Elementary excitations in the Δ chain

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We clarify elementary excitations in the Δ chain. They are found to be ''kink''-''antikink''-type domain wall excitations to the dimer singlet ground state. The characters of a kink and an antikink are quite different in this system: a kink has no excitation energy and is localized, while an antikink has a finite excitation energy and propagates. The excitation energy of a kink-antikink pair consists of a finite-energy gap and a kinetic energy due to the free motion of the antikink. Variational wave functions for an antikink are studied to clarify its propagating states. All the numerical results are explained consistently based on this picture. At finite temperatures, thermally excited antikinks are moving in regions bounded by localized kinks. The origin of the low-temperature peak in the specific heat reported previously is explained and the peak position in the thermodynamic limit is estimated.

I. INTRODUCTION

Recently, much interest is focused on systems whose classical (mean-field) ground states exhibit an infinite number of local continuous degeneracies due to frustration(''floppy'' systems). In such a system, construction of the linear spin-wave theory based on one of the classical ground states leads to at least one spin-wave mode whose frequency vanishes for all wave vectors (zero-energy mode). The zero-energy mode corresponds to local deformation of a spin configuration that does not raise the energy. The set of the ground state configurations is a manifold with dimensions proportional to the system size. The classical ground state thus may be considered as disordered. We can find examples of floppy spin systems in all dimensions.[1] It is an interesting and a challenging problem to investigate how the quantum effects manifest themselves in such spin systems. The central issue is whether quantum effects lift the ground state degeneracy and select some long-range order. Also the low-energy excitation spectrum is of interest, since it may lead to peculiar thermodynamic properties.

A typical example of such systems is the antiferromagnetic Heisenberg (AFH) model on the *kagomé* lattice. Intensive studies[2–13] on this system have been inspired by the experiments on the ^{3}He layer adsorbed on graphite[14,15] and also on the compound $SrCr_8Ga_4O_{19}$.[16] What mainly have been concerned with are the existence of a double peak in the specific heat at low temperatures and whether a magnetic order is realized in the ground state or not. Several approximate analyses[7–9] have been done but they are still far from giving a common understanding on the ground state property. Numerical studies on finite systems support the existence of the double peak.[2,3,12,13]

In this paper we study a simple one-dimensional floppy system called the Δ chain.[17,18] We consider that this model shares general features of quantum floppy systems, and an understanding of its properties might give some insight into that of the *kagomé* antiferromagnet. Theoretical interest on the Δ chain itself is also enhanced by its experimental realization.[19] The ground state of this system is exactly known to be a dimer state.[20,21] One of the authors (K.K.) examined the low-lying excitations and the specific heat in a previous paper.[22] The numerical diagonalization study of small clusters (up to 20 spins) exhibited that the low-lying excitation modes in the periodic chains are almost dispersionless. The first and the second lowest mode were revealed to converge to dispersionless modes with the same energy in the thermodynamic limit. The specific heat was shown to have a double peak in common with the *kagomé* antiferromagnet. This double peak structure was also observed recently by a Monte Carlo method[23] and by a recursion method.[24]

The dispersionless aspect of excitations may be considered to imply immediately their localization and hence very weak size-dependence of various quantities. The energy gap obtained by numerical diagonalizations,[22] however, does exhibit fairly large size dependence. Also a broad bump of the spin correlation was observed between the most distant spin pairs in the lowest triplet excitations.[25] These results suggest that the excited states are not localized. We solve this puzzle and clarify the character of low-lying excited states in the following sections by mainly employing numerical diagonalization of finite size systems. Elementary excitations are revealed to be ''kink''-''antikink''-type domain walls created in the singlet dimer ground state. An antikink is shown to move freely in a region bounded by kinks at both ends. The kinetic energy of an antikink leads to the size dependence of the energy gap. On the other hand, a kink is localized and gives the dispersionless property to a kink-antikink pair excitation mode.

Properties of an isolated kink and an antikink, and also interactions between them will be discussed in Sec. II. In

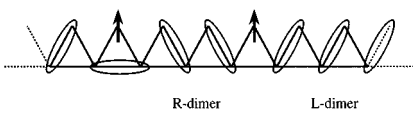

FIG. 1. An excited state of the periodic Δ chain. The up spin that has a dimer singlet pair in its triangle is what we call a ''kink'' and the other one is an ''antikink.''

Sec. III, we show that the size dependence of the energy gap in the periodic chain agrees with that of the kinetic energy of an antikink. The specific heat due to kink-antikink excitations is discussed in Sec. IV, and the position of the low-temperature peak in the thermodynamic limit is estimated. Conclusion is given in Sec. V.

II. ELEMENTARY EXCITATIONS

A. Introduction of a kink and an antikink

The Δ chain is described by the following Hamiltonian:

$$H=\sum_{i=1}^{N} h_i , \tag{1}$$

where

$$h_i=\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i}+\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+1}+\mathbf{S}_{2i-1}\cdot\mathbf{S}_{2i+1}. \tag{2}$$

$\mathbf{S}_i$ is the spin with size 1/2 at the site i and N denotes the number of triangles in the chain.

