Boundary Resonances in $S=1/2$ Antiferromagnetic Chains Under a Staggered Field

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(Received 4 December 2011; revised manuscript received 27 June 2012; published 10 December 2012)

We develop a boundary field theory approach to electron spin resonance in open $S = 1/2$ Heisenberg antiferromagnetic chains with an effective staggered field. In terms of the sine Gordon effective field theory with boundaries, we point out the existence of boundary bound states of elementary excitations, and modification of the selection rules at the boundary. We argue that several "unknown modes" found in electron spin resonance experiments on $KCuGaF_6$ [I. Umegaki, H. Tanaka, T. Ono, H. Uekusa, and H. Nojiri, Phys. Rev. B **79**, 184401 (2009)] and Cu-PM [S. A. Zvyagin, A. K. Kolezhuk, J. Krzystek, and R. Feyerherm, Phys. Rev. Lett. **93**, 027201 (2004)] can be understood as boundary resonances introduced by these effects.

DOI: 10.1103/PhysRevLett.109.247603 PACS numbers: 76.30.−v, 02.30.Ik, 75.10.Jm, 75.25.−j

Introduction.—Impurities often introduce new aspects in physics, Kondo effect being a notable example. In particular, impurity effects in strongly correlated systems are currently among central topics in condensed matter physics. Although the standard perturbation theory can fail, there are a number of powerful theoretical approaches to strongly correlated systems, especially in one dimension. Impurity effects in gapless one-dimensional systems have been vigorously studied in terms of boundary conformal field theory. In contrast, impurity effects in gapped one-dimensional systems received much less attention, with the exception of the edge states in the $S = 1$ Haldane gap phase [1–3].

On the other hand, integrable models and field theories have been successfully applied to many gapped one-dimensional systems. In quantum magnetism, a field-induced gap in $S = 1/2$ Heisenberg antiferromagnetic (HAFM) chains is described in terms of a quantum sine Gordon field theory [4–6]; the one-dimensional Ising chain with critical transverse field and a weak longitudinal field realizes a quantum field theory with E_8 symmetry [7,8]. Experimental studies indeed found elementary excitations predicted by these integrable field theories. Application of integrable field theories to impurity and boundary effects in gapped one-dimensional strongly correlated systems is an interesting but largely unexplored subject.

In this Letter, we present a theory of electron spin resonance (ESR) in $S = 1/2$ HAFM chains in a staggered field with boundaries, which may be realized by nonmagnetic impurities. The low-energy effective theory of the system is the quantum sine Gordon field theory with boundaries. In fact, this theory is integrable even in the presence of a boundary, and boundary bound states (BBS) of elementary excitations have been found in the exact solution [9–14]. The existence of BBS, and modification of the selection rules, imply extra resonances in addition to those in the bulk. ESR measurements on corresponding systems $KCuGaF_6$ [15] and $[\mathrm{PM\text{-}Cu(NO_3)_2(H_2O)2}]_n$ (PM denotes pyrimidine, abbreviated as Cu-PM) [16,17] had found several resonances that could not be accounted for by the theory. We argue that several of those resonances can be successfully identified in terms of the boundary sine Gordon field theory.

Boundary sine Gordon field theory.—We consider a semiopen chain with the Hamiltonian

$$\mathcal{H} = \sum_{j<0}[J\boldsymbol{S}_j \cdot \boldsymbol{S}_{j-1} - \mu_B \boldsymbol{H}\cdot \mathbf{g}\cdot \boldsymbol{S}_j + (-1)^j \boldsymbol{D}\cdot \boldsymbol{S}_j \times \boldsymbol{S}_{j-1}], \tag{1}$$

which models one side of an infinite chain broken by a nonmagnetic impurity at $j = 0$. $\mathbf{g}$ is the g tensor of localized spins, and μ_B is Bohr magneton.

The Zeeman energy can be represented as $-\mu_B \sum_{j,a,b} H^a [g^u_{ab} + (-1)^j g^s_{ab}] S^b_j$. Hereafter, we assume that $g^u_{ab} g\delta_{ab}$ and $|g^s_{ab}| \ll g$, and employ a unit $\hbar = k_B = g\mu_B = 1$.

We consider $\boldsymbol{H} = H\hat{z}$ applied along the z direction ($\hat{z}$ is a unit vector in the z direction). The last term of (1) is the staggered Dzyaloshinskii-Moriya (DM) interaction. This can be eliminated by a staggered rotation of spin about the direction of $\boldsymbol{D}$ by angle $(-1)^j\alpha/2$, where $\alpha = \tan^{-1}(|\boldsymbol{D}|/J)$ where j is the site index.

