The study of spin-spin correlations in quasi-one-dimensional Heisenberg antiferromagnetic clusters

Yong-Jun Liu$^{1,2}$ and Chang-De Gong$^{3,1}$

$^1$National Key Laboratory of Solid States of Microstructure, Nanjing University, Nanjing 210093, PRC
$^2$Complexity Science Center, Yangzhou University, Yangzhou 225002, PRC
$^3$CCAST (World Laboratory), P.O. Box 8730, Beijing 100080, China

For a class of quasi-one-dimensional clusters, by using exact diagonalization, we study the effect of side spins on the spin-spin correlations on chain. Our calculations show that the side spins added in the same sublattice can effectively strengthen the spin-spin correlations in large distance region and make the change tend to flat. It is exactly proved that periodically adding side spins can set up magnetic long-range orders in the ground state. Also we investigate the effect of the density of side spins on correlation strength. The case that two sublattices have different localized spins is discussed.

Spin-spin correlation and magnetic long-range order (LRO) are of fundamental importance for quantum spin systems. They have been studied by many analytical and numerical works. For the bipartite Heisenberg antiferromagnetic (AF) systems, the spin-spin correlations of any two sites in the ground state (GS) always are AF, i.e. the correlation functions are positive when two sites belong to the same sublattice whereas negative the different sublattices. However, it is not sufficient to set up the AF LRO. The dimensionality of system is one of the key factors. It has been rigorously proved that there exists Néel order in the GS of the three-dimensional system, whereas no Néel order for the one-dimensional one. Although there is no magnetic LRO for one- and two-dimensional (1D and 2D) Heisenberg antiferromagnets at temperature $T > 0$ by Mermin-Wagner theorem. $T = 0$ may be the critical point. When the localized spin $S > 1$, it has been proved that the GS of the 2D Heisenberg antiferromagnet has Néel order. Notwithstanding the rigorous proof of Néel order when $S = \frac{1}{2}$ has not been established until now, many numerical and analytical works support its existence at $T = 0$.

The situation of quasi-one-dimensional (QOD) systems may be diverse due to their various geometric structures. The discovery of a heavy-fermion phenomenon in the Ce-doped Neodymium cuperate has led to an increasing interest in the study of strongly correlated electrons coupled antiferromagnetically to magnetic moments. W. Zhang et al. have investigated the case of a single magnetic impurity and found that the spin-spin correlation function between the impurity spin and spins in the chain extends over long range. Obviously, the magnetic LRO cannot be established through adding a single impurity spin to an 1D chain. The situation may change when impurity spins are periodically added to the chain in a special way. In this paper, by using exact diagonalization, we investigate a class of QOD Heisenberg AF clusters, in which there are some impurity spins sit beside an 1D finite chain (we call them as side spins), and explore the effects of side spins on spin-spin correlations. Our numerical results indicate that the spin-spin correlations in the region of large distances can be enhanced by adding side spins in the same sublattice. When periodically adding side spins, the decay of spin-spin correlations with distances slows down and becomes obviously flat in the range of large distances. For infinite 1D chains, it is analytically proved that adding side spins can set up magnetic LROs. Also, we investigate the variation of magnetic LROs with the density of side spins, and find that the decay of ferromagnetic (F) LRO is faster than that of AF LRO.

We investigate the spin $\frac{1}{2}$ Heisenberg AF system with interactions of nearest neighbors, whose Hamiltonian reads

$$H = J \sum_{\langle i,j \rangle} \vec{S}(i) \cdot \vec{S}(j),$$

where $J > 0$. $(i, j)$ denotes the sum over pairs of nearest neighbors. The spin-spin correlation can be written as

