Numerical evidences of spin-1/2 chain approaching spin-1 chain

Hsiang-Hsuan Hung\textsuperscript{1} and Chang-De Gong\textsuperscript{2,1,3}

\textsuperscript{1}National Key Laboratory of Solid State Microstructure and Department of Physics, Nanjing University, Nanjing 210093, China\textsuperscript{2}
\textsuperscript{Chinese Center of Advanced Science and Technology (World Laboratory) P.O. Box 8730, Beijing 100080, China and\textsuperscript{3}}
Department of Physics, The Chinese University of Hong Kong, Hong Kong, China

Abstract

In this article, we study the one dimensional Heisenberg spin-1/2 alternating bond chain in which the nearest neighbor exchange couplings are ferromagnetic (FM) and antiferromagnetic (AF) alternatively. By using exact diagonalization and density matrix renormalization groups (DMRG) method, we discuss how the system approaches to the AF uniform spin-1 chain under certain condition. When the ratio of AF to FM coupling strength $\alpha (\alpha = J_{AF}/J_{F})$ is very small, the physical quantities of the alternating bond chain such as the spin-spin correlation, the string correlation function and the spin density coincide with that of the AF uniform spin-1 chain. The edge state problem is discussed in the present model with small $\alpha$ limit. In addition, the Haldane gap of the AF uniform spin-1 chain is 4-times of the gap of the system considered.
Haldane argued that the elementary excitation spectrum in the one dimensional (1-D) antiferromagnetic Heisenberg (AFH) spin system with integer spin is gapful (massive) whereas for the system with half-integer spin is gapless (massless). Furthermore, the spin-spin correlation in the ground state for 1-D AFH spin-1 systems should have the exponential decay behavior due to the gapful excitation energy. By contrary, in 1-D AFH spin-1/2 systems, the spin-spin correlation function exhibits power law decay behavior due to the gapless excitation energy. There are many numerical studies to investigate this conjecture. On the other hand, the spin gap has been observed in the compound NENP[Ni(C$_2$H$_8$N$_2$)$_2$NO$_2$ClO$_4$] through the susceptibility measurement by inelastic neutron scattering experiment.

Among different studies of the Haldane problem in AFH spin-1 chain, the interested one is given by AKLT model. This model gave a simple picture for the ground state of 1-D AFH spin-1 system. Each S=1 spin was viewed as a triplet state of two spins with $S = 1/2$. According to this picture, only two end spins of the open AKLT chain are left and form two "free" $S = 1/2$ spins which are called the edge state and all the other $S = 1/2$ spins form RVB type spin singlet state between nearest neighbor spins. In the thermodynamic limit, the spin-1 chain is fourfold degeneracy due to the two $S = 1/2$ spins. This picture was observed experimentally and discussed theoretically. For an open spin-1 chain the Haldane gap is the difference between the lowest eigen-energy in subspace $S^z_{tot} = 0$ (or $S^z_{ot} = 1$) and $S^z_{ot} = 2$. Although spin-1 chain is a disorder system, it still has a hidden order, the corresponding order parameter proposed by M.den Nijs and K. Rommelse is represented by the string correlation defined in the later discussion. Since after, the numerical studies have been performed for 1-D spin-1 Heisenberg model and have proven that the systems really posses the hidden order.

In this article the Haldane problem is studied from another reversed approach. We start from a 1-D AFH spin chain with $S = 1/2$, the exchange couplings between nearest neighbor spins take $J_1$ and $J_2$ alternatively as shown in Fig.1. The Hamiltonian is

$$H = J_1 \sum_{<i\in \text{odd}>} \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_{<j\in \text{even}>} \vec{S}_j \cdot \vec{S}_{j+1}$$

(1)

This model which is called alternating bond chain has been studied in detail. In general, the excitation spectrum of this model is gapful except the case of $J_1 = J_2$, i.e. it reduced to the uniform spin-1/2 chain. We may ask the questions that, what is the relation between the Haldane gap and the gap of model (1), and how can we understand the edge state of AKLT
model in a reasonable way. For definiteness, we are interested in the special case, where \( J_1 < 0 \) (ferromagnetic coupling FM) and \( J_2 > 0 \) (antiferromagnetic coupling AF). We define a parameter \( \alpha = |J_2/J_1| \) and explore how the magnetic behavior of the system evolves with the parameter \( \alpha \). We use two numerical techniques including the exact diagonalization method up to the system \( N=32 \) (\( N \) is the number of sites) with periodic boundary condition and DMRG method[16] to even more large system (\( N=360 \)) with open boundary condition.