Under an applied field, this transformation leaves a staggered field $\boldsymbol{h} \sim \boldsymbol{H} \times \boldsymbol{D}/2$, which is perpendicular to $\boldsymbol{H}$ and to $\boldsymbol{D}$ [5,6]. Together with the staggered field due to the staggered component of the g tensor, the effective model may be given by

$$\mathcal{H} = \sum_{j<0}[J\boldsymbol{S}_j \cdot \boldsymbol{S}_{j-1} - HS^z_j - h(-1)^j S^x_j], \tag{2}$$

keeping only the most important terms. $h = c_s H$ is the effective staggered field, approximately perpendicular to the applied field; the direction of the staggered field is chosen to be the x axis. c_s depends both on the staggered DM interaction and on the staggered part of g tensor g^s_{ab}. Using bosonization formulas,

$$S^z_x \sim m + \frac{1}{2\pi R}\partial_x \phi + C^z_s(-1)^x \cos(\phi/R + Hx), \quad (3)$$

$$S^\pm_x \sim e^{\pm 2\pi R i \tilde{\phi}}[C^\perp_s(-1)^x + C^\perp_u \cos(\phi/R + Hx)], \quad (4)$$

at low temperature $T \ll J$, the model (2) is mapped to a boundary sine Gordon (BSG) field theory, defined by the action

$$\mathcal{A} = \int_{-\infty}^{\infty} dt \int_{-\infty}^{0} dx \bigg[\frac{1}{2}\bigg\{\frac{1}{v^2}(\partial_t \tilde{\phi})^2 - (\partial_x \tilde{\phi})^2\bigg\} - C^\perp_s h \cos(2\pi R \tilde{\phi})\bigg]. \quad (5)$$

v is the spin-wave velocity. The fields ϕ and $\tilde{\phi}$ are dual and compactified as $\phi \sim \phi + 2\pi R$ and $\tilde{\phi} \sim \tilde{\phi} + 1/R$; m is the uniform magnetization density and the nonuniversal constants $C^z_{u,s}$ and $C^\perp_{u,s}$ are determined numerically [18]. The bulk operator $\cos(2\pi R\tilde{\phi})$, which represents the transverse staggered magnetization, is relevant in the renormalization group sense. Thus it induces a finite mass (excitation gap), as it was observed in the experiments [5,6]. The bulk gap is stable against dilute nonmagnetic impurities.

In the absence of the staggered field term, the field ϕ obeys the Dirichlet boundary condition $\phi(x = 0, t) =$ const [19]. This is equivalent to the Neumann boundary condition in terms of the dual field:

$$\partial_x \tilde{\phi}(x, t)|_{x=0} = 0. \quad (6)$$

Inclusion of the staggered field could change the boundary condition; in fact, the staggered field in the bulk would also induce the corresponding operator $\cos(2\pi R\tilde{\phi})$ at the boundary. If this boundary perturbation is dominant, $\tilde{\phi}$ would obey the Dirichlet boundary condition. However, since $\cos(2\pi R\tilde{\phi})$ is, as a boundary operator, (nearly) marginal in a renormalization group, its effects are negligible at the energy scale set by the bulk spin gap. Thus, for a small staggered field h, the boundary condition can still be regarded as the Neumann on $\tilde{\phi}$.

Energy spectrum.—The elementary excitation of the bulk sine Gordon field theory includes soliton (denoted by S) and antisoliton ($\bar{S}$) with the same mass M. A soliton and antisoliton carry soliton charge $Q = +1$ and $Q = -1$, respectively. Additional particles called breathers are generated as bound states of a soliton and an antisoliton [20,21]. There can be several different kinds of breathers B_n with the mass $M_n = 2M\sin(n\pi\xi/2)$, for $n = 1, 2, \ldots, \lfloor \xi^{-1} \rfloor$. Here $\lfloor\cdot\rfloor$ is the floor function. Breathers have zero soliton charge. The soliton charge is conserved in the bulk sine Gordon field theory. For the case of our interest, that is experimental situations in $KCuGaF_6$ and Cu-PM, the parameter $\xi = 1/(2/\pi R^2 - 1)$ satisfies $\xi < 1/3$. In particular, $\xi \approx 1/3$ in the low field limit $H \to 0$.

