Finite Size Scaling for Low Energy Excitations in Integer Heisenberg Spin Chains

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In this paper we study the finite size scaling for low energy excitations of $S = 1$ and $S = 2$ Heisenberg chains, using the density matrix renormalization group technique. A crossover from $1/L$ behavior (with $L$ as the chain length) for medium chain length to $1/L^2$ scaling for long chain length is found for excitations in the continuum band as the length of the open chain increases. Topological spin $S = 1/2$ excitations are shown to give rise to the two lowest energy states for both open and periodic $S = 1$ chains. In periodic chains these two excitations are “confined” next to each other, while for open chains they are two free edge $1/2$ spins. The finite size scaling of the two lowest energy excitations of open $S = 2$ chains is determined by coupling the two free edge $S = 1$ spins. The gap and correlation length for $S = 2$ open Heisenberg chains are shown to be 0.082 (in units of the exchange $J$) and 47, respectively.

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Since Haldane pointed out the difference between integer and half integer Heisenberg spin chains [1], the richness of the physics in the Heisenberg model has attracted intensive attention. It was conjectured [1] that the ground state of integer spin chains has an exponentially decaying correlation and a nonzero energy gap for excitations, in contrast to the ground state for half integer spin chains with a zero energy gap. Like valence bond solid picture [2], excitations are shown to be responsible for them. We show explicitly that the two spin $1/2$ edge states are “confined” to each other in PBC chains. The finite size scaling of the two lowest excitation energies in $S = 2$ OBC chains is also determined by their free edge $S = 1$ spins. The gap and correlation length for $S = 2$ Heisenberg chains are shown to be 0.082(3) (in units of the exchange $J$) and 47(3), respectively. We also point out that a reasonable scaling for the first excited state (the bottom of the continuum band) of $S = 2$ PBC chains is of exponential type in analogy with $S = 1$ PBC chains.

We apply the density matrix renormalization group (DMRG) method [13] to calculate the lowest energies for Heisenberg chains using the Hamiltonian:

$$H = \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (1)$$

(The above equation is for OBC. The Hamiltonian for PBC chains is obtained by adding the term $\mathbf{S}_L \cdot \mathbf{S}_1$ to Eq.(1).) We use the DMRG infinite chain algorithm to calculate the low energy spectrum for both OBC chains and PBC chains [13]. By keeping 300 optimized states, we calculate the energies $E_0^{P1}$ for the ground state and $E_1^{P1}$ for the first excited state in $S = 1$ PBC chains up to length $L = 36$. The largest truncation errors in calculations are $9 \times 10^{-8}$ for $E_0^{P1}$ and $5 \times 10^{-7}$ for $E_1^{P1}$, respectively. By keeping 200 optimized states, we calculate the energies $E_0^{O1}$ for the ground state and $E_1^{O1}$ for the first excited state of $S = 1$ OBC chains up to length $L = 42$. The largest truncation errors in the calculations are $2 \times 10^{-11}$ for $E_0^{O1}$ and $1 \times 10^{-13}$ for $E_1^{O1}$. By keeping 150 optimized states, we calculate also the energies $E_2^{O1}$, $E_3^{O1}$, and $E_4^{O1}$ for the low-lying states of total spin $S_{tot}^{O1} = 2$, 3, and 4, respectively for $S = 1$ OBC chains up to length $L = 100$. $E_1^{P1}$ and $E_2^{P1}$ are then calculated for chain lengths up to $L = 250$. The largest truncation errors occurred in these calculations are $1 \times 10^{-12}$. 



\[ \text{arXiv:cond-mat/9610100v1 11 Oct 1996} \]
2 \times 10^{-10}, \ 1 \times 10^{-9}, \text{ and } 6 \times 10^{-9} \text{ for } E_0^{O1}, \ E_1^{O1}, \ E_2^{O1}, \text{ and } E_3^{O1}, \text{ respectively. By keeping 250 optimized states, we calculate the energies } E_0^{O2}, \ E_1^{O2}, \ E_2^{O2}, \text{ and } E_3^{O2} \text{ for } S = 2 \text{ OBC chains up to length } L = 150, \text{ and they are corresponding to the lowest energy states with total spin } S_z^{\text{tot}} = 0, 1, 2, \text{ and } 3, \text{ respectively. The largest truncation errors in the calculations are } 1 \times 10^{-6}, \ 2 \times 10^{-7}, 4 \times 10^{-8}, \text{ and } 7 \times 10^{-8} \text{ for } E_0^{O2}, \ E_1^{O2}, \ E_2^{O2}, \text{ and } E_3^{O2}, \text{ respectively. The analysis of these numerical results is straightforward, and we will show them in detail in the following.}