We first explain the ground state of this system and then forward to the explanation of elementary excitations. Under periodic boundary conditions, the ground state is the perfect singlet dimer state, since the ground state of the local Hamiltonian h_i is realized by pairing any two of three spins into the singlet state. The twofold degenerate ground states are written as

$$\psi_g^L=[1,2]\otimes[3,4]\otimes[5,6]\otimes\cdots\otimes[2N-1,2N],$$

$$\psi_g^R=[2,3]\otimes[4,5]\otimes[6,7]\otimes\cdots\otimes[2N,1]. \tag{3}$$

Here $[i,j]$ denotes the singlet dimer of the spins at the site i and j, i.e., $[i,j]=(\alpha_i\beta_j-\beta_i\alpha_j)/\sqrt{2}$, where $\alpha_i(\beta_i)$ is the state with $S_i^z=1/2(-1/2)$. They are schematically depicted in Fig. 1. We call a dimer located on the left(right) side of a triangle an L dimer (R dimer) and hence the state $\psi_g^L(\psi_g^R)$ an L-dimer (R-dimer) state. These two states are linearly independent but not orthogonal to each other for finite N. They become orthogonal in the limit where $N\rightarrow\infty$. The existence of the excitation energy gap above the ground state was rigorously shown.[20,21]

Under open boundary conditions, the ground state of a system with N triangles is highly degenerate since a ground state consists of N singlet dimers and one free spin. A dimer configuration is uniquely determined by fixing the position of the free spin, which plays a role of a domain wall between an L-dimer state and an R-dimer state. The number of possible positions for a free spin in the ground state is equivalent to the number of sites, and therefore $2N+1$ different dimer configurations can be considered. However, those $2N+1$ states are linearly dependent, since only two out of three dimer configurations in a triangle are linearly independent. The dimensions of the ground state reduce to $2\times(N+1)$;[20,21] only one positional freedom per triangle is allowed.

Let us consider a simple trial excited state in a periodic chain constructed by changing one dimer singlet in the ground state into a triplet state. Then the expectation value of the excitation energy ΔE is identical to the singlet-triplet gap; $\Delta E=1$. Since the energy gap is known as $\Delta E\sim 0.22$ in the thermodynamic limit,[22] the lowest excited state is not such a simple state. In fact, the above state is not an eigenstate and the two spins coupled to a triplet are separated when the Hamiltonian is operated. The average excitation energy may decrease if the two spins are apart as depicted in Fig. 1. Each of two spins is regarded as a domain wall between an L-dimer and an R-dimer state. We show in the following that isolated domain walls are the elementary excitations in this system.

A domain wall which has L dimers on the left side and R dimers on the right has a singlet dimer in its own triangle, and thus is the ground state of the local Hamiltonian h_i. We call this type of a domain wall a ''kink.'' A free spin appearing in the ground state of the open Δ chain is a domain wall of this type. Therefore the excitation energy of a kink is null. There is ambiguity in the definition of the position of a kink, since ground states with different positions of the free spin are not orthogonal to each other. Let us consider a kink as a state where a free spin is located at the top of a triangle as depicted in Fig. 1 for a convention. Then the overlap between the states with an up(or a down)-spin at the ith and the jth($i\neq j$) triangle is $-(-2)^{-|i-j|}$. We treat a kink as a localized object since the state with a kink alone is an eigenfunction of the system, although its position is not a good quantum number due to the nonorthogonality.

We call another type of a domain wall an ''antikink,'' which has R dimers on the left side and L dimers on the right. The state with an antikink at the ith triangle is not a ground state of h_i as the triangle cannot accommodate a singlet dimer. A finite energy is necessary to excite an antikink. It spreads out to other triangles and propagates among them. The energy of an antikink is lowered by this motion, which will be discussed in the next subsection.

Both a kink and an antikink have a spin 1/2 as a whole, and must appear alternatively. Elementary excitations in the Majumdar-Ghosh model is known as propagating domain walls.[26,27] They are also kink-antikink-type domain walls. The physical properties of a kink and an antikink are same in this model, since they are transformed to each other by symmetry operations. On the other hand, the properties of a kink and those of an antikink are quite different in the Δ chain: kinks are localized and antikinks move about in a region bounded by two localized kinks. In the following, we study first an isolated antikink and then the interaction between a kink and an antikink.

B. An isolated antikink

An antikink is necessarily accompanied by a kink in a periodic chain and it is not easy to extract the properties of an isolated antikink because the translational symmetry mixes the states with different positions of a kink and an antikink. We can solve this difficulty by considering open systems as shown in Fig. 2(a), which we call ''open-A'' systems. In this subsection we treat only open-A systems.

