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Spin-correlation function of the $S=1$ antiferromagnetic Heisenberg chain at $T=0$

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The correlation function $\rho(l)=\langle S_i^z S_{i+l}^z\rangle$ is calculated for the spin-1 Heisenberg antiferromagnetic chain ($H=J\sum_i \mathcal{S}_i\mathcal{S}_{i+1}$, $\mathcal{S}_{N+1}\equiv\mathcal{S}_1$) at the ground state. Using the Monte Carlo method of Hirsch, Sugar, Scalopino, and Blankenbecler, we find that $\rho(l)$ decays exponentially in contrast to the $S=\frac{1}{2}$ case where $\rho(l)$ decays algebraically. This fact coincides with Haldane's prediction and recent numerical calculations. We calculate the upper bound of elementary excitation from the structure factor using a variational method which resembles the Feynman theory for elementary excitation of liquid ^{4}He.

Since Haldane's theory in 1983,[1] the ground-state and elementary excitations of the antiferromagnetic Heisenberg (AFH) chain has been investigated by many theorists[1-11] and experimentalists.[12,13] In contrast to the ferromagnetic case, the system shows different behaviors for integer S and half-odd integer S. The simplest case is $S=\frac{1}{2}$ which can be solved by the Bethe ansatz method. It was established that the elementary excitation is gapless. It is expected that the spin-correlation function of the ground state decays algebraically.[14] The exact numerical method has been applied to $S=\frac{1}{2}$ finite chains up to $N=24$.[15-17] Monte Carlo (MC) analysis of the correlation function has been done for a longer chain with $N=40$.[18]

For the $S=1$ case the exact numerical method is applied up to $N=16$,[19] but the existence of Haldane's gap is not clear for such short chains. Takada and co-worker,[8,9] applied the transfer matrix method for infinite length and finite temperature. Extrapolating to the $T=0$ case, they obtained positive results for Haldane's gap. Recently, Nightingale and Blote[10] calculated the lowest energies of the total $S^z=0$ and the total $S^z=1$ case for $N=32$ using a kind of MC method. The energy difference is 0.41 J in the limit of $N\to\infty$ and Haldane's gap was confirmed. Then it seems that the MC method is a powerful tool to investigate the AFH chain. Unfortunately, the method used by Nightingale and Blote is not appropriate to calculate the correlation function. Therefore, we use the Monte Carlo (MC) method proposed by Hirsch, Sugar, Scalapino, and Blanckenbecler (HSSB).[20] The application of the HSSB MC method to the $S=1$ AFH chain was first done by Sogo and Uchinami.[21] They calculated the spontaneous order of the antiferromagnetic chain and obtained a negative result for the existence of Haldane's gap. But in our analysis, the HSSB MC method gives positive results for Haldane's prediction.

In this paper, we retry the HSSB MC calculation for the $S=1$ Heisenberg antiferromagnet and analyze the two-point correlation function $\rho(l)\equiv\langle S_i^z S_{i+l}^z\rangle$ and its Fourier transform $S(q)$. We write the Hamiltonian as follows:

$$H=J\sum_{i=1}^{N}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z)+D\sum_{i=1}^{N}(S_i^z)^2. \quad (1)$$

Using the HSSB decomposition we get the following equation for the partition function Z:

$$Z\simeq \mathrm{Tr}(V_1V_2)^L, \quad (2)$$

$$V_1=\prod_{n=\text{odd}}\exp(-\Delta\tau H_{n,n+1}),$$

$$V_2=\prod_{n=\text{even}}\exp(-\Delta\tau H_{n,n+1}), \quad (3)$$

$$\Delta\tau=\beta/L, \quad (4)$$

$$H_{n,n+1}=J(S_n^xS_{n+1}^x+S_n^yS_{n+1}^y+\Delta S_n^zS_{n+1}^z)+D/2[(S_n^z)^2+(S_{n+1}^z)^2]. \quad (5)$$

