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A note on Haldane's conjecture

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Abstract

According to Haldane's conjecture, there is a spin gap of the excitation spectrum in integer Heisenberg spin chains whereas half-integer spin chains have a gapless excitation spectrum. In an earlier publication (Hung and Gong 2005 *Phys. Rev.* B **71** 054413), the Haldane gap and other properties of the spin-1 system are explained using a spin-1/2 alternating bond chain model. The ferromagnetic–ferromagnetic–antiferromagnetic Heisenberg spin-1/2 chain is expected to behave similarly to the uniform spin-3/2 Heisenberg chain for strong ferromagnetic coupling. And the general nonuniform spin-1/2 chain may be used to explain the properties of the integer and half-integer high spin-S chains, consistently. In this paper, we provide a detailed numerical verification for the above problems.

(Some figures in this article are in colour only in the electronic version)

In 1983, Haldane [1] claimed that the integer spin antiferromagnetic Heisenberg (AFH) chains have a gap in the excitation spectrum and an exponential decay of the ground state spin correlation function. However, the spectrum of the half-integer spin AFH chain is gapless and the decay of the ground state spin correlation follows a power law. Since then, there has been a lot of work investigating this conjecture, by studying the uniform AFH chains [2–4] and other modulated spin chains [5–7].

Recently the Haldane problem was studied taking another, reverse approach by Hung and Gong [8]. They used the Heisenberg spin-1/2 alternating bond chain [9] (ABC) in which the nearest neighbor exchange couplings are ferromagnetic (FM) J_1 and antiferromagnetic (AF) J_2, alternately. Hereafter this is taken as the period-2 ABC. And they provide numerical evidence for the period-2 ABC approaching the uniform spin-1 AFH chain with the same AF coupling J_2 when the ratio of AF to FM coupling strengths is small enough, and explain a possible origin of the Haldane gap in the uniform spin-1 AFH chain, which is four times the gap of the period-2 ABC.

The ferromagnetic–ferromagnetic–antiferromagnetic Heisenberg spin-1/2 chain is expected to behave similarly to the uniform spin-3/2 Heisenberg chain for strong ferromagnetic coupling [10]. In this paper, we try to give a numerical verification that the spin-1/2 ABC can also approach the half-integer spin AFH chain and explain its gapless excitation spectrum. Then we can say that the Haldane problem can be completely approached by the nonuniform spin-1/2 ABC model.

For discussion of the aforementioned problem, we define the period-n ABC model as follows. Each spin-$n/2$ site in the uniform spin-$n/2$ AFH chain is replaced by a FM multimer or a subchain composed of n $s = 1/2$ spins, between any two nearest neighboring (n.n.) spins $s = 1/2$ in each subchain connected with FM bonds, and the AF couplings exist between the edge spins of two n.n. subchains. The idea of representing spin-$n/2$ operators as the sums of $2n$ spin-1/2 ones has been applied widely for Haldane chains [8, 11, 12]. The model Hamiltonian is

$$H = J_1 \sum_{i/n\notin N^*} \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_{i/n\in N^*} \vec{S}_i \cdot \vec{S}_{i+1}. \qquad (1)$$

Here S_i denotes a spin-1/2 operator at site i. N^* denotes the set of positive integers. If i/n is not an integer, i.e., spins $\vec{S}_i$ and $\vec{S}_{i+1}$ belong to the same subchain, the couplings are J_1 (<0). Otherwise, if i/n is an integer, the couplings are J_2 (>0). Also we define the parameter $\alpha \equiv |J_2/J_1|$, and consider only the case of the small α limit. We will set $|J_1| \equiv 1$ and the energy is measured in units of $|J_1|$. In the case of $S = 3/2$, we have the ferromagnetic–ferromagnetic–antiferromagnetic trimerized spin-1/2 Heisenberg chain [10]. Later we call this the J_1–J_1–J_2 model or the period-3 ABC (figure 1).

In this paper, the above questions will be answered through numerical calculation by using the density matrix renormalization group (DMRG) method [13]. For the case

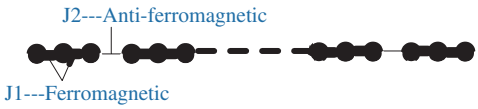

Figure 1. The structure of the J_1–J_1–J_2 model.

