LOGARITHMIC CORRECTIONS FROM FERROMAGNETIC
IMPURITY ENDING BONDS OF OPEN ANTIFERROMAGNETIC
HOST CHAINS

Jizhong Lou
Institute of Theoretical Physics,
P.O. Box 2735, Beijing 100080, People’s Republic of China,

Jianhui Dai
Zhejiang Institute of Modern Physics, Zhejiang University,
Hangzhou 310027, People’s Republic of China,

Shaojin Qin, Zhaobin Su
Institute of Theoretical Physics,
P.O. Box 2735, Beijing 100080, People’s Republic of China

and

Lu Yu
Institute of Theoretical Physics,
P.O. Box 2735, Beijing 100080, People’s Republic of China

and

The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

MIRAMARE – TRIESTE
June 2000
Abstract

We analyze the logarithmic corrections due to ferromagnetic impurity ending bonds of open spin 1/2 antiferromagnetic chains, using the density matrix renormalization group technique. A universal finite size scaling $\sim \frac{1}{L \log L}$ for impurity contributions in the quasi-degenerate ground state energy is demonstrated for a zigzag spin 1/2 chain at the critical next nearest neighbor coupling and the standard Heisenberg spin 1/2 chain, in the long chain limit. Using an exact solution for the latter case it is argued that one can extract the impurity contributions to the entropy and specific heat from the scaling analysis. It is also shown that a pure spin 3/2 open Heisenberg chain belongs to the same universality class.
The logarithmic corrections due to marginally irrelevant operators\(^1\) complicate greatly the comparison of experiments and numerical simulation results for finite size systems with analytical calculations. However, a careful analysis in some specific cases may yield useful information on the low energy excitation spectrum and relevant physical quantities. In this Report, we consider the finite size scaling for open spin 1/2 antiferromagnetic (AF) chains with ferromagnetic (FM) coupling at the ending bonds. This system exhibits the same behavior as a Kondo impurity coupled ferromagnetically to a Luttinger liquid.\(^2\)–\(^5\) In these systems the Kondo screening is not complete, and the ground state is quasi-degenerate, \(i.e.\) the level spacing is vanishing faster than \(1/L\), where \(L\) is the system size. Recently, some exactly solvable models belonging to this class have been found, and the impurity entropy as well as specific heat has been obtained through thermodynamic Bethe ansatz\(^4\)–\(^6\). We will show in this report the universal behavior of logarithmic corrections for this class of systems and, using the exact solution, we will argue that one can extract from the scaling analysis the impurity contributions to the entropy and specific heat when the exact solutions are not available. We will also show that a pure open spin 3/2 AF chain (without additional FM ending bonds) belongs to the same universality class.

The impurity effects in spin 1/2 Heisenberg AF chains have been discussed extensively in Ref. 7. The logarithmic corrections to scaling functions for spin 1/2 Heisenberg chains have been discussed in recent papers.\(^8\)–\(^\infty\) Those corrections are due to bulk marginally irrelevant operators, although their manifestations depend on boundary conditions.\(^9\) Instead, we will carry out a detailed numerical analysis of the finite size scaling for the ground state near-degeneracy and low energy spectrum of open \(s = 1/2\) spin chains due to FM ending bonds. To the best of our knowledge, this issue has not been addressed numerically up to now. We first consider the following Heisenberg chain with next nearest neighbor coupling, or equivalently, a zigzag chain:

\[
H = \sum_{i=2}^{L-2} S_i \cdot S_{i+1} + J_{2c} \sum_{i=2}^{L-3} S_i \cdot S_{i+2} + H_{imp},
\]

\[
H_{imp} = -S_1 \cdot S_2 - S_{L-1} \cdot S_L,
\]

where \(L\) is the chain length and \(S_i\) is the \(s = 1/2\) spin on site \(i\). We draw the system in Fig. 1. The nearest neighbor coupling is set to \(J = 1\) and the next nearest neighbor coupling is set to the critical value\(^12\) \(J_2 = J_{2c} = 0.2411\). The two ending bonds are FM \(J' = -1\), and the ending sites are impurity spins, also \(s = 1/2\). There are no logarithmic corrections due to zero initial bulk marginal coupling at the critical value \(J_2 = J_{2c}.\)\(^13,14\) Therefore, all logarithmic corrections in our calculations are coming entirely from the boundary effects.

