Local magnetic structures induced by inhomogeneities of the lattice in $S = 1/2$ bond-alternating chains and response to time-dependent magnetic field with a random noise

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Abstract

We study effect of inhomogeneities of the lattice in the $S = 1/2$ bond-alternating chain by using a quantum Monte Carlo method and an exact diagonalization method. We adopt a defect in the alternating order as the inhomogeneity and we call it “bond impurity”. Local magnetic structures induced by the bond impurities are investigated both in the ground state and
at very low temperatures. The local magnetic structure can be looked on as an effective $S = 1/2$ spin and the weakness of the interaction between the local structures causes the quasi-degenerate states in the low energy. We also investigate the force acting between bond impurities and find that the force is generally attractive. We also study the dynamical property of the local magnetic structure. While the local magnetic structure behaves as an isolated $S = 1/2$ spin in the response to a time-dependent uniform field, it is found to be robust against the effect of a random noise applied at each site individually in the sweeping field.
I. INTRODUCTION

The low dimensional quantum spin chains exhibit a wide variety of peculiar properties. Properties of magnetizations induced by inhomogeneities of interaction have been extensively studied. Eggert and Affleck \cite{1, 2} studied spin structure in the open uniform system of $S = 1/2$ Heisenberg antiferromagnetic (HAF) chains, where edges cause the inhomogeneity. Laukamp, et al. also studied the same problem by a DMRG method \cite{3}. There the finite size effect at very low temperatures was not clear. We clarified the temperature dependence of the magnetic structure of the open uniform $S = 1/2$ HAF chain and found the new aspect and finite size effects \cite{4}. While the local susceptibility profile is quite similar to each other at modestly low temperatures regardless of whether the number of spins is even or odd, the profile is very different from each other at very low temperatures. We also studied magnetic structures due to various spatial configurations with one or two bond impurities in the uniform system of $S = 1/2$ HAF chains \cite{4}. There “bond impurity” means a bond with a strength different from those in the bulk. The impurity in the uniform chain causes the division of magnetic structure into domains. There we found that each domain behaves almost independently at modestly low temperatures. However, the interaction between the domains is found to be not negligible at very low temperatures.

Various studies of impurity effect in the $S = 1$ AF chain have been also done. The existence of the edge state was pointed out in the AKLT \cite{5} chain and this edge state in the $S = 1$ AF chain has been studied in detail by numerical method \cite{6, 7}, where the singlet and triplet (Kennedy triplet) states become degenerate in the thermodynamic limit (the four-fold degeneracy). The energy structure due to an $S = 1/2$ impurity was observed in Cu-doped NENP by ESR measurement \cite{8}. A doping of an impurity of $S = 1/2$ causes interesting energy structures \cite{8, 9}. The possibility of the impurity induced long range order has been emphasized. However, it was found that although each of the local structures induced by $S = 1/2$ impurities is robust against the temperature, the correlation between the local structures is very weak at finite temperatures because of the quasi degenerate
energy structure [11].

In this paper we study bond-impurity effects in the bond-alternating chain, where “bond impurity” means a defect of the alternating order. In the bond-alternating system, spins tend to form a dimer state at the strong bond. Therefore, a finite energy gap exists between the ground state and excitation states and the correlation length is finite [12]. The role of the bond impurity is very different from that in the uniform chain. The impurity in the bond-alternating system induces a localized magnetic structure around it and the weak interaction between the local structures results in the quasi-degenerate states in the low energy as the case of $S = 1$ chains.

We also study the force acting between the impurity bonds by investigating the dependence of the ground state energy on the distance between the impurities. The force due to the spin interaction is found to be generally attractive regardless of the type of impurities.

Recently the quantum dynamics in the microscopic or nanoscale systems has received much attention, because the technology in microscopic processing makes remarkable progress and the analyses in microscale or nanoscale phenomena have become possible. At sufficiently low temperatures quantum dynamical effects are important. Among the quantum phenomena in microscale or nanoscale, the concept of quantum tunneling of the magnetization (QTM) has become a topic of much interest. The tunneling dynamics has been studied from view point of the nonadiabatic transition [13–15]. The feature of the nonadiabatic transition is easily analyzed in pure system. However in realistic situations disturbance usually exists. The noise effect in the nonadiabatic transition is a quite interesting problem [16,17]. We study dynamical aspect of the local magnetic structure by investigating the response of the magnetization to a sweeping magnetic field. The structure behaves as an effective $S = 1/2$ spin and shows the same response to the uniform field as an $S = 1/2$ free spin. However, the local magnetic structure shows a different response in a sweeping magnetic field when random noises exist individually at sites. Solving the time-dependent Schrödinger equation, the effect of noise to the tunneling ratio is analyzed. In the uniform field the behavior of magnetization is described by the Landau-Zener-Stückelberg (LZS) formula [18,20]. We
investigate how the noise disturbs the quantum process. Such study would provide a basic information for the manipulation of microscopic or nanoscale magnetic devices in the future.