We discuss the case $D=0$ and $\Delta=1$ setting $L=32$ or 64, $N=32$ or 64, $\Delta\tau=0.2$, and $J=1$. Then T/J becomes 1/6.4 or 1/12.8. This can be regarded effectively as zero temperature. A Metropolis algorithm is adopted to perform the MC simulation. A Monte Carlo state is represented by a set of $N\times 2L$ spins $S_{i,j}$ ($i=1,\ldots,N$, $j=1,\ldots,2L$). The Boltzmann weight is given by

$$W(\{S_{i,j}\})=\prod_{i+j=\text{even}}a(S_{i,j},S_{i+1,j},S_{i,j+1},S_{i+1,j+1}), \quad (6a)$$

$$a(\alpha,\beta,\gamma,\delta)\equiv\langle\alpha,\beta|\exp(-\Delta\tau H_{i,i+1})|\gamma,\delta\rangle, \quad (6b)$$

where $S_{i,j}$ takes $2S+1$ values $S,S-1,\ldots,-S$. The correlation function of the quantum system at the temperature β^{-1} is given by the correlation function of classical spins $S_{i,j}$:

$$\rho(l)\equiv N^{-1}\sum_{i=1}^{N}\langle S_i^zS_{i+1}^z\rangle=(2NL)^{-1}\sum_{i,j}\langle S_{i,j}S_{i+l,j}\rangle. \quad (7)$$

The Fourier transform of $\rho(l)$ is the structure factor $S(q)$:

$$S(q)\equiv\sum_{l=1}^{N}e^{iql}\rho(l)=(2L)^{-1}\sum_{j=1}^{2L}\langle|S_{q,j}|^2\rangle,\quad q=2\pi n/N, \quad (8)$$

$$S_{q,j}=N^{-1/2}\sum_{m=1}^{N}e^{iqm}S_{m,j}. \quad (9)$$

We use (8) and (9) rather than (7) to calculate the correlation function. In the sequence of the MC calculation we calculate $S_{q,j}$ by the fast Fourier transformation. After MC calculation of $S(q)$ we calculate $\rho(l)$ by the inverse

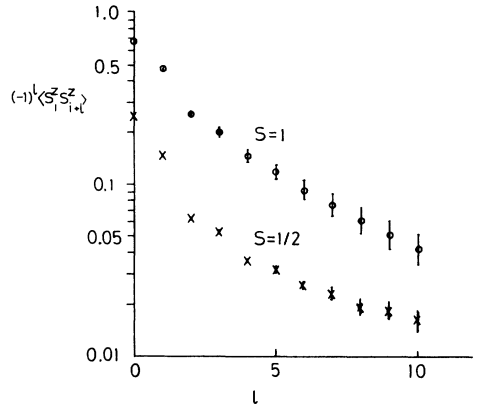

FIG. 1. Longitudinal spin-correlation function $(-1)^l\langle S_i^z \times S_{i+l}^z\rangle$ is plotted as a function l in semilog plot. Crosses are for the $S=\frac{1}{2}$ AFH chain and circles are for $S=1$. Apparently, the $S=1$ data are nearly on a straight line and the $S=\frac{1}{2}$ data are on a logarithmic line.

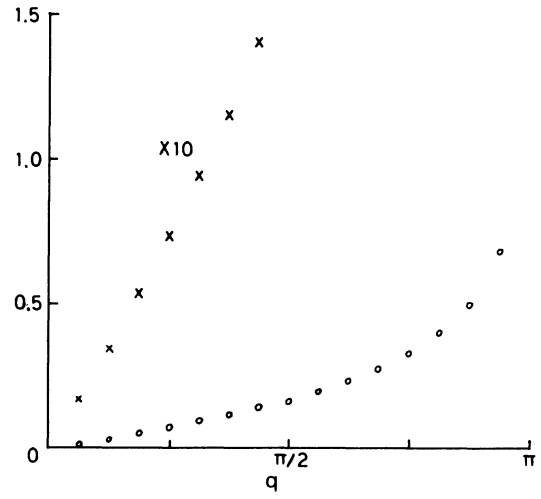

FIG. 3. Structure factor $S(q)$ of the $N=32$, $S=\frac{1}{2}$ AFH chain at the ground state. Circles give its net values. Crosses are ten times the net values. For small q, $S(q)$ behaves as $|q|$.

Fourier transformation. This process is faster than the calculation which uses Eq. (7).