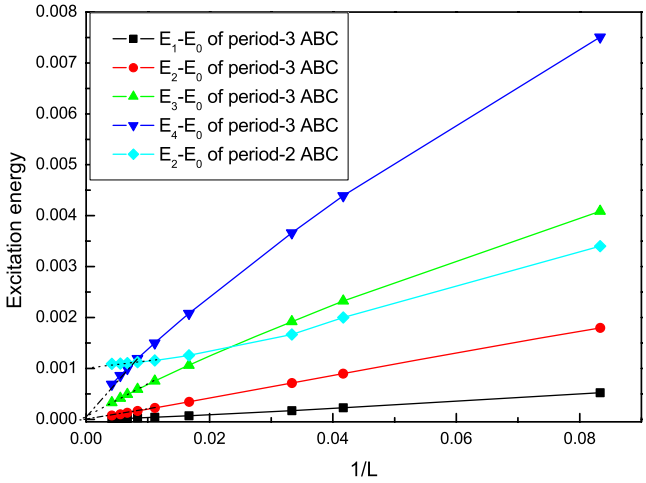

Figure 2. The excitation energy $E_m - E_0$ of the period-3 ABC at $\alpha = 0.01$ as a function of the inverse chain length $1/L$. Also shown is the excitation energy $E_2 - E_0$ of the period-2 ABC. Dotted lines are guides to the eye. They are straight lines fitted to the last few points.

of $S = 3/2$, the physical properties of the period-3 ABC are calculated and, making a comparison with those of the uniform AF J_2 spin-3/2 model, we find that they approach each other in the small α limit. In addition, in the small α limit the ratio of $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for the AF coupled pairs in the period-3 ABC and $\langle S_i \cdot S_{i+1}\rangle^{s=3/2}$ for the uniform spin-$n/2$ AFH chain is $1/3^2$. And the dimerization parameter $q(x) = \langle S_{xn} \cdot S_{xn+1} - S_{(x-1)n} \cdot S_{(x-1)n+1}\rangle$ of the AF coupled bond that is number x counting from the end of the chain for the ground states of the period-n ($n = 2, 3, 4, 5$) ABC will also be examined.

Figure 2 shows the excitation energies $E_m - E_0$ (m = 1–4) as a function of the inverse chain length L^{-1} for the case of $\alpha = 0.01$. E_m is the lowest energy in the subspace $S^z_{\rm tot} = m$. The calculations are performed for the open spin chains with even numbers of sites, i.e., L can take the values 12, 24, 30, 60, 90, 150, 180, and 240 consecutively. Thus the ground state is in the $S^z_{\rm tot} = 0$ subspace. $M = 128$ states are retained in the DMRG calculation. The truncation error is about 10^{-12}, and the energies are well converged. For comparison, the excitation energy $E_2 - E_0$ of the period-2 (spin-1) ABC is plotted in the same diagram. It is gapped, and approaches 0.001 in the thermodynamic limit. In contrast, in the case of the period-3 ABC, $E_m - E_0$ is a monotonically decreasing function of L and approaches zero in the large L limit in all four cases. So the excitation spectrum of the model period-3 ABC is gapless in the thermodynamic limit ($L \to \infty$).

Next, the expectation values of the z component of the spin $\langle S^z_i\rangle$ at each site i of the period-3 ABC with $L = 180$ lattice sites, $\alpha = 0.01$ and an open boundary condition in

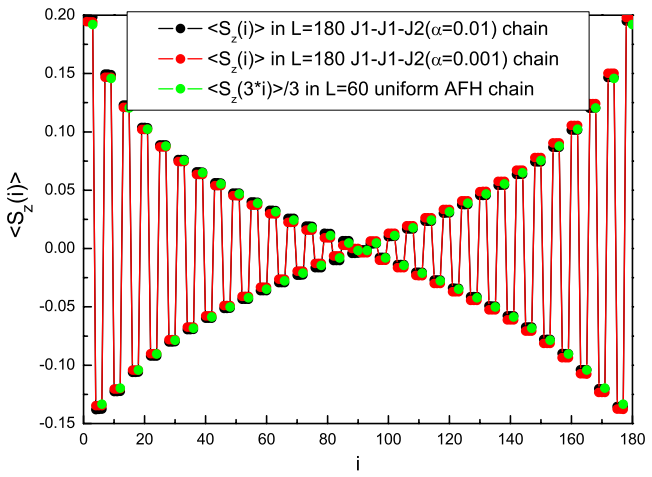

Figure 3. The expectation value $\langle S^z_i\rangle$ in subspace $S^z_{\rm tot} = 1$ for the $L = 180$ J_1–J_1–J_2 chain at $\alpha = 0.01$, in comparison of that for the $L = 60$ uniform AFH spin-3/2 chain.