This paper is organized as follows. In the next section, we explain briefly the method used in this study. In Sect. II, effects of bond impurities on the magnetic structure in bond-alternating chains are studied. In Sect. IV, we study the force between bond impurities. In Sect. V, we investigate the response of the magnetization to a sweeping field. Sect. VI is devoted to the summary and discussion.

**II. MODEL AND METHOD**

The Hamiltonian treated in the present paper is given as

$$\mathcal{H} = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1},$$

where $\mathbf{S}_i = (S^x_i, S^y_i, S^z_i)$ are the $S = 1/2$ spin operators at the site $i$. We study the bond-alternating chain where $J_{i,i+1}$ changes alternately among $J_1$ (a strong bond) and $J_2$ (a weak bond). Here we consider defects of the order in the alternation which cause inhomogeneities of the lattice. We call this inhomogeneity “bond impurity”. To study low temperature properties of the model, we mainly use the loop algorithm with continuous time quantum Monte Carlo method (LCQMC) [21,22]. This method overcomes the problem of long auto-correlation in Monte Carlo update and allows us to study systems at very low temperatures. In the present work, we performed $10^5$ Monte Carlo steps (MCS) for getting equilibrium of the system and $10^6$ MCS to obtain quantities in the equilibrium state. Here a MCS means an update of the whole spins.

We can not specify the value of the magnetization $M_z$ in a standard LCQMC because the number of world line and the winding number are updated automatically in this method. Here we adopt a modified method, where we perform the standard LCQMC and store the data separately according to the $M_z$ space. Thus we can obtain a physical property in the specific $M_z$ space. This method worked successfully in the study of the site impurity problem.
(S = 1/2 spin) in the S = 1 HAF chain [11] and the bond impurity problem in the uniform S = 1/2 HAF chain [4].

In order to study the response of the magnetization of a local magnetic structure to a sweeping field, we investigate the dynamics of spins under a time-dependent external field with a random noise. The Hamiltonian is given by

\[ H = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\Gamma \sum_i S_i^x - \sum_i (H(t) + h_i(t)) S_i^z, \]

(2)

where \( \Gamma \) is transverse field, \( H(t) \) is a time-dependent external field and \( h_i(t) \) is a random noise applied to each site individually. When the uniform external field is swept, dynamics of the magnetization of a local magnetic structure (effective S = 1/2 spin) is the same as that of a free S = 1/2 spin regardless of the interaction \( \{J_{ij}\} \) among spins in the lattice.

The time dependence of the magnetization is obtained by the time-dependent Schrödinger equation (TDSE)

\[ i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H|\Psi(t)\rangle, \]

(3)

where \( |\Psi(t)\rangle \) denotes the wave function of the spin system at time \( t \). We set \( \hbar = 1 \). Equation (3) is solved using the fourth-order fractal decomposition [23],

\[ e^{-itH} = [S_2(-itp_2)]^2 S_2(-it(1 - 4p_2))[S_2(-itp_2)]^2, \]

(4)

where \( S_2(x) = e^{x^2/2}e^{x^2}e^{x^2/2} \) putting \( \mathcal{H}_1 = \sum_i J_{i,i+1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\Gamma \sum_i S_i^x, \mathcal{H}_2 = -\sum_i (H(t) + h_i(t)) S_i^z \) and \( p_2 = (4 - 4\frac{1}{4})^{-1} \).

First we set the applied field to its minimum value \( H(t = 0) = -H_0 < 0 \) and put the system in the ground state for this field and then sweep the filed as

\[ H(t) = -H_0 + ct. \]

(5)

We provide a random noise \( \{h_i(t)\} \) by a Langevin equation (Ornstein-Ulenbeck process),

\[ h(t) = -\gamma \dot{h}(t) + \eta(t). \]

(6)

Here \( \eta(t) \) is a white gaussian noise,
\[ \langle \eta(t) \rangle = 0 \quad \text{and} \quad \langle \eta(0)\eta(t) \rangle = A^2 \delta(t), \]  

(7)

where \( A \) is amplitude, \( \gamma \) is damping factor and \( \tau = 1/\gamma \). Thus obtained random process \( h(t) \) has the properties

\[ \langle h(t) \rangle = 0 \quad \text{and} \quad \langle h(0)h(t) \rangle = \frac{A^2}{2\gamma} \exp\left( -\frac{t}{\tau} \right). \]  

(8)

The dynamics of magnetization is obtained as

\[ M(t) = \langle \Psi(t)| \sum_i S^z_i |\Psi(t) \rangle. \]  

(9)

If the magnetic field changes rather slowly, i.e., the sweep rate is rather small, \( |\Psi(t)\rangle \) changes adiabatically. In this case the state stays in the ground state of the system with the field \( H(t) \) and the magnetization follows the value of the corresponding ground state. When the sweeping rate becomes large the system cannot follow the change completely and the nonadiabatic transition occurs. The probability to stay in the ground state was given by LZS formula as

\[ p = 1 - \exp\left( -\frac{2\pi \Gamma^2}{c} \right). \]  

(10)

When the effect of noise does not become negligible, the noise disturbs the quantum process and this probability changes \[16\]. We find a difference between the response of the magnetization of local magnetic structure (effective \( S = 1/2 \) spin) and that of a free \( S = 1/2 \) spin.