The correlation function $\rho(l)$ is given in Fig. 1 for the $S=\frac{1}{2}$ and $S=1$ cases. In the $S=1$ case $(-1)^l\rho(l)$ decays exponentially. In the $S=\frac{1}{2}$ case, it decays as $1/l$. The statistical error becomes larger as l increases. Our estimation of the correlation length ξ has a large error:

$$\xi=5.5\pm 2. \tag{10}$$

This value is not far from Takada's[9] estimation $(1/\xi\simeq 0.12)$ which is obtained by the transfer matrix method.

The elementary excitation of the AFH chain is expected to have the following approximate form:

$$\varepsilon(q)=c(\sin^2 q+\xi^{-2})^{1/2}. \tag{11}$$

Here, q is momentum of the excitation and c is the so-called light velocity of the system. In the region where q is far from 0 or π, $\varepsilon(q)$ is approximately $c|\sin q|$. According to the spin-wave theory, $\epsilon(q)$ is $2SJ|\sin q|$. Then the spin-wave value of c is $2J$ for the $S=1$ case. Using Eq. (11) we have

$$\varepsilon(\pi)=c/\xi\simeq 0.36J. \tag{12}$$

This value is very near to Nightingale and Blote's calculation of the gap, $0.41J$. The real light velocity is slightly larger than the spin-wave value $2J$. From Parkinson and Bonner's[6] numerical data for the $N=14$ chain, we estimate that c is about $2.7J$. This enhancement of light velocity occurs in the $S=\frac{1}{2}$ AFH chain where the spin-

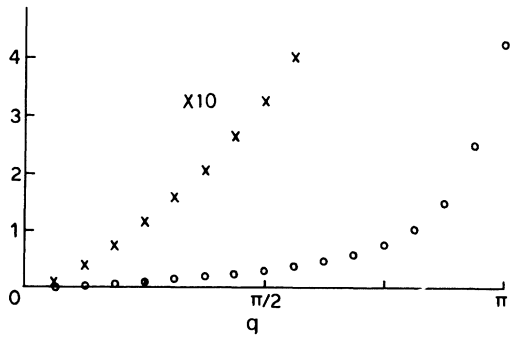

FIG. 2. Structure factor $S(q)$ of the $N=32$, $S=1$ AFH chain at the ground state. Circles give its net values. Crosses are ten times of net values. For small q, $S(q)$ behaves as q^2.

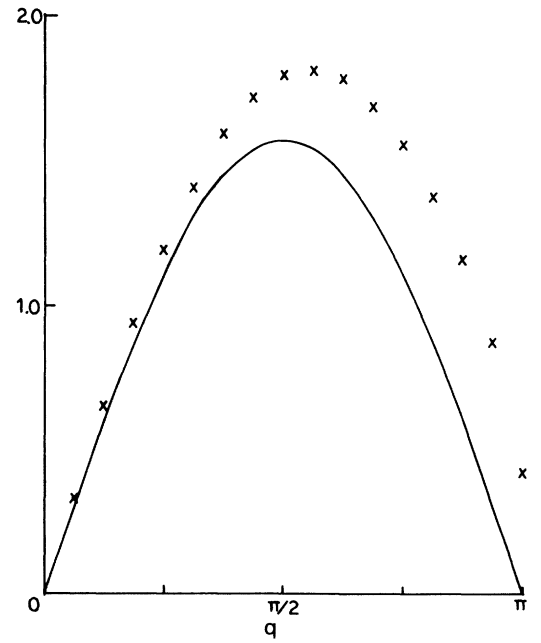

FIG. 4. Elementary excitation $\varepsilon(q)$ and $g(q)$ defined in Eq. (13) for the $S=\frac{1}{2}$ AFH chain in units of J. Solid line is $\varepsilon(q)$ which is taken from des Cloiseaux and Pearson's solution (Ref. 22) $[\varepsilon(q)=(J\pi/2)|\sin q|]$. Crosses are $g(q)$ for the $N=32$ chain.

wave value of c is J instead of the exact value $c=\pi J/2$ (Ref. 22).