Fortunately, the BSG theory (5) with the Neumann boundary condition (6) is still integrable [9]. An analysis of the *boundary S* matrices implies [9–12,22] the existence of the BBS with the mass

$$M_{\mathrm{BBS}} = M\sin(\pi\xi), \quad (7)$$

for $\xi < 1/2$. Therefore, the BBS with $M_{\mathrm{BBS}} \sim \sqrt{3}M/2$ does exist in the low field limit of the present system. The BBS of soliton, antisoliton, and first breather turn out to be identical and there is only one type of BBS. This is another manifestation of the soliton charge nonconservation at the boundary.

Thus the analysis of the BSG theory predicts a new excited state, which is a BBS, at the energy M_{BBS} lower than the bulk gap M. In fact, in an earlier numerical study of an open chain based on a density matrix renormalization group, Lou *et al.* [23,24] had found such an excited state localized near the boundary. They called it a midgap state. Figure 1 shows a comparison of the soliton (12) and BBS (7) masses to the numerically obtained bulk gap and the energy of the midgap state in Refs. [23,24]. Here we used $M \approx 1.85(h/J)^{2/3}[\ln(J/h)]^{1/6}$ appropriate for $H = 0$, which was used in Refs. [23,24]. The excellent agreement between the two energies means that the midgap state found in the density matrix renormalization group calculation was nothing but a BBS.

While it was pointed out in Refs. [23,24] that the midgap state is localized near the boundary, physical understanding of its origin has been lacking. The analogy to the edge state in the Haldane phase is clearly inappropriate, since the $S = 1/2$ HAFM in a staggered field is topologically trivial. With the present identification of the midgap state with the BBS, the BSG theory is established as an effective theory describing the boundary physics of the system. This is essential in understanding the ESR spectra.

Electron spin resonance.—Next we discuss the ESR spectrum, which is given by $I(\omega) \propto \omega\chi''_{\mathrm{phys}}(q = 0, \omega)$. Here, χ'' is an imaginary part of the dynamical susceptibility χ. $\chi_{+-}(q, \omega) = -G_{S^+S^-}(q, i\omega = \omega + i\epsilon)$ where

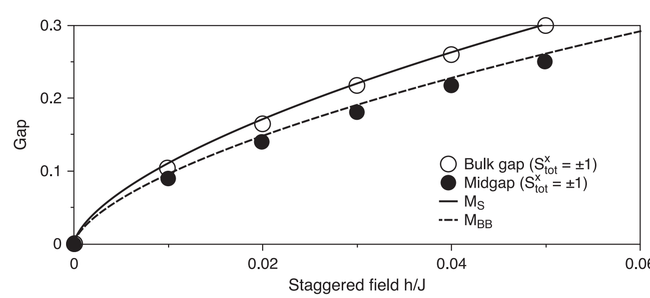

FIG. 1. Numerically obtained bulk gap (open circles) and midgap (solid circles) in Ref. [23] are compared with the soliton mass M and the BBS mass M_{BBS} (7).

positive infinitesimal ϵ is the analytic continuation of the temperature Green's function $G_{S^+S^-}(q, i\omega)$. The staggered rotation of spins by angles $(-1)^j\alpha/2$ to eliminate the DM interaction mix the uniform ($q = 0$) and the staggered ($q = \pi$) components. The physical susceptibility $\chi''_{\rm phys}(q = 0, \omega)$ is

$$\chi''_{\rm phys}(0, \omega) \sim \chi''_{+-}(0, \omega) + \left(\frac{D_z}{J}\right)^2 \chi''_{+-}(\pi, \omega), \qquad (8)$$

where D_z is the z component of the DM vector $\boldsymbol{D}$ parallel to the applied field. On the right-hand side, we dropped the longitudinal susceptibility $\chi_{zz}(q = \pi, \omega)$ because it contains the same resonances as those in the transverse part $\chi_{+-}(q = 0, \omega)$, and merely modifies their intensities.