At first, in the case of large \( \alpha \) limit, the two nearest neighbor spins connected with AF bond will form an AF singlet dimer and the 1-D chain reduces to \( N/2 \) \( S=0 \) dimers connected with FM bond. As well known that the first excited state is the state in which one of the \( N \) \( S=0 \) dimers is excited to become a triplet, i.e. the excitation energy is \( \Delta = J_2 \). In opposite case of small \( \alpha \) limit, the two nearest neighbor spins connected with a FM bond will form a FM triplet dimer and the AF coupling exists between triplet dimers. Thus we can image that the system will behave like an AFH uniform spin-1 chain. In the following discussion we will argue this imagination through some physical properties calculation for Hamiltonian (1) in the small \( \alpha \) cases and compare them with corresponding properties of the 1-D AFH spin-1 chain.

We find that all the properties for the two systems coincide with each other in the small \( \alpha \) limit. In Fig.2, the exact diagonalization result of the model (1) for the spin-spin correlation on 32 sites is shown by solid circles. The plateaus in the spin-spin correlation occur at the pairs of site. Within each pair the spins couple each other with the FM interaction. This means that in small \( \alpha \) limit each pair of spins (\( S = 1/2 \)) corresponds to a FM triplet dimer as mentioned above. The spin-spin correlation of the AF uniform spin-1 chain on 16 sites is also shown in the same figure for comparison. (The data of spin-1 chain should be reduced by a factor 4 in comparison with the data of model (1).[5]) It can be seen that when \( \alpha = 0.01 \) the locus of plateaus of model (1) approaches to that of the AF uniform spin-1 chain.

Beside the spin-spin correlation, the string correlation of the alternating bond chain also shows Haldane-like behavior. We define the string correlation of model (1) as follows

\[
\vartheta^z_{alt}(j) = \left\langle (S^z_1 + S^z_2) \exp[i\pi \sum_{k=1}^{j-1} (S^z_{2k-1} + S^z_{2k})] (S^z_{2j-1} + S^z_{2j}) \right\rangle
\]

where \( \langle .. \rangle \) means taking the average over the ground state of the model considered. This is a simple generalization of the definition of the string correlation of integer spin S
\[ \psi_{z/S}(j) = \left( S^z_i \exp \left[ i \frac{\pi}{S} \sum_{k=1}^{j-1} S^z_k \right] S^z_j \right) \]  

(3)

In considering the two spins with FM coupling in a \( S = 1/2 \) alternating bond chain will form a triplet dimer in small \( \alpha \) limit, which is corresponding to a spin-1 chain. The numerical results of the string correlation for two models are shown in Fig.3. We can see that upon decreasing \( \alpha \), the string correlation of the alternating bond chain is closer and closer to that of the AF uniform spin-1 chain.

In addition to the spin-spin and the string correlations, the average of \( z \)-component of spin at each site \( \langle S^z_i \rangle \) of the alternating bond chain will also show the ”edge state” with average spin at the ”end sites” proposed by AKLT model. In the following discussion we will understand what do the ”edge state” and ”end sites” mean in our approach: From \( S = 1/2 \) model (1) to an uniform spin-1 chain. We now calculate the \( \langle S^z_i \rangle \) of model (1) in subspace \( S^z_{\text{tot}} = 1 \) by using DMRG method and consider open boundary condition for both systems. In Fig.4 (a) the results are shown for the system with \( N=60 \) lattice sites and \( \alpha = 0.01 \). It is clear that the two spins with the FM coupling are pairing to triplet dimers, while the coupling between nearest neighbor dimers is AF. The average value \( \langle S^z_i \rangle \) for the two spins in each dimer are nearly the same, e.g. each spin of the edge dimer gives \( \langle S^z_1, 2 \rangle \approx 0.27 \).