III. BOND IMPURITY IN BOND-ALTERNATING CHAINS

We investigate models with bond alternation, \( \cdots J_1 J_2 J_1 J_2 \cdots \), where \( J_1 > J_2 \). Here we study the effect of a defect in the alternation, such as \( \cdots J_1 J_2 J_1 J_2 J_1 J_2 J_1 J_2 J_1 \cdots \). As mentioned in the introduction, the alternating chain has an energy gap between the ground state and the first excited state and the spin correlation length is finite. These features are similar to those in the \( S = 1 \) AF Heisenberg model which is a Haldane system. As we see
below, in the present chain, the edge state strongly depends on the bond structure at the edge. Thus we study the following four cases of the configurations of bonds:

(a) the two strong bonds are at the center and the edges terminate with a strong bond,
(b) the two strong bonds are at the center and the edges terminate with a weak bond,
(c) the two weak bonds are at the center and the edges terminate with a weak bond,
and
(d) the two weak bonds are at the center and the edges terminate with a strong bond.

Here we take the strong bond to be $J_1 = 1.3$ and the weak bond to be $J_2 = 0.7$, where the correlation length is estimated as $\xi \simeq 0.82$ (see Appendix). Here we take $k_B$ as a unit of energy ($k_B = 1$). These four models have odd number of spins and their ground state is doublet according to the Lieb-Mattis theorem \[24\]. We performed simulations at $T = 0.01$ in the $M_z = 1/2$ space to study magnetic structures in the low energy state. The magnetization profiles $\{m_i\}$ of (a)-(d) are drawn in Fig. 1, where $m_i = \langle S_i^z \rangle$ and $\langle \rangle$ denotes the canonical average at a given temperature. A magnetization is induced locally around the impurity. First we consider the cases where the bonds at edges are strong, i.e., model (a) and (d). If we allocate a singlet pair at each strong bond, a structure with neighboring two strong bonds remains at the center in the model (a), while one site remains in the model (d). The magnetization of $M_z = 1/2$ is assigned in the remaining part at the center of the lattices to induce a local magnetic structure. Because the edge bonds are strong, no magnetization is induced at the edges. Figures 1(a) and (d) are considered to describe well the magnetization profiles of the ground state since these are gapful systems without quasi-degenerate states within a subspace with a fixed magnetization (i.e., $M_z = 1/2$). We find that $M_z$ is distributed only into the $\pm 1/2$ space through all Monte Carlo steps in the simulations.

In the models (b) and (c), when we allocate singlet state at the strong bond, there are three positions for magnetic moments, i.e., the center and both edges. Indeed in both models (b) and (c), magnetizations are induced around the impurity and both the edges. In order to study the distribution of magnetization in the lattice, we introduce the summation of the
magnetization per site from the left edge site

\[ M_z(j) = \sum_{i=1}^{j} m_i. \]  

(11)

We show this quantity for the model (b) in Fig. 2. There the values of the left plateau and right plateau are 0.166 and 0.333, respectively. From this figure we find a spin 1/6 locates at each local structure. This deceptive fractional magnetization is considered to come from mixing of states.

Looking on the local magnetic structure as an effective \( S = 1/2 \) spin interacting by an exchange \( \tilde{J} \), this system is modeled by a three-site Heisenberg model

\[ H = \tilde{J} S_1 \cdot S_2 + \tilde{J} S_2 \cdot S_3. \]  

(12)

In the \( M_z = 1/2 \) space the eigenvalues and the eigenvectors are

\[ E_1 = -\tilde{J}, \quad |\phi_1\rangle = \frac{1}{\sqrt{6}}(|++-\rangle - 2|--\rangle + |+++\rangle), \]

\[ E_2 = 0, \quad |\phi_2\rangle = \frac{1}{\sqrt{2}}(|++-\rangle -|--\rangle), \]

\[ E_3 = \tilde{J}/2, \quad |\phi_3\rangle = \frac{1}{\sqrt{3}}(|++-\rangle + |+-+\rangle + |--\rangle). \]  

(13)

The expectation values of magnetization of spins in each state are

\[ \langle \phi_1 | S^z_1 | \phi_1 \rangle = \langle \phi_1 | S^z_3 | \phi_1 \rangle = 1/3 \quad \text{and} \quad \langle \phi_1 | S^z_2 | \phi_1 \rangle = -1/6, \]

\[ \langle \phi_2 | S^z_1 | \phi_2 \rangle = \langle \phi_2 | S^z_3 | \phi_2 \rangle = 0 \quad \text{and} \quad \langle \phi_2 | S^z_2 | \phi_2 \rangle = 1/2, \]

\[ \langle \phi_3 | S^z_1 | \phi_3 \rangle = \langle \phi_3 | S^z_2 | \phi_3 \rangle = \langle \phi_3 | S^z_3 | \phi_3 \rangle = 1/6. \]  