We use the following relations for the two lowest energies in } S = 1 \text{ Heisenberg chains (to be explained later)}:

\begin{align}
E_0^{P1} &= e_0 L + a_0^{P1} e^{-L/\xi_1}/\sqrt{L}, \\
E_1^{P1} &= e_0 L + \Delta_1 + a_1^{P1} e^{-L/\xi_1}/\sqrt{L}, \\
E_0^{O1} &= e_0 (L-1) + \Delta_0 + a_0^{O1} e^{-(L-1)/\xi_1}, \\
E_1^{O1} &= e_0 (L-1) + \Delta_0 - \frac{1}{4} a_0^{O1} e^{-(L-1)/\xi_1}.
\end{align}

(2)

for PBC (the first two equations) and OBC (the last two relations), respectively. It is more convenient to introduce

\begin{align}
f_1(L) &= -(E_0^{P1} - e_0 L)/\sqrt{L} = -a_0^{P1} e^{-L/\xi_1}, \\
f_2(L) &= (E_1^{P1} - e_0 L - \Delta_1)/\sqrt{L} = a_1^{P1} e^{-L/\xi_1}, \\
f_3(L-1) &= -(E_0^{O1} - e_0 (L-1) - \Delta_0) = -a_0^{O1} e^{-(L-1)/\xi_1}, \\
f_4(L-1) &= E_0^{O1} - e_0 (L-1) - \Delta_0 = -\frac{1}{4} a_0^{O1} e^{-(L-1)/\xi_1}.
\end{align}

(3)

Hence the ratio of the constants is } -\frac{1}{4} \text{ and the coupling constant } J_{\text{eff}} \sim e^{-(L-1)/\xi_1}. \text{ It is very interesting to note that } a_1^{P1}/a_0^{O1} \sim -1/3 \text{ in Eq.(2), which means that the singlet and triplet combinations of the two topological spin 1/2 excitations are also responsible for the two lowest states for PBC chains, with a coupling constant } J_{\text{eff}} \sim e^{-L/\xi_1}/\sqrt{L}. \text{ An important question is where are these topological excitations located. For OBC chains they are exactly pinned at the edges. One might think that these two states are pushed away as far as possible from each other for PBC chains. However, this is not true: they are “confined”, sitting next to each other \cite{17}. These two excitations will interact with each other in “both directions”, a direct coupling of the order of } J \text{ which is responsible for the Haldane gap, and an indirect coupling via virtual spin-wave excitations around the spin chain which is proportional to } J_{\text{eff}} \sim \exp(-L/\xi_1)/\sqrt{L} \text{ Fig.3.}

The exponential term } e^{-L/\xi_1}/\sqrt{L} \text{ in } E_0^{P1} \text{ and } E_1^{P1} \text{ is in agreement with previous exact diagonalization results} \cite{6}. \text{ By studying chain length longer than the one used in exact diagonalization, we have shown that } E_0^{O1} \text{ and } E_1^{O1} \text{ have the same scaling behavior as for the spin-spin correlation} \cite{18-19}, \text{ instead of a net exponential } e^{-L/\xi_1}. \text{ We point out that } E_1^{O1} \text{ is the bottom of the one magnon band and has a zero kinetic energy since } w(k) \sim (k-\pi)^2 \text{ Fig.4, therefore its scaling is different from the } 1/L^2 \text{ behavior expected for other single or multi-magnon states in PBC chains as well as the magnon states in OBC chains.}

Our numerical results are plotted in Fig.1 as ln } f_i(L) \text{ v.s. } L \text{ in comparison with Eq.(3). From fitting we obtain the site energy } e_0 = -1.401484(1), \text{ correlation length } \xi_1 = 6.00(4), \text{ energy gap } \Delta_1 = 0.4104892(2), \text{ and edge state energy for OBC chains } \Delta_0 = -0.1931661(1). \text{ The constants are of similar precision for } \xi_1, a_0^{P1} = -1.33(1), a_1^{O1}/a_0^{O2} = -0.33(2), \text{ and } a_0^{O1} = -0.50(2).