![Fig. 1 Lou et al. PRB](image)

**FIG. 1.** Open zigzag spin chain with coupling \(J\) and \(J_2\) for nearest and next nearest neighbors, respectively. Two ending impurity spins couple to the bulk by a FM bond \(J' < 0\).
A pure open zigzag chain without $H_{\text{imp}}$ has the same low energy spectrum as the pure open $s = 1/2$ chain when $0 < J_2 < J_{2c}$. There is a unique ground state with total spin $S = 0$, and one first excited state of spin $S = 1$, with excitation energy scaled as $\pi v/L$ for finite size chains, where $v$ is the spin velocity. For the zigzag chain shown in Fig. 1 with FM ending bonds, the ending spins are not fully screened, and there is an RKKY coupling between them scaled as $J_{RKKY}(L) = \frac{a}{L \log L}$ in the large $L$ limit. The two ending impurity spins form a singlet and a triplet with energy spacing $J_{RKKY}(L)$. We identify the following low energy states:

1. Two quasi-degenerate ground states: One is composed of the bulk $S = 0$ state and singlet impurity state with energy $E_0^\text{O}$; the other is formed by the bulk $S = 0$ state and the triplet impurity state with energy $E_1^\text{O}$. We take $J_{RKKY}(L) = E_1^O - E_0^O$ as the definition of $J_{RKKY}(L)$.

2. Four quasi-degenerate first excited states with excitation energy scaled as $\pi v/L$. One is composed of the bulk $S = 1$ state and singlet impurity state with energy $E_1^\text{I}$. The other three are formed by the bulk first excited $S = 1$ state and triplet impurity state with energies $E_1^\text{I}E_1^\text{II}$, $E_1^\text{I}E_1^\text{II}$, and $E_1^\text{I}E_1^\text{II}$, for the total spin $S = 2, 1, 0$, respectively. Due to the bulk $S = 1$ excitation propagating in-between the ending spins, the energy difference $E_1^\text{II} - E_1^\text{I}$ is not the same as $J_{RKKY}(L)$.

We use density matrix renormalization group (DMRG) method to calculate low energy levels for the above Hamiltonian. By keeping $m = 150$ states, the truncation error is as small as $10^{-7}$. We study even length chains only. The low-lying excitation energies are plotted vs $1/\log L$ in Fig. 2. In Fig. 2a we see the ground state is degenerate at the scale of the graph. The first four excitation energies scale to $\pi v/L$. They correspond to $E_2^\text{II}, E_1^\text{I}, E_1^\text{II}$, and $E_0^\text{I}$, respectively, from bottom up. We note the ratio between the two energy spacings $E_0^\text{I} - E_1^\text{II}$ and $E_1^\text{I} - E_2^\text{II}$ is approximately 1:2, which indicates these excitations can be identified as due to coupling of the bulk $S = 1$ state and impurity triplet state. The next group of six energy levels scales to $2\pi v/L$. They are composed of the impurity singlet/triplet states and the two bulk levels scaled as $2\pi v/L$ of spin $S = 0$ and $S = 1$. We have drawn guiding lines to separate these two groups of lowest excitations. In Fig. 2b, we magnify the scale of the energy spacing for the quasi-degenerate ground states to show the scaling $E_1^O - E_0^O = J_{RKKY}(L) \sim \frac{1}{L \log L}$. Since there are no bulk logarithmic corrections involved at the critical coupling $J_{2c}$ for zigzag chains, the logarithmic term appears solely due to the Kondo impurity effect. If the ending bound coupling $J' = 0$, the end impurity spins are decoupled from the bulk and the ground state is exactly degenerate. The impurity has nonzero entropy at zero temperature. When $J' < 0$, the ground state and low energy spectrum have an asymptotic degeneracy and the energy difference between these quasi-degenerate states scales as $\frac{1}{L \log L}$. This has been very clearly seen for the ground state. The zero temperature entropy will change, as we shall argue, depending on the coefficient $a$ in the ground state energy scaling $J_{RKKY}(L) = \frac{a}{L \log L}$. We will see that this logarithmic scaling behavior due to boundary spins is universal for systems composed of Kondo impurities ferromagnetically coupled to Luttinger liquids, even when there are also logarithmic corrections due to bulk marginally irrelevant operators.
FIG. 2. Excitation energies times the chain length, \((E^K_f - E^Q_0)L\), vs \(1/\log L\) are plotted in figure (a) for the zigzag chain shown in Fig. 1. Scaling for the quasi-degenerate ground state, \((E^Q_f - E^Q_0)L\) vs \(1/\log L\), is plotted in figure (b) along with a fitting line.
FIG. 3. Excitation energies times the chain length, \((E^K_i - E^K_0)L\), vs \(1/\log L\) are plotted in figure (a) for spin 1/2 Heisenberg AF chain with FM ending bonds. Scaling for the quasi-degenerate ground state, \((E^Q_1 - E^Q_0)L\) vs \(1/\log L\), is plotted in figure (b) along with a fitting line.

