Topological effects at short antiferromagnetic Heisenberg chains

Jizhong Lou[1], Shaojin Qin[1], Tai-Kai Ng[2], Zhaobin Su[1]
[1]*Institute of Theoretical Physics, P O Box 2735, Beijing 100080, P R China*
[2]*Department of Physics, Hong Kong University of Science and Technology, Hong Kong*
(June 22, 2000)

The manifestations of topological effects in finite antiferromagnetic Heisenberg chains is examined by density matrix renormalization group technique in this paper. We find that difference between integer and half-integer spin chains shows up in ground state energy per site when length of spin chain is longer than $\sim \xi$, where $\xi \sim \exp(\pi S)$ is a spin-spin correlation length, for spin magnitude S up to 5/2. For open chains with spin magnitudes $S = 5/2$ to $S = 5$, we verify that end states with fractional spin quantum numbers S' exist and are visible even when the chain length is much smaller than the correlation length ξ. The end states manifest themselves in the structure of the low energy excitation spectrum.

PACS Numbers: 75.10.Jm, 75.40.Mg

The importance of topological term in antiferromagnetic spin chains was first pointed out by Haldane by mapping the Heisenberg model onto nonlinear σ-model (NLσM)[1,2]. As a direct manifestation of the topological effect, Haldane pointed out that (infinite) integer spin chains have a gap in their excitation spectrum, whereas half-integer spin chains are gapless. The gap Δ in integer spin chains scale as $\Delta \sim Je^{-\pi S}$, where J is the exchange coupling, and S the spin magnitude. Topological effect is expected to manifest itself also at properties not directly related to excitation spectrum, for example, oscillation in ground state energies as S changes from half-integer to integer[3]. More recently Ng pointed out that end states appear as lowest energy excitations in long open spin chains[4,5] due to the same topological term, and the structure of end states spectrum is determined by the spin magnitude S of the spin chain. In this paper we shall study numerically the manifestation of topological effect in finite spin chains with short lengths.

Naively, we expect that difference between integer and half-integer spin chains becomes unobservable when $L \leq \xi \sim e^{\pi S}$, when the Haldane gap energy is comparable with the lowest spinwave excitation energy of the finite spin chain and becomes unobservable. If this is the case, then we expect that the topological effect will be hard to observe for spin chains with large value of spin magnitude S, where the correlation lengths are very long. However, the derivation of the NLσM assumes only that the length scale is much larger than lattice spacing and the topological term exists as long $L >> 1$, independent of the correlation length ξ. Therefore, we expect that topological effect may manifest itself in some properties of spin chain even when chain length L is less than ξ, as long as $L >> 1$. In this paper, we shall study two properties of finite spin chains: the ground state energy and the end states. We find that oscillation in ground state energies between integer and half-integer spin chains is indeed observed numerically when chain length $L \geq \xi$. However the topological end states are much more robust and appear in finite spin chains even when $L << \xi$.

We use the DMRG method[6] to calculate the ground state energy per site for antiferromagnetic Heisenberg open chains with Hamiltonian

$$H = \sum_{j=1}^{L-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \tag{1}$$

where the chain length is L and $\mathbf{S}$ is spin operator. First we consider the large L limit. In this limit the ground energy $e_0(S)$ can be obtained accurately as half of the difference of the energies for length L and $L+2$ chain in DMRG method[7]. We keep $m = 500$ states in DMRG, and the biggest truncation error is 10^{-6}. We obtain the following converging results for thermodynamic limit from data of L up to several thousands:

S	$e_0(S)$	S	$e_0(S)$
0.5	-0.4431471	1.0	-1.4014841
1.5	-2.8283304	2.0	-4.76124365
2.5	-7.1922313	3.0	-10.1237525
3.5	-13.5553061	4.0	-17.486892
4.5	-21.918498	5.0	-26.850118

The ground state energy for $S = 1/2$ chain is exactly known, with $e_0(0.5) = 1/4 - \ln(2) \sim -0.4431471$. The energy for $S = 1$ chain has also been obtained to very high accuracy[7], where $e_0(1) = -1.401484038971$. In a paper demonstrating the $k = 1$ $SU(2)$ WZW low energy behavior of $S = 3/2$ chain[8], the ground state for it has been accurately obtained, with $e_0(1.5) = -2.82833$. The energy for $S = 2$ chain was obtained in another paper demonstrating its massive relativistic low energy property[9], $e_0(2) = -4.761244$. Our calculation is in agreement with these earlier studies[10].

