We investigate the long-distance asymptotic behavior of the dimer correlations in the spin-1/2 alternating XY chain both at $T = 0$ and at sufficiently low-temperatures. The correlations consist of the dimer long-range order part and the exponentially decaying one. Although the dimer long-range order takes the different values depending on the choice of the spin pairs, the behavior in the decaying term is same irrespective of the choice of spin pairs.
The spin-Peierls phase transition has been studied as one of the attracting problems by many theoretical and experimental physicists. Some physicists attempted to understand the mechanism of the spin-Peierls phase transition by investigating the spin-1/2 alternating quantum Heisenberg chain. This system is thought to represent the spin degree of freedom of the organic compounds which fall into the spin-Peierls state at sufficiently low-temperatures. The degree of the bond alternations is treated as a given parameter, though it should be determined so as to minimize the total energy.

The spin-1/2 alternating $XY$ chain has been studied as one of the exactly solvable models for the spin-Peierls state. The Hamiltonian is

$$H = J \sum_{j=1}^{N} [1 + (-1)^j \delta] \left( S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right),$$

where $N$ is the system size which is assumed to be even and $\delta$ generates the bond alternation. Here we only show the typical previous works on this model in the following. Pincus [1] first calculated the excitation spectrum by using the Jordan-Wigner transformation. He [1] pointed out that the finite energy gap is generated above the ground state as far as $\delta > 0$. Since then the physical quantities, such as the longitudinal spin correlations $\langle S_j^z S_j^z \rangle$ and susceptibility, have been evaluated by various methods. The long-distance asymptotic behavior of the longitudinal spin correlations was exactly obtained both at $T = 0$ and at sufficiently low-temperatures by one of the present authors (K.O.). [2,3] He [2,3] obtained the correlation length and the pre-exponential factor exactly.

The purpose of the present paper is to exactly estimate the long-distance asymptotic behavior of the dimer correlations both at $T = 0$ and at sufficiently low-temperatures. The definition of the dimer correlation is given as the sum of the dimer long-range order part and the exponentially decaying one; (ii) It takes different value of the dimer long-range order depending on the choice of the spin pairs; (iii) It exhibits same behavior both in the correlation length and the pre-exponential factor irrespective of the choice of the spin pairs.

The organization of the present paper is in the following. We first show the diagonalization procedure of the spin-1/2 quantum $XY$ chain with bond alternation. We secondly show the long-distance asymptotic behavior of the two-point correlation functions of fermion operators at $T = 0$ and at sufficiently low-temperatures. Thirdly we estimate the long-distance asymptotic behavior of the dimer correlations both at $T = 0$ and at sufficiently low-temperatures.

Let us begin with the diagonalization procedure. On the first step, we rewrite the Hamiltonian (1) into the fermion representation by the following Jordan-Wigner transformation

$$S_{2j-1}^z = a_{2j-1} K(2j - 1) = \{S_{2j-1}^-\}^\dagger,$$

$$S_{2j-1}^z = a_{2j-1}^\dagger a_{2j-1} - \frac{1}{2},$$

$$K(2j - 1) = \exp \left[ i \pi \sum_{l=1}^{j-1} a_{2l-1}^\dagger a_{2l-1} + i \pi \sum_{l=1}^{j} b_{2l}^\dagger b_{2l} \right],$$

$$S_{2j}^z = b_{2j}^\dagger K(2j) = \{S_{2j}^-\}^\dagger, S_{2j}^z = b_{2j} b_{2j} - \frac{1}{2},$$

$$K(2j) = \exp \left[ i \pi \sum_{l=1}^{j} a_{2l-1} a_{2l-1} + i \pi \sum_{l=1}^{j} b_{2l} b_{2l} \right],$$

The degree of the bond alternation is treated as a given parameter, though it should be determined so as to minimize the total energy.
where $a_l$ and $b_m$ are the fermion operators and $K(l)$ is the kink operator. By this transformation, the Hamiltonian (1) is rewritten into

$$H = J(1 - \delta) \sum_{j=1}^{N/2} (a_{2j-1}^\dagger b_{2j} - a_{2j-1}b_{2j}^\dagger) + J(1 + \delta) \sum_{j=1}^{N/2} (a_{2j+1}^\dagger b_{2j} - a_{2j+1}b_{2j}^\dagger).$$

(8)

On the next step, we transform the model Hamiltonian by use of the canonical transformation after the Fourier transformation:

$$a_k = \frac{1}{\sqrt{2}}(\alpha_k + \beta_k)e^{-i\theta_k}, \quad b_k = \frac{1}{\sqrt{2}}(\alpha_k - \beta_k)e^{-i\theta_k},$$

(9)

$$\tan 2\theta_k = -\delta \tan k,$$

(10)

where

$$a_k = \frac{1}{N} \sum_k e^{ik(2j-1)}a_{2j-1}, \quad b_k = \frac{1}{N} \sum_k e^{ik2j}b_{2j}.$$  