The structure factor $S(q)$ is related to the elementary excitation $\varepsilon(q)$. At $q=0$, $S(q)$ becomes zero. Near $q=\pi$, $S(q)$ diverges logarithmically for the $S=\frac{1}{2}$ case. But for the $S=1$ case, it has a Lorenzian peak at $q=\pi$. In the same way as Feynman's[23] variational theory for excitation spectrum of liquid ^{4}He, we get the following inequality:

$$\varepsilon(q)\leq g(q)\equiv 2J(1-\cos q)[-\rho(1)]/S(q)\,. \tag{13}$$

Assume that $|\psi\rangle$ is the ground-state wave function of the Hamiltonian H. Consider the trial wave function with momentum q:

$$S^z_q|\psi\rangle\equiv N^{-1/2}\sum_{m=1}^{N} e^{iqm}S^z_m|\psi\rangle\,. \tag{14}$$

Then we have

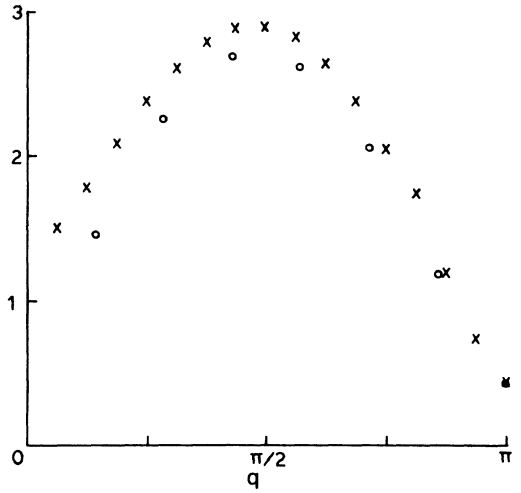

FIG. 5. Elementary excitation $\varepsilon(q)$ and $g(q)$ defined in (13) for $S=1$ AFH chain in units of J. Circles are elementary excitation with total spin one and momentum q of the $N=14$ chain which is taken from the Parkinson and Bonner's table in Ref. 6. Crosses are $g(q)$ for the $N=32$ chain.

$$\begin{aligned}\varepsilon(q)=[\varepsilon(q)+\varepsilon(-q)]/2 &\leq \frac{1}{2}\frac{\langle\psi|S^z_{-q}HS^z_q+S^z_qHS^z_{-q}|\psi\rangle}{\langle\psi|S^z_{-q}S^z_q|\psi\rangle}-E_0\\ &=-\frac{1}{2}\frac{\langle\psi|[S^z_{-q},[H,S^z_q]]|\psi\rangle}{\langle\psi|S^z_{-q}S^z_q|\psi\rangle}=\frac{J(1-\cos q)\left\{-N^{-1}\sum_i\langle S^x_iS^x_{i+1}+S^y_iS^y_{i+1}\rangle\right\}}{S(q)}\\ &=2J(1-\cos q)[-\rho(1)]/S(q)\,.\end{aligned} \tag{15}$$

Thus we get Eq. (13). A similar inequality was obtained by Hohenberg and Brinkman.[24] The numerator of Eq. (13) behaves as q^2 near $q=0$. Then $S(q)$ for the $S=1$ Heisenberg antiferromagnet should behave as q^α ($\alpha\geq 2$) because $\varepsilon(q)$ is bounded from below. This can be seen from Fig. 2 where $S(q)$ is plotted for the $N=32$, $S=1$ AFH chain. In fact, $S(q)$ behaves as q^2 near $q=0$. On the other hand, $S(q)$ for the $S=\frac{1}{2}$ case behaves as $|q|$ as shown in Fig. 3. Thus the behavior of $S(q)$ is different for the $S=\frac{1}{2}$ and 1 cases. As shown in Fig. 4, the inequality (13) stands very well for the $S=\frac{1}{2}$ case. Here, $g(q)$ and $\varepsilon(q)$ are almost the same near $q=0$. In Fig. 5, we plot $g(q)$ for the $S=1$ and $N=32$ cases. We have no data on $\varepsilon(q)$ for such a long chain. As a comparison, we plot $\varepsilon(q)$ for the $N=14$ case from Ref. 6. In conclusion, it is expected that the system has an elementary excitation assumed in Eq. (11). This excitation resembles the mode of des Cloiseaux and Pearson[22] for the $S=\frac{1}{2}$ chain but is different near $q=0$ and π.

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