In this system, two additional edge bonds have strong tendency to form dimer singlet states and they force the left(right)-hand side of the system to be in the $R(L)$-dimer state. Then inconsistency of the dimer configurations results in an antikink to appear in the middle of the chain. Thus we expect only an antikink to exist in the ground state of an

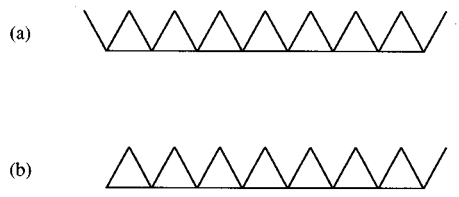

FIG. 2. (a) "Open-A" system. (b) "Open-B" system.

open-A system. We confirm this speculation and clarify the properties of an isolated antikink through numerical and variational analyses. The energy of an antikink δE is obtained from the total energy E of the system with N triangles as $\delta E = E + 3(N+2)/4$.

Figure 3 shows the nearest-neighbor spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ and the local magnetization $\langle S_i^z \rangle$ in the lowest two states of an "open-A" system with $S^z = 1/2$. We consider the ground state first. It is seen that the spin correlations at the both edge bonds are very close to the value of a dimer singlet state $-3/4$, while those of the bonds next to the edges almost vanish. These features show that the both edges are almost in the perfect dimer states. We notice that the state close to the left(right) edge is approximately the $R(L)$-dimer state. As the position of a bond approaches the center, the singlet coupling becomes weak and finally the phase changes at the center. Since the L dimers are located in the right-hand side of the domain wall, we may conclude that there is an antikink. The local magnetization oscillates extended to the whole system, and its amplitude has a broad maximum in the middle of the system.

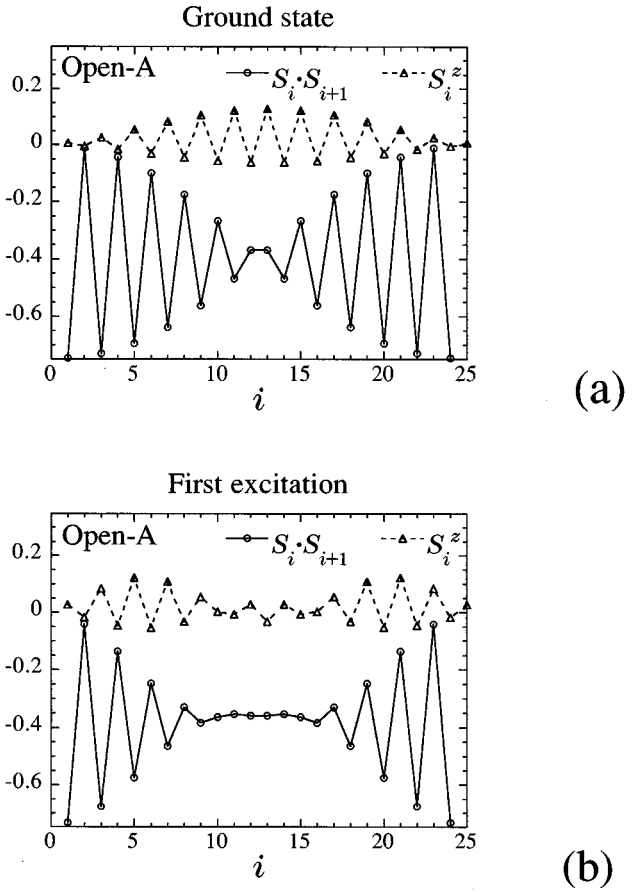

FIG. 3. The nearest-neighbor spin correlations and the local magnetization in the open-A system with 11 triangles (25 spins). Data for the lowest two states are shown.

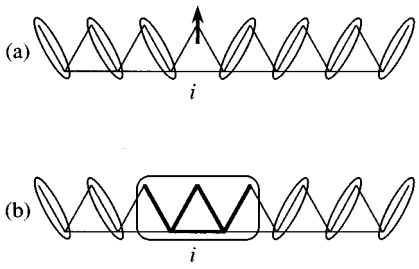

FIG. 4. (a) A basis state for the 1-spin variation. (b) A basis state for the 5-spin variation.

In the first excited state, the profile of the magnetization has two bellies at about a quarter of the system size from both edges and a node at the center. If we assume that the local magnetization reflects the probability of existence of an antikink, the above result suggests that the wave function of an antikink is something like a sine function with a node at the center. The spin correlation profile is very flat with its value ~ -0.35 in the middle region. The correlation at a bond is averaged to be $-3/8$ if the probability for an antikink to be at the left of the bond is equal to that at the right. So the result is consistent with a wave function of an antikink which has a node in the center and two bellies. We see in the following that our speculation on the wave function is correct by comparing the diagonalization results with those by a simple trial functions.