Upon entering into the interior of the chain, the \( \langle S^z_i \rangle \) decreases. At the two centre dimers, the \( \langle S^z_i \rangle \) are zero. Increasing the size of the chain to \( N=120 \), we can see from Fig.4(b) that: i) the average value of \( \langle S^z_i \rangle \) in each dimer is nearly equal to the corresponding one in the case of \( N=60 \), and takes nearly the same value irrespective to \( \alpha = 0.01 \) or \( \alpha = 0.001 \). The loci of dimers are well-coincident with the \( \langle S^z_i \rangle/2 \) of the uniform spin-1 system, e.g. for \( \alpha = 0.001 \), the \( \langle S^z_1 + S^z_2 \rangle \approx 0.531 \) for the edge dimer of model (1), it’s considerably close to the value (0.532) of the end spin in the AFH spin-1 chain calculated by S.R.White. ii) more dimers of spins located in the middle part of the chain with \( \langle S^z_i \rangle \approx 0 \). From these results, we conclude that the ”edge state” in the AFH spin-1 system is actually the state of edge dimer in model (1).

In addition, from Fig.4(c), we can see that as the \( N \) increases further, such as \( N=240 \) and 360, the two side regions where the \( \langle S^z_i \rangle \neq 0 \) change little because they come from the ”surface” effect. So, we may image that, in the limit of \( N \rightarrow \infty \), \( N_0/N \rightarrow 1 \). (\( N_0 \) is the number of sites in the middle part.) The effect is due to the spin disturbance which
is happened at the surface (surface mode) and the penetration depth $\xi$ of the disturbance is independent of the system size, but it will depend on $\alpha$. The decay behavior of $\langle S_i^z \rangle$ away from the end point of the chain in model (1) as shown in Fig.4(c) can be fitted by the exponential form $|\langle S_i^z \rangle| = |\langle S_0^z \rangle|e^{-\xi}$. In the small $\alpha$ region, $\xi$ decreases upon increasing $\alpha$ and the relation between $\xi$ and $\alpha$ is approximately linear. Through numerical calculations, we could conclude that $\xi \simeq 12$ as $N \to \infty$ and $\alpha \to 0$. The penetration depth $\xi$ is approximately the double of the decay length of the AFH spin-1 chain [3] and this is because two spins connected with a FM coupling of model (1) correspond to a $S=1$ spin of the AFH spin-1 chain. These conclusions support AKLT model but it should be noted that: i) the edge state in which the average value of end spin equal to nearly $S/2$ is valid for both the AFH uniform spin-1 system and $S = 1/2$ system of model (1) as state above, i.e. it is not necessary explained by AKLT model in general. ii) The side region, originating from "surface" effect, is finite and independent of the system size.

At last, we turn to study the excitation energy $\Delta_{1/2}$ of model (1) in small $\alpha$ limit, $\Delta_{1/2}$ is defined as $\Delta_{1/2} = E_1 - E_0$, where $E_0$ and $E_1$ are the energies of ground state and the lowest excite state of model (1) with periodic boundary condition respectively. For open boundary condition, one must define the gap $\Delta_{1/2}$ ($\Delta_1$) of the alternating bond chain (the uniform spin-1 chain) as the difference between the lowest-lying states with $S_T = 2$ and $S_T = 0$ (or, $S_T = 2$ and $S_T = 1$). As a matter of fact, the two gaps of model (1): $\Delta_{1/2} = E_2 - E_0$ and $\Delta_{1/2} = E_2 - E_1$ are equal. The $\Delta$ for both the $S = 1/2$ model (1) with $J_1 = 1$, $J_2 = \alpha = 0.002$ and the AFH spin-1 system with the same $J_2$ (i.e. The Hamiltonian of the spin-1 chain is $H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$, here $J = J_2$) are shown in Fig.5. In the thermodynamic limit ($N \to \infty$), the excitations of both systems through above definition are gapful. (For the spin-1 chain, $\Delta_1 = \Delta_{Haldane}J$, $\Delta_{Haldane} \sim 0.41, \Delta_{1/2} \sim 0.02$) This is the so called Haldane gap and, however, the gap of the uniform spin-1 system is nearly 4-times of the gap of model (1). If we recalculate $\Delta_1$ for the AF uniform spin-1 system with $J = J_2 = \alpha/4$ and its locus is denoted by stars, then we find that they nearly complete coincide with the corresponding locus of model (1). The appearance of factor 4 is due to the following reason. The ground state energy of model (1) is

$$E_0 = \langle 0 | H | 0 \rangle = J_1 \sum_{i \in \text{odd}} \langle \vec{S}_i \cdot \vec{S}_{i+1} \rangle_0 + J_2 \sum_{j \in \text{even}} \langle \vec{S}_j \cdot \vec{S}_{j+1} \rangle_0$$