subspace $S^z_{\rm tot} = 1$ are shown in figure 3. We can see that (i) the expected spin values for the FM trimers coincide well with $\langle S^z_i\rangle$ for the uniform spin-3/2 AFH chain (e.g., for $\alpha = 0.01$, $\langle S^z_1 + S^z_2 + S^z_3\rangle \sim 0.588\,53$ for the edge trimer of the period-3 ABC, which is very close to the value (0.576 18) for the end spin of the uniform spin-3/2 AFH chain); (ii) the expectation values $\langle S^z_i\rangle$ for the three spins in each trimer are nearly the same, irrespective of whether $\alpha = 0.01$ or 0.001. We conclude that the edge state of the uniform spin-3/2 AFH chain is actually the state of the edge trimer in the period-3 ABC. Like those for open uniform $S > 1/2$ AFH chains [14], the first excited states consist of spin excitations localized around edges of spin chains. But the decay length is three times the decay length of the spin-3/2 AFH chain. This is a surface state due to the quantum many-body effect.

The expectation values of the local bond strengths $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for all FM trimers are equal to 0.25, while the expectation value of the local AF bond strength is around 0.314 and has a dimerization character. Upon decreasing the value of α, $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for the AF coupled pairs in the period-3 ABC will approach $\langle S_i \cdot S_{i+1}\rangle^{s=3/2}$ for the uniform spin-3/2 AFH chain scaled down by a factor of $1/3^2$ more and more closely, as in figure 4(a). In the small α limit ($\alpha < 0.001$), they are actually equal.

As regards the ratio of $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for AF coupled pairs in a general period-n ABC and $\langle S_i \cdot S_{i+1}\rangle^{S=n/2}$ for the uniform spin-$n/2$ AFH chain, it is $1/n^2$ numerically for even higher spin chains. As shown in figure 4(b), the ratio of the calculated results for $\langle S_i \cdot S_{i+1}\rangle^{s=2}$ for an $L = 60$ $S = 2$ AFH chain and $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for the $L = 240$ period-4 ABC ($\alpha = 0.001$) is 16, while the ratio of $\langle S_i \cdot S_{i+1}\rangle^{s=5/2}$ for an $L = 60$ $S = 2.5$ AFH chain and $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for the $L = 300$ period-5 ABC ($\alpha = 0.001$) is 25. It should be recalled that, in the uniform spin-$n/2$ AFH chain, the AF exchange interactions act between the n interior electrons (spin-1/2 ones), and therefore all n interior electrons of each atom contribute to the AF exchange energy. In other words, for any two nearest neighbor atoms, there are n^2 pairs of electrons