$$\Delta(R_i - R_j) = \langle G | \vec{S}(i) \cdot \vec{S}(j) | G \rangle.$$

Here, $R_i$ and $R_j$ are the coordinates of sites $i$ and $j$ respectively, and $|G\rangle$ represents the GS. Let $\vec{i}$ denote the site by the $i$th site of the chain. At first, we consider a finite chain of 23 sites under free boundary conditions and study the effect of a single side spin on the spin-spin correlations. By exact diagonalization, we calculate $\Delta(R_i - R_j)$ for site 2 (i.e. $j = 2$ and $i = 3, 4, 5, ...$), and the numerical results are shown in Fig. 2, here the side spin is placed at site 2, 3 and 4 respectively (see Fig 1.(a)). When the side spin is added on site 3, $\Delta(R_i - R_j)$ becomes weaker than that of the pure 1D chain. Namely, the side spin weakens the spin-spin correlations. But, when the side spin is at site 2 (or 4), $\Delta(R_i - R_j)$ becomes stronger in the region of large distances. In this case, the side spin strengthens the spin-spin correlations for most of $(R_i - R_j)$. When a single side spin is placed at sites 5, 7, 9 and 11 respectively, our calculations show that the effect of the side spin is similar to that of the side spin at site 3. And, when the side spin is placed at site 6, 8, 10 and 12 respectively, it is similar to that of the side spin at site 2.
Under the periodic boundary conditions, the case of a single side spin has been studied by Monte Carlo simulations and the spin correlation function is found to extend over long range. For such a system, the GS always takes the lowest possible total spin (LTS) no matter where the side spin is attached. But the situation for a finite chain under free boundary conditions becomes little complicated. The finite chain can be divided into two ‘sublattices’ as doing for infinite systems. Sites 1, 3, 5, ..., 21 and 23 belong to sublattice A, and sites 2, 4, 6, ..., 20 and 22 sublattice B (Fig. 1(a)). Adding the single side spin at different sites can leads to the GS taking different values. When the side spin sits by the site of sublattices B, it belongs to sublattice A. By Lieb-Mattis theorem, the GS has the global spin 1 and is 3-fold degenerate. In other words, the GS takes a higher total spin than its lowest possible value. But, when the side spin sits by the site on sublattices A, it belongs to sublattice B. The GS takes the LTS zero. Our calculations show that the effect of a single side spin depends on where the side spin is. In other words, the total spin of the GS is related to the behaviors of spin-spin correlations. One important question concerned is how the spin correlations change when more side spins are added. When the side spins added are in the same sublattice, the total spin of the GS becomes higher, and the difference between it and the lowest possible total spin larger. From the above calculations, we speculate that $\Delta(R_i - R_j)$ will become stronger in the region of large distances.

For further details, we consider the cases of two side spins. If adding two side spins at site 2 and 4, the GS has the global spin $\frac{4}{3}$ while the lowest possible total spin is $\frac{3}{2}$. But, if adding two side spins by site 2 and 3, the GS takes the lowest possible total spin $\frac{5}{2}$. From the above notion, one can speculate that spin-spin correlations will become stronger and decay more slowly. Approximately, we can fit the spin-spin correlations in exponential way, $g(R) \sim (R/k)^{-\lambda}$, where $C$ is coefficient and $\lambda$ the correlation length. We calculate $\lambda$ by $\Delta(R_0 - R_2)$ and $\Delta(R_0 - R_3)$. The numerical results are plotted in Fig. 3. Our calculations show that periodically adding side spins in the same sublattice can obviously enhance the spin-spin correlations in the large distance region. And, as the density of side spins increasing, spin-spin correlations become stronger and decay more slowly. Approximately, we can fit the spin-spin correlations in exponential way, $g(R) \sim (R/k)^{-\lambda}$, where $C$ is coefficient and $\lambda$ the correlation length. We calculate $\lambda$ by $\Delta(R_0 - R_2)$ and $\Delta(R_0 - R_3)$. For the bare chain of 21 sites, $\lambda = 9.30$. But, for the above three cases, $\lambda = 51.38, 77.27$ and 7345.38. It shows that the large distance behavior of spin-spin correlations is enhanced by adding side spins. Especially, $\lambda \sim 10^3$ for the third case. It is much larger than the correlation length of bare chain, even the size of system. Consequently, side spins can slow down effectively the decay and make the variation become flat in the region of large distances (Fig. 3). It seems to exist the AF LRO.

Now, we turn to consider an infinite QOD system, which is constructed by periodically adding side spins in the same sublattice (Fig. 1(b)). The total number of sites is $N = K(l + 2)$, here $K$ denotes the number of cells and $l$ the number of sites on chain between every two side spins. $l$ must take odd, i.e. $l = 2k + 1$, here $k = 0, 1, 2, ...$. Supposing the side spin is in sublattice A, the number of sites of sublattice A is $N_A = K(l + 3)/2$ and that of sublattice $B N_B = K(l + 1)/2$. By the Lieb-Mattis theorem, the global spin of the GS is

$$\Lambda = K |(k + 2)S_A - (k + 1)S_B|,$$

(2)

where $S_A$ and $S_B$ are the values of localized spins on sublattice A and B respectively. To investigate the existence of magnetic LRO, one needs to calculate the quantity

$$g(q) = \langle G \mid \hat{S}(\mathbf{q}) \cdot \hat{S}(\mathbf{q}) \mid G \rangle .$$

(3)