The energies can be compared with a $1/S$ expansion:

$$e_0(S) = -S^2 + (2/\pi - 1)S + a_0 + a_1/S + \ldots, \tag{2}$$

where the first two terms were obtained from spin-wave theory[11]. In Fig. 1 we plot $-S^2 - (1 - 2/\pi)S - e_0(S)$ as a function of $1/S$. Our numerical result shows clearly the oscillatory nature of $e_0(S)$ between integer and half integer spin chains and $e_0(S)$ cannot be fitted by a single monotonic function of $1/S$. Assuming that the oscillatory behaviour is coming from topological terms in $NL\sigma M$ we expect that the oscillatory part of the ground state energy scales as $exp(-\pi S)$ and is nonanalytic in a $1/S$ expansion. This is indeed consistent with our numerical result as can be seen from the fitting in Fig. 1.

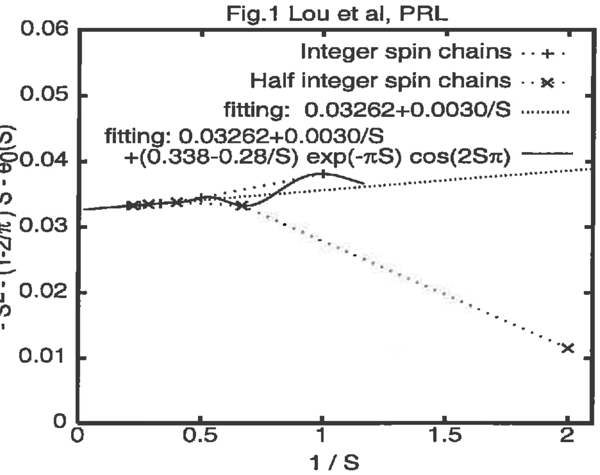

FIG. 1. Ground state energy for antiferromagnetic Heisenberg chains. $-S^2-(1-2/\pi)S-e_0(S)$ vis $1/S$ is plotted and fit by polynomial of $1/S$. The ground state energies for integer spin chains and half integer spin chains cannot be fitted by a single monotonic curve. The difference decreases to zero very fast as S increases. We note that the $S=1/2$ point is not used in the fitting process

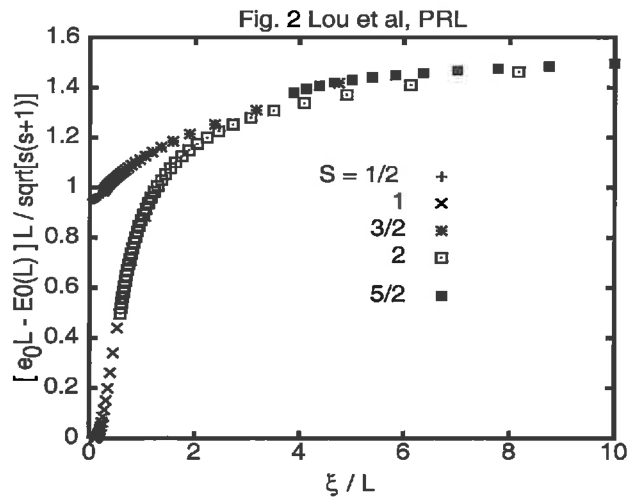

FIG. 2. Finite size scaling for ground state energy $E0(L)$ for antiferromagnetic Heisenberg chains. $(e_0-E0/L)/\sqrt{S(S+1)})$ versus inverse of the renormalized length L/ξ is plotted for $S=1/2,1,3/2,2,$ and $5/2$ with approximated values of $\xi=2,6.3,19,49,$ and 140, respectively. Integer S and half-integer S chains behave differently in finite size scaling, but the difference vanishes for small L when $\xi/L\geq 1$,

As is shown in Fig. 1, for $S\geq 3$, the energy differences between integer and half integer spin chains due to topological effects are very weak. To examine the chain length dependence of ground state energy we plot in Fig. 2 the the length dependence of the finite length correction of the ground state energy $L*(e_0*L-E0(L))/\sqrt{S(S+1)})$ versus the inverse of renormalized length L/ξ for various value of spin magnitude S up to $S=5/2$. The correlation lengths are estimated independently through various fittings and the scaling behaviour is insensitive to the fluctuation in values of ξ within ~ 10 percent. $E0(L)$ is computed using DMRG method for chains with periodic boundary condition (PBC). It is clear from the figure that the ground state energies of integer and half-integer spin chains behave differently in finite size scaling, and the difference vanishes as $L\leq\xi$, in agreement with naive expectation based on Haldane gap argument.