(14)

Similarly to the case of local magnetic structures induced by \( S = 1/2 \) impurities in the \( S = 1 \) HAF model in the finite temperatures [11], the interaction between the local magnetic structures in this case is expected to be very weak, i.e., \( \tilde{J} \ll 1 \) and also to become exponentially small with the distance, which is due to the gapful nature. Although there are energy gaps between the state \( |\phi_1\rangle, |\phi_2\rangle \), and \( |\phi_3\rangle \), these states are considered to be almost degenerate even at the temperature \( T = 0.01 \). In such a case three states in the \( M_z = 1/2 \) space
appear in equal probability, and the expectation values are given by an equal-weight average in the three state. That is, \( \langle S^z_1 \rangle, \langle S^z_2 \rangle, \) and \( \langle S^z_3 \rangle \) are given by \((1/3 + 0 + 1/6)/3 = 1/6,\)
\((-1/6 + 1/2 + 1/6)/3 = 1/6,\) and \((1/3 + 0 + 1/6)/3 = 1/6,\) respectively. These values correspond to the observed deceptive fractional magnetization.

In order to confirm the above modeling we perform the following two investigations. First, we investigate a short chain of \( L = 21 \) by the diagonalization method in order to check that the ground state of the type (b) is represented by the \( |\phi_1\rangle \) of the three-spin model. Because the length of the chain is short, we choose a chain of a shorter correlation length. Namely, we set \( J_1 = 2 \) and \( J_2 = 0.5, \) respectively (\( \xi \ll 1 \)). Figure \( 3 \) (a) shows the magnetization profile in the ground state of this model, and Fig. \( 3 \) (b) shows the summation of the magnetization from the left edge site (Eq. (11)). The net magnetization around the right and the left edge is positive and that around the impurity site is negative. The value for the left plateau is about 1/3 which corresponds to \( \langle \phi_1|S^z_1|\phi_1\rangle \). The value of the second plateau is about 1/6, which also corresponds to \( \langle \phi_1|S^z_1|\phi_1\rangle + \langle \phi_1|S^z_2|\phi_1\rangle \). Thus the ground state \( |\phi_1\rangle \) represents well that of the type (b) model.

Second, to confirm the quasi-degeneracy in the model (b), we check the distribution of \( M_z \) in the Monte Carlo simulation, which is shown in Fig. \( 4 \). Here the distribution for \( M_z = 3/2 \) is about 12.5 %. Because there are three states in the \( M_z = 1/2 \) space and one state in the \( M_z = 3/2 \) space in the three-spin model, this distribution indicates that these four states are equally populated and that \( T = 0.01 \) is much higher than the energy gaps between these four states. In the three-spin model the eigenvalue of the state of \( M_z = 3/2 \) is \( \tilde{J}/2 \), while the eigenvalues of the state of \( M_z = 1/2 \) are \( -\tilde{J}, 0, \) and \( \tilde{J}/2 \) (Eq. (13)). In the \( M_z = 3/2 \) space we observe \( S = 1/2 \) moment at each local structure as shown in Figs. \( 5 \) (a) and (b), which represents the state \( |++\rangle \) in the effective three-site model. The values \( \{m_i\} \) are almost three times as large as those of Fig. \( 1 \) (b). In principle we can obtain the energy gap from the temperature dependence of the distribution [11]. However it is too small to detect here.

We find a similar scenario for the model (c). Thus we conclude that in bond-alternating
systems, local magnetic structures are induced by a bond impurity or weak edge bonds as an effective $S = 1/2$ spin and they behave almost independently.

Now let us examine more detailed structures of the local magnetic structures. In the case (a) a negative magnetization appears at the middle site, while in the case (d) a positive magnetization appears there. The interaction of the three spins at the center of the model (a) is approximately represented as the three-spin model with the strong bonds (Eq. (12)). Here the magnetizations at the center of the model (a) are distributed as about $(1/3, -1/6, 1/3)$. On the other hand in the model (d) a spin at the center is isolated from the others.

Finally we consider the quasi-degenerate structure of the model (b) (similarly (c)). We found that the impurity-induced local structures in the bond-alternating system can be well described by the effective spin model with small $\tilde{J}$. In order to break a singlet pair a finite energy is necessary which causes the gapful nature of the model. The degree of freedom of induced structures without breaking singlet pairs causes the quasi-degenerate states. In the Haldane system in the open boundary condition, the interaction between the edge magnetic moments brings the singlet and triplet states which is called Kennedy triplet at the low energy. In the $S = 1$ Haldane systems with $S = 1/2$ impurities, doping impurities causes a quasi degenerate low energy structure \[\text{[11]}\]. Similar situation exists in the models (b) and (c). In these cases, according to the above mentioned three spin model, two doublets ($S=1/2$) and one quartet ($S=3/2$) state lie at the low energy as shown in Fig. 6.