$\hat{S}(\mathbf{q}) = \frac{1}{\sqrt{N}} \sum_j \hat{S}(j) \exp(i\mathbf{q} \cdot j)$. $\mathbf{q}$ is a reciprocal vector. The criterion of magnetic LROs is that $g(q) \geq O(N)$ at some $q$. If $g(Q) \geq O(N)$, here $Q = (\pi, \pi, ..., \pi)$, there exists AF LRO. If $g(0) \geq O(N)$, there exists F LRO. Following the approaches developed by G. S. Tian [12,13], one can obtain

$$g(Q) > g(0) = \frac{\Lambda^2 + \Lambda}{N} .$$

(4)

We discuss the case that the sites on two sublattices have the equal localized spin, i.e. $S_A = S_A = S$. From equation (2), we readily obtain $\Lambda = NS/(l + 2)$. As long as $l$ is finite, it is always true that

$$g(Q) > g(0) > O(N).$$

(5)

From these inequalities, one can conclude that AF and F LROs coexist in the GS, and the former is predominant. In other words, side spins set up magnetic LROs.
Obviously, although there always exist magnetic LROs for finite $l$, both of F and AF correlation strengths will depend on the density of side spins, which is defined as $\eta \equiv 1/(l + 2)$. We introduce the following two quantities to measure F and AF correlation strengths respectively,

$$\Gamma_F \equiv \frac{1}{N^2} \sum_{i,j} \langle G | \vec{S}(i) \cdot \vec{S}(j) | G \rangle,$$

(6)

and

$$\Gamma_{AF} \equiv \frac{1}{N^2} \sum_{i,j} \lambda_{ij} \langle G | \vec{S}(i) \cdot \vec{S}(j) | G \rangle,$$

(7)

where $\lambda_{ij} = 1$ when sites $i$ and $j$ belong to the same sublattice and $\lambda_{ij} = -1$ when sites $i$ and $j$ the different sublattices. $\Gamma_F$ and $\Gamma_{AF}$ will decrease as $l$ increasing. When $l$ reaches to the infinite, the system changes into an 1D chain and the magnetic LROs vanish (i.e. $\Gamma_F = \Gamma_{AF} = 0$). Possibly, the variation speeds of $\Gamma_F$ and $\Gamma_{AF}$ are different. We calculate the ratio $\rho \equiv \Gamma_F/\Gamma_{AF}$ for $l = 1, 3$ and $5$, and plot the data in Fig. 4. $\rho$ decreases as $\eta$ decreasing approximately in the linear way. Then the decay speed of F correlation strength is faster than that of AF correlation strength. In other words, the ferrimagnetism becomes weaker and weaker as the density of side spins decreasing.

Ref. [13] has proved that the GS of 1D Heisenberg AF chain has magnetic LROs when its two sublattices have unequal localized spins. It is interesting to investigate the QOD system with unequal localized spins. From equation (2) and (4), we can conclude that if

$$\frac{S_A}{S_B} = \frac{k + 1}{k + 2},$$

(8)

g(0) = 0 due to $\Lambda = 0$. It means that there is no F LRO. The simplest case is $S_A = \frac{1}{2}$, $S_B = 1$ and $l = 1$. One can give a spin picture of the GS in valence-bond version. The spin on sublattice $B$ can be divided into two $\frac{1}{2}$ spins. One of them forms a singlet with the nearest side spin, and the other combines with its nearest neighbor on chain. We think this kind of configurations governs the physics of the GS. And it is responsible for the F LRO to vanish. Although we have not exactly proved that the AF LRO can not exist in the GS of such systems, we believe it is true. But, if $S_A/S_B \neq (k + 1)/(k + 2)$, the AF and F LROs coexist in the GS.

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Figure Captions:

Fig. 1: (a) the 1D Heisenberg AF chain. (b) the QD Heisenberg AF chain. There are $l$ sites between site $P_1$ and $P_2$, and $l = 2k + 1$, here $k = 0, 1, 2$...

Fig. 2: Spin-spin correlations between site 2 and others (see Fig. 1(a)) for these cases: no side spin (square); single side spin at site 2 (cross +), 3 (circle) and 4 (cross ×) respectively; two side spins at sites 2 and 4 (triangle); two side spins at sites 2 and 3 (diamond). Here, $R = R_i - R_2$. The length of chain is 23.

Fig. 3: Spin-spin correlations between site 2 and others (see Fig. 1(a)) for these cases: bare chain of 21 sites (square); 4 side spins at sites 2, 8, 14 and 20 on a chain of 21 sites (diamond); 5 side spins by site 2, 6, 10, 14 and 18 on a chain of 19 sites (triangle); 8 side spins by site 2, 4, 6, 8, 10, 12, 14 and 16 on a chain of 17 sites (solid circle). Here, $R = R_i - R_2$.

Fig. 4: $\rho$ vs. $\eta$. The solid line is obtained by fitting $\rho$ in linear way.
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Fig. 1
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Fig. 2
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Fig. 3
Fig. 4