It was pointed out in Ref. [4] that topological effect also leads to appearance of end states in open spin chains. For integer spin chains with length $L>>\xi$ end spins with magnitude $S/2$ appear at each end of spin chain and are coupled to each other with effective Hamiltonian

$$H_{eff}=J(L)\mathbf{S'}_1\cdot\mathbf{S'}_L, \qquad (3)$$

where $\mathbf{S'}_1$ and $\mathbf{S'}_L$ are the two end spins on the ends of the open chain. $J(L)\sim Je^{-L/\xi}$ is positive for even L and negative for odd L. For half-integer spin chains end spins with magnitude $(S-1/2)/2$ appear and are coupled to each other with same effective Hamiltonian (3) except that $J(L)\sim\frac{J}{L\ln(L)}$ for large L. Notice that bulk spin-wave excitations have energies scale as $\sim 1/L$ for large L and the lowest spin excitations of both integer and half-integer open spin chains are end-spin excitations when L is large enough. Note that end states for $S=1$[7,12] and $S=3/2,2$[13] open chains have been observed numerically in long chains $L>>\xi$ with properties in agreement with end state theory[4]. The question of interests here is whether these end states remain robust as spin value S increases, with length of spin chains reduce to $L<\xi$. We expect that the end states may stay robust because in general energy level crossings have to occur if end states are moved out of the low energy excitation spectrum. We shall show in the following that end states are observed as lowest energy excitations in open spin chains for large spin magnitude S up to 5 with chain lengths much smaller than ξ.

We consider spin chains with spin magnitudes $5/2\leq S\leq 5$ and with even number of sites with chain lengths from $L=4$ to 30. Notice that by restricting ourselves to chains with large value of S and short lengths ≤ 30 we are always in the limit $L \leq \xi$ in our numerical study. By keeping $m = 450$ states in DMRG. We calculate the lowest energy states in sectors with $S_z^{tot} = 0, 1, \ldots, S+1$. The biggest truncation error is 10^{-4} for $S = 5$. According to end state theory, the lowest $2S' + 1$ states in the excitation spectrum should have $S^{tot} = 0, 1, \ldots, 2S'$ in increasing order of energy, where $S' = S/2$ for integer spin chains and $S' = (S - 1/2)/2$ for half-integer chains, the bulk spinwave spectrum appears only above these states.

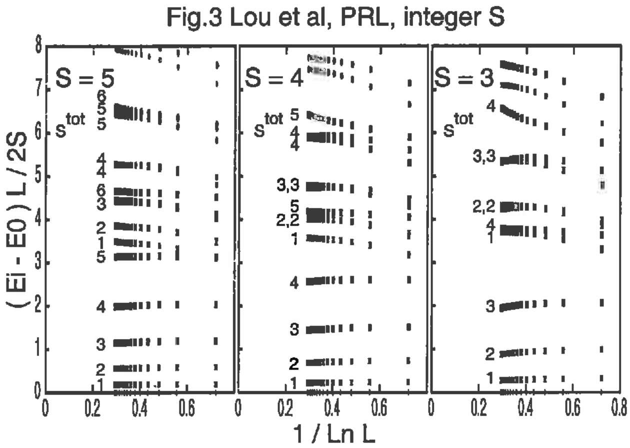

FIG. 3. Low energy excitations times chain length for integer spin $S = 3$ to 5 open chains. The ground state is of total spin $S^{tot} = 0$. The $S+1$ lowest excited states from low energy to high energy are $S^{tot} = 1, \ldots, S$, and $S^{tot} = 1$ from bottom to top.

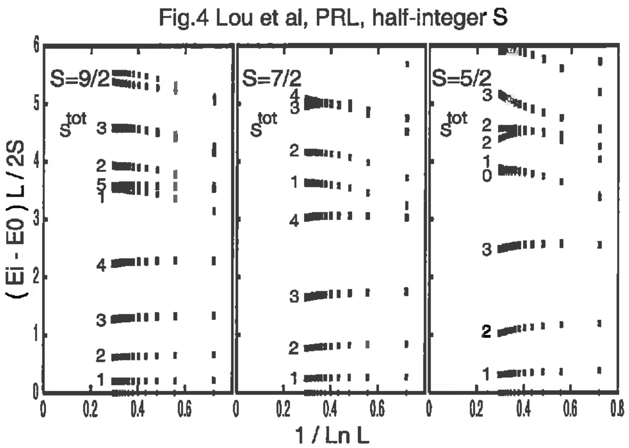

FIG. 4. Low energy excitations times chain length for half-integer spin $S = 5/2$ to $S = 9/2$ open chains. The ground state is of total spin $S^{tot} = 0$. The $S - 1/2$ lowest excited states from low energy to high energy are $S^{tot} = 1, \ldots, S - 1/2$.