where $|0\rangle$ is the ground state.
From Fig.6(a) we can see that the mean value of local bond strength $\langle S_i \cdot S_{i+1} \rangle_{S=1/2}$ of all pairs of spins coupled with a FM interaction equal to 0.25 and contributes an energy $0.25J_1$. In same, the mean value of all pairs of spins coupled with a AF interaction is equal to $-0.35$ and contributes an energy of $0.35J_2$. In small $\alpha$ limit, all the pairs with FM coupling form the triplet dimers, and between the dimers, there exist weak AF interactions. Now let us consider the lowest excite state. It is obviously that if we change the spin state of a triplet dimer as a whole, the energy cost is about $4 \times 0.35J_2$. This is much lower than the excitation energy in which only single one spin state is changed. This is about $2(0.25J_1 + 0.35J_2)$. So the gap of model (1) should be approximately written as $\Delta_{1/2} \simeq 4 \times 0.35J_2$. In similar consideration, the excitation energy of the AFH uniform spin-1 system is $\Delta_1 \simeq 4J\langle S_i \cdot S_{i+1} \rangle_{S=1} = 4 \times 1.40J_2$ (see Fig.6(b)). Therefore we have got the relation $\Delta_1 = 4\Delta_{1/2}$ or equivalently the $J_2$ in the spin-1 system effectively equals to 4 times of $J_2$ in model (1). In addition, like the AFH spin-1 systems, the excitation of model (1) between the lowest-lying $S_T = 1$ and $S_T = 0$ states is gapless due to the four-fold degenerate ground state generated by two free spins of ends of systems.

In summary, we presented numerical results of model (1) and compare with the AFH uniform spin-1 chain. From the spin-spin correlation and the string correlation, the system with small $\alpha$ has Haldane-like behavior. The plateaus of the spin-spin correlation and the spin density of model (1) with small $\alpha$ display that spins coupled with a FM interaction form a FM triplet dimer. The edge state of model (1) is also observed and $\langle S_1^z + S_2^z \rangle$ of model (1) is nearly equal to $\langle S_1^z \rangle$ of the AFH spin-1 chain. Furthermore, the penetration depth $\xi$ of model (1) is the double of the decay length of the AFH spin-1 chain and then the lattice constant of AFH spin-1 chain is equivalent to the double of that of model (1). In addition, we find that the gap of model (1) with small $\alpha$ is not only finite but it’s also a quarter of the Haldane gap of the AFH uniform spin-1 chain. This is because the energy cost for changing the state of the triplet dimer as a whole is less than that for changing only one spin of the triplet dimer and the local bond strength of the AFH uniform spin-1 chain is 4-times of that of model (1).


Acknowledgments

The authors are grateful for the support from the Ministry of Science and Technology of China under Grant No. NKBRSF-G19990646

Figure 1: The structure of an alternating bond chain.

Figure 2: The spin-spin correlation of the ground state of the alternating bond chain (N=32) with periodic boundary condition. It shows many plateaus. In each plateau, the two spins have the same spin correlations.

Figure 3: The string correlation of the alternating bond chain (N=32) with periodic boundary condition.

Figure 4: The spin density of an alternating bond chain in subspace $S^z_{tot} = 1$ in two cases: (a) $\alpha = 0.01$, $N = 60$, (b) $\alpha = 0.01$ and $\alpha = 0.001$, $N = 120$. The data $\langle S^z_i \rangle/2$ corresponds to the AFH spin-1 chain with $N=60$. (c) The comparison between several cases with different numbers of sizes, each locus corresponds to a half of different N.

Figure 5: $\Delta_{1/2}$ is the gap of model (1) with open (or periodic) boundary condition and $\alpha = 0.002$; $\Delta_1$ is the Haldane gap of the AF uniform spin-1 chain with $J = J_2 = 0.002$ (or 0.0005).

Figure 6: (a) The comparison of the local bond strength $L(i)$ of the ground state between model (1) of 120 sites with $\alpha = 0.001$ and the AF uniform spin-1 chain of 60 sites. $L(i)$ are $\langle S_i \cdot S_{i+1} \rangle_{S=1/2}$ and $\langle S_{i/2} \cdot S_{i/2+1} \rangle_{S=1/4}$ for model (1) and the AFH spin-1 chain, respectively. (b) The local bond strength $\langle S_i \cdot S_{i+1} \rangle_{S=1}$ of the ground state of the AF uniform spin-1 chain with $N=60$.