The local magnetic structures in the present model are well isolated. Therefore we can locate such magnetic structures as we desire. In Fig. 6 we show the magnetization profile for a model which has five positions of induced structures. This configuration is obtained at a very low temperature in the space of the total magnetization $M_z = 1/2$. Each moment almost behaves independently. Thus magnetization at each location is given by an average over all the possible states. In the present case, $\langle S_i \rangle = 1/10$ $(i = 1 - 5)$. Furthermore we confirmed that the distribution of magnetization $P(M_z)$ is given by a binomial distribution

$$P(M_z) = \frac{1}{2^5} \frac{5!}{(5 - 2|M_z|)! (2|M_z|)!}.$$ (15)
IV. FORCE BETWEEN TWO DEFECTS IN AN ALTERNATING CHAIN

When a bond-alternating system has impurities, what kind of interaction does exist between them, attractive or repulsive? If we allow positions of impurities to move, the distance between impurities is distributed in the canonical distribution according to the interaction between the impurities in the thermal equilibrium at a given temperature [4]. We study the force between the bond impurities in this section. We estimate the ground state energies of the spin system in various fixed configurations of bonds and compare the ground state energies as a function of the distance between the bond impurities. Namely, we study effective interaction between the impurities due to the spin interaction.

In the alternate chain (\(\cdots J_1J_2J_1J_2\cdots\)), the system may have a pair of defects by shifting a position of a strong bond by one.

\[
\cdots J_1J_2J_1J_2J_1J_2\cdots. \quad (16)
\]

If we shift the position furthermore, the system has a configuration

\[
\cdots J_1J_1J_2J_1J_2J_1\cdots, \quad (17)
\]

etc. We study dependence of the energy on the distance (\(\Delta_a\)) between the positions of \(J_1J_1\) and \(J_2J_2\). We define \(\Delta_a = 0\) for the case of no defect, \(\Delta_a = 1\) for the configuration (16), \(\Delta_a = 2\) for the configuration (17) and so on. In Fig. 8 (a) we plot the ground state energy as a function of \(\Delta_a\) obtained by exact diagonalization for \(L = 24\) with \(J_1 = 2\) and \(J_2 = 1\) in the periodic boundary condition (PBC). This combination of \(J_1\) and \(J_2\) is used throughout this section. The ground state energy becomes greater as \(\Delta_a\) becomes larger. Therefore we find an attractive force between the impurities (\(J_1J_1\) and \(J_2J_2\)).

Next another situation is considered. If one \(J_2\) is exchanged by \(J_1\) in the alternating chain, the system has a configuration

\[
\cdots J_1J_2J_1J_2J_1\cdots. \quad (18)
\]
We define $\Delta_b = 0$ for the configuration (18). Shifting a position of a $J_1$ by one, the system has two $J_1J_1$ pairs and has a configuration,

$$
\cdots J_1J_1J_2J_1J_1 \cdots \tag{19}
$$

We define this distance between $J_1J_1$ and $J_1J_1$ as $\Delta_b = 1$. Furthermore, $\Delta_b = 2$ is defined for the configuration (20) and etc.

$$
\cdots J_1J_1J_2J_1J_2J_1 \cdots \tag{20}
$$

The ground state energies are shown as a function of $\Delta_b$ in Fig. 8 (b). We also study the interaction between $J_2J_2$ and $J_2J_2$, where we define $\Delta_c$ in the same way exchanging the role of $J_1$ and $J_2$. We plot the ground state energies as a function of $\Delta_c$ in Fig. 8 (c). In all cases, we observe that the ground state energy increases as the distance becomes larger. Thus an attractive force acts between the impurities regardless of their type.

V. RESPONSE OF THE LOCAL MAGNETIC STRUCTURE TO THE MAGNETIC FIELD

In this section we investigate the response of the magnetization of a local magnetic structure (effective $S = 1/2$ spin) induced by a bond impurity and of a free $S = 1/2$ spin to a time-dependent magnetic field with a random noise.

First let us consider the response of the magnetization of a free $S = 1/2$ spin. The Hamiltonian without noise is given by

$$
\mathcal{H}(t) = 2\Gamma S_x - (-H_0 + ct)S_z. \tag{21}
$$

This system is two-level system whose energy levels are shown in Fig. 8 as a function of $H$, where the avoided level crossing occurs near $H = 0$. If $H_0 \gg \Gamma > 0$, the ground state consists primarily of the $M_z = -1/2$ state at $t = 0$. The probability for the system to end up in the $M_z = 1/2$ state (i.e., the probability to change its magnetization) at $t = \infty$ is given by Eq. (10)
Next we consider the case of a local magnetic structure (effective \( S = 1/2 \)) on a lattice. Because we can treat a limited number of spins in the scheme of Eq. (3), we adopt here the minimum model of (d) in Fig. 1, where the system consists of five sites and we take \( J_1 = 1.0 \) and \( J_2 = 0.5 \). This system is the minimum bond-alternating model with a \( J_2J_2 \) bond impurity. This system is looked on as an effective \( S = 1/2 \) spin. When the noise \( \{ h_i(t) \} \) does not exist, dynamics of the system is generally the same as that of a free \( S = 1/2 \) spin as far as we concern the states in an \( S = 1/2 \) space. It is easily understood as follows. Adopting \( \{ |+\rangle, |-\rangle \} \) as the basis set, the matrix representation of Eq. (22) is

\[
\mathcal{H} = \begin{pmatrix}
-H/2 & \Gamma \\
\Gamma & -H/2
\end{pmatrix}.
\]  