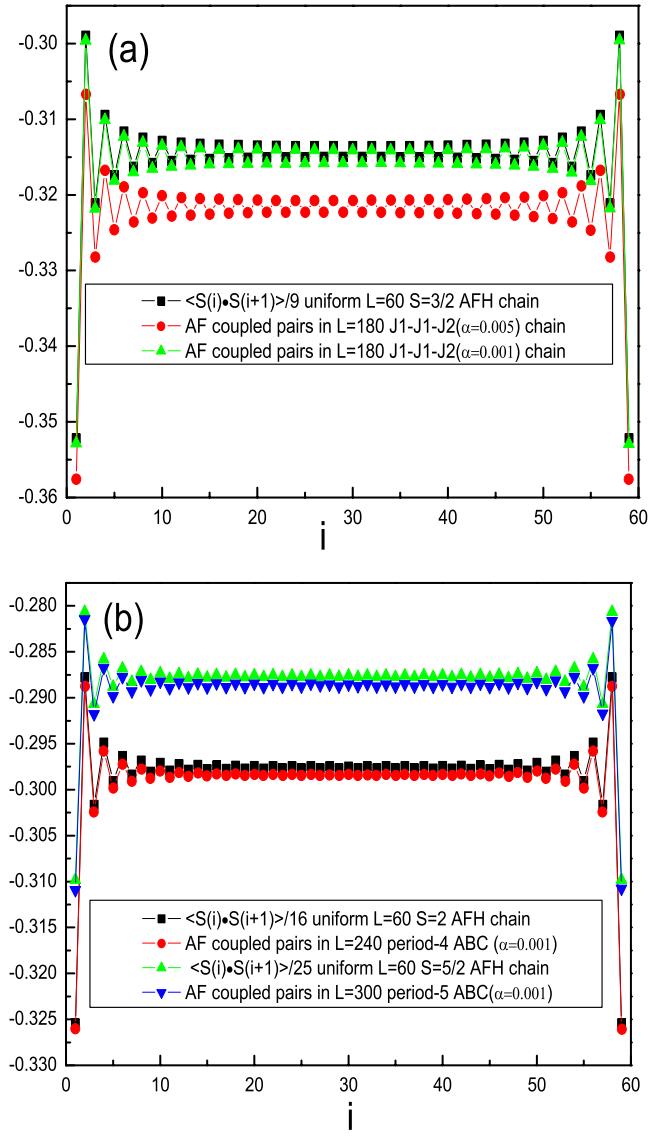

Figure 4. (a) The comparison of the local bond strength of the AF coupled pairs for the $L = 180$ period-3 ABC at $\alpha = 0.005, 0.001$ and $\langle S_i \cdot S_{i+1}\rangle^{s=3/2}/9$ for the $L = 60$ uniform AFH spin-3/2 chain in the ground state. (b) The result for the $L = 240$ period-4 ABC and the $L = 300$ period-5 ABC at $\alpha = 0.001$, and the corresponding $\langle S_i \cdot S_{i+1}\rangle^{s=n/2}/n^2$ for the uniform AFH spin-$n/2$ ($n = 4, 5$) chain in the ground state.

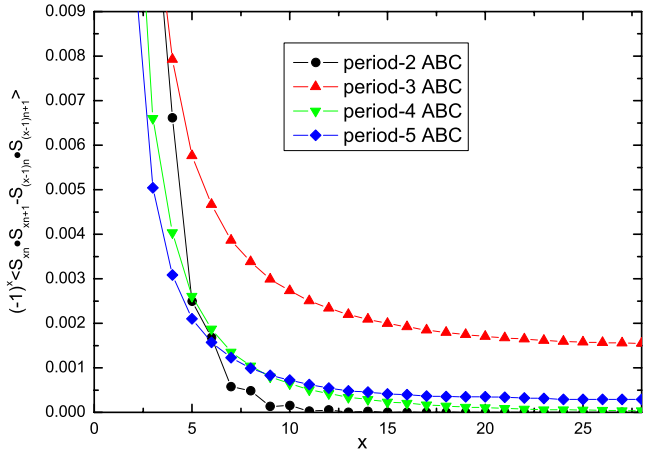

Figure 5. The dimerization strength $|q(x)| = |\langle S_{xn} \cdot S_{xn+1} - S_{(x-1)n} \cdot S_{(x-1)n+1}\rangle$ of the AF coupled bond that is number x counting from the end of the chain for the period-n (2, 3, 4, 5) ABC of length $n \times 60$ at $\alpha = 0.001$.

participating in the AF interaction, while in the equivalent ABC model, the AF exchange interactions only act between one pair of electrons. So in the calculation of the AF exchange energy, as well as the local bond strength of the systems, there is a factor $1/n^2$.

The dimerization parameter $q(x) = \langle S_{xn} \cdot S_{xn+1} - S_{(x-1)n} \cdot S_{(x-1)n+1}\rangle$ [14] of the AF coupled bond that is number x counting from the end of the chain for the ground states of the general period-n ABC is shown in figure 5. For even n, $q(x)$ decays exponentially as the AF coupled bond moves into the interior. $q(x) = \mathrm{e}^{-x/\xi}$; here ξ is multimer length dependent. For example, ξ is 1.85 for the period-2 ABC and 4.81 for the period-4 ABC. For odd n, $q(x)$ decays following a power law into the interior of the period-n ABC. $q(x) = x^{-\beta}$; here the exponent β is also multimer length dependent. β is 1.23 for the period-3 ABC and 1.61 for the period-5 ABC. Similar behavior has been previously observed for the uniform Heisenberg chain. From figure 8 of [14], it has been seen that there is a huge difference in behavior of the dimerization parameter between integer and half-integer open AFH chains. So the huge difference in behavior of $q(x)$ between even and odd n reflects another aspect: that the period-n ABC may approach a uniform spin-$n/2$ AFH chain.

In summary, numerical results for the period-3 ABC are presented and compared with ones for the uniform spin-3/2 AFH chain. We deduce that the excitation spectrum for the period-3 ABC is gapless in the small α limit. The spin density and the local bond strength of the period-n ABC ($n = 2, 3, 4, 5$) are equal to the corresponding properties of the uniform spin-$n/2$ AFH model in the small α limit ($\alpha < 0.001$) only if $\langle S_i \cdot S_{i+1}\rangle^{s=1/2}$ for the AF coupled pairs in the period-n ABC is replaced by the product of $1/n^2$ and $\langle S_i \cdot S_{i+1}\rangle^{S=n/2}$ for the uniform spin-$n/2$ AFH model. Combining this with Hung and Gong's result [8], we may conclude that a general period-n Heisenberg spin-1/2 alternating bond chain in the strong FM limit can be used to approach a uniform spin-$n/2$ AFH chain and to describe Haldane's problem completely.

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