Localization length of a soliton from a non-magnetic impurity in a general double-spin-chain model

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A localization length of a free-spin soliton from a non-magnetic impurity is deduced in a general double-spin-chain model ($J_0$-$J_1$-$J_2$-$J_3$ model). We have solved a variational problem which employs the nearest-neighbor singlet-dimer basis. The wave function of a soliton is expressed by the Airy function, and the localization length ($\xi$) is found to obey a power law of the dimerization ($J_2 - J_3$) with an exponent $-1/3$: $\xi \sim (J_2 - J_3)^{-1/3}$. This explains why NaV$_2$O$_5$ does not show the antiferromagnetic order, while CuGeO$_3$ does by impurity doping. When the gap exists by the bond-dimerization, a soliton is localized and no order is expected. Contrary, there is a possibility of the order when the gap is mainly due to frustration.

75.10.Jm, 75.50.Ee, 75.30.Hx

A possibility of the superconductivity upon doping carriers to the spin-ladder system has attracted much interest to the quasi-one dimensional quantum spin system these years. Without the doping, the ground state of the spin-ladder has strong singlet-dimer correlations along the rung pairs. It leads to the finite energy gap and no long-range magnetic order. Many intensive investigations were done in the course of doping impurities to the spin-gapped systems after this prediction. As its byproduct, an unexpected anomaly was found. That is, the long-range antiferromagnetic (AF) order appears by doping non-magnetic impurities to a spin-gapped material. Copper sites of the base compound, SrCu$_2$O$_3$, is replaced with non-magnetic zinc atoms. The impurity destroys the spin gap with only 1% concentration, and causes the AF order at low temperature. This doping effect suddenly became a big topic both experimentally and theoretically. The similar phenomena was also observed in inorganic spin-Peierls compound, CuGeO$_3$. This compound can be explained theoretically by the one-dimensional frustrated spin system with a ratio of the next-nearest-neighbor to the nearest-neighbor interaction $\alpha \sim 0.35$. Thus, the origin of the gap is frustration. On the other hand, another spin-Peierls compound NaV$_2$O$_5$ has not shown the antiferromagnetic order by the Na depletion, while the energy gap disappear. The origin of the gap of this system is the bond-dimerization. We can attribute this difference to the origin of the gap.

Generally, one non-magnetic impurity atom destroys one singlet dimer pair, and makes one free spin-$1/2$. We call it a soliton hereafter. Solitons should interact with each other to be ordered antiferromagnetically. Thus, a localization length of a soliton, $\xi$, should exceed a mean distance between impurities. Up to now, an explicit expression for the wave function of a soliton or for its localization length has not given analytically. Theoretical investigations have been done mainly by numerical methods. In this paper, we deduce $\xi$ as a function of the strength of interaction bonds in a general double-spin-chain model by using a variation which employs the nearest-neighbor singlet-dimer basis. The result explains why a soliton localizes in the system whose energy gap exists by the bond-dimerization.

We consider the following spin Hamiltonian as the base system under the open boundary conditions:

$$\mathcal{H} = \sum_{n=1}^{N} \left( J_0 \sigma_n \cdot \sigma_{n+1} + J_1 \tau_n \cdot \tau_{n+1} + J_2 \sigma_n \cdot \sigma_{n+1} + J_3 \tau_n \cdot \tau_{n+1} \right)$$

FIG. 1. (a) Shape of the a general double spin-chain model with a single non-magnetic impurity at the origin, $\sigma_0$. (b) An equivalent bond-depleted model to the site-depleted model (a). Soliton sites are indicated by numbers. (c) A schematic picture for the variational basis $\psi_i$ for $i = -1$. An ellipse denotes a singlet-dimer state.

Figure (a) shows the shape of the lattice. A non-magnetic impurity is located at the $\sigma_0$-site. This site-depleted lattice is equivalent to the bond-depleted lattice as shown in Fig. (b), if we shift spins on the left side of the impurity by one lattice spacing to the right and exchange the upper and the lower chain. We make
a variational analysis to this bond-depleted model. The ground state of the base system has a strong nearest-neighbor singlet-dimer correlation when it has a finite energy gap. We consider this picture remains valid even after an impurity is doped, i.e., the ground state can be described in terms of one soliton and 2N nearest-neighbor singlet-dimer states. Far-nearest dimer states are neglected. In this sense, the analysis is variational. This soliton approach has already succeeded in explaining properties of the low-lying states in the fully-frustrated system. The present approximation is good as long as the nearest-neighbor interactions, J2 and J3 dominate the other bonds.