(22)

Noting that \( \sum_i J_{i,i+1} S_i \cdot S_{i+1} \) and \( 2\Gamma \sum_i S_i^z - H(t) \sum_i S_i^z \) commute, the matrix representation of Eq. (2) in the total \( S = 1/2 \) space is given by

\[
\mathcal{H} = \begin{pmatrix}
-H/2 + \text{const.} & \Gamma \\
\Gamma & -H/2 + \text{const.}
\end{pmatrix},
\]  

(23)

adopting \( \{ |S_{\text{tot}} = 1/2, M_z = 1/2 \rangle, |S_{\text{tot}} = 1/2, M_z = -1/2 \rangle \} \) as the basis set. The constant in Eq. (23) does not depend on \( H(t) \). Thus the dynamics is independent of the number of sites and the combination of \( \{ J_{ij} \} \).

In the experimental situation, however, noise usually has an influence on the system. If a random noise is applied to each site, the term \( -\sum_i (H(t) + h_i(t)) S_i^z \) does not commute with \( (S_{\text{tot}})^2 = (\sum S_i)^2 \), and therefore the dynamics would be changed when the interaction \( \{ J_{ij} \} \) and the system size are varied.

It would be expected that the effect of noise is reduced as the system size becomes large and a local magnetic structure (effective \( S = 1/2 \) spin) consisting of some number of spins is less sensitive to such a random noise than a free \( S = 1/2 \) spin. In order to study effects of the noise we investigate the following properties.

First let us study the broadening of the level due to the noise. For a single spin the energy level with a noise is given by

\[
E_\pm = \frac{1}{2} \sqrt{(2\Gamma)^2 + (h(t))^2}
\]  

(24)
and the energy gap is given by

\[ \Delta E = \sqrt{(2\Gamma)^2 + (h(t))^2} \]  

(25)

for \( H(t) = 0 \). Thus using the distribution of \( h(t) \) (a gaussian distribution with the variance \( A^2/2\gamma \) in Eq. (2)), we can calculate the mean \( \langle \Delta E \rangle \) and the width \( \delta E = \sqrt{\langle (\Delta E)^2 \rangle - \langle \Delta E \rangle^2} \), which are listed in Table I. For the local magnetic structure, we calculate the energy gap in a noise by a perturbation method. That gives

\[ \Delta E = 2\Gamma + \frac{2|\langle \phi_1^{(0)}|V_1|\phi_2^{(0)} \rangle|^2}{E_2^{(0)} - E_1^{(0)}} + \text{contributions from higher levels,} \]  

(26)

where \( E_1^{(0)} \) and \( \phi_1^{(0)} \) (\( E_2^{(0)} \) and \( \phi_2^{(0)} \)) are the eigenstate of the ground state (the first exited state) of the non perturbed hamiltonian. The term \( V_1 \) is \( \sum_i h_i S_i^z \). Noting that

\[ \langle |\langle \phi_1^{(0)}|V_1|\phi_2^{(0)} \rangle|^2 \rangle = \sum_i \langle h_i^2 \rangle |\langle \phi_1^{(0)}|S_i^z|\phi_2^{(0)} \rangle|^2, \]  

(27)

we can calculate \( \langle \Delta E \rangle \) from the distribution of \( \{h_i\} \), which are also listed in Table I.

For large values of \( A \), we obtain the energies by diagonalizing the hamiltonian Eq. (2) and obtained \( \langle \Delta E \rangle \) and \( \delta E \) numerically from 500 samples of \( \{h_i\} \), which are also listed in Table I. Thus we find the noise causes almost the same effect on the broadening of the energy levels at \( H(t) = 0 \) in both systems, i.e., a single spin and a local magnetic structure, which is not in accordance with the above expectation.

Second, we investigate the dynamical properties of the both systems. In particular, we study the time evolution of magnetization under the sweeping field with a noise. We set parameters \( \Gamma = 0.02, H_0 = 0.5, c = 0.0005, t_{max}=2000, \) and \( dt = 0.01 \). In this parameter set the probability \( p \) in Eq. (10) is nearly 1.