Numerical results of open-A systems suggest that an antikink behaves like a free particle propagating in the whole system, since the data are consistent with that the wave function of an antikink is a sine function in terms of the position. In order to check the validity of this picture, we have made a variational analysis.[28] We take the state where an antikink consists of one free spin as the first trial function. Then the variational basis is the set of $\psi_i^{(1)}$ which consists of $(N+1)$ dimer singlet pairs and the one free spin located at the top of the ith triangle as depicted in Fig. 4(a). The dimension of the basis is $N+2$ since the free spin may occupy the sites at the edges. These basis functions are not orthogonal to each other and satisfy the following relations.

$$\langle \psi_i^{(1)} | \psi_j^{(1)} \rangle = \left(-\frac{1}{2} \right)^{|i-j|}, \tag{4}$$

$$\langle \psi_i^{(1)} | H | \psi_j^{(1)} \rangle = -\frac{3}{4} [(N+2) \langle \psi_i^{(1)} | \psi_j^{(1)} \rangle - \delta_{ij}]. \tag{5}$$

Here, δ_{ij} is the Kronecker δ. The trial function $\Psi_{\mathrm{var}}^{(1)}$, which is assumed as

$$\Psi_{\mathrm{var}}^{(1)} \equiv \sum_{i=0}^{N+1} C_i \psi_i^{(1)}, \tag{6}$$

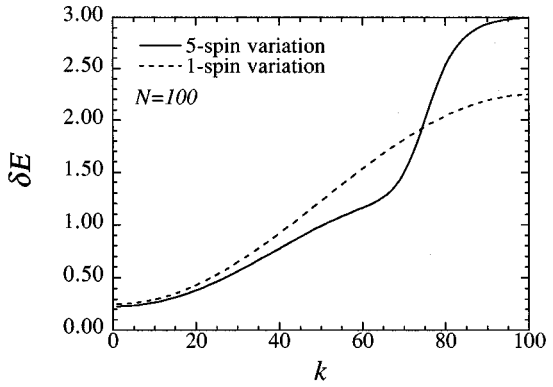

FIG. 5. The excitation energy δE obtained by the 5-spin variation is plotted together with that by the 1-spin variation.

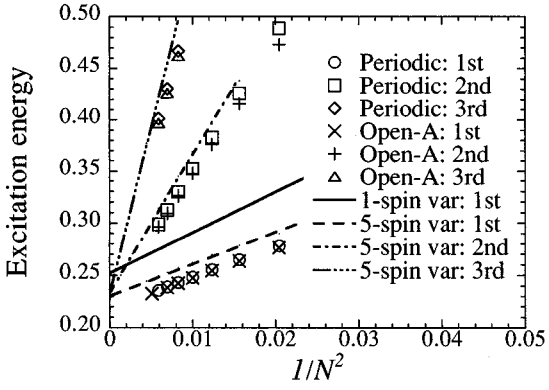

FIG. 6. Excitation energies of the lowest three excited states of the periodic chain in the $S=1$ subspace are plotted against $1/N^2$ together with those of the open-A system obtained by numerical diagonalization and the variation.

is determined as an eigenfunction of the matrix $\langle \psi_i^{(1)} | \psi_j^{(1)} \rangle$ $(0 \leqslant i,j \leqslant N+1)$. In the limit of infinite N we can neglect the boundary effect, and the eigenfunction is easily obtained as $C_i \propto (-1)^i \sin qi$ with the excitation energy $\delta E_{\text{1-spin}} = 5/4 - \cos q$. For a finite N, we have solved the eigenvalue problem numerically and have found that the kth state $(k=1,2,\ldots)$ and its antikink energy is well approximated by

$$C_i \propto (-1)^i \sin \frac{\pi k (i+3/2)}{N+4} \tag{7}$$

and

$$\delta E_{\text{1-spin}} = \frac{5}{4} - \cos \frac{\pi k}{N+4}. \tag{8}$$

The variational energy gap converges to $\delta E_{\text{1-spin}} = 0.25$ as $N \to \infty$. The fact that the true energy gap converges to about 0.22 implies that the above choice of the variational basis is too simple to describe an antikink. We have to take into account of the fact that a free spin spreads out to neighboring triangles destroying singlet dimers nearby.

As an improved trial function, we have employed $\Psi_{\text{var}}^{(5)}$ which is given by Eq. (6) with $\psi_i^{(1)}$ replaced with $\psi_i^{(5)}$, which consists of $(N-1)$ dimer singlet pairs and the ground state of the cluster with five spins as depicted in Fig. 4(b). We numerically diagonalized the effective Hamiltonian for $\Psi_{\text{var}}^{(5)}$. The wave functions for the lowest levels are well approximated by the expression (7), which is consistent with the numerical results of the local magnetization shown in Fig. 3. There is no qualitative difference between the 1-spin variational wave functions and the 5-spin ones. The variational energy by $\Psi_{\text{var}}^{(5)}$ is lower than that by $\Psi_{\text{var}}^{(1)}$ for low-lying states $(k \ll N)$ as shown in Fig. 5. It leads to the energy gap $\Delta E_{\text{5-spin}} \sim 0.23$ in the limit $N \to \infty$. The 5-spin variational energy, however, rapidly increases as k approaches N and exceeds the 1-spin variational energy, which implies that the 5-spin wave function is not a good approximation in the high momentum region. This is because we only took into account the *ground state* of the 5-spin Hamiltonian. In the high momentum region the 1-spin variational function seems to be a better approximation than the 5-spin one.