The variational basis is as depicted in Fig. 3 (c) and is written as follows.

\[ \psi_i = [\sigma_{-N}, \tau_{-N}] \cdots [\tau_{i-1}, \sigma_i] \uparrow_i [\tau_{i+1}, \sigma_{i+1}] \cdots [\tau_N, \sigma_N], \]

where \( i > 0 \), and \( [a, b] = (\uparrow_a \downarrow_b - \downarrow_a \uparrow_b)/\sqrt{2} \) denotes the singlet-dimer state. We convention that the spin-\( a \) is always located in the upper chain, and the spin-\( b \) in the lower chain. The basis \( \psi_i \) for \( i < 0 \) is defined in the same way. A location of a soliton \( \uparrow_i \) is restricted within the upper chain, thus there are \( (2N + 1) \) different states. Note that a state with a soliton in the lower chain can be expanded in a linear combination of states with a soliton in the upper chain. The present variational basis is not orthogonal to each other and satisfies the following relation:

\[ \langle \psi_i | \psi_j \rangle = \left( \frac{1}{2} \right)^{|i - j|}. \]  

The matrix elements of the Hamiltonian, \( \langle \psi_i | \mathcal{H} | \psi_j \rangle \), take different forms in regard to a sign of \( i \) and \( j \):

\[
\langle \psi_i | \mathcal{H} | \psi_j \rangle \bigg/ \left( -\frac{3}{4} \langle \psi_i | \psi_j \rangle \right) =
\begin{align*}
&= -\max(i, j)(J_2 - J_3) + |i - j|(J_2 - J_1 - J_0) \\
&\quad + 2N J_2 + J_0(1 - \delta_{i,j}),
&\text{for} \max(i, j) \geq 0 \text{ and } \min(i, j) \geq 0, \tag{3}
\end{align*}

\[
= |i - j|(J_3 - J_1 - J_0) + 2N J_2 - J_3 + 2(J_1 + J_0),
&\text{for} \max(i, j) > 0 \text{ and } \min(i, j) < 0, \tag{4}
\]

\[
= -\min(i, j)(J_3 - J_1 - J_0) + 2N J_2 + J_0 + 2J_1 - J_3,
&\text{for} \max(i, j) = 0 \text{ and } \min(i, j) < 0, \tag{5}
\]

\[
= \max(i, j)(J_2 - J_3) + |i - j|(J_3 - J_1 - J_0) \\
&\quad + 2N J_2 + 2J_1 - J_3 - J_i \delta_{i,j},
&\text{for} \max(i, j) < 0 \text{ and } \min(i, j) < 0, \tag{6}
\]

where \( \max(i, j) = i \) for \( i > j \), \( \min(i, j) = i \) for \( i < j \), and \( \delta_{i,j} \) is the Kronecker delta. The constant energy term is lower in the case of \( i, j \geq 0 \) than that in \( i, j \leq 0 \), when \( J_1 < J_3 \). This makes a soliton confined within the region of positive sites in the low-energy limit. Therefore, an impurity acts as a potential barrier to a soliton.

Our task is to find a function, \( \Psi_{\text{var}} = \sum_i C_i \psi_i \), that minimizes the energy expectation,

\[ E_{\text{var}} = \frac{\langle \Psi_{\text{var}} | \mathcal{H} | \Psi_{\text{var}} \rangle}{\langle \Psi_{\text{var}} | \Psi_{\text{var}} \rangle} = \sum_{i,j} C_i C_j \langle \psi_i | \mathcal{H} | \psi_j \rangle. \]  

If we diagonalize the denominator and rewrite the numerator with its eigenfunction, this variational problem is transformed into a simple eigenvalue problem. We first solve this transformed eigenvalue problem by the numerical diagonalization for a finite system with \( N = 200 \). After that, we give an analytic solution in the continuous limit, \( N \to \infty \), when the wave number of the lowest energy state is zero.