We show the low energy excitation spectrum for open integer spin chains in Fig. 3. Starting from the ground state energy $E0$, we label the i^{th} excited states' energy as Ei. For integer spin chains, we find indeed that the lowest $S+1$ energy levels are ordered in sequence with $S^{tot} = 0, 1, \ldots, S$ from ground state to the S^{th} excited states. Above this series of states, spinwave excitations appear, starting with total spin $S^{tot} = 1$. The corresponding low energy spectrum for open half integer spin chains is shown in Fig. 4, and the same structure is observed- the lowest $S + 1/2$ energy levels are ordered in sequence with $S^{tot} = 0, 1, \ldots, S - 1/2$ from ground state to the $(S - 1/2)^{th}$ excited states. Above these series of states, spinwave excitations appear. These are exactly the spectra predicted by the end state theory.

To examine the nature of these low lying states further we investigate the validity of Eq. (3) in describing the energies of these states. It is easy to show that Eq. (3) predicts that the number series $y(i) = (Ei - E0)/(E1 - E0)$ for the end states is given by the simple mathematical expression $y(i) = i(i+1)/2$, independent of chain lengths L and spin magnitude S.

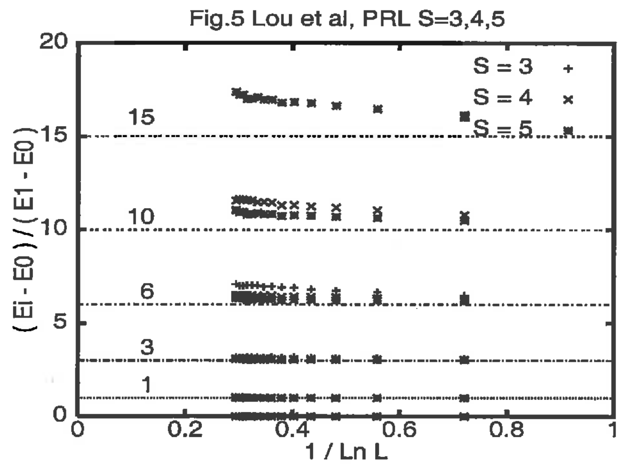

FIG. 5. Edge excitation energy for integer spin chains.

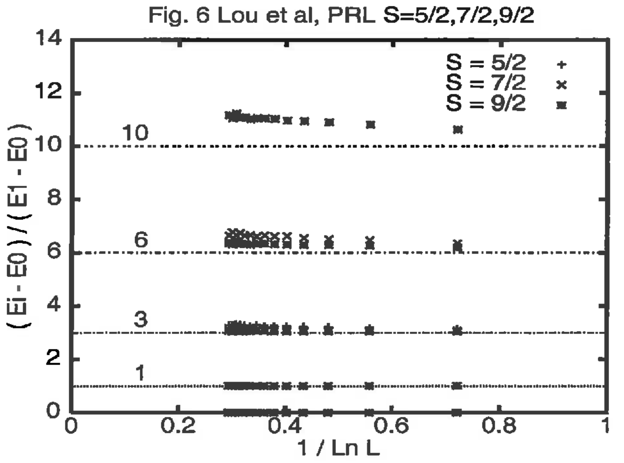

FIG. 6. Edge excitation energy for half integer spin chains.

In Fig. 5 and Fig. 6, we plot respectively, $y(i)$ for the $2S'$ lowest energy levels given by DMRG versus $1/\ln L$ for integer spin chain and half integer spin chains. It is clear that Eq. (3) describes quite well the qualitative behaviour of the lowest $2S'$ states of the excitation spectra for all chains with different spin values and lengths under investigation, despite that we are already in the $L < \xi$ limit.

Summarizing, we study in this paper using DMRG method several manifestions of topological effect in finite Heisenberg spin chains. We confirm the oscillation of ground state energies between integer and half-integer spin chains. The magnitude of the oscillatory part of ground state energies goes down very rapidly as S increases and is consistent with an $e^{-\pi S}$ behaviour. The oscillation becomes unobservable when chain length L decreases to less than ξ, in agreement with argument based on Haldane gap. We have also study open spin chains where topological effect also manifest itself as end states. Surprisingly, we find strong numerical evidence that end states stay robust as chain length L's decrease and are observable even when $L << \xi$. Our result confirms the theoretical expectation that the topological effect is a robust property of quantum spin chains and exists as long as chain length $L >> 1$, independent of the appearance of Haldane gap in the excitation spectrum.