(11)

Here the summation runs over the first Brillouin zone and $\alpha_k$ and $\beta_k$ are also the fermion operators. By use of the above relations, the model Hamiltonian is diagonalized as

$$H = J \sum_k \omega_k \alpha_k^\dagger \alpha_k - J \sum_k \omega_k \beta_k^\dagger \beta_k,$$

(12)

$$\omega_k = \sqrt{1 - (1 - \delta^2) \sin^2 k}.$$  

(13)

We can see from (12) and (13) that the ground state is defined as the half-filled state and that non-zero $\delta$ value generates the energy gap above the ground state. It also indicates that the Luttiger liquid state which is the ground state of the spin-$1/2$ uniform $XY$ chain is changed into the effective dimer state as far as $\delta > 0$. The support for the above statements is, as Okamoto [2] calculated, obtained by the long-distance asymptotic behavior of the longitudinal spin correlation function $\langle S_z^i S_z^j \rangle$. He showed that the correlation length becomes finite when $\delta$ is non-zero value.

Then we show the long-distance asymptotic behavior of the following two-point correlation functions of fermion operators $g(2m+1)$ which is given by

$$g(2m+1) = \langle a_{2j-1}^\dagger b_{2j+2m}^\dagger \rangle = -\langle a_{2j-1}^\dagger b_{2j+2m} \rangle = \frac{1}{2}(1 + \delta)L(2m) + \frac{1}{2}(1 - \delta)L(2m + 2),$$

(14)

where

$$L(2m)_{T=0} = \frac{1}{2N} \sum_k \frac{\cos 2km}{\sqrt{1 - (1 - \delta^2) \sin^2 k}},$$

(15)

$$L(2m)_{T \neq 0} = \frac{1}{4N} \sum_k \frac{\cos 2km}{\sqrt{1 - (1 - \delta^2) \sin^2 k}} \tanh \left( \frac{\omega_k}{2T} \right).$$

(16)
Here $T = T/J$. The long-distance asymptotic behavior of $L(2m)_{T=0}$ and $L(2m)_{T\neq 0}$ is exactly estimated by Okamoto.[2,3] Here we only write down the asymptotic form of $L(2m)_{T=0}$ without entering into the details of the derivation.

$$L(2m)_{T=0} \sim \frac{(-1)^m}{2\sqrt{\pi \delta}} \frac{1}{\sqrt{m}} \exp \left[-ma_{T=0}\right],$$

where

$$a_{T=0} = \frac{1}{\xi_{T=0}} \log(1+\delta) - \log(1-\delta).$$

Here $\xi_{T=0}$ is the correlation length. When $\delta = 0$, the correlation length becomes infinite, which suggests the power-law behavior of $L(2m)_{T=0}$.

We show the long-distance asymptotic behavior of $L(2m)_{T\neq 0}$ at sufficiently low temperatures:

$$L(2m)_{T\neq 0} \sim \frac{(-1)^m 2\tilde{T} u_1^m}{\sqrt{\delta^2 + (1 + \delta^2)\pi^2 \tilde{T}^2 + \pi^4 \tilde{T}^4}},$$

where

$$u_1 = \frac{1 + \delta^2 + 2\pi^2 \tilde{T}^2 + 2\sqrt{\delta^2 + (1 + \delta^2)\pi^2 \tilde{T}^2 + \pi^4 \tilde{T}^4}}{1 - \delta^2}.$$

The above result gives the reasonable value at sufficiently low temperatures, because the temperature dependence is evaluated by the most contributing pole at sufficiently low temperatures. If we expand the correlation length around $T = 0$, the derivation of the correlation length at low temperatures can be estimated.

The dimer correlations (Fig.1) are expressed by use of $g$'s as follows;

$$D(2j - 1 : 2j - 1 + 2m)$$
$$\equiv \langle T(2j - 1, 2j)T(2j - 1 + 2m, 2j + 2m) \rangle$$
$$= [g(1)]^2 - g(1 + 2m)g(1 - 2m),$$

where

$$T(l, m) = S^+_l S^-_m + S^-_l S^+_m.$$
The dimer correlations are sum of the dimer long-range order parts and the exponentially decaying ones. We should notice that the correlations have the same correlation length and the same pre-exponential factor though they have different values of the dimer long-range order. The correlation length of the dimer correlations is exactly equal to that of the longitudinal spin correlations derived by Okamoto.[2] That is, the correlation length is given as

\[ \xi_{T=0} = \frac{1}{\log(1+\delta) - \log(1-\delta)}. \] (24)

The correlation length grows from 0 to \(\infty\) with the decrease in the parameter \(\delta\) from 1 to 0. At \(\delta = 1\) where the system is the ensemble of the interacting two-spin systems, it is natural that there is no correlation between the different spin pairs. In particular, both in \(\delta \to 0\) limit and in \(\delta \to 0\) limit the correlation length behaves as

\[ \xi_{T=0} \to \frac{1}{\log[2(1-\delta)]}, \quad (\delta \to 0) \] (25a)
\[ \to \frac{1}{2\delta}, \quad (\delta \to 1) \] (25b)

Finally at \(\delta = 0\) where the system is reduced the spin-1/2 uniform XY chain, the correlation length becomes infinity.