Let us first review the ESR in the bulk, in the limit of $T \to 0$. The uniform part $\chi''_{+-}(0, \omega)$ reflects transitions caused by the operator

$$S^{\pm}_{q=0} \sim e^{\pm 2\pi R i\tilde{\phi}} \cos(\phi/R + Hx). \qquad (9)$$

The operator $\cos(\phi/R)$ changes the soliton charge by ± 1 and thus must create at least one soliton or antisoliton. The other factor $e^{\pm 2\pi R i\tilde{\phi}}$ can create any number of excitations with zero soliton charge in total. Thus ESR induced by the operator (9) with the lowest possible energy corresponds to the creation of a single soliton or antisoliton. It should be noted also that the factor Hx in the cosine causes the shift of the momentum with H. That is, the created soliton or antisoliton should carry the momentum H. Thus the ESR due to a single soliton or antisoliton creation is at frequency $\omega = E_S \equiv \sqrt{M^2 + H^2}$. There are also resonances due to (9) at higher energies, corresponding to the creation of additional elementary excitations.

Next we turn to the staggered part $\chi''_{+-}(q = \pi, \omega)$, which reflects transitions caused by the operator

$$S^{\pm}_{q=\pi} \sim e^{\pm 2\pi R i\tilde{\phi}}. \qquad (10)$$

This carries zero soliton charge, and thus the simplest excitation induced by this operator is the creation of a single breather B_n. This leads to the resonances at $\omega = M_n$.

Now let us discuss the boundary effects on ESR. Here we discuss the ESR spectrum based on the physical picture, leaving systematic formulations to the Supplementary Material [25].

First we consider the contribution of the staggered part $\chi''_{+-}(q = \pi, \omega)$. The simplest excitation created by the operator (10) is a single breather. In the presence of the boundary, the first breather can form the BBS. Thus the resonance with the lowest energy in the presence of the boundary is given by $\omega = M_{\rm BBS}$. Creation of a breather not bounded at the boundary and the BBS is also possible, leading to the resonance at $\omega = M_{\rm BBS} + M_n$.

In order to understand the boundary effects on ESR, we need to clarify the issue of the momentum conservation.

TABLE I. Typical resonance modes in $\chi''_{+-}(q = 0, \omega)$. Resonances shown in the second row are absent at $T = 0$. The soliton resonance E_S is accompanied with all bulk resonances. On the other hand, E_S does not necessarily appear in the boundary resonances. In fact, some boundary resonances are involved with a novel resonance E_n instead of E_S.

	Bulk	Boundary
$T = 0$	$\omega = E_S, E_S + M_n$	$\omega = E_n, E_S + M_{\rm BBS}, E_n + M_{\rm BBS}$
$T > 0$	$\omega = \lvert E_S - M_n \rvert$	$\omega = E_n - M_{\rm BBS}$

In general, total momentum is conserved due to the translation invariance of the system. In the presence of the boundary, the translation invariance is lost and the total momentum is no longer conserved. Nevertheless, the momentum is still important in discussing ESR spectra, because the momentum of each elementary excitation is conserved or reversed in a scattering with another elementary excitation, or in a reflection at the boundary. Thus, once created, the set of momenta of elementary excitations is conserved, up to the sign of each momentum.

The existence of the boundary has an interesting effect, in addition to the contribution of the BBS, on the ESR spectrum. Although the expectation of the operator $\cos(\phi/R)$ vanishes in the bulk, it is nonvanishing [26,27] near a boundary with the Dirichlet boundary condition on ϕ [equivalent to the Neumann boundary condition (6) on $\tilde{\phi}$]. This reflects ϕ taking a fixed value at the boundary. Thus, *in the vicinity of the boundary*, the leading contribution from the uniform part is effectively given by the operator $S^{\pm}_{q=0} \sim e^{\pm 2\pi R i\tilde{\phi}} \cos(Hx)$, which creates excitations with zero soliton charge, in contrast to the original one (9). This is another consequence of violation of soliton charge conservation at the boundary. The created excitations should carry the total momentum $\pm H$, up to the uncertainty $\sim 1/l_p$. Here l_p is the pinning length scale, namely $\phi(x) \sim$ const if $|x| < l_p$.

Thus, the simplest among the possible ESR processes due to this operator is the creation of a single breather B_n with momentum $\pm H$. This corresponds to the frequency

$$E_n = \sqrt{M_n^2 + H^2}. \qquad (11)$$

The resonance at E_n with $n > 1$ was absent in the bulk and is a new feature due to the boundary. We emphasize that

TABLE II. Typical resonance modes in $\chi''_{+-}(q = \pi, \omega)$. Breather masses are directly measured in the bulk part. The BBS mass itself appears in the boundary resonances. Equation (8) shows that intensities of these modes are smaller than those in Table I by $(D_z/J)^2$.