FIG. 2. The ground-state wave function obtained by numerical diagonalization of the variational problem for (a): \( J_0 = 0.35 \), (b): \( J_0 = 0.5 \), and (c): \( J_0 = 0.7 \). \( J_3 \) is set unity and \( J_1 = J_0 \). The strength of the dimerization \( J_2 - J_3 = 2.441 \times 10^{-4} \). Solid lines in (a) and (b) are the asymptotic form of the Airy function.
Figure 2 shows behaviors of the ground-state wave function. We set \(J_3\) unity and vary \(J_0 = J_1\) as (a): \(J_0 = 0.35\), which corresponds to \(\text{CuGeO}_3\); (b): \(J_0 = 0.5\), the Majumdar-Ghosh model; and (c): \(J_0 = 0.7\), which is in the incommensurate phase. Since our analysis is base on the nearest-neighbor singlet-dimer state, the results in the incommensurate phase is not beyond the speculation level. For \(J_0 \leq 0.5\), the wave function of the non-dimerized case \((J_2 = J_3)\) is the sine-function with a phase shift caused by the impurity. The phase shift decreases with a decrease of \(J_1\), since the effective potential barrier at the impurity increases, and it becomes an open edge at \(J_1 = 0\). A soliton can be regarded as a free particle in a potential well in this case. When the dimerization is switched on, the wave function suddenly collapse to the impurity and exhibits an exponential decay. The strength of the dimerization, \(J_2 - J_3\), is only \(2.441 \times 10^{-4}\) in this figure. Therefore, a soliton becomes localized even with a sufficiently weak dimerization. It can be noticed that the wave function is more localized in the case \(J_0 = 0.5\) as compared with that of \(J_0 = 0.35\). We will clarify this \(J_0\)-dependence of \(\xi\) in the analytic solution. In the case of \(J_0 = 0.7\), the wave function exhibits an oscillation with an incommensurate wave number, \(k_{\text{inc}}\), and is already localized without the dimerization. The dimerization effect only decreases a fraction of the localization length. Since the origin of the localization in \(J_0 \leq 0.5\) can be attributed to the bond-dimerization alone, the localization phenomenon in the incommensurate phase is considered quite different from the former ones. We leave to clarify this problem for the future investigation.

The variational problem can be solved analytically by the Fourier transformation, since the denominator is diagonalized in the \(N \to \infty\) limit. Therefore, we rewrite the problem with a new basis, \(|\phi_k\rangle = \sum_n \exp[ik n]|\psi_n\rangle\). The basis relation becomes

\[
|\phi_k|\psi_i\rangle = \frac{3}{5 - 4 \cos k} \delta_{k,l} + O(1/N).
\]

The leading and the second terms of the diagonal part of the Hamiltonian, \(\mathcal{H}_{k,k} \equiv \langle \phi_k | \mathcal{H} | \phi_k \rangle\), are

\[
\mathcal{H}_{k,k} = \frac{9}{4} \frac{(J_2 - J_3)}{5 - 4 \cos k} \frac{N^2}{2N + 1} \left[ \frac{3 (J_2 - J_0 - 2J_1)}{5 - 4 \cos k} + \frac{3 (J_2 - J_0 - 2J_1)}{N} \right] + \frac{3 (J_2 - J_3)}{4} \frac{J_0 + J_1}{(5 - 4 \cos k)^2} \frac{N}{2N + 1},
\]

where we have dropped the constant term, \(2NJ_2\). The leading term of the off-diagonal part, \(\mathcal{H}_{k,l}\), is

\[
\mathcal{H}_{k,l} = -\frac{3}{4} \frac{2N + 1}{2N + 1} \left[ \frac{\text{4N} \cos((k+l)N)}{5 - 4 \cos k} \right] + \frac{3}{2} \frac{1}{5 - 4 \cos k} \frac{1 - \cos((k+l)N)}{1 - \cos(k-l)N}.
\]

The off-diagonal parts are always smaller than the diagonal parts by an order of \(N\).

Before proceeding to the solution, we list several notices. First, the wave number of the ground state must be zero, because we consider the continuous limit, \(N \to \infty\) and \(k \to 0\). In the case of \(J_0 = J_1\), and \(J_2 = J_3\), the wave number that minimizes the variational energy, \(k_{\text{inc}}\), is zero for \(J_1/J_2 < 9/17\), and otherwise it is given by

\[
\cos k_{\text{inc}} = \frac{1}{4} \left( 5 - \sqrt{9(2J_1 - J_2)/J_1} \right).
\]

This incommensurate point was also obtained by the variational matrix-product ansatz. Secondly, we find the diagonal part diverge for \(J_2 - J_3 \neq 0\). In order to avoid this divergence, we introduce a cutoff factor to the momentum as \(k \to k + i\delta\), which has no effect to the physical results by taking a limit \(\delta \to 0\) after \(N \to \infty\).