We have also checked that the behaviors of the local magnetization estimated by the 1-spin variation quantitatively agree well with those of the numerically-exact results for the lowest three states (not shown in the figure). The size dependence of the variational energy is shown in Fig. 6 and is compared with the diagonalization results. All the data show almost linear dependence on N^{-2}. It is seen that the slope of the results of the 5-spin trial function agrees very well with the diagonalization results. Another important fact shown in this figure is that the behavior of the eigen energy of the open-A system agrees with that of the excitation energy of the periodic system. A low energy excitation of the periodic system is considered to be a kink-antikink pair excitation but the above result implies that the excitation energy is mainly determined by a freely moving antikink.

C. Kink-antikink interaction

In this subsection, we investigate the wave function of a kink and the interaction between a kink and an antikink. For this purpose we study the excited states of finite clusters as depicted in Fig. 2(b), which we call "open-B" systems. The L-dimer state is the unique ground state of this open-B system. Hence low energy excitations in this system necessarily involve a kink and an antikink and the open boundary conditions make each of them visible as shown below.

We first consider the first excited state. This is a triplet state and we show the nearest-neighbor spin correlation $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle$ and the local magnetization $\langle S_i^z \rangle$ in the state with $S^z = 1$ in Fig. 7. The numerical results show that the leftmost bond forms a complete triplet state for all system sizes, i.e., $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 1/4$ (note that $\mathbf{S}_1 \cdot \mathbf{S}_2$ commutes with the Hamiltonian). The data for the three leftmost spins approach the limiting values when $N \to \infty$ as $\langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle \to -1/2$, $\langle S_1^z \rangle = \langle S_2^z \rangle \to 1/3$, and $\langle S_3^z \rangle \to -1/6$. In fact the difference from the limiting values is almost negligible in the data of the system with $N=11$ (not shown in the figure). This result implies that the total wave function reduces to a direct product of the wave function of these three spins given by the following equation and that of the remaining $(2N-1)$ spins in the limit $N \to \infty$.

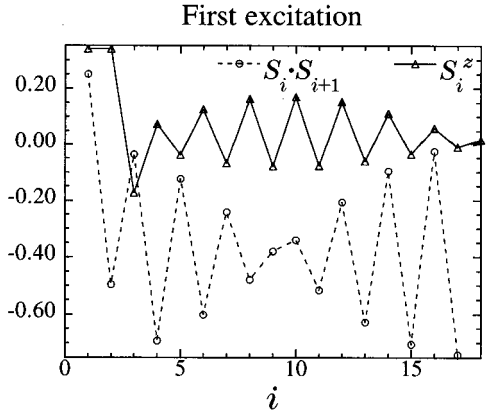

FIG. 7. The nearest-neighbor spin correlation and the local magnetization of the first excited state of the ''open-B'' system with 18 spins.

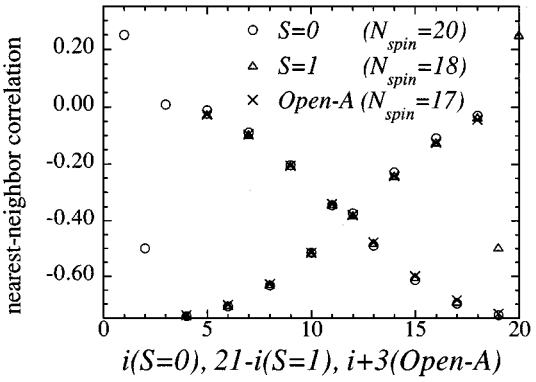

FIG. 8. The nearest-neighbor correlations of the ground state in the open-A system under the magnetic field, and those of the first excited state in the open-B system with $S=0$ and $S=1$. The number of spins are as denoted in the figure. The profile is depicted from the left for the $S=0$ state and the open-A ground state, while its mirror image is depicted for the $S=1$ state.

$$\psi_{\text{kink}}=[\alpha_1(\alpha_2\beta_3-\beta_2\alpha_3)+\alpha_2(\alpha_1\beta_3-\beta_1\alpha_3)]/\sqrt{6}. \quad (9)$$

Therefore a kink is localized in the leftmost triangle though it is a linear combination of the wave function with two different positions of a free spin.

An antikink is distributed in the rest part of the system which corresponds to an open-A system with $N-2$ triangles. It also feels a magnetic field at the 4th and 5th site caused by a magnetization $\langle S_3\rangle\sim -1/6$ of the kink at the third site. Otherwise the antikink is freely propagating in this region. The domain wall profile shown in Fig. 7 is fairly well reproduced by that of the open-A system with 6 triangles and under a magnetic field $-1/6$ at the site 1and 2. Almost complete reproduction of the profile is made by adjusting the magnetic field to be -0.225, which implies that the antikink feels a larger effective field due to the overlap of the wave function with that of the kink for finite N. The antikink is pulled to the left by this effective interaction between a kink and an antikink. Since the leftmost triangle is occupied by a kink, the region for the motion of an antikink in the system with N triangles is same with that in a open-A system with $N-2$ triangles. The interaction with a kink attracts the wave function of an antikink, and as a result, an antikink feels a larger region for its motion. The wave function in the $S=1$ subspace roughly corresponds to that in the open-A system with $N-1$ triangles.