As was mentioned, the responses of the magnetization are the same in both systems when a random noise is not applied. Time evolution without noise is shown by thin dotted lines in Figs. (10) (a)-(c). Next we investigate the dynamics with the random field (Eq. (3)). We observe the three cases changing the amplitude \( A \) of noise (Eq. (4)); (a) \( A = 0.01 \), (b) \( A = 0.02 \) and (c) \( A = 0.03 \). The value of \( \gamma \) is fixed at 0.1. The lowest two energy levels
for the model of the five spins with a random noise \( \{ h_i(t) \} \) for case (b) are illustrated as a function of time in Fig. [1]. It should be noted that under a random noise the dynamics does not obey simple LZS transition.

Figure [10] (a) shows \( M(t) \) in the noise of a small amplitude (\( A = 0.01 \)). The transition probabilities for a local magnetic structure (effective \( S = 1/2 \) spin) and an \( S = 1/2 \) free spin are very close to each other at this small amplitude and the probabilities are reduced by a little amount from the probability of the pure system (i.e., \( h_i(t) = 0 \)). Increasing the amplitude to \( A = 0.02 \) (Fig. [10] (b)), \( M(t) \) at the final state is more reduced. We find that \( M(t) \) at the final state for a local magnetic structure is larger than that of a free spin. In \( A = 0.03 \) (Fig. [10] (c)) the difference becomes more distinct.

The reduction of \( M(t) \) by field fluctuation corresponds to the reduction of \( p \) in Eq. (10), which has already pointed out for a single spin by Y. Kayanuma and H. Nakayama [16]. Our results are qualitatively consistent with their results.

We conclude that the transition probability \( p \) is different between a local magnetic structure (effective \( S = 1/2 \) spin) and a free \( S = 1/2 \) spin under a sweeping field with a random noise in the individual site. \( M(t) \) at the final state for a local magnetic structure is larger than that of a free spin, which indicates that a local magnetic structure induced by an impurity is less sensitive to the noise. This is in accordance with our expectation. This feature may be due to this bulky structure of the local magnetic structure. From this observation we may expect that local magnetizations are easier to manipulate than single spins in a field with noise. Detail analysis for the noise dependence will be reported elsewhere.

VI. SUMMARY AND DISCUSSION

Effects of bond impurities were investigated in the bond-alternating chain, where the role of the bond impurity is very different from that in the uniform chain and rather similar to that of the site impurity of the Haldane systems because of the gapful nature. While the bond impurity in the uniform chain causes the division of magnetic structure into domains,
the bond impurity in the bond-alternating chain induces a magnetic structure around it. It was found that induction of magnetic moments at edges depends on whether the edge bonds are strong or weak. In the bond-alternating chain, the local magnetic structures behave almost independently even at very low temperatures, contrary to the case of the uniform chain.

We showed that a local magnetic structure induced by a bond impurity can be looked on as an effective $S = 1/2$ spin. It was found that these local structures interact with one another by very small effective couplings $\tilde{J}$, which causes the quasi-degenerate states in the low energy.

We also studied the force acting between these defects of alternation. In the bond-alternating chain two kinds of defects, $J_1 J_1$ and $J_2 J_2$ exist. We investigated the forces between $J_1 J_1$ and $J_1 J_1$, between $J_2 J_2$ and $J_2 J_2$, and between $J_1 J_1$ and $J_2 J_2$. It turned out that the forces are generally attractive regardless of the type of impurities.

We considered what property is different between the local magnetic structure (effective $S = 1/2$ spin) induced by an impurity and a free $S = 1/2$ spin. It has been found that the noise has almost the same effect on the broadening of the energy levels in both systems. However, we found a difference in the response of the magnetization to a time-dependent magnetic field with a random noise. That is, the local magnetic structure is found to be more robust against noise applied at each site individually. We hope that this work is a starting research concerned with the manipulation of microscopic or nanoscale magnet and to be applied to the technology of manipulation of a microscopic or nanoscale magnetic device. We also hope that the present study helps to analyze the magnetic properties at low temperatures such as observed by NMR measurement.

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APPENDIX A: THE CORRELATION LENGTH OF BOND-ALTERNATING CHAIN \((S = 1/2)\)

We determined the correlation length of HAF bond-alternating chain \((S = 1/2)\) in the ground state as a function of the ratio \(J_1/J_2\). We calculated the correlation function for various ratios \((J_1/J_2)\) and estimated the correlation length using the relation

\[
\ln\langle S^z_i S^z_j \rangle = \text{constant} - \frac{r_{ij}}{\xi},
\]

where \(r_{ij}\) denotes the distance between site \(i\) and site \(j\), and \(\xi\) denotes the correlation length of the system. We treated periodic chains with 60 sites and simulations were performed at \(T = 0.01\) in the \(M_z = 0\) space. We show the correlation lengths for various ratios \((J_1/J_2)\) in Table II. Here we adopt the length of a pair of bonds for \(J_1\) and \(J_2\) to be a unit length, i.e., this unit is double of the bond length.
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FIGURES

FIG. 1. Magnetization profiles \( \{m_i\} \) of the models (a)-(d) at \( T = 0.01 \) in the \( M_z = 1/2 \) space. (a) and (c) contain 63 sites and (b) and (d) contain 65 sites. The diamonds denote the strength of bonds \( \{J_{i,i+1}\} \), those at high positions denote \( J_1 \) and those at the low positions denote \( J_2 \). Details are shown in text.