We rewrite the matrix elements and pick up only the leading term of the off-diagonal part and terms up to \(k^2\) in the diagonal part. Then, we have the continuous limit of the Hamiltonian \(\mathcal{H}_{k,l}\):

\[
\mathcal{H}_{k,l} = \left[ \text{const.} + \frac{(J_0 + J_1)}{4} + \frac{9}{J_2 - J_1 - J_0} \left( \frac{k^2}{2N + 1} \right) \right] \delta_{k,l} - \frac{3}{4} \frac{J_2 - J_3}{(5 - 4 \cos k)^2} \frac{N}{2N + 1},
\]

where the constant term is \((3J_1 + 6J_0 - 3J_2)/8\). Apart from this constant term, the Hamiltonian is equivalent to the following in the real space representation:

\[
\mathcal{H}_{C} = -\frac{d^2}{dx^2} + \frac{3}{4} (J_2 - J_3) |x| \exp[-|x|].
\]

Here, \(x\) is the distance from the impurity, and \(m\) is an effective mass of a soliton given by

\[
m^{-1} = (J_0 + J_1) + 2(3J_2 - J_3).\]

We take the limit \(\delta \to 0\) at this stage. The first term of the eq. (13) is the kinetic energy of a soliton, and the second term is the triangular potential which comes from the bond-dimerization. By a scale transformation, \(X = \theta x\), the eigenvalue equation \(H_c \Psi = E_c \Psi\) becomes

\[
\left[ -\frac{d^2}{dX^2} + (X - E') \right] \Psi = 0,
\]

where \(E' = E_c \times 2m \theta^2\) with \(\theta^3 = 3m(J_2 - J_3)/2\). A solution of this equation is known as the Airy function, \(\Psi = \text{Ai}(X - E')\), with the first eigenvalue \(E' = 2.338\). Then, the energy, \(E_c\), and the localization length, \(\xi\), of a soliton is estimated as

\[
E_c = \frac{E'}{2m \theta^2} = 1.532 \times m^{-1/3} (J_2 - J_3)^{2/3},
\]

\[
\xi \sim (3 + E') \theta^{-1} = 4.663 \times m^{-1/3} (J_2 - J_3)^{-1/3}.
\]

The numeric factor, \((3 + E')\), is determined since the Airy function decays exponentially for large \(X\) as
and $A_0(3) \sim 0.01$. We plot this asymptotic form in Fig. 3(a) and (b) and compare with the numerical solution. The agreements are excellent, even though we have neglected the impurity term of the off-diagonal matrix elements in the analytic solution. As depicted in Fig 3(b), the $J_0$- and the $J_1$-bond vanish and the $J_2$-bond changes to the $J_1$ at the impurity site. This means the effective mass given by eq. (14) is reduced to $m = 9J_1$ only at this site. Therefore, the impurity attracts a soliton. The analytic localization length, eq. (27), should be modified as $\xi - a$ by a some constant term $a$ regarding the phase shift. We will determine $a$ by fitting $\xi - a$ to the numerical results of the variation in the following, since the phase shift cannot be obtained by the present analysis.

Figure 3 compares the analytic results of $\xi$ to those obtained by the numerical diagonalization. The numerical data are estimated at the point where the absolute value of the normalized wave function $|\Psi_{\text{var}}(\xi)|$ becomes smaller than 0.01. Analytic data depicted by lines are $\xi - a$ with $a = 5.5$. This small subtraction merely improves the fit in a small-$\xi$ region, $\xi \leq 20$. It does not influence the asymptotic form of $\xi$ which is in a power law with an exponent $-1/3$. We have checked this behavior remains in a wide region of $0 < J_0/J_3 < 0.5$. We can also predict the strength of the dimerization, $\delta = (J_2 - J_3)/2$, in CuGeO$_3$ by a plot of $J_0$ at 0.35 of this figure. Since the AF order appears at the 2% doping but disappears at the 1%, $\xi$ would be $12.5 < \xi < 25$, which roughly corresponds to $0.003 \leq \delta \leq 0.025$.

In summary, we have given an explicit expression for the localization length of a soliton when a non-magnetic impurity is doped in a general double-spin-chain model. The expression (17) classifies the behavior of a soliton by the origin of the energy gap. When the gap originates in the bond-dimerization, a soliton is strongly localized near the impurity, which means there expects no antiferromagnetic order. On the other hand, a soliton can interact with another soliton when the gap is formed mainly by frustration, since $\xi$ diverges. This result explains why NaV$_2$O$_5$ does not exhibit the AF order by the Na depletion, while CuGeO$_3$ does by the Zn doping. The present analysis clarified that the motion of a soliton is well-described by a quantum particle in a potential well. A soliton is confined to one side of the impurity by the potential barrier proportional to $J_3 - J_1$, and thus, it can penetrate to the other side as $J_1$ approaches $J_3$. It also feels a triangular potential which is an outcome of the bond-dimerization. We conclude that this triangular potential is the cause of the localization of a soliton in the dimer phase. Another type of the localization was also found in the incommensurate phase. It occurs irrespective of the bond-dimerization. Derivation of the interaction between solitons and the localization problem in the incommensurate phase are left for the future investigations.

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