We have also obtained the lowest singlet excited state in the subspace where the edge bond forms a triplet state. We find that the results at the leftmost triangle is almost same with those in the corresponding triplet states. On the other hand, the results on the right side of the system are different from those in the the triplet states; the domain wall profile is shifted to the right by nearly *one triangle* compared to that in the triplet states. This is the effect of the exchange interaction with the kink, which acts as a repulsion in the singlet state. The antikink in the singlet state is repelled stronger by the kink than that in the triplet state because the state must be orthogonal to the ground state. As a result, it is nearly prohibited for the antikink to occupy the site 4 in the singlet state. Therefore, the wave function of an antikink in the $S=0$ subspace roughly corresponds to that in the open-A system with $N-3$ triangles under an adequate magnetic field. Figure 8 shows the nearest-neighbor correlations of the ground state of the open-A system with N triangles under the magnetic field $+0.320$, that of the $S=0$ excited state of the open-B system with $N+3$ triangles, and the mirror image of the profile of the $S=1$ excited state of the open-B system with $N+1$ triangles for $N=7$. They agree surprisingly well in the central region of the antikink. We may conclude by this evidence that the wave functions of an antikink in these three states are approximately equal.

We have examined higher excited states up to the fourth in the subspace of $S^z=1$ (not shown in the figure). We found that a kink is located in the nth triangle in the nth excited state and the left side of that triangle is in the L-dimer state. Therefore the wave function of the nth state is nothing but a direct product of the wave function of the L-dimer state of $n-1$ triangles and that of the first excited state of a smaller open-B system with $N-(n-1)$ triangles.

We have studied the interaction between a kink and an antikink when only one antikink is on the right side of the kink. In periodic systems and/or higher excitations, an antikinks exists also on the left side of a kink. We expect that a kink will be localized even when antikinks exist at both sides. Its wave function, however, would be different from that studied above which is asymmetric with respect to the inversion. The ferromagnetic nature of the interaction is deduced from the fact that the lowest excited state of the periodic systems is singlet.

III. SIZE DEPENDENCE OF THE ENERGY GAP

In the previous section, we focused on a kink and an antikink as elementary excitations and clarified their individual characteristics and the interaction between them. We found that the excitation energy of the system is determined mainly by the excited antikink. The antikink is described as a particle propagating freely in a region bounded by kinks and/or boundaries. If the region of its motion is bounded by a kink, it feels an exchange field which modifies its wave function. The expectation value of the exchange interaction is usually very small, since the probability for a kink and an

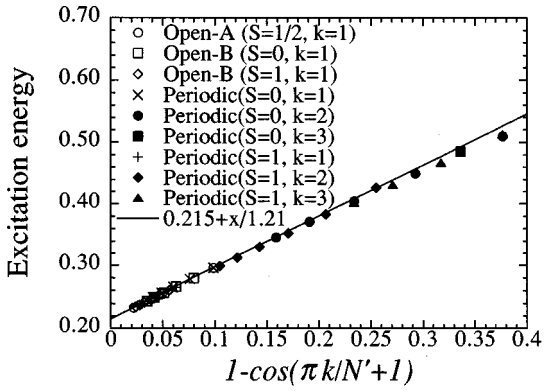

FIG. 9. Excitation energy of all the systems considered in this paper are plotted against $1-\cos\pi k/(N'+1)$. Definition of $N'=N+\Delta N$ is described in the text. The least-square fitting gives $\epsilon_0=0.215$ and $m=1.21$.

antikink to be at the nearest neighbor triangles is very small. The effect of the interaction appears rather as a change in the effective length of the region of motion for the antikink. We therefore postulate that the excitation energy of the system is given by the energy of a freely propagating antikink as a first approximation. Then the excitation energy may be written as

$$\delta E=\epsilon_a=\epsilon_0+\frac{1}{m}\left(1-\cos\frac{\pi k}{N'+1}\right). \tag{10}$$

Here ϵ_a denotes the energy of an antikink, m its mass, $k-1$ stands for the number of nodes in the wave function, and N' the effective length of the region where the antikink propagates. The creation energy ϵ_0 of an antikink is equal to the excitation energy gap of the Δ chain in the thermodynamic limit. Of course, the cosine form in Eq. (10) is an approximate form only valid in the region where $\pi k/(N'+1)$ is small compared to unity. We treat only such cases. In this section, we show that the excitation energies in the periodic systems as well as those in the open systems considered in the previous section are well described by Eq. (10). We examine δE of the ground state of the open-A systems, the first excited state of the open-B systems with $S=0$ and that with $S=1$ and the lowest three excited states of the periodic systems with $S=0$ and those with $S=1$ in the subspace with zero total momentum. We assume that Eq. (10) with $k=1$ expresses δE of the ground state of the open-A systems, the first excited state of the open-B system with $S=0$ and that with $S=1$. The first, the second, and the third excited states of the periodic systems with $S=0$ and $S=1$ are also assumed to be expressed by Eq. (10) with $k=1,2$, and 3, respectively. The parity of these states are consistent with this assignment (parity = even for $k=1$ and 3; parity = odd for $k=2$).