We consider now an open spin 1/2 AF Heisenberg chain with impurity ending bonds described by the Hamiltonian

\[
H = \sum_{i=2}^{L-2} \mathbf{S}_i \cdot \mathbf{S}_{i+1} - \mathbf{S}_1 \cdot \mathbf{S}_2 - \mathbf{S}_{L-1} \cdot \mathbf{S}_L.
\]  

(2)

The nearest neighbor coupling is set to \(J = 1\) and the FM coupling \(J'\) for the ending spin is set to \(J' = -1\). For a pure spin 1/2 open chain without FM impurity bonds, the ground state energy scales as \(E = e_0 L + e_1 - \frac{\pi v}{24L} [1 + b/\log^2(L) + \ldots]\), where \(e_0\) is the site energy, \(e_1\) is the boundary energy, and \(v\) is the spin velocity for spin 1/2 Heisenberg chain. The logarithmic correction appears here due to the bulk marginally irrelevant operator. We will demonstrate the ground state energy has one more term \(L/\log L\) in its finite size scaling due to FM Kondo coupling:

\[
E^Q_1 = e_0 L + e_1 - \frac{\pi v}{24L} + \frac{a}{L \log L} + \ldots.
\]  

(3)

We calculate the energy levels by using DMRG method for even length chains. We keep \(m = 200\) states and the truncation error is of the order \(10^{-9}\). The ground state is the same as for Hamiltonian (1), with energy \(E^K_0\). The energy levels \(E^K_i\) are also labeled the same way. We plot the excitation energies \((E^K_i - E^K_0)L\) vs \(1/\log L\) in Fig. 3a. In Fig. 3b, the scaling \(E^Q_1 - E^Q_0 \sim \frac{0.6}{L \log L}\) is exhibited. The first excited states are four-fold degenerate as we analyzed before for the zigzag chains. We have drawn guiding lines in Fig. 3 to group these first excited states together. For the low energy spectrum, the excitations are again composed of the combined impurity and bulk spin states. The logarithmic scaling behavior of a standard Heisenberg chain due to FM impurity bonds is identical to that of zigzag chain, as the correction due to the bulk marginally irrelevant operator is of higher order.
FIG. 4. Energy of one of the quasi-degenerate ground states with total spin $S = 1$ $E^O_1$, obtained from the exact solution is plotted vs $\frac{1}{L \log L}$ along with the fitting line.

On the other hand, the model has been solved exactly using the Bethe Ansatz, we can extract its ground state energy from the exact solution. We calculate, using the Bethe Ansatz equations of Ref. 5, the energy $E^O_1$ of $S = 1$ state for system size up to more than four thousands sites. (We have not yet obtained the energy for another degenerate ground state with lower energy $E^O_0$ from the Bethe ansatz equations.) Following Eq.(3), we plot $E^O_1 - e_0 L + \frac{\pi v}{24L}$ vs $\frac{1}{L \log L}$ in Fig. 4, where the site energy $e_0 = 1/4 - \log 2$, and the spin velocity $v = \pi / 2$. We obtain $E^O_1 - e_0 L + \frac{\pi v}{24L} = 0.787984 + \frac{0.66}{L \log L}$ by the least square fitting. Based on Eq.(3), we have $e_1 = 0.787984$. We obtain also the scaling $J_{RKKY}(L) \sim \frac{0.66}{L \log L}$ from the exact solution, to be compared with an almost identical fitting of the DMRG data (coefficient $a = 0.6$ instead of 0.66 in the scaling formula $J_{RKKY}(L) = \frac{a}{L \log L}$). Therefore, we conclude that the quasi-degenerate ground state and low-lying excitations of Luttinger liquids with FM Kondo impurities can be indeed described by this logarithmic scaling function.

Moreover, using the exact solution, the impurity entropy and specific heat can be expressed in terms of the coefficient $a$ in the above finite size scaling. If two systems have the same ground state degeneracy and the same low-energy excitation spectrum, the thermodynamic properties at very low temperatures should also be identical to each other. Using this argument, we can estimate the impurity entropy and specific heat from the finite size scaling analysis of the energy spectrum even in the case when the exact solution is not available (e.g. the zigzag chain considered earlier). Using the same argument we will discuss another related system, an open spin 3/2 AF chain without additional FM ending bonds.
The spin 3/2 chain has been shown to have the same low energy physics as for spin 1/2 chain.\textsuperscript{17} When the chain is open, there are effective edge $s' = 1/2$ spins left at the ends of the chain.\textsuperscript{18} It was shown earlier\textsuperscript{19} that the energy spacing between the two degenerate ground states scales as $\frac{1}{\log L}$. However, the scaling of the low energy spectrum is very difficult to study and the logarithmic corrections are big.\textsuperscript{17} Following the way of dealing with such edge spins for integer spin chains,\textsuperscript{20} it was proposed to treat them as impurity spins ferromagnetically coupled to the bulk spin excitations.\textsuperscript{19} Unlike the previous cases, there are no additional FM impurity bonds at the ends of spin 3/2 chains. Now we calculate the scaling of the ground state energy spacing $J_{RKKY}(L) = \frac{a}{L \log L}$ by DMRG. We keep $m = 1000$ states in DMRG and the truncation error is $10^{-6}$. We calculate only a few low energy levels and plot the excitation energies times length vs $1/\log L$ in Fig. 5. We obtain the coefficient $a = 3.9$ in scaling $J_{RKKY}(L) = \frac{a}{L \log L}$. With the known spin velocity $v = 3.87$ for spin 3/2 chain,\textsuperscript{17} we obtain a nonzero entropy at zero temperature. Its exact value can be expressed in term of $a$ analytically when exact solution is available. (Non-zero impurity entropy is also predicted in Takhatajan-Babujian spin-3/2 chain with spin-1/2 boundary impurities, where Bethe ansatz solution is available.\textsuperscript{6}) We hope such a nonzero entropy at zero temperature can be measured in quasi-one-dimensional spin 3/2 materials such as $CsVCl_3$ (Ref. 21), $AgCrP_2S_6$ (Ref. 22), etc.