[1] F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983); Phys. Lett. 93A, 464 (1983).
[2] M. P. Nightingale and H. W. J. Blöte, Phys. Rev. B 33, 659 (1986).
[3] S. R. White and D. A. Huse Phys. Rev. B 48, 3844 (1993).
[4] T. Kennedy, J. Phys. Condens.Matter 2, 5737 (1990).
[5] O. Golinelli, Th. Jolicoeur and R. Lacaze, Phys. Rev. B 50, 3037 (1994).
[6] Ulrich Schollwöck, Olivier Golinelli and Thierry Jolicoeur, Phys. Rev. B 54, 4038 (1996).
[7] J.P. Renard et al, Europhys. Lett. 3, 945 (1987).
[8] I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987).

[9] S. H. Glarum, S. Geschwind, K. M. Lee, M. L. Kaplan, and J. Michel, Phys. Rev. Lett. 67, 1614 (1991).

[10] M. Hagiwara et al, Phys. Rev. Lett. 65, 3181 (1990).

[11] Shaojin Qin, Tai-Kai Ng and Zhao-Bin Su, Phys. Rev. B 52, 12844 (1995).

[12] M. den Nijs and K. Rommelse, Phys. Rev. B 40, 4709 (1989).

[13] S. M. Girvin and D. P. Arovas, Phys. Scr. T27, 156 (1989); Y. Hatsugai, J. Phys. Sco. Jpn. 61, 3856 (1992); Y. Hatsugai and M. Kohmoto, Phys. Rev. B 44, 11789 (1991).

[14] F. C. Alcaraz and Y. Hatsugai, Phys. Rev. B 46, 13914 (1992).

[15] J. C. Bonner and H. W. J. Blöte, Phys. Rev. B 25, 6959 (1982).

[16] S. R. White, Phys. Rev. Lett. 69, 2863 (1992); S. R. White, Phys. Rev. B 48, 10345 (1993).
Fig. 1  H.H. Hung & C.D. Gong

\[ J_1 = \text{Ferromagnetic} \]

\[ J_2 = \text{Anti-ferromagnetic} \]
Periodic BC

- $N=32, \alpha=0.01$
- $N=32, \alpha=0.1$
- $\triangle$ AF uniform spin1 chain ($N=16$)

Fig. 2  H.H. Hung & C.D. Gong
Fig. 3  H.H. Hung & C.D. Gong

periodic BC

N=32 alternating bond chain:
- ■ $\alpha=0.005$
- ∗ $\alpha=0.01$
- ○ $\alpha=0.025$
- ▲ $\alpha=0.05$
- ◇ $\alpha=0.075$
- + $\alpha=0.1$
- --- AF uniform spin-1 chain (N=16)
Fig. 4 (a)  H.H. Hung & C.D. Gong

alternating bond chain, Open BC

$\alpha = 0.01$, $N = 60$, $S_{tot}^z = 1$
Open BC, $S_{tot}^z = 1$

alternating bond chain $N=120$

- $\alpha = 0.01$
- $\alpha = 0.001$

AF uniform spin-1 chain ($N=60$, $<S_i^z>/2$)

Fig. 4 (b)  H.H. Hung & C.D. Gong
alternating bond chain
Open BC, $\alpha=0.01$, $S^z_{\text{tot}}=1$

Fig. 4 (c) H.H. Hung & C.D. Gong
\[ \Delta = \frac{1}{N} \alpha = 0.002, \quad \Delta_{1/2} = E(S_T = 1) - E(S_T = 0) \]

\[ \Delta = \frac{1}{2} = E(S_T = 2) - E(S_T = 0) \]

\[ \Delta = \frac{1}{2} = E(S_T = 2) - E(S_T = 1) \]

\[ \Delta_1, J = 0.002, \text{AFH spin-1 chain} \]

\[ \Delta_1, J = 0.0005, \text{AFH spin-1 chain} \]
(a) $L(i) = \langle S_i S_{i+1} \rangle_{S=1/2}$, $\alpha = 0.001$, $L = 120$

$\quad$ $L(i) = \langle S_{i/2} S_{i/2+1} \rangle_{S=1/4}$ spin-1 chain

(b) AF uniform spin-1 chain

Fig. 6  H.H. Hung & C.D. Gong