 \) for \( S = 3/2 \) chain and \( \epsilon_0 = -4.7068 \) for \( S = 2 \) chain.

Summarizing, in this paper we have performed numerical studies on low energy properties of finite quantum spin chains with spin values \( S = 1/2, 1, 3/2, 2 \) using the Density-Matrix Renormalization Group techniques which has been applied successfully to study \( S = 1/2 \) and \( S = 1 \) spin chains. We find that all the results we obtained are consistent with the edge states picture conjectured by Ng [8]. In particular, we present for the first time numerical evidence for existence of edge states in \( S = 3/2 \) and \( S = 2 \) finite quantum spin chains. The dimmerization parameter \( q(i) \)'s for the ground states are also studied where the huge difference in behavior between integer and half-integer spin chains is pointed out.

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**FIG. 1.** The excitation energy \( E_n - E_0 \) for even \( S = 1 \) chain as function of chain length \( L \). The black circles, black squares, and black triangles are for \( E_1 - E_0, E_2 - E_0 \), and \( E_3 - E_0 \) respectively.

**FIG. 2.** The excitation energy \( E_n - E_0 \) for even \( S = 2 \) chain as function of chain length \( L \). The open circles, black circles, black squares, and black triangles are for \( E_1 - E_0, E_2 - E_0, E_3 - E_0, \) and \( E_4 - E_0 \) respectively.

**FIG. 3.** The excitation energy \( E_n - E_0 \) for even \( S = 1/2 \) chain as function of inverse chain length \( 1/L \). The black circles, black squares, and black triangles are for \( E_1 - E_0, E_2 - E_0, \) and \( E_3 - E_0 \) respectively. The dashed lines are \( E_n - E_0 = n^2 \pi/L \).

**FIG. 4.** The excitation energy \( E_n - E_0 \) for even \( S = 3/2 \) chain as function of inverse chain length \( 1/L \). The open circles, black circles, black squares, and black triangles are for \( E_1 - E_0, E_2 - E_0, E_3 - E_0, \) and \( E_4 - E_0 \) respectively.
FIG. 5. The configuration $< S_i^z >$ for the lowest states of $S = 1/2, 1, 3/2, 2$ chains with $S^\text{tot}_z = 1$ and length $L = 100$. The zero point for $S = 1/2, 1, 3/2, 2$ chains are shifted to 4, 3, 2, 1 respectively. The circles, black circles, black squares, and black triangles are for the $< S_i^z >$ of chains with $S = 1/2, 1, 3/2, 2$ respectively.