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

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Abstract
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 the chain. Our calculations show that side spins added in the same sublattice can effectively strengthen the spin–spin correlations in the large-distance region and make the change tend to flatten. It is exactly proved that periodically adding side spins can set up magnetic long-range order in the ground state. We also investigate the effect of the density of side spins on correlation strength. The case where 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 in 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 they are negative for different sublattices. However, it is not sufficient to set up the AF LRO. The dimensionality of the system is one of the key factors. It has been rigorously proved that there exists Néel order in the GS [1] of the three-dimensional system, whereas there is no Néel order for the one-dimensional one. Although there is no magnetic LRO for one- and two-dimensional Heisenberg AFs at temperature $T > 0$ by the Mermin–Wagner theorem [2], $T = 0$ may be the critical point. When the localized spin $S \geqslant 1$, it has been proved that the GS of the two-dimensional Heisenberg AF has Néel order [3]. 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 $T = 0$ [4].

The situation of quasi-one-dimensional (Q1D) systems may be diverse due to their various geometric structures. The discovery of a heavy-fermion phenomenon in the Ce-doped neodymium cuprate [5] has led to an increasing interest in the study of strongly correlated

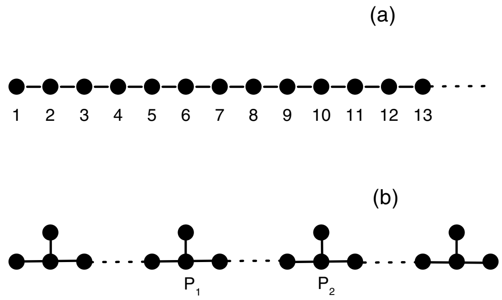

Figure 1. (a) The one-dimensional Heisenberg AF chain. (b) The Q1D Heisenberg AF chain. There are l sites between site P_1 and P_2, and $l = 2k + 1$, where $k = 0, 1, 2, \ldots$.

electrons coupled antiferromagnetically to magnetic moments [6–9]. Zhang *et al* [7] 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 a one-dimensional 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 Q1D Heisenberg AF clusters, in which there are some impurity spins beside a one-dimensional finite chain (we call them 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 distance slows down and becomes obviously flat in the range of large distances. For infinite one-dimensional chains, it is analytically proved that adding side spins can set up magnetic LRO. Also, we investigate the variation of magnetic LRO 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 neighbours, whose Hamiltonian reads

$$H = J \sum_{(i,j)} \vec{S}(i) \cdot \vec{S}(j) \tag{1}$$

where $J > 0$. (i, j) denotes the sum over pairs of nearest neighbours. The spin–spin correlation can be written as $\Delta(R_i - R_j) \equiv \langle G|\vec{S}(i) \cdot \vec{S}(j)|G\rangle$. Here, R_i and R_j are the coordinates of sites i and j respectively, and $|G\rangle$ represents the GS. Let $\bar{i}$ denote the site by the ith 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 $i = 3, 4, 5, \ldots$), and the numerical results are shown in figure 2, where the side spin is placed at site $\bar{2}$, $\bar{3}$ and $\bar{4}$ respectively (see figure 1(a)). When the side spin is added on site $\bar{3}$, $\Delta(R_i - R_j)$ becomes weaker than that of the pure one-dimensional chain. That is, the side spin weakens the spin–spin correlations. However, when the side spin is at site $\bar{2}$ (or $\bar{4}$), $\Delta(R_i - R_j)$ 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 $\bar{5}$, $\bar{7}$, $\bar{9}$ and $\overline{11}$, our calculations show that the effect of the side spin is similar to that of the side spin at site $\bar{3}$. Moreover, when the side spin is placed at site $\bar{6}$, $\bar{8}$, $\overline{10}$ and $\overline{12}$, it is similar to that of the side spin at site $\bar{2}$.