This work is partially supported by Chinese Natural Science Foundation, HKUGC under RGC grant HKUST6143/97P. T.K. Ng acknowledge the hospitality of the Issac Newton Institute for Mathematical Sciences at which this paper is partly written.

---

[1] F.D.M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).

[2] see I. Affleck, in *Field Theory Methods and Quantum Critical Phenomena*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1990) for a review.

[3] S. C. Zhang, H. J. Schulz, and Timothy Ziman, Phys. Rev. Lett. **63**, 1110 (1989).

[4] T.K. Ng, Phys. Rev. B **52**, 555(1994).

[5] I. Affleck, T. Kennedy, E.H. Lieb and H. Tasaki, Phys. Rev. Lett. **59**, 799 (1987); Commun. Math. Phys. **115**, 477 (1988).

[6] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993); R. M. Noack and S. R. White, "The density matrix renormalization group" in *Lecture Note in Physics:* Density-Matrix Renormalization, Eds. I. Peschel, X. Wang, M. Kaulke and K. Hallberg, Springer (1999).

[7] S. R. White and D. A. Huse, Phys. Rev. B **48** 3844 (1993).

[8] K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. **76**, 4955 (1996).

[9] S. Qin, X. Wang and Lu Yu, Phys. Rev. B **56**, 14251(1997).

[10] H. Q. Lin, Phys. Rev. B **42**, 6561(1990).

[11] P. W. Anderson, Phys. Rev. **86**, 694 (1952).

[12] T. Kennedy, J. Phys: Cond. Matter **2**, 5737 (1990).

[13] S. Qin, T.K. Ng, and Z.B. Su, Phys. Rev. B **52**, 12844(1995); S. Qin, Y.L. Liu, and Lu Yu, *ibid.* **55**, 2721(1997).

Recent Newton Institute Preprints

NI00001-SMM **KZ Markov**
Justification of an effective field method in elasto-statics of heterogeneous solids

NI00002-SCE **YY Lobanov and VD Rushai**
Studying the evolution of open quantum systems via conditional Wiener integrals

NI00003-SCE **J-G Wang and G-S Tian**
Spin and charged gaps in strongly correlated electron systems with negative or positive couplings

NI00004-SCE **FV Kusmartsev**
Conducting electron strings in oxides

NI00005-ERN **SG Dani**
On ergodic Z^d actions on Lie groups by automorphisms

NI00006-SMM **V Nesi and G Alessandrini**
Univalence of σ-harmonic mappings and applications

NI00007-SCE **X Dai, T Xiang, T-K Ng et al**
Probing superconducting phase fluctuations from the current noise spectrum of pseudogaped metal-superconductor tunnel junctions

NI00008-ERN **B Hasselblatt**
Hyperbolic dynamical systems

NI00009-SCE **J Lou, S Quin, T-K Ng et al**
Topological effects at short antiferromagnetic Heisenberg chains

NI00010-SCE **V Zlatić and J Freericks**
Theory of valence transitions in Ytterbium-based compounds

NI00011-ERN **A Iozzi and D Witte**
Cartan-decomposition subgroups of SU(2,n)

NI00012-ERN **D Witte and L Lifschitz**
On automorophisms of arithmetic subgroups of unipotent groups in positive characteristic

NI00013-ERN **D Witte**
Homogeneous Lorentz manifold with simple isometry group

NI00014-SGT **R Uribe-Vargos**
Global theorems on vertics and flattenings of closed curves

NI00015-SGT **EA Bartolo, P Cassou-Nogués, I Luengo et al**
Monodromy conjecture for some surface singularities

NI00016-SGT **IG Scherbak**
Boundary singularities and non-crystallographic Coxeter groups

NI00017-SGT **K Houston**
On the classification and topology of complex map-germs of corank one and $\mathcal{A}_e$-codimension one

NI00018-SGT **PJ Topalov and VS Matveev**
Geodesic equivalence via integrability

NI00019-GTF **S Friedlander**
On vortex tube stretching and instabilities in an inviscid fluid

NI00020-SGT **VD Sedykh**
Some invariants of admissible homotopies of space curves

NI00021-SGT **IA Bogaevsky**
Singularities of linear waves in plane and space

Information about Newton Institute Preprints is also available at
`http://www.newton.cam.ac.uk/preprints.html`