The interpretation of OBC results is obvious: } E_0^{O1} \text{ and } E_1^{O1} \text{ are the energies of the singlet and triplet combinations of the two spin 1/2 edge states, respectively.

\begin{align}
E_0^{O2} - E_0^{O1} &= a_0^{O2} e^{-(L-1)/\xi_2}, \\
E_2^{O2} - E_1^{O2} &= 2a_0^{O2} e^{-(L-1)/\xi_2},
\end{align}

(4)

where the correlation length } \xi_2 = 47(3) \text{ and constant } a_0^{O2} = 0.060(5). \text{ The DMRG data are plotted in compar-

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig1.png}
\caption{The logarithm of the energy expressions in Eq.(3) for the two lowest energy states of } S = 1 \text{ spin chains as functions of chain length } L.
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig2.png}
\caption{The logarithm of the energy spacings (Eq.(4)) for the three lowest energy states in } S = 2 \text{ spin chains as functions of chain length } L. \text{ Diamonds are for } \ln (E_1^{O2} - E_0^{O2}), \text{ and crosses are for } \ln (E_2^{O2} - E_1^{O2}).
\end{figure}
ison with the above equation in Fig.2 as $\ln(E_{1}^{O2} - E_{0}^{O2})$ and $\ln(E_{2}^{O2} - E_{1}^{O2})$ v.s. $L - 1$. These asymptotic expressions come from the coupling of two spin $S = 1$ edge spins in $S = 2$ OBC chains [13]. From these energies we have calculated the site energy for $S = 2$ Heisenberg chains $\epsilon_0 = -4.76125(5)$ by $E_0^{O2}(L + 2) - E_0^{O2}(L)$ analysis [10].

$$E_n^{O1} - E_1^{O1} = (n - 1)\Delta_1 + \frac{a_1^{O1}}{L - 1}(1 + \frac{b_1^{O1}}{\ln(L - 1)}),$$

where $n = 2, 3, 4$ correspond to one, two, and three magnon band bottoms, respectively. We plot in Fig.3 $(L - 1)(E_2^{O1} - E_1^{O1} - \Delta_1)$, $(L - 1)(E_3^{O1} - E_2^{O1} - 2\Delta_1)$, and $(L - 1)(E_4^{O1} - E_1^{O1} - 3\Delta_1)$ v.s. $1/\ln(L - 1)$ for $S = 1$ OBC chains with medium chain length, $L = 20$ to 100, which is more than ten times the correlation length $\xi_1$. The ratios of the constants are $a_3^{O1}/a_2^{O1} \approx 4$, $a_4^{O1}/a_2^{O1} \approx 9$, and $b_4^{O1} \approx b_3^{O1} \approx b_2^{O1}$. For long chains, $L > 100$, the expected scaling term $1/L^2$ [10] for $E_n^{O1} - E_1^{O1}$ shows up. In Fig.4, using again the plot $(L - 1)(E_2^{O1} - E_1^{O1} - \Delta_1)$ v.s. $1/\ln(L - 1)$ for chain length $L = 20$ to 250, we show the crossover from the behavior given by Eq.(5) for medium chain length to $E_2^{O1} - E_1^{O1} = \Delta_1 + \frac{\partial_1}{L - 1}$ for long chain length. We point out that the crossover occurs within a rather narrow range in $1/L$ plot in Fig.4. For $S = 2$ OBC chains, we use medium chain length expressions similar to the ones for $S = 1$ chains,

$$E_3^{O2} - E_2^{O2} = \Delta_2 + \frac{a_3^{O2}}{L - 1}(1 + \frac{b_3^{O2}}{\ln(L - 1)}),$$

where the gap turns out to be $\Delta_2 = 0.082(3)$ and constants $a_3^{O2} = 2.8(2)$ and $b_3^{O2} = 5.9(4)$. We plot in Fig.5 $(L - 1)(E_3^{O2} - E_2^{O2} - \Delta_2)$ v.s. $1/\ln(L - 1)$ for chain length up to $L = 150$. As we show in Fig.5, the medium chain length behavior extends to chain length $L = 150$ and bigger. For the chain lengths we have studied, which is more than three times the correlation length, the leading term $1/L$ in Eq.(6) is still dominant. In analogy to $S = 1$ chains [13], the long length asymptotic expression for $S = 2$ OBC chains is expected to be $1/L$ as well [2], and the crossover between the medium length and long length behavior should occur for longer chain lengths.