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 a long

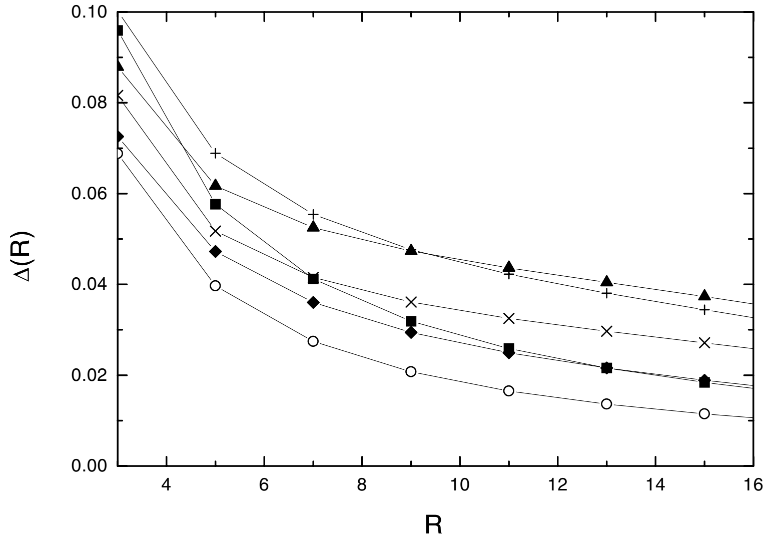

Figure 2. Spin–spin correlations between site 2 and others (see figure 1(a)) for these cases: no side spin (square); single side spin at site $\bar{2}$ (cross +), $\bar{3}$ (circle) and $\bar{4}$ (cross ×); two side spins at sites $\bar{2}$ and $\bar{4}$ (triangle); two side spins at sites $\bar{2}$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

range [7]. For such a system, the GS always takes the lowest possible total spin (LTS) no matter where the side spin is attached. However, the situation for a finite chain under free boundary conditions becomes a little complicated. The finite chain can be divided into two 'sublattices' as for infinite systems. Sites 1, 3, 5, ..., 21 and 23 belong to sublattice A, and sites 2, 4, 6, ..., 20 and 22 sublattice B (figure 1(a)). Adding the single side spin at different sites can leads to the GS taking different values. When the side spin sits by a site of sublattice B, it belongs to sublattice A. By the Lieb–Mattis theorem [10], the GS has the global spin 1 and is threefold degenerate. In other words, the GS takes a total spin higher than its lowest possible value. However, when the side spin sits by a site of sublattice 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 behaviours 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 LTS 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 sites $\bar{2}$ and $\bar{4}$, the GS has the global spin $\frac{3}{2}$ while the LTS is $\frac{1}{2}$. However, if adding two side spins by sites 2 and 3, the GS takes the LTS $\frac{1}{2}$. From the above notion, one can speculate that spin–spin correlations will become stronger if adding two side spins at sites $\bar{2}$ and $\bar{4}$, whereas they will become weaker for sites $\bar{2}$ and $\bar{3}$. We calculate the spin–spin correlations between site 2 and others. The numerical results are shown in figure 2. They agree with the above speculation.

Also, we calculate spin–spin correlations for the following three cases (see figure 1(a)): (1) four side spins sitting at sites $\bar{2}$, $\bar{8}$, $\overline{14}$ and $\overline{20}$ on a finite chain of 21 sites; (2) five side spins sitting at sites $\bar{2}$, $\bar{6}$, $\overline{10}$, $\overline{14}$ and $\overline{18}$ on a finite chain of 19 sites; (3) eight side spins sitting at