In Fig. 9, we show the plot of δE versus $1-\cos[\pi k/(N'+1)]$, where $N'=N+\Delta N$ is chosen so that all the data fall onto one curve. ΔN is a correction to N induced by the boundary effect and/or the interaction with kinks. It is remarkable that all data lie on a curve. This is a clear and strong evidence for that the excitation energy is mainly contributed by an antikink. For the open-A systems we take $\Delta N=3$ for a convention. Then the best choice of ΔN for other cases are shown in Table I.

TABLE I. ΔN for the systems we considered.

System	ΔN
open-A	3
open-B $(S=0)$	0.8
open-B $(S=1)$	2.3
Periodic $(S=0,k=1)$	-3.0
Periodic $(S=0,k=2)$	-3.0
Periodic $(S=0,k=3)$	-2.8
Periodic $(S=1,k=1)$	-0.2
Periodic $(S=1,k=2)$	-0.4
Periodic $(S=1,k=3)$	-0.5

Let us try to understand the above results in an intuitive way. In open-B systems, a kink occupies the leftmost triangle. Then the region allowed for an antikink to move is assumed to be equivalent to an open-A system with less triangles by two. The attractive interaction elongates the effective region for $S=1$ state, and repulsive interaction and the requirement of the orthogonality to the ground state shortens it for $S=0$. We see from the numerical results (Table I) that the effect of the interaction amounts to $1.3(-0.2)$ triangles for $S=1(0)$. It amounts to $-0.2(-3)$ triangles for $k=1$ and $S=1(0)$ states in the periodic systems, since the allowed region for an antikink is equivalent to an open-A system with less triangles by three. The difference of the effect of the interaction and/or the orthogonality between the open-B systems and the periodic systems is not clarified yet at present. The least-square extrapolation by using all the data in the figure gives the creation energy ϵ_0 in the limit $N\to\infty$ and the mass of an antikink m. They are

$$\epsilon_0=0.215 \tag{11}$$

and

$$m=1.21. \tag{12}$$

IV. THE LOW-TEMPERATURE SPECIFIC HEAT

In this section, we show that the elementary excitations discussed in the previous sections generate the low-temperature peak in the specific heat. First we calculate the specific heat of a finite system by numerical diagonalization, and examine whether the result can be reproduced by the elementary excitation with the spectrum given by Eq. (10) with the parameters (11) and (12). We consider a periodic system with 8 triangles ($N=8$). All the 2^{16} states can be diagonalized numerically, and thus the exact specific heat is obtained as shown in Fig. 10. Now we calculate the specific heat due to kink-antikink excitations. We take only low-lying states into account, i.e., the ground state (doubly degenerate), all the states with one pair of a kink and an antikink, and some states with two pairs. Among the states with two kink-antikink pairs, we take those where the distance between two kinks are largest. We treat the states with two kink-antikink pairs as two independent pairs for simplicity.

The expectation values of energy are calculated by the excitation energy given by Eq. (10) with the values of ϵ_0 and m given by Eqs. (11) and (12). The specific heat is calculated by differentiating the energy with respect to the temperature

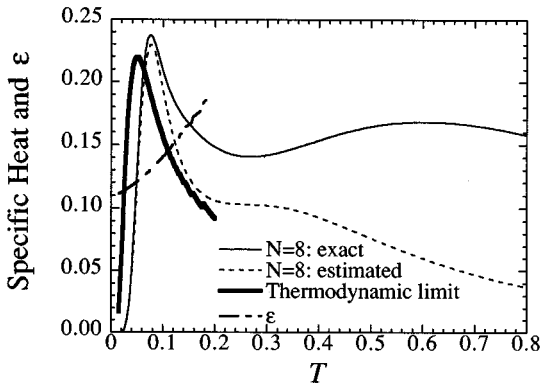

FIG. 10. Temperature dependence of the specific heat. Numerically exact results (solid line) and the approximate results (dashed line) for the $N=8$ periodic system are plotted together with the one estimated in the thermodynamic limit (bold line). Excitation energy in the Schottky-type specific heat $\epsilon=\langle\epsilon_a\rangle_\beta/2$ is also plotted.

numerically. The result coincides with the exact specific heat at low temperatures as shown in Fig. 10. The peak position and the low-temperature side of the peak are correctly reproduced. The peak height is a little smaller than the exact value. The approximate result gives much smaller value than the exact one at higher temperatures because of the negligence of higher excited states. We may conclude that the low-temperature peak is caused by the low-lying kink-antikink excitations whose spectrum is described by Eq. (10).