In summary, we have carried out a detailed analysis of the low energy spectrum of FM Kondo impurity in Luttinger liquids, or equivalently, an open spin 1/2 AF Heisenberg chain. We have shown this class of models has a universal logarithmic quasi-degeneracy in the low energy states due to the RKKY interaction between the unscreened edge spins. We argue that nonzero entropy at zero temperature can be obtained for FM Kondo impurity system by studying the finite size scaling of the ground state energies.

\textit{Acknowledgments} J. Lou and S. Qin would like to thank Prof. T.K. Ng for valuable discussions. This work is partially supported by Chinese Natural Science Foundation.
References

1. J. L. Cardy, J. Phys. A19, L1093 (1986).

2. D.-H. Lee and J. Toner, Phys. Rev. Lett. 69, 3378 (1992); A. Furusaki and N. Nagaosa, Phys. Rev. Lett. 72, 892 (1994).

3. P. Fröjd and H. Johannesson, Phys. Rev. Lett. 75, 300 (1995).

4. Y. Wang, J. Dai, Z. Hu and F.-C. Pu, ibid. 79, 1901 (1997); J. Dai and Y. Wang, Phys. Rev. B 60, 12309 (1999).

5. Y. Wang, Phys. Rev. B 56, 14045 (1997).

6. J. Dai, Y. Wang and U. Eckern, Phys. Rev. B 60, 6594 (1999).

7. S. Eggert and I. Affleck, Phys. Rev. B46, 10866 (1992).

8. V. Barzykin and I. Affleck, cond-mat/9810075.

9. I. Affleck and S. Qin, J. Phys. A32, 7815 (1999).

10. V. Brunel, M. Boucquet and Th. Jolicoeur, Phys. Rev. Lett. 83, 2821 (1999).

11. S. -W. Tsai and J. B. Marston, cond-mat/0001275.

12. K. Okamoto and K. Nomura, Phys. Lett. A169, 433 (1992).

13. F.D.M. Haldane, Phys. Rev. B 25 4925 (1982); ibid. 26, 5257 (1982).

14. I. Affleck, D. Gepner, H.J. Schulz and T. Ziman, J. Phys. A22, 511 (1989).

15. 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 Notes in Physics: Density-Matrix Renormalization, Eds. I. Peschel, X. Wang, M. Kaulke and K. Hallberg, Springer (1999).

16. E. S. Sorensen, S. Eggert, and I. Affleck, J. Phys. A26, 6757 (1993).
17 K. Hallberg, X. Q. G. Wang, P. Horsch, and A. Moreo, Phys. Rev. Lett. 76, 4955 (1996).

18 T.K. Ng, Phys. Rev. B 52, 555(1994).

19 S. Qin, T.K. Ng, and Z.B. Su, Phys. Rev. B 52, 12844 (1995).

20 E. S. Sorensen and I. Affleck, Phys. Rev. B 49, 15771 (1994).

21 S. Itoh, K. Kakurai, Y. Endoh, and H. Tanaka, Physica B213&214, 161 (1995).

22 H. Mutka, C. Payen, P. Molinie, and R. S. Ecclestone, Physica B213&214, 170 (1995).
Fig. 5 Lou et al., PRB

fitting line: $3.9 \times$

$y = 1 / \log L$
Fig. 4 Lou et al., PRB

exact solution

$0.787984 + 0.66x$

$x = 1 / L / \log L$
energy spacing between two degenerate ground states times chain length

Fig. 3b Lou et al., PRB
energy spacing between two degenerate ground states times chain length

Fig 2b Lou et al., PRB
excitation energy times the chain length

Fig. 2a Lou et al., PRB
Fig. 1 Lou et. al. PRB