	Bulk	Boundary
$T = 0$	$\omega = M_n, M_n + M_m$	$\omega = M_{\rm BBS}, M_n + M_{\rm BBS}$
$T > 0$	$\omega = M_n - M_m \ (n > m)$	$\omega = M_n - M_{\rm BBS}$

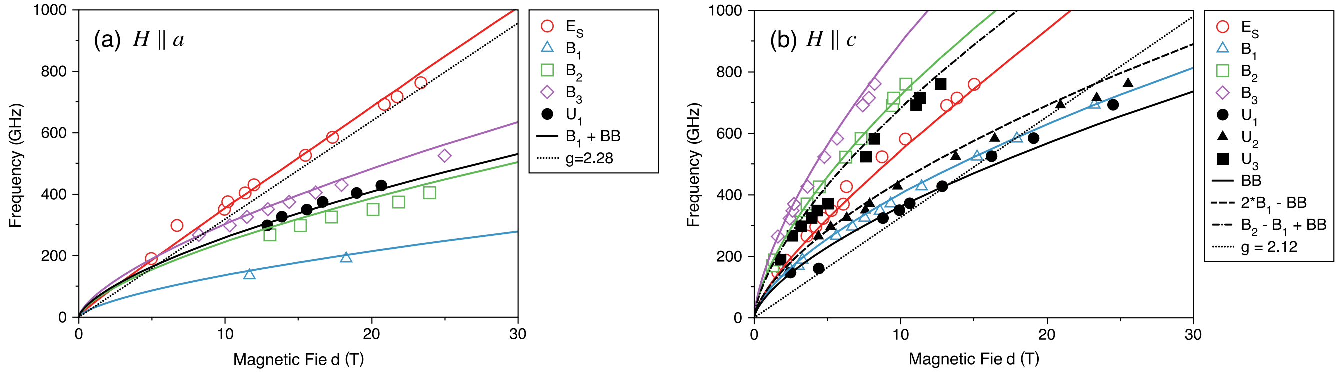

FIG. 2 (color online). Frequency vs field diagrams of ESR in $KCuGaF_6$ [15] for (a) $H \parallel a$ and (b) $H \parallel c$ configurations. The dotted line is high temperature paramagnetic resonance $\omega = H$. Open symbols and filled symbols represent bulk modes and "unknown modes." E_S, B_1, B_2, B_3 denotes resonances $\omega = E_S$, M_1, M_2, M_3 by a soliton S and breathers B_n. An antisoliton $\bar{S}$ also leads to $\omega = E_S$. The labels U_1, U_2, U_3 are "unknown" peaks found in Ref. [15]. (a) The configuration $H \parallel a$ bears the smallest $h = c_s H$ with the coefficient $c_s = 0.031$. An excitation $\omega = M_1 + M_{\rm BBS}$ is found in addition to the bulk excitations. (b) We have the largest staggered field, $c_s = 0.178$, when $H \parallel c$. This large c_s makes the rich kinds of boundary modes detectable. The labels BB, $2^*B_1 - \rm BB$, $B_2 - B_1 + \rm BB$ denote $\omega = M_{\rm BBS}$, $2M_1 - M_{\rm BBS}$, $M_2 - M_1 + M_{\rm BBS}$.

these new resonances do *not* simply follow from the existence of the midgap state numerically found in Refs. [23,24]. In fact, the resonance frequency E_n does not explicitly contain the energy $M_{\rm BBS}$. This shows the necessity of the BSG framework to fully understand the physics at the boundary.

At finite temperatures, additional resonances may be observable. When the initial state contains the BBS as a thermal excitation, a resonance at $\omega = M_n - M_{\rm BBS}$ exists, corresponding to annihilation of the BBS and creation of a breather B_n. Similarly, when the initial state contains B_1, the resonance at $\omega = M_n - M_1 + M_{\rm BBS}$ corresponds to the creation of B_n and binding of B_1 at the boundary. These resonances are contained in the staggered part $\chi''_{+-}(\pi, \omega)$. The uniform part also contains, at finite temperatures, additional resonances.

Typical resonance modes are summarized in Tables I and II. Note that intensities of resonances due to the staggered part $\chi''_{+-}(q = \pi, \omega)$ and $\chi''_{zz}(q = \pi, \omega)$ are suppressed by the factor $(D_z/J)^2$ in (8), compared to those from the uniform part $\chi''_{+-}(q = 0, \pi)$.