Next we estimate the specific heat in the thermodynamic limit. We consider the system at low temperatures where the thermal excitations are described by kinks and antikinks. Let us first consider the case where the mass m is infinite. In this case, antikinks are localized with the excitation energy ϵ_0. This system is thermodynamically equivalent to that where independent kinks and antikinks have the excitation energy $\epsilon_0/2$, and it shows a Schottky-type specific heat with an excitation energy $\epsilon=\epsilon_0/2$. If m is finite, the excitation energy of an antikink ϵ_a depends on the length L of the region of the motion and also on the level k as $\epsilon_0+(1/m)\times(1-\cos[\pi k/L])$. In order to obtain thermodynamic quantities, we must average them over all states with possible values of L and k. Instead of doing this summation, we estimate the specific heat in an approximate way. We assume that the thermal excitations of kink-antikink pairs at a temperature $T\equiv\beta^{-1}$ are regulated by the averaged antikink energy defined by

$$\langle\epsilon_a\rangle_\beta=\frac{\Sigma_{k=1}^{l}E_k\exp[-\beta E_k]}{\Sigma_{k=1}^{l}\exp[-\beta E_k]},\quad E_k=\epsilon_0+\frac{1}{m}\left(1-\cos\frac{\pi k}{l}\right). \tag{13}$$

Here the integer l is the average distance between two excited kinks, i.e., the length of the region where an antikink can move. We have neglected the effects of interactions between kinks and antikinks. This may be justified if $l\gg1$, which will be shown to be the case below. We assume that the specific heat is written as a Schottky-type one as

$$C(T)=\frac{(\beta\epsilon)^2\exp[\beta\epsilon]}{(1+\exp[\beta\epsilon])^2},\quad \epsilon=\langle\epsilon_a\rangle_\beta/2. \tag{14}$$

The average length l, which is equal to the distance between two antikinks, is given by

$$l=\mathrm{int}(\exp[\beta\langle\epsilon_a\rangle_\beta]), \tag{15}$$

since an antikink is excited with the probability $\exp[-\beta\langle\epsilon_a\rangle_\beta]$. We can solve self-consistent equations (13) and (15) by iteration for a given T. Then with obtained $\langle\epsilon_a\rangle_\beta$, we can calculate the specific heat at the temperature through Eq. (14). We have employed the parameters given by Eqs. (11) and (12) and plotted the obtained specific heat in Fig. 10. The peak position shifts from the finite-size result toward the low temperature and locates at $T\sim0.05$. The profile of the peak is very steep on its low-temperature side but it has a tail on the other side. These features are common with the numerical results of finite-size systems. This agreement implies that above approximation is correctly taking into account of the temperature dependence of $\langle\epsilon_a\rangle_\beta$. The approximation is based on the idea that an antikink can be treated as a localized object after averaging the kinetic energy in $\langle\epsilon_a\rangle_\beta$. We consider that this picture is a good approximation if the discreteness of the antikink kinetic energy is negligible and the motion of antikinks is well thermalized. In fact, the average antikink energy $\langle\epsilon_a\rangle_\beta$ obtained in the above calculation turns out to be 0.244 at $T\sim0.05$, the peak position of the specific heat. Therefore the averaged kinetic energy $\langle\epsilon_a\rangle_\beta-\epsilon_0=0.029$ is larger than $T/2=0.025$, the classical thermal average of the kinetic energy. The result implies that the phase space of the l states is well thermalized at this temperature. The average distance between antikinks, l, is estimated as ~130, which is much greater than unity. The average kinetic energy is much smaller than the creation energy at this temperature range. Above results indicate that our approximate scheme is a consistent one and is correctly describing the thermodynamics of the system in the temperature region of the peak in the specific heat.

V. CONCLUSION

In the previous sections, we have clarified the elementary excitations in the Δ chain to a great extent. They are two types of domain walls called a kink and an antikink. A kink is essentially localized in a finite range (about one triangle). An antikink propagates with kinetic energy within a region bounded by kinks. The dispersionless mode found previously[22] originates in the localized character of a kink. The low-temperature peak in the specific heat is caused by thermal excitations of kinks and antikinks. The peak position is mainly determined by the creation energy of the antikink, while its kinetic energy causes the size dependence of the excitation energies as well as the broadening of the peak of the specific heat.

Above understanding of the Δ chain might give some insight into the properties of the *kagomé* antiferromagnet. Though the dimensionality of two systems are different, they have some common features. Both systems have macroscopically degenerate classical ground states and show the second peak in the specific heat at low temperatures. The low-temperature peak in the specific heat is observed in finite

kagomé antiferromagnets.[2,11–13] The uniform susceptibility seems to decrease suddenly at the same temperature.[11,13] In the Δ chain, the spin gap corresponds to the first excitation gap. Above similarities suggest that the elementary excitations with a *spin gap* in both systems may have common characters that create the second peak of the specific heat. Recently, Zeng and Elser[12] investigated the *kagomé* antiferromagnet by dimer calculations. Their results support this speculation, but further investigation on the *kagomé* antiferromagnet is necessary for a concrete understanding of the system.

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