One way to explain the $1/L$ scaling in the medium range is to consider the energy dispersion [9] $\Delta(k) = \sqrt{\Delta^2 + (vk)^2}$ for a magnon with wave vector $k$. This expression has also been suggested for such gapped systems using nonlinear sigma models [21]. For OBC chains with big length $L$, one can expand the $(vk)^2$ term and get the $1/L^2$ scaling. So it is in agreement with our calculation and previous studies [1]. The leading finite size scaling term would be $1/L$ only when $\Delta^2 \ll (2\pi v/L)^2$. The shape of the curve $\sqrt{\Delta^2 + (2\pi v/L)^2}$ v.s. $L$ is consistent with $E_2^{O1} - E_1^{O1}$ (see Fig.4), but it cannot fit $E_2^{O2} - E_1^{O2}$ for the medium size well, for instance, $L \sim 20$ to 90 for $S = 1$ OBC chains. We suggest that further studies on the medium size behavior of $S = 1$ and $S = 2$ chains are needed, especially because it is relevant to experiment on chains with typical doping (of the order of one percent).

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**FIG. 3.** The excitation energies for the bottoms of one, two, and three magnon bands of medium length $S = 1$ OBC chains (Eq.(5)). We plot $[E_n^{O1} - E_1^{O1} - (n - 1)\Delta_1]/(L - 1)$ v.s. $1/\ln(L - 1)$ for medium lengths $L = 20$ to 100.

**FIG. 4.** The excitation energies for the bottom of one magnon band of medium length and long length $S = 1$ OBC chains. We plot $(E_2^{O1} - E_1^{O1} - \Delta_1)/(L - 1)$ v.s. $1/\ln(L - 1)$ for medium lengths $L = 20$ to 100, and for long lengths $L = 100$ to 250. The crossover from $(E_2^{O1} - E_1^{O1} - \Delta_1)/(L - 1) \approx a_2^{O1}(1 + b_2^{O1}/\ln(L - 1))$ for medium lengths (dashed line) to $(E_2^{O1} - E_1^{O1} - \Delta_1)/(L - 1) = 74.7/(L - 1)^2$ for long lengths (full line) [13] is evident. The bottom of the magnon dispersion $E_1^{O1} = \sqrt{\Delta^2 + (2.49\pi/L)^2}$ [13] is also plotted (dotted line).

As for excitations in the continuum, we first describe the medium length scaling behavior for integer spin OBC chains. For $S = 1$ chains, we use the following energy expression for medium length:
The leading order scaling $1/L$ for medium chain length has been found numerically in recent studies \cite{11,12} for $S = 2$ Heisenberg chains under various boundary conditions. Given the decreasing of the gap equal to, or more rapid than, the inverse of chain length $1/L$, our calculation gives a lower bound $0.082(3)$ for the gap of $S = 2$ chain. In a previous work \cite{12}, a similar lower bound $0.085(5)$ was also given for the gap using a different boundary condition \cite{11,12}. Since the lower bound of the gap is finite, the existence of a nonzero gap in $S = 2$ Heisenberg chain has been proved by numerical calculations, and therefore, Haldane’s conjecture is verified also for $S = 2$ chain. Moreover, the calculated gap is also in agreement with an earlier calculation in Ref. \cite{14} and a recent experiment \cite{23}. We emphasize that the gap calculation in the present paper disagrees with some other studies \cite{14,11}. This discrepancy may arise from the different scalings used, such as $1/L^2$ scaling \cite{11} for the gap of short $S = 2$ PBC chain, where an exponential type scaling is more appropriate.