Comparison with experiments.—Thus several novel resonances, which are absent in the bulk, are derived from the BSG theory. They indeed match the "unknown" resonances observed previously in ESR spectra on $KCuGaF_6$ (Fig. 2) and Cu-PM (Fig. 3). Here the uniform field effect is taken into account in the soliton-antisoliton mass [28],

$$M = \frac{2v}{\sqrt{\pi}} \frac{\Gamma(\xi/2)}{\Gamma((1+\xi)/2)} \left[\frac{\Gamma(1/(1+\xi))}{\Gamma(\xi/(1+\xi))} \frac{C_s^{\perp} \pi}{2v} c_s H \right]^{(1+\xi)/2}. \tag{12}$$

While the ratio $c_s = h/H$ can in principle be determined by the staggered DM interaction and g tensor, we use the value obtained by fitting experimental data.

Each figure shows different resonances, though. The difference between the spectra in two materials can be understood in terms of the different magnitude of the DM interaction. The coefficient c_s at its maximum is larger (0.178) in $KCuGaF_6$ compared to 0.083 in Cu-PM. While precise estimates of the DM interaction and the staggered g tensor are not available, the staggered DM interaction is presumably larger in $KCuGaF_6$. This leads to larger mixing of the staggered part $\chi''_{+-}(q = \pi, \omega)$. Thus it is natural that the resonances due to the mixings are observed only in $KCuGaF_6$ (Fig. 2). We note that the simplest possible BBS contribution at $\omega = M_{\rm BBS}$ is not observed for $H \parallel a$ in Fig. 2(a). This is presumably because only two of the frequencies used in the experiments can detect the resonance below the bulk resonance at $\omega = M_1$. On the other hand, in the Cu-PM with a smaller DM interaction, only the contributions from the uniform part are observed (Fig. 3). We conjecture that, with more careful examination

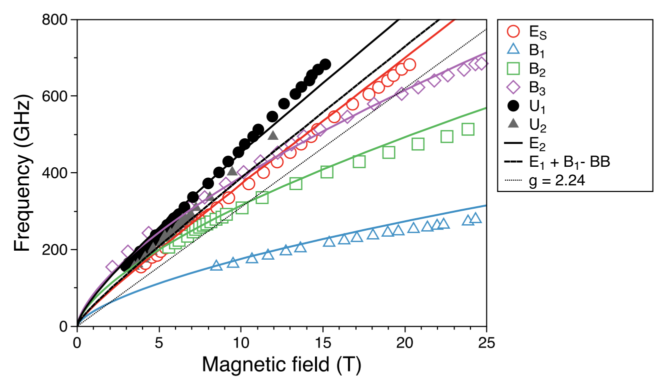

FIG. 3 (color online). Frequency vs field diagrams of ESR in Cu-PM [16]. Two "unknown" peaks U_1 and U_2 are attributed to $\omega = E_2$, $E_1 + M_1 - M_{\rm BBS}$, respectively, where E_n is defined in Eq. (11). These boundary modes appear in $\chi''_{xx}(q = 0, \omega)$.

of the spectra, more resonances due to the BBS will be found in experiments.

Conclusions.—We point out the existence of BBS and modification of the selection rules at boundaries of the $S = 1/2$ antiferromagnetic chain in an effective staggered field, in terms of the BSG theory (5). The boundary effects can account for the mysterious "unknown modes" found in two compounds $KCuGaF_6$ [15] and Cu-PM [16,17].

In the compound $KCuGaF_6$, magnetic ions Cu^{2+} and nonmagnetic ions Ga^{3+} form a pyrochlore lattice. Magnetically, the compound $KCuGaF_6$ is effectively regarded as $S = 1/2$ HAFM chains of Cu^{2+} ions. However, since Cu^{2+} and Ga^{3+} ions occupy equivalent positions, an intersite mixing of them can occur in the course of syntheses [29]. We speculate that the intersite mixing brings about nonmagnetic impurities in spin chains. We expect that a few percent of the nonmagnetic impurities would lead to observation of the boundary resonances as discussed in this Letter. Our picture may be verified experimentally by controlling the density of nonmagnetic impurity, which will change the intensity of boundary resonances.

The authors thank P. Bouillot, T. Giamarchi, S. Takayoshi, H. Tanaka, I. Umegaki, and S. Zvyagin for fruitful discussions. This work is partly supported by the Global COE Program "The Physical Sciences Frontier" (S. C. F.), and KAKENHI Grant No. 50262043 from MEXT of Japan.

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