FIG. 2. Summation of magnetization per site from the left edge site for the model (b).

FIG. 3. (a) Magnetization profile \( \{m_i\} \) of a bond-alternating chain of the type (b) in Fig. 1 with \( L = 21 \). The strong and weak bonds are \( J_1 = 2 \) and \( J_2 = 0.5 \), respectively. (b) Summation of magnetization per site from the left edge site.

FIG. 4. Distribution of \( M_z \) for the model (b) in Fig. 1.

FIG. 5. (a) Magnetization profile \( \{m_i\} \) for the model (b) in Fig. 1 in the \( M_z = 3/2 \) space at \( T = 0.01 \). (b) Summation of magnetization per site from the left edge site.

FIG. 6. Low energy structure of the model (b).

FIG. 7. Magnetization profile \( \{m_i\} \) for a model which has five positions of induced moments in the \( M_z = 1/2 \) space at \( T = 0.01 \) with \( L = 101 \). The diamonds denote the strength of bonds \( \{J_{i,i+1}\} \), those at high positions denote \( J_1 \) and those at the low positions denote \( J_2 \).

FIG. 8. Ground state energy as a function of (a) \( \Delta_a \), (b) \( \Delta_b \) and (c) \( \Delta_c \) obtained by the exact diagonalization (\( L = 24 \), PBC).

FIG. 9. Avoided level crossing.
FIG. 10. Time evolution of magnetization. Thin dotted line denotes the magnetization without noise. Thick line denotes the magnetization of a local magnetic structure (effective $S = 1/2$ spin) with a random noise (averaged over 500 samples $\{h_i\}$). Thick dotted line denotes the magnetization of a free $S = 1/2$ spin with a random noise (averaged over 500 samples $\{h_i\}$). (a) $A = 0.01, \gamma = 0.1$, (b) $A = 0.02, \gamma = 0.1$, (c) $A = 0.03, \gamma = 0.1$

FIG. 11. Energy structure of the two level system with a random noise for $A = 0.02, \gamma = 0.1$. 
TABLES

TABLE I. Average energy gaps $\langle \Delta E \rangle$ and their widths $\delta E$ for several values of $A/\sqrt{2\gamma}$. (1), (5), and (9) mean a single free spin, the minimum model consisting of 5 spins, and the next minimum model consisting of 9 spins of the type (d) in Fig. 1, respectively. The subscript $p$ denotes that the quantities are obtained by the perturbation method and the subscript $d$ denotes that the quantities are obtained by the exact diagonalization method.

TABLE II. Correlation length $\xi$ as a function of the ratio of the $J_1/J_2$ in the bond-alternating chain ($S = 1/2$)
Fig. 1 (a) M. Nishino, et al.
Fig. 1 (b) M. Nishino, et al.
Fig. 1 (c) M. Nishino, et al.
Fig. 1 (d) M. Nishino, et al.
Fig. 2 M. Nishino, et al.
Fig. 3 M. Nishino, et al.
Fig. 4  M. Nishino, et al.
Fig. 5 M. Nishino, et al.
Fig. 6 M. Nishino, et al.
Fig. 7  M. Nishino, et al.
$E(H)$

$H$

$1 - p$

$\Delta E = 2\Gamma$

Fig. 9 M. Nishino, et al.
Fig. 10(b) M. Nishino, et al.
Fig. 11 M. Nishino, et al.
Table I

| $A/\sqrt{\gamma}$ | $\Delta E_d(1)$ | $\delta E_d(1)$ | $\Delta E_p(5)$ | $\Delta E_d(5)$ | $\delta E_d(5)$ | $\Delta E_p(9)$ | $\Delta E_d(9)$ | $\delta E_d(9)$ |
|-------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 0.01              | 0.0412          | 0.0016          | 0.0412          | 0.0016          | 0.0412          | 0.0016          | 0.0413          | 0.0017          |
| 0.02              | 0.0445          | 0.0056          | 0.0450          | 0.0054          | 0.0450          | 0.0054          | 0.0446          | 0.0058          |
| 0.03              | 0.0486          | 0.0105          | 0.0513          | 0.0111          | 0.0514          | 0.0111          | 0.0492          | 0.0112          |
| 0.04              | 0.0542          | 0.0157          | 0.0601          | 0.0169          | 0.0602          | 0.0169          | 0.0546          | 0.0171          |
| 0.05              | 0.0609          | 0.0222          | 0.0714          | 0.0213          | 0.0716          | 0.0213          | 0.0605          | 0.0233          |

Table II

| $J_1/J_2$ | 1.2 | 1.3 | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 | 1.9 | 2.0 |
|-----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| $\xi$     | 2.02| 1.51| 1.31| 1.18| 1.01| 0.93| 0.84| 0.80| 0.77|