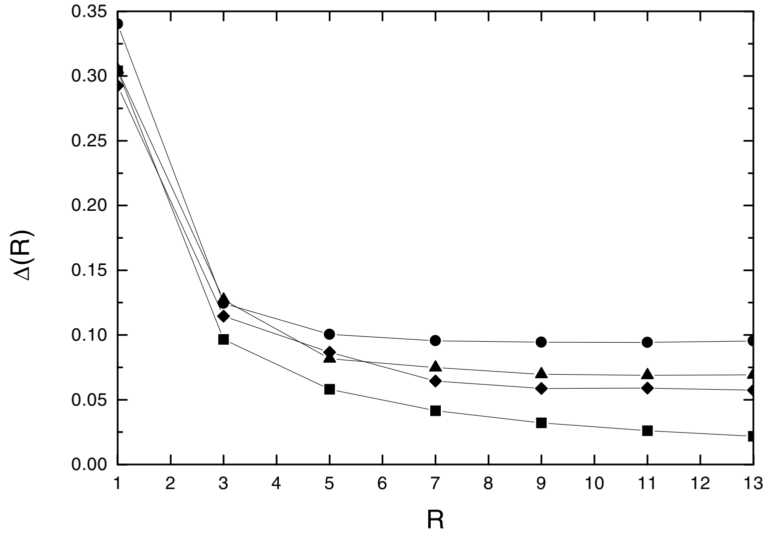

Figure 3. Spin–spin correlations between site 2 and others (see figure 1(a)) for these cases: bare chain of 21 sites (square); four side spins at sites $\bar{2}$, $\bar{8}$, $\overline{14}$ and $\overline{20}$ on a chain of 21 sites (diamond); five side spins by sites $\bar{2}$, $\bar{6}$, $\overline{10}$,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

sites $\bar{2}$, $\bar{4}$, $\bar{6}$, $\bar{8}$, $\overline{10}$, $\overline{12}$, $\overline{14}$ and $\overline{16}$ on a finite chain of 17 sites. Their GSs have the global spins $S^T = \frac{5}{2}$, 3 and $\frac{9}{2}$ respectively. The numerical results are plotted in figure 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. Moreover, as the density of side spins increases, spin–spin correlations become stronger and decay more slowly. We can approximately fit the spin–spin correlations in an exponential way, i.e. $\Delta(R_i - R_j) = C\exp(-|R_i - R_j|/\zeta)$, where C is a coefficient and ζ the correlation length. We calculate ζ by $\Delta(R_9 - R_2)$ and $\Delta(R_{15} - R_2)$. For the bare chain of 21 sites, $\zeta = 9.30$. However, for the above three cases, $\zeta = 51.38$, 77.27 and 7345.38. This shows that the large-distance behaviour of spin–spin correlations is enhanced by adding side spins. In particular, $\zeta \sim 10^3$ for the third case. This is much larger than the correlation length of the bare chain, or even the size of the system. Consequently, side spins can effectively slow down the decay and make the variation become flat in the region of large distances (figure 3). There seems to exist AF LRO.

Now, we turn to consider an infinite Q1D system, which is constructed by periodically adding side spins in the same sublattice (figure 1(b)). The total number of sites is $N = K(l+2)$, where K denotes the number of cells and l the number of sites on the chain between every two side spins. l must be odd, i.e. $l = 2k+1$, where $k = 0, 1, 2, \ldots$. 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 [10], the global spin of the GS is

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

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

$$g(\boldsymbol{q}) \equiv \langle G|\vec{S}(-\boldsymbol{q}) \cdot \vec{S}(\boldsymbol{q})|G\rangle. \tag{3}$$

$\vec{S}(\boldsymbol{q}) = 1/\sqrt{N}\sum_j \vec{S}(j)\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{j})$; $\boldsymbol{q}$ is a reciprocal vector. The criterion of magnetic LRO is that $g(\boldsymbol{q}) \geqslant \mathrm{O}(N)$ at some $\boldsymbol{q}$. If $g(\boldsymbol{Q}) \geqslant \mathrm{O}(N)$, where $\boldsymbol{Q} = (\pi, \pi, \ldots, \pi)$, there exists