Next we discuss the dimer long-range order terms. As we mentioned above, the dimer long-range order takes different value by the choice of the spin pairs because it is constructed by the product of the nearest neighbor correlations. The explicit forms of dimer long-range order are represented by use of the complete elliptic integrals of first and second kinds as follows.

\[ [g(1)]^2 = \frac{1}{\pi^2(1+\delta)^2} \left[ \delta K\left(\sqrt{1-\delta^2}\right) + E\left(\sqrt{1-\delta^2}\right) \right], \] (26)
\[ [g(-1)]^2 = \frac{1}{\pi^2(1-\delta)^2} \left[ -\delta K\left(\sqrt{1-\delta^2}\right) + E\left(\sqrt{1-\delta^2}\right) \right], \] (27)

where

\[ K(\lambda) = \int_0^\pi \frac{dk}{\sqrt{1-\lambda^2\sin^2 k}}, \] (28)
\[ E(\lambda) = \int_0^\pi dk\sqrt{1-\lambda^2\sin^2 k}. \] (29)

Here we examine the dimer long-range order both in \(\delta \to 0\) limit and in \(\delta \to 1\) limit. In \(\delta \to 0\) limit, we see

\[ \lim_{m \to \infty} \frac{D(2j-1 : 2j-1+2m)}{\pi^2} = \frac{4}{\pi^2} (1 + \delta \log \delta), \] (30a)
\[ \lim_{m \to \infty} \frac{D(2j : 2j+2m)}{\pi^2} = \frac{4}{\pi^2} (1 - \delta \log \delta), \] (30b)
\[ \lim_{m \to \infty} \frac{D(2j-1 : 2j+2m)}{\pi^2} = \frac{4}{\pi^2} \left(1 - (\delta \log \delta)^2/2\right), \] (30c)

and in \(\delta \to 1\) limit

\[ \lim_{m \to \infty} \frac{D(2j-1 : 2j-1+2m)}{\pi^2} = (1 - \delta)^2, \] (31a)
\[ \lim_{m \to \infty} \frac{D(2j : 2j+2m)}{\pi^2} = 4 - 2(1 - \delta^2), \] (31b)
\[ \lim_{m \to \infty} \frac{D(2j-1 : 2j+2m)}{\pi^2} = 2(1 - \delta). \] (31c)
Then we discuss the temperature dependence of the dimer correlations by using (19) and (20). As we have stated above, (19) and (20) are suitable in the sufficiently low temperature region. The results are

\[
D(2j - 1 : 2j - 1 + 2m) \sim [g(1)_{T \neq 0}]^2 + \frac{T^2}{8\pi} \exp \left[ -2m/\xi_{T \neq 0} \right],
\]

\[
D(2j : 2j + 2m) \sim [g(-1)_{T \neq 0}]^2 + \frac{T^2}{8\pi} \exp \left[ -2m/\xi_{T \neq 0} \right],
\]

\[
D(2j - 1 : 2j + 2m) \sim g(1)_{T \neq 0}g(-1)_{T \neq 0} + \frac{T^2}{8\pi} \exp \left[ -(2m + 1)/\xi_{T \neq 0} \right],
\]

where

\[
\xi_{T \neq 0} = \xi_{T = 0} \left( 1 - \frac{\pi^2 T^2}{\delta} \right).
\]

Here \(\xi_{T \neq 0}\) denotes the correlation length at sufficiently low temperatures. We can see that the \(\xi_{T \neq 0} < \xi_{T = 0}\) due to the thermal effects. It means that there is no second-order phase transition at finite temperatures, as the Mermin-Wagner theorem guarantees. The correlations at sufficiently low temperatures have similar character in comparison with those at \(T = 0\). That is, the dimer long-range order takes different value depending on the choice of spin pairs, but the exponential decaying part has the same behavior in the correlation length and pre-exponential factor in each correlation.

In summary, we obtain the following statements: (i) The dimer long-range order takes the different values depending on the choice of spin pairs; (ii) The behavior in the decaying term is same irrespective of the choice of spin pairs, both at \(T = 0\) and at sufficiently low temperatures.

References

1. P. Pincus, Solid State Commun. 9, 71 (1971).
2. K. Okamoto, J. Phys. Soc. Jpn. 57, 2947 (1988).
3. K. Okamoto, J. Phys. Soc. Jpn. 59, 4286 (1990).
Figure Caption

Fig.1 Three kinds of the dimer correlations. (a),(b) and (c) correspond to eq.(21a),(21b) and (21c), respectively.