To conclude we have performed a systematic study of finite size scaling behavior for the energy spectrum of integer spin chains ($S = 1, 2$), using the DMRG technique. This analysis shows that the lowest excitations are due to the “edge” states for both OBC and PBC chains. As for excitations in the continuum a crossover from $1/L$ behavior for medium chain length to $1/L^2$ behavior for long chain length has been demonstrated. Using this analysis, a reliable estimate for the gap and correlation length in $S = 2$ chains has been obtained.

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\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig5.png}
\caption{The excitation energies for the bottom of one magnon band of medium length $S = 2$ OBC chains (Eq.(6)). We plot $(E_{02}^S - E_{02}^S - \Delta_2)(L-1)$ vs. $1/\ln(L-1)$ for lengths $L = 50$ to 150.}
\end{figure}

[1] F.D.M. Haldane, Phys. Lett. 93A, 464(1983); Phys. Rev. Lett. 50, 1153(1983).
[2] I. Affleck, T. Kennedy, E.H. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799(1987); Commun. Math. Phys. 115, 477(1988).
[3] T.K. Ng, Phys. Rev. B 50, 555(1994).
[4] I. Affleck, Phys. Rev. B 43, 3215(1991); A.M. Tsvelik, Phys. Rev. B 42, 10499(1990).
[5] Y. Ajiro, T. Goto, H. Kikuchi, T. Sakakibara, and T. Inami, Phys. Rev. Lett. 63, 1424(1989); K. Katsumata, H. Hori, T. Takeuchi, M. Date, A. Yamagishi, and J.P. Renard, Phys. Rev. Lett. 63, 86(1989).
[6] O. Golinelli, Th. Jolicoeur, and R. Lacaze, Phys. Rev. B 50, 3037(1994); a collection of references on gap of $S = 1$ spin chains is listed therein.
[7] J.P. Renard, M. Verdaguer, L.P. Regnault, W.A.C. Erke lens, J. Rossat-Mignod, and W.G. Stirling, Europhys. Lett. 3, 945(1988); W.J.L. Buyers, R.M. Morra, R.L. Armstrong, M.J. Hogan, P. Gerlach, and K. Hirikawa, Phys. Rev. Lett. 56, 371(1986).
[8] S. Qin, T.K. Ng and Z-B. Su, Phys. Rev. B 52, 12844 (1995).
[9] E.S. Sorensen and I. Affleck, Phys. Rev. Lett. 71, 1633(1993).
[10] S. Yamamoto, Phys. Rev. Lett. 75, 3348(1995); a collection of references on gap in $S = 2$ spin chains is listed therein.
[11] Y. Nishiyama, K. Totsuka, N. Hatano, and M. Suzuki, J. Phys. Soc. Japan 64, 414(1995).
[12] U. Schollwöck and Th. Jolicoeur, Europhys. Lett. 30, 449(1996).
[13] G. Sun, Phys. Rev. B 51, 8370(1995).
[14] J. Deisz, M. Jarrell, and D.L. Cox, Phys. Rev. B 48, 10227(1993).
[15] S.R. White, Phys. Rev. Lett. 69, 2863(1992), Phys. Rev. B 48, 10345 (1993).
[16] S.R. White and D.A. Huse, Phys. Rev. B 48 3844(1993).
[17] I. Affleck, Phys. Rev. Lett. 54, 966 (1985).
[18] We thank T.K. Ng for suggesting this interpretation.
[19] We thank I. Affleck for pointing out this possibility.
[20] S. White, preprint cond-mat/9604129.
[21] E.S. Sorensen and I. Affleck, Phys. Rev. B 51, 16115(1995); W. Wang, S. Qin, Z.Y. Lu, Lu Yu, and Z.B. Su, Phys. Rev. B 53, 40(1996); X. Wang and S. Mallwitz, Phys. Rev. B 53, 492(1996).
[22] In [3], a rather peculiar boundary condition has been used and the authors have argued that their boundary condition is appropriate. From another point of view, the boundary acts as an impurity for the chain and thus the lowest excitation energy should be less than or equal to the Haldane gap of the chain in certain situations [3,21]. So the lowest excitation energy is the lower bound of the Haldane gap in such systems.
[23] G.E. Granroth, M.W. Meisel, M. Chaparala, B.H. Ward and D.R. Talham, (unpublished).