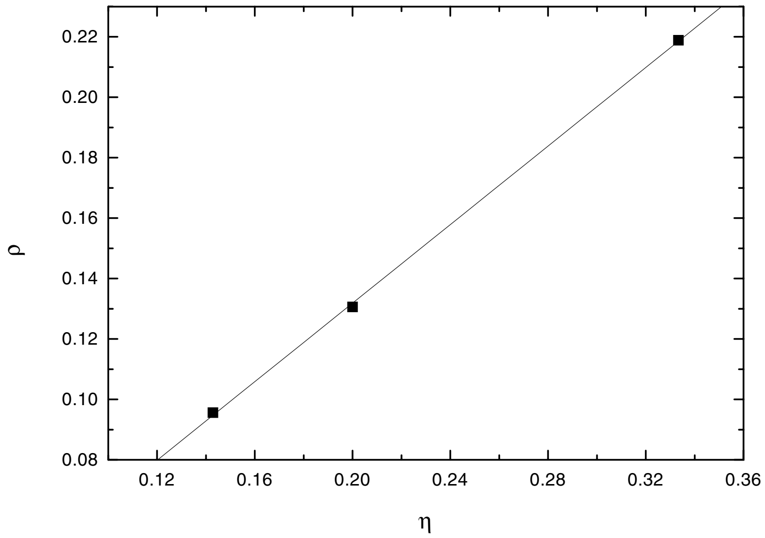

Figure 4. ρ versus η. The solid line is obtained by fitting ρ in a linear way.

AF LRO. If $g(\mathbf{0}) \geqslant O(N)$, there exists F LRO. Following the approaches developed by Tian [12, 13], one can obtain

$$g(\boldsymbol{Q}) > g(\mathbf{0}) = \frac{\Lambda^2 + \Lambda}{N}. \tag{4}$$

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

$$g(\boldsymbol{Q}) > g(\mathbf{0}) > O(N). \tag{5}$$

From these inequalities, one can conclude that AF and F LRO coexist in the GS, and the former is predominant. In other words, side spins set up magnetic LRO.

Obviously, although there always exists magnetic LRO for finite l, both 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:

$$\Gamma_F \equiv \frac{1}{N^2} \sum_{i,j} \langle G|\vec{S}(i) \cdot \vec{S}(j)|G\rangle \tag{6}$$

and

$$\Gamma_{AF} \equiv \frac{1}{N^2} \sum_{i,j} \lambda_{ij} \langle G|\vec{S}(i) \cdot \vec{S}(j)|G\rangle \tag{7}$$

where $\lambda_{ij} = 1$ when sites i and j belong to the same sublattice and $\lambda_{ij} = -1$ when sites i and j belong to different sublattices. Γ_F and Γ_{AF} will decrease as l increases. When l reaches infinity, the system changes into a one-dimensional chain and the magnetic LRO vanishes (i.e. $\Gamma_F = \Gamma_{AF} = 0$). Possibly, the variation speeds of Γ_F and Γ_{AF} are different. We calculate the ratio $\rho \equiv \Gamma_F/\Gamma_{AF}$ for $l = 1, 3$ and 5, and plot the data in figure 4. ρ decreases as η decreases in an approximately 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 decreases.

Reference [13] has proved that the GS of the one-dimensional Heisenberg AF chain has magnetic LRO when its two sublattices have unequal localized spins. It is interesting to investigate the Q1D system with unequal localized spins. From equations (2) and (4), we can conclude that if

$$\frac{S_{\mathrm{A}}}{S_{\mathrm{B}}} = \frac{k+1}{k+2} \tag{8}$$

$g(\mathbf{0}) = 0$ since $\Lambda = 0$. This means that there is no F LRO. The simplest case is $S_{\mathrm{A}} = \frac{1}{2}$, $S_{\mathrm{B}} = 1$ and $l = 1$. One can give a spin picture of the GS in the valence-bond version. The spin on sublattice B can be divided into two spins $\frac{1}{2}$. One of them forms a singlet with the nearest side spin, and the other combines with its nearest neighbour on the chain. We think this kind of configuration governs the physics of the GS, and it is responsible for the F LRO vanishing. Although we have not exactly proved that the AF LRO cannot exist in the GS of such systems, we believe it is true. However, if $S_{\mathrm{A}}/S_{\mathrm{B}} \neq (k+1)/(k+2)$, the AF and F LRO